CLASSES OF GRAPHS HAVING EXTREMAL TOPOLOGICAL INDICES

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DECLARATION

I, Mr. **Naveed Akhter** Registration No. **66-GCU-PHD-SMS-13** student at **Abdus Salam School of Mathematical Sciences GC University** in the subject of **Mathematics,** year of admission **2013**, hereby declare that the matter printed in thesis titled

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Date Signature of Student

Dedicated

To My Family

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Abstract

Now a days graph theory is one of the prime objects of study in discrete mathematics. It has applications in diverse fields which include chemistry, linguistics, computer science, natural science, operations research and electrical engineering. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. The advantage of topological indices is in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR). Zagreb indices, were introduced 43 years ago by I. Gutman and N. Trinajstić [21]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [3, 49]. In 1975, Randić proposed a structural descriptor called branching index [43] that later became the well-known Randić index (product-connectivity index), which is the most used molecular descriptor in QSPR and QSAR studies[49, 29]. The sum-connectivity index was proposed in [63] and it was found that the sum-connectivity index and the product-connectivity index correlate well among themselves and with the π-electronic energy of benzenoid hydrocarbons [36]. Many applications of the sum-connectivity index may be found in [37]. Recently, this concept was extended to the general sum-connectivity index in [64].

Chapter one of this dissertation briefly describes some basic definitions and notations of graph theory which we used in our research.

In chapter two we briefly introduce elements of chemical graph theory and some topological indices whose extremal properties we discuss in next chapters.

In chapter 3, using a graph transformation and several inequalities, in the class of n-vertex connected bicyclic graphs G with $n \geq 4$, we determine the unique graph minimizing the general sum-connectivity index for $-1 \leq \alpha < 0$.

In chapter 4 we deduced upper and lower bounds of $M_1(G)$ and an upper bound

of $M_2(G)$ in k-apex trees. We proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 5$, the graph $K_k + S_{n-k}$ maximizes the first and second Zagreb indices. We also proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 3k$ the graph G that has $n - 2k + 2$ vertices of degree 2 and $2k - 2$ vertices of degree 3 minimizes the first Zagreb index.

In chapter 5 we obtained explicit expressions for minimal first general Zagreb index $Z_p(G)$ for $p > 1$, which directly can be extended for $\gamma > 2$, where γ is the cyclomatic number of G.

In chapter 6 we determined the extremal values of the Narumi-Katayama, first Zagreb and second Zagreb indices of connected (n, n_1)-graphs with fixed cyclomatic number and showed that these bounds are tight.

Chapter 1

Fundamental Concepts

1.1 Introduction

In this chapter we present some basic concepts and results related to graphs. In our work we are dealing with finite, simple and connected graphs.

1.2 Preliminaries

A *graph* G is a triple consisting of a *vertex* set $V(G)$, an *edge* set $E(G)$ and a relation that assigns each edge with two vertices. The two vertices associated with an edge are called its *end points*. The number of elements in $V(G)$ is called *order* of the graph G and number of elements in $E(G)$ is called its *size*. In this dissertation the order and size of the graph are usually denoted by n and by m, respectively. A graph of zero order and zero size is known as *null* graph. A graph of order one is called *trivial* graph. A graph of finite order and finite size is called *finite* graph. In a graph G two vertices a and b are said to be *adjacent* if they are ends of an edge. Two adjacent vertices are also know as *neighbours* of each other. If vertex a is an endpoint of edge e, then a and e are *incident*. An edge having same end points is called a *loop*. Two edges with same end points are called parallel edges. A graph having no loop or parallel edges is called a *simple* graph. An edge e in a graph G with end points a and b is denoted as $e = ab$. The set of neighbours of a vertex a is called *nighbourhood* of a and is denoted by $N(a)$. The number of elements in $N(a)$ is called *degree* of vertex a and is denoted by $d_G(a)$ or $d(a)$. A vertex of degree zero is called an *isolated* vertex. A vertex of degree one is called *pendent* vertex. An edge whose one end is a pendent vertex is called a *pendent edge*. The maximum and minimum degrees of vertices of a graph G are denoted by ΔG and δG, respectively. If in a graph G, $\delta G = \Delta G = t$, then the graph G is called t-regular graph. If G is a simple graph of order n and a is any vertex of G, then the following inequalities hold:

$$0 \leq \delta G \leq d(a) \leq \Delta G \leq n - 1.$$

The degree of vertices and the number of edges of a graph G are related by the following result.

Proposition 1.2.1. *[57] If G is a graph, then*

$$\sum_{a \in V(G)} d(a) = 2m.$$

Corollary 1.2.2. *The number of vertices of odd degree in a graph is always even.*

The join of two vertex-disjoint graphs G and H is the graph $G+H$ with $V(G+H) = V(G) \cup V(H)$ and the edges of $G + H$ are all edges of graphs G and H and the edges obtained by joining each vertex of G with each vertex of H. A graph H is called *subgraph* of the graph G, if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If a graph H is a subgraph of the graph G, then we write $H \subseteq G$ and say that "G contains H". If $V(H) = V(G)$ then the subgraph H is called *spanning* subgraph of the graph G. A subgraph H of a graph G is called *induced subgraph*, if for every $a, b \in V(H)$ and $ab \in E(G)$ then $ab \in E(H)$. Figure 1.1 is an example of a graph and its spanning subgraph. A graph H is called a *proper subgraph* of the graph G, if either $V(H)$ is a

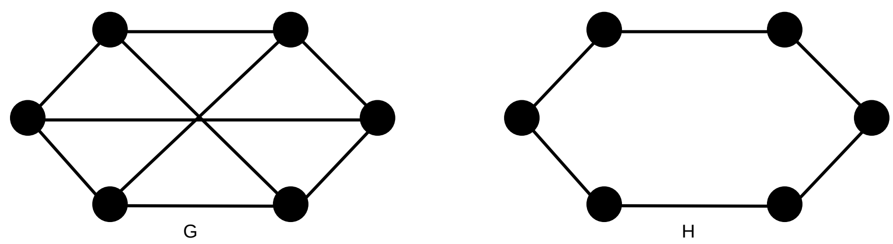

Figure 1.1: Graph G and its spanning subgraph H

proper subset of $V(G)$ or $E(H)$ is a proper subset of $E(G)$. If e is an edge of the graph G, then the graph $G-e$, obtained by deleting edge e from G is called *edge-deleted* subgraph. If a is a vertex of the graph G, then the graph $G-a$, obtained by deleting vertex a and all edges incident to a is called *vertex-deleted* subgraph.

1.3 Connected Graphs

A graph P of order n, with vertex set $\{a_1, a_1, \ldots, a_n\}$ and edge set $\{a_1a_2, a_2a_3, \ldots, a_{n-1}a_n\}$ is called a *path*. The vertices a_1 and a_n are called *end vertices* of the path P. A path of order n is denoted by P_n. Figure 1.2 is an example of path of order six. The number of edges in a path is called its *length*. The length of a path of order n is $n-1$. Two vertices a and b in a graph G are called *connected* if there exists a path in G whose end vertices are a and b. A graph G is said to be *connected* if any two distinct vertices in G are connected. If a graph G is not connected it is called *disconnected*. In a connected graph the shortest lenght of the paths with end points a and b is called the *distance* between vertices a and b and is denoted by $d(a, b)$. The *diameter* of a graph G is denoted by $d(G)$ and is defined as $d(G) = \max\{d(a, b) : a, b \in V(G)\}$.

A connected subgraph of G that is not a proper subgraph of any other connected subgraph of G is called a *component* of G. A graph G is then connected if and only if

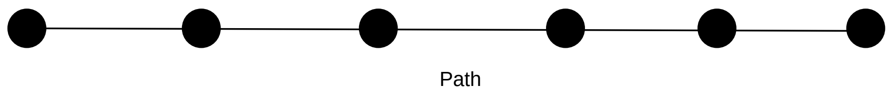

Figure 1.2: Path of order six

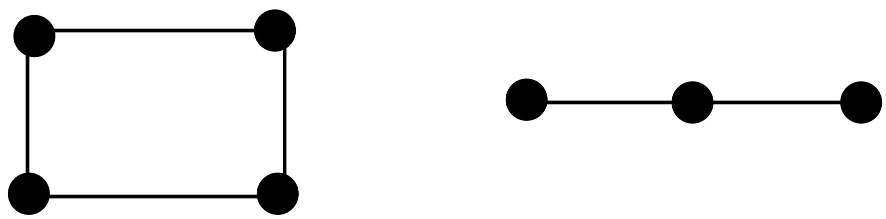

Figure 1.3: A disconnected graph with two components

it has exactly one component. The path is an example of a connected graph. Figure 1.3 is an example of a disconnected graph.

Proposition 1.3.1. *[57] Every graph with order n and size m has at least $n - m$ components.*

Theorem 1.3.2. *[6] Suppose G is a graph of order three or more, then G is connected if and only if G contains two distinct vertices a and b such that $G - a$ and $G - b$ are connected.*

1.4 Some Classes of Graphs

In the study of graphs, we see that certain graphs are encountered often and it is useful to be familiar with such graphs. In many cases a special notation is reserved for such graphs.

We have already seen that paths are a special kind of graphs. A graph C of order $n(n \geq 3)$, with vertex set $\{a_1, a_1, \ldots, a_n\}$ and edge set $\{a_1a_2, a_2a_3, \ldots,$

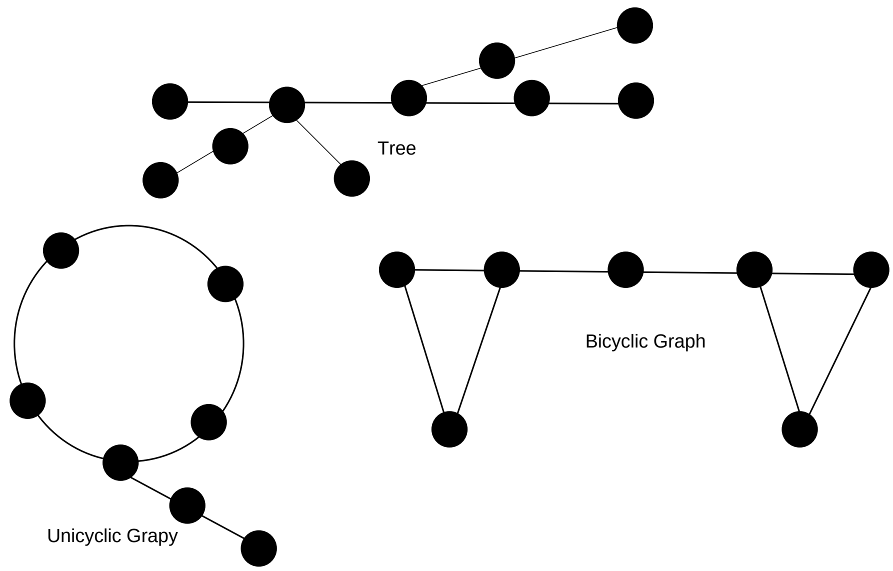

Figure 1.4: An example of tree, unicyclic and bicyclic graphs

$a_{n-1}a_n, a_na_1\}$ is called a *cycle*. A cycle of order n is denoted by C_n. A cycle of even order is called *even cycle* while a cycle of odd order is called an *odd cycle*. A graph having no cycle is called *acyclic* graph. An acyclic connected graph is known as a *tree*. Paths are trees and a tree T is a path if and only if $\Delta T = 2$. In a graph two cycles having at least one distinct vertex are called independent cycles. In a graph G of order n and size m, the number $\gamma = m - n + 1$ (number of independent cycles in G) is called the *cyclomatic* number. The graphs with $\gamma = 0, 1, 2$ are called trees, *unicyclic* graphs and *bicyclic* graphs respectively. Figure 1.4 shows a tree, a unicyclic graph and a bicyclic graph. The size of a tree of order n is $n-1$. The sizes of unicyclic and bicyclic graphs of order n are n and $n+1$, respectively.

A tree of order n is called a *star* if there exist a vertex a such that $d(a) = n - 1$. A star graph of order n is denoted by S_n. A graph G is called a *complete* graph if any two vertices of it are connected by an edge. A complete graph of order n is denoted by K_n. A complete graph of order n has $\frac{n(n-1)}{2}$ edges. A graph G is called

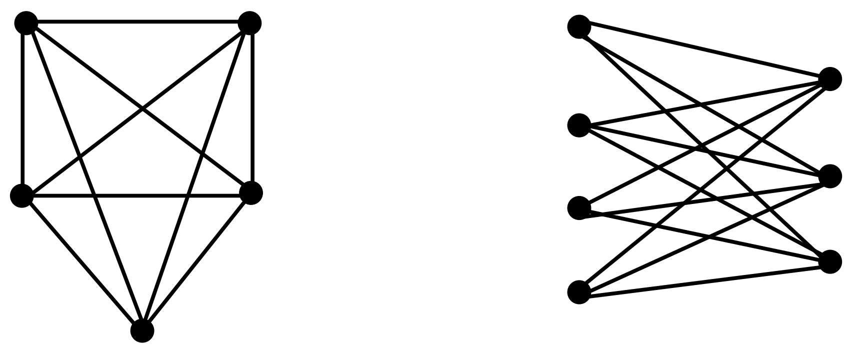

Figure 1.5: Complete and complete bipartite graphs

bipartite graph if its vertex set $V(G)$ can be partitioned into two disjoint subsets A and B such that every edge has one end in the set A and the other end in the set B. If every vertex of the set A is connected with every vertex of the set B, then the bipartite graph G is called *complete bipartite* graph. A complete bipartite graph in which $|A| = l$ and $|B| = t$ is denoted by $K_{l,t}$. Star of order n is also a complete bipartite graph and therefore can be written as $K_{1,n-1}$. Figure 1.5 shows a complete graph and a complete bipartite graph.

Theorem 1.4.1. *[6] A graph is bipartite if and only if it contains no odd cycle.*

Theorem 1.4.2. *[6] A graph is a tree if and only if any two distinct vertices of it are connected by a unique path.*

A graph G is called an *apex tree* [60] if it contains a vertex x such that $G - x$ is a tree. The vertex x is called an *apex vertex* of G. Note that a tree is always an apex tree, hence a non-trivial apex tree is an apex tree which itself is not a tree. For any integer $k \geq 1$ the graph G is called k*-apex* tree if there exists a subset X of $V(G)$ of cardinality k such that $G - X$ is a tree and for any $Y \subset V(G)$ and $|Y| < k$, $G - Y$ is not a tree. A vertex in X is called k*-apex vertex.* Clearly, 1-apex trees are precisely

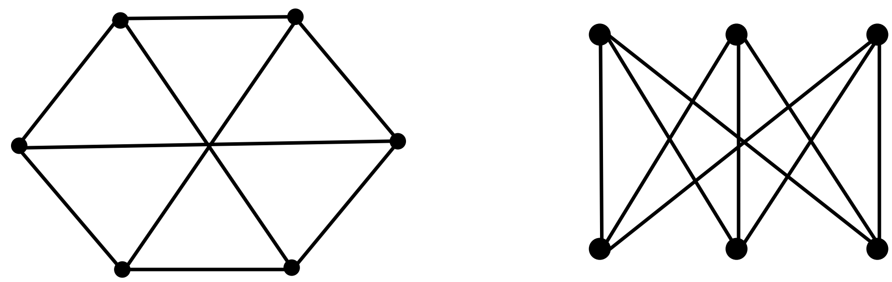

Figure 1.6: Two isomorphic graphs

non-trivial apex trees. Apex trees and k-apex trees were introduced in [58] under the name quasi-tree graphs and k-generalized quasi-tree graphs, respectively.

1.5 Isomorphic Graphs

Two graphs G and H are said to be *isomorphic* if there exists a bijection $f : V(G) \to V(H)$ such that $ab \in E(G)$ if and only if $f(a)f(b) \in E(H)$. The function which shows that two graphs are isomorphic is called an *isomorphism*. If G and H are isomorphic graphs then we write $G \cong H$. If there is no isomorphism between two graphs then they are called *non-isomorphic* graphs. The graphs in Figure 1.6 are isomorphic.

Theorem 1.5.1. *[6] If G and H are isomorphic graphs, then the degrees of vertices of G are same as the degrees of vertices of H.*

The *complement* of a graph G is the graph $\bar{G}$ such that $V(G) = V(\bar{G})$ and for any pair $a, b \in V(G)$, $ab \in E(G)$ if and only if $ab \notin E(\bar{G})$.

Theorem 1.5.2. *[6] Two graphs are isomorphic if and only if their complements are isomorphic.*

Chapter 2

Topological Indices

2.1 Chemical Graph Theory

Chemical graph theory is the branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [5]. The pioneers of the chemical graph theory are Alexandru Balaban, Ante Graovac, Ivan Gutman, Haruo Hosoya, Milan Randić and Nenad Trinajstić [42] (also Harary Wiener and others).

Many, yet not all, chemical substances consist of molecules. The fact that molecules have a "structure" is known since the middle of the 19th century. Since then, one of the principal goals of chemistry is to establish relations between the chemical and physical properties of substance and the structure of the corresponding molecules. Countless results along these lines have been obtained, and their presentation comprises significant parts of textbooks of organic, inorganic and physical chemistry, not to mention treatises on theoretical chemistry.

The vast majority of such "chemical rules" are qualitative in nature. A century-long tendency in chemistry is to go a step further and to find quantitative relations of the same kind. Here, however, one encounters a major problem. Molecular structure is a non-numerical notion. The measured physico-chemical properties of substances are quantities that are expressed by numbers (plus units, plus experimental errors).

Hence, to find a relation between molecular structure and any physico-chemical property, one must somehow transform the information contained in the molecular structure into a number. There have been many attempts in this direction. One group of researchers uses so-called topological indices.

2.2 Topological Indices

If we represent atoms in a structural formula of a chemical compound by vertices and covalent bonds by edges then the corresponding graph is know as *molecular graph*. A *topological index* is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. The advantage of topological indices consists in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships ($QSPR$) and in Quantitative Structure Activity Relationships ($QSAR$)[13, 15]. Topological indices found broad applications in the correlation and prediction of several molecular properties [3, 47] and also in tests of similarity and isomorphism [14, 46]. In this chapter we will discuss some topological indices.

2.2.1 General Sum-connectivity Index

The *Randić* index (product-connectivity index) is one of the most used topological index in structure-property and structure-activity relationship studies [19, 20, 33, 41, 44, 45, 49]. The Randić index $R(G)$ of a graph G was proposed by Randić [43] in 1975 and was defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$

Motivated by the Randić's definition of product-connectivity index, the *sum-connectivity* index of a graph G was proposed in [63] and was defined as

$$\chi(G) = \sum_{ab \in E(G)} \frac{1}{\sqrt{d(a) + d(b)}}.$$

The applications of the sum-connectivity index have been investigated in [36]. This idea of sum-connectivity index was extended to general sum-connectivity index by B. Zhou and N. Trinajstić [64] and was defined as

$$\chi_\alpha(G) = \sum_{ab \in E(G)} (d(a) + d(b))^\alpha.$$

In what follows we will present some results about graphs having maximum or minimum general sum-connectivity index in various classes of connected graphs for some values of the parameter α.

In the paper proposing new index $\chi_\alpha(G)$ [64] Zhou and Trinajstić proved the following result:

Theorem 2.2.1. *Let T be a tree with $n \geq 4$ vertices. If $\alpha > 0$ then:*

$$2.3^\alpha + (n-3)4^\alpha \leq \chi_\alpha(T) \leq (n-1)n^\alpha,$$

where left equality holds if and only if $T = P_n$ and right equality holds if and only if $T = K_{1,n-1}$. If $\alpha < 0$ then the above inequalities on $\chi_\alpha(G)$ are reversed, where the upper bound holds for $\alpha \geq 1 - \frac{log2}{log(\frac{4}{3})} \approx -1.4094$.

Minimum value of $\chi_\alpha(T)$ for trees of given diameter and $-1 \leq \alpha < 0$ has been deduced in [56] using graph transformations and some parametric inequalities:

Theorem 2.2.2. *For every $-1 \leq \alpha < 0$ in the set of trees T having order $n \geq 3$ and diameter equal to d $(2 \leq d \leq n-1)$, $\chi_\alpha(T)$ is minimum if and only if $T = S_{n,n-d+1}$.*

The extremal connected bicyclic graphs of order n for $\alpha \geq 1$ were deduced in [48] and [51] as follows:

Theorem 2.2.3. *The unique graph with the largest general sum-connectivity index for $\alpha \geq 1$ among all connected bicyclic graphs of order n, consists of two triangles having a common edge and other $n-4$ pendent edges incident to a vertex of degree three of this graph.*

Theorem 2.2.4. *The set of graphs which minimize the general sum-connectivity index in the set of the connected bicyclic graphs of order n for $\alpha \geq 1$ is $A \cup B$, where A is the set of graphs consisting of two vertex disjoint cycles C_p and C_q, joined by a path P_r and B the set of those graphs formed by two cycles C_{p+r} and C_{q+r}, having in common a path P_r, provided $r \geq 2$.*

We have determined the minimum general sum-connectivity index for bicyclic graphs of order $n \geq 4$ for $-1 \leq \alpha < 0$ in Chapter 3.

2.2.2 Zagreb Indices

The first and second Zagreb indices of a graph G, denoted $M_1(G)$ and $M_2(G)$, respectively are defined as:

$$M_1(G) = \sum_{a \in V(G)} (d(a))^2$$

$$M_2(G) = \sum_{ab \in E(G)} d(a)d(b).$$

These indices were defined by Trinajstić and Gutman [21]. They found that the total π-electron energy depends on these two indices. Balaban et al. [3] named $M_1(G)$ and $M_2(G)$ as the first Zagreb-Group index and the second Zagreb-Group index, respectively. These names were later abreviated as first Zagreb index and second Zagreb index [49]. Main properties of these indices were summarized in [18, 40]. In what follows we will present some results about graphs having maximum or minimum Zagreb indices in various classes of connected graphs.

A vertex in a tree is called a stem vertex if it has incident pendent edges. The minimum trees with given number of pendent vertices for M_1 and M_2 were deduced by Gubko [22] as follows:

Theorem 2.2.5. *For any tree T with $n_1 \geq 2$ pendent vertices $M_1(T) \geq 9n_1 - 16$ if n is even. The equality holds if every non-pendent vertex of T is of degree 4. If n_1 is odd, then $M_1(T) \geq 9n_1 - 15$, and the equality holds if T is a tree with all non-pendent vertices having degree 4 except the one of degree 3.*

Theorem 2.2.6. *For any tree T with $n_1 > 8$ pendent vertices $M_2(T) \geq 11n_1 - 27$. The equality holds if each stem vertex in T has degree 4 or 5 while other non-pendent vertices have degree 3. At least one such tree exists for any $n_1 \geq 9$.*

Gutman et al. [24] generalized the Gubko's result for any graph with n_1 pendent vertices with a fixed value of cyclomatic number. They also deduced minimum graphs of order n having n_1 pendent vertices with a fixed value of the cyclomatic number as follows:

Theorem 2.2.7. *Let G be a connected graph with n_1 pendent vertices and cyclomatic number γ. Then*

$$M_1(G) \geq 9n_1 + 16(\gamma - 1).$$

Equality holds if and only if all non-pendent vertices of G are of degree 4, provided such graphs exist.

Corollary 2.2.8. *If graphs, specified in Theorem 2.2.7, for which the equality ($M_1 = 9n_1 - 16$) holds, do not exist, then*

$$M_1(G) \geq 9n_1 + 16(\gamma - 1) + 1.$$

Equality holds if and only if one non-pendent vertex of G is of degree 3 and all other non-pendent vertices are of degree 4, and/or one non-pendent vertex of G is of degree 5 and all other non-pendent vertices are of degree 4, provided such graphs exist.

Theorem 2.2.9. *Let T be a tree of order n with n_1 pendent vertices. Then*

$$M_1(T) \geq 4n - 6 + (n + n_1 - 4)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor - (n - n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor^2.$$

Equality is attained if and only if T consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor - n_1 + 2$ vertices of degree $t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$ and $n_{t+1} = n - 2 - (n - n_1)\left\lfloor \frac{n-2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Theorem 2.2.10. *Let U be a unicyclic graph of order $n \geq 3$ with $n_1 \geq 0$ pendent vertices. Then*

$$M_1(U) \geq 4n + (n + n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor - (n - n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor^2.$$

Equality is attained if and only if U consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor - n_1$ vertices of degree $t = \left\lfloor \frac{n}{n-n_1} \right\rfloor + 1$ and $n_{t+1} = n - (n - n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Theorem 2.2.11. *Let B be a bicyclic graph of order $n \geq 4$ with $n_1 \geq 0$ pendent vertices. Then*

$$M_1(B) \geq 4n + 6 + (n + n_1 + 4)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor - (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor^2.$$

Equality is attained if and only if B consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor - n_1 - 2$ vertices of degree $t = \left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 1$ and $n_{t+1} = n + 2 - (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Also for any value of γ greater than 2, structural characterization of $\gamma-$cyclic graphs of order n with n_1 pendent vertices, minimal first Zagreb index can be achieved in a fully analogous manner.

In Chapter 4 we have determined upper and lower bounds of $M_1(G)$ and an upper bound of $M_2(G)$ in k-apex trees. The corresponding extremal k-apex trees are also characterized in each case.

The *first general Zagreb* index $Z_p(G)$ for $p \in R$ is defined as

$$Z_p(G) = \sum_{v \in V(G)} d(v)^p.$$

The first general Zagreb index seems to have been first considered and named by Lie et al.[34, 35]. Obviously, the first Zagreb index $M_1(G)$ is a special case of the first general Zagreb index Z_p for $p = 2$. The case for $p = 3$ has been discussed in [21] and was ignored in all later considerations and applications of Zagreb indices. In Chapter 5 we deduce the minimal first general Zagreb index for trees, unicyclic and bicyclic graphs of order n with n_1 pendent vertices.

2.2.3 Degree-Product Indices

In 1984, Narumi and Katayama [39] established a definition "*simple topological index*":

$$NK(G) = \prod_{v \in V(G)} d(v).$$

In recent works on this graph invariant [23, 30, 55], the name Narumi-Katayama index is being used. In [62] You and Liu deduced extremal $NK(G)$ of trees, unicyclic graphs with given diameter and vertices and the minimal $NK(G)$ of bicyclic graphs with given vertices. Todeschini et al. [52, 53] have recently proposed to consider the multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to:

$$\begin{aligned} \prod\nolimits_1 (G) &= \prod_{v \in V(G)} d(v)^2, \\ \prod\nolimits_2 (G) &= \prod_{uv \in E(G)} d(u)\, d(v) = \prod_{v \in V(G)} d(v)^{d(v)}. \end{aligned}$$

The properties of these "multiplicative Zagreb indices" have not been studied so far, and in Chapter 6 we attempt to contribute towards their better understanding.

Chapter 3

Bicyclic Graphs having Minimum General Sum-Connectivity Index for $-1 \leq \alpha < 0$

Du, Zhou and Trinajstić [11] proved that in the set of n-vertex connected unicyclic graphs, G with $n \geq 3$, for $-1 \leq \alpha < 0$, the graph consisting of a triangle and $n-3$ pendent vertices adjacent to the same vertex of this triangle is the unique graph with the minimum general sum-connectivity index $\chi_\alpha(G)$.
The problem of maximizing the general sum-connectivity index for connected bicyclic graphs for $\alpha \geq 1$ was considered in [48]. In this chapter, using a graph transformation and several inequalities, we show that in the class of n-vertex connected bicyclic graphs, G with $n \geq 4$, the graph consisting of two triangles having a common edge and $n-4$ pendent vertices adjacent to the same vertex of degree three of this graph is the unique graph minimizing the general sum-connectivity index for $-1 \leq \alpha < 0$ [2].

3.1 Preliminary results

In [11] a graph transformation was defined (it will be denoted t_1-transform), which strictly decreases the general sum-connectivity index of a graph for $\alpha < 0$ as follows: Let u, v be two adjacent vertices of a graph G such that $N(u) = \{v, z_1, \ldots, z_p\}, N(v) = \{u, w_1, \ldots, w_s\}$, where $\{z_1, \ldots, z_p\} \cap \{w_1, \ldots, w_s\} = \emptyset, p \geq 0$ and $s \geq 1$. By removing edges $vw_1, vw_2, \ldots, vw_s$ and adding new edges $uw_1, uw_2, \ldots, uw_s$ a new graph is produced, which is denoted $t_1(G)$.

Lemma 3.1.1. *[11] If $\alpha < 0$ then $\chi_\alpha(t_1(G)) < \chi_\alpha(G)$.*

Lemma 3.1.2. *Let G be a bicyclic graph and C a chordless cycle of G of length greater than or equal to four. Then there exists an edge $uv \in E(C)$ such that $(N(u)\backslash\{v\}) \cap (N(v)\backslash\{u\}) = \emptyset$.*

Proof. Suppose that $uv, vw \in E(C)$ such that $(N(u)\backslash\{v\}) \cap (N(v)\backslash\{u\}) \neq \emptyset$ and $(N(v)\backslash\{w\}) \cap (N(w)\backslash\{v\}) \neq \emptyset$. This implies the existence of a triangle T_1 having an edge uv and a triangle T_2 with an edge vw in G. We deduce that $T_1 \neq T_2$, since otherwise $V(T_1) = V(T_2) = \{u, v, w\}$, which contradicts the hypothesis that C is chordless. Therefore $V(T_1) = \{u, v, t_1\}$ and $V(T_2) = \{v, w, t_2\}$, where $t_1 \neq w$ and $t_2 \neq u$. If $t_1 \neq t_2$ then T_1, T_2 and C are linearly independent, which contradicts the property that G is bicyclic. It follows that $t_1 = t_2$ and by denoting $t_1 = t_2 = t$, C is the cycle u, v, w, t, u having the chord vt, a contradiction. Consequently, $(N(u)\backslash\{v\}) \cap (N(v)\backslash\{u\}) = \emptyset$ or $(N(v)\backslash\{w\}) \cap (N(w)\backslash\{v\}) = \emptyset$. $\square$

Lemma 3.1.3. *If $-1 \leq \alpha < 0$ then the functions $\zeta(x) = -(x+6)^\alpha + x(x+3)^\alpha - x(x+4)^\alpha$ and $\lambda(x) = (x+4)^\alpha - 3(x+6)^\alpha + x(x+3)^\alpha - x(x+5)^\alpha$ are strictly increasing for $x \geq 0$.*

Proof. We have $\zeta(x) = h(x) - h(x+1)$, where $h(x) = (x+4)^\alpha + (x+5)^\alpha + x(x+3)^\alpha$ and we get $h''(x) = \alpha(\alpha-1)(x+4)^{\alpha-2} + \alpha(\alpha-1)(x+5)^{\alpha-2} + (x\alpha(\alpha+1) + 6\alpha)(x+3)^{\alpha-2} <$

$\alpha(x(\alpha+1)+2(\alpha+2))(x+3)^{\alpha-2}<0$. Since $h(x)$ is strictly concave, it follows that $\zeta(x)$ is strictly increasing for $x \geq 0$.

Similarly, $\lambda(x)=\eta(x)-\eta(x+2)+\psi(x)$, where $\eta(x)=x(x+3)^{\alpha}+2(x+5)^{\alpha}+(x+4)^{\alpha}$ and $\psi(x)=2(x+7)^{\alpha}-2(x+6)^{\alpha}$ is strictly increasing. Also, $\eta(x)$ is strictly concave since $\eta''(x)<\alpha(\alpha+1)(x+3)^{\alpha-1}$. □

3.2 Main Results

For $n \geq 4$ let $\mathcal{A}(n)$ denote the set of n-vertex connected bicyclic graphs consisting of two triangles ABC and BCD having a common edge BC and $n-4$ pendent vertices adjacent to some vertices of these triangles. Similarly, let $\mathcal{B}(n)$ be the set of connected bicyclic graphs of order $n \geq 5$ constructed from two triangles ABC and CDE with a common vertex C and $n-5$ pendent vertices adjacent to some vertices A, B, C, D, E. First we shall find the graphs from these two classes having minimum general sum-connectivity index. In this section we suppose that $-1 \leq \alpha < 0$.

Lemma 3.2.1. *Let $G_1 \in \mathcal{A}(n)$ be such that in B, C, A, D are adjacent p, q, s, t pendent vertices, respectively $(p+q+s+t=n-4)$. We move p pendent edges from B to C and denote the resulting graph by G_2. If $p, q \geq 1$ then $\Delta=\chi_{\alpha}(G_1)-\chi_{\alpha}(G_2)>0$.*

Proof. We have $\Delta=\gamma(p,q,s)+\gamma(p,q,t)+p((p+4)^{\alpha}-(p+q+4)^{\alpha})+q((q+4)^{\alpha}-(p+q+4)^{\alpha})$, where $\gamma(p,q,s)=(p+s+5)^{\alpha}-(s+5)^{\alpha}+(s+q+5)^{\alpha}-(s+p+q+5)^{\alpha}$ and $\gamma(p,q,t)=(p+t+5)^{\alpha}-(t+5)^{\alpha}+(t+q+5)^{\alpha}-(t+p+q+5)^{\alpha}$. We deduce $\gamma(p,q,s)=\rho(s+5)-\rho(s+q+5)$, where $\rho(x)=(x+p)^{\alpha}-x^{\alpha}$ is strictly concave. It follows that $\gamma(p,q,s)$ is strictly increasing in s, having a minimum for $s=0$. Similarly, $\gamma(p,q,t)$ is strictly increasing in t and reaches its minimum for $t=0$. Hence $\Delta \geq 2((p+5)^{\alpha}-5^{\alpha}+(q+5)^{\alpha}-(p+q+5)^{\alpha})+p((p+4)^{\alpha}-(p+q+4)^{\alpha})+q((q+4)^{\alpha}-(p+q+4)^{\alpha})$. Since the function $x^{\alpha}-(x+q)^{\alpha}$ is strictly decreasing for

$q \geq 1$, it follows that $(p+4)^\alpha - (p+q+4)^\alpha > (p+5)^\alpha - (p+q+5)^\alpha$; similarly, $(q+4)^\alpha - (p+q+4)^\alpha > (q+5)^\alpha - (p+q+5)^\alpha$, which yields $\Delta > E(p,q) - 2 \cdot 5^\alpha$, where $E(p,q) = (p+2)(p+5)^\alpha + (q+2)(q+5)^\alpha - (p+q+2)(p+q+5)^\alpha$. Let $\varphi(x) = x(x+3)^\alpha$; this function is strictly concave since $\varphi''(x) < 0$ for $-1 \leq \alpha < 0$. We can write $(p+2)(p+5)^\alpha - (p+q+2)(p+q+5)^\alpha = \varphi(p+2) - \varphi(p+q+2)$, which is strictly increasing in $p \geq 0$ for fixed $q, q > 0$. Consequently, for any $p \geq 1$ we have $E(p,q) > E(0,q) = 2 \cdot 5^\alpha$, which yields $\Delta > 0$. □

Lemma 3.2.2. *Let $G_1 \in \mathcal{A}(n)$ be such that in A, D, C are adjacent p, q, r pendent vertices, respectively $(p+q+r = n-4)$. We move p pendent edges from A to C and q pendent edges from D to C and denote the resulting graph by G_2. If $p+q \geq 1$ then $\Delta = \chi_\alpha(G_1) - \chi_\alpha(G_2) > 0$.*

Proof. In this case $\Delta = (p+5)^\alpha - 5^\alpha + (q+5)^\alpha - 5^\alpha + (r+6)^\alpha - (p+q+r+6)^\alpha + (p+r+5)^\alpha - (p+q+r+5)^\alpha + (q+r+5)^\alpha - (p+q+r+5)^\alpha + p(p+3)^\alpha + q(q+3)^\alpha + r(r+4)^\alpha - (p+q+r)(p+q+r+4)^\alpha$. This expression is symmetric in p and q. By selecting only terms depending of p in Δ and denoting $p = x$ we obtain the following function $f(x) = (x+5)^\alpha + x(x+3)^\alpha + (x+r+5)^\alpha - 2(x+q+r+5)^\alpha - (x+q+r+6)^\alpha - (x+q+r)(x+q+r+4)^\alpha$. We shall prove that $f(x)$ is strictly increasing for $x \geq 0$. Its derivative equals $f'(x) = \alpha(x+5)^{\alpha-1} + \alpha(x+r+5)^{\alpha-1} - 2\alpha(x+q+r+5)^{\alpha-1} - \alpha(x+q+r+6)^{\alpha-1} + (x(\alpha+1)+3)(x+3)^{\alpha-1} - (x(\alpha+1)+q(\alpha+1)+r(\alpha+1)+4)(x+q+r+4)^{\alpha-1}$. We have $\alpha(x+r+5)^{\alpha-1} \geq \alpha(x+5)^{\alpha-1}$ and equality holds only for $r = 0$. By denoting $q+r = y$, we deduce that the partial derivative of $f'(x)$ relatively to $y \geq 0$ equals

$$\alpha[-2(\alpha-1)(y+x+5)^{\alpha-2} - (\alpha-1)(y+x+6)^{\alpha-2} - (y+x+4)^{\alpha-2}(y(\alpha+1)+x(\alpha+1)+8)]$$

$$> -\alpha(y+x+4)^{\alpha-2}(y(\alpha+1)+x(\alpha+1)+3\alpha+5) > 0$$

for $-1 \leq \alpha < 0$. Hence the smallest value of $f'(x)$ is reached for $q = r = 0$ and this is $-\alpha(x+6)^{\alpha-1} + (x(\alpha+1)+3)(x+3)^{\alpha-1} - (x(\alpha+1)+4)(x+4)^{\alpha-1}$, which equals

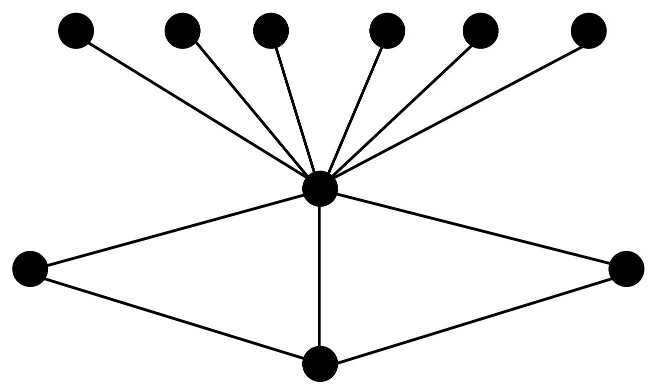

Figure 3.1: Graph having minimal general sum-connectivity index in $\mathcal{A}(10)$

the derivative of the function $-(x+6)^\alpha + x(x+3)^\alpha - x(x+4)^\alpha$. By Lemma 3.1.3 this derivative is strictly positive for $x \geq 0$, which implies $f'(x) > 0$ for $x \geq 0$. By the symmetry of Δ in p and q it follows that Δ is strictly increasing in both $p \geq 0$ and $q \geq 0$, the minimum value being reached for $p = q = 0$, hence $\Delta \geq 0$. Since $p + q \geq 1$ it follows that $\Delta > 0$. □

As a consequence of Lemmas 3.2.1 and 3.2.2 one deduces that in the set $\mathcal{A}(n)$ the unique graph having minimum general sum-connectivity index consists of two triangles having a common edge and $n - 4$ pendent vertices adjacent to a vertex of degree three of this graph. It can be obtained from the n-vertex star $K_{1,n-1}$ by adding two edges having a common extremity (a path P_3) and will be denoted by $K_{1,n-1} \oplus P_3$. Figure 3.1 is an example of a graph in $\mathcal{A}(10)$ having minimal general sum-connectivity index.

As a by-product we get the following corollary:

Corollary 3.2.3. *For every natural numbers p, r, s, t and $-1 \leq \alpha < 0$ the following inequality holds:*

$$(p+s+5)^\alpha+(p+t+5)^\alpha+(r+s+5)^\alpha+(r+t+5)^\alpha+(p+r+6)^\alpha-2(p+r+s+t+5)^\alpha-(p+r+s+t+6)^\alpha+p(p+4)^\alpha+r(r+4)^\alpha+s(s+3)^\alpha+t(t+3)^\alpha-(p+r+s+t)(p+r+s+t+4)^\alpha \geq 2\cdot 5^\alpha.$$

Equality is reached only for $p = s = t = 0$ or $r = s = t = 0$.

Proof. Consider a graph in $\mathcal{A}(n)$ having p, r, s, t pendent vertices adjacent to vertices B, C, A and D, respectively. By transfering pendent edges from A, B, D in C the general sum-connectivity index decreases and this fact is expressed by this inequality. □

Now we shall deduce the extremal graph in the set $\mathcal{B}(n)$.

Lemma 3.2.4. *Let $G_1 \in \mathcal{B}(n)$ be such that in A, B, C are adjacent p, q, r pendent vertices, respectively. We move one pendent edge from A to B and denote the resulting graph by G_2. If $1 \le p \le q$ then $\Delta = \chi_\alpha(G_1) - \chi_\alpha(G_2) > 0$.*

Proof. We get $\Delta = \chi_\alpha(G_1) - \chi_\alpha(G_2) = (p+r+6)^\alpha + (q+r+6)^\alpha - (p+r+5)^\alpha - (q+r+7)^\alpha + p(p+3)^\alpha + q(q+3)^\alpha - (p-1)(p+2)^\alpha - (q+1)(q+4)^\alpha = \eta(p) - \eta(q+1)$, where $\eta(x) = h(x) - h(x-1)$ and $h(x) = x(x+3)^\alpha + (x+r+6)^\alpha$. $h(x)$ is strictly concave for $x \ge 0$ and $-1 \le \alpha < 0$ since

$$h''(x) = (2\alpha(x+3) + \alpha(\alpha-1)x)(x+3)^{\alpha-2} + \alpha(\alpha-1)(x+r+6)^{\alpha-2}$$

$$< \alpha(x(\alpha+1) + \alpha + 5)(x+3)^{\alpha-2} < 0.$$

It follows that $\eta(x)$ is strictly decreasing in $x \ge 1$. This implies $\Delta > 0$ since $1 \le p < q+1$ by hypothesis. □

Consequently, the minimum general sum-connectivity index in the class $\mathcal{B}(n)$ will be reached only for those graphs having pendent edges incident only to vertices B, C and E.

Lemma 3.2.5. *Let $G_1 \in \mathcal{B}(n)$ be such that in B, C, E are adjacent p, r, q pendent vertices, respectively $(p+q+r = n-5)$. We move p pendent edges from B to C and q pendent edges from E to C and denote the resulting graph by G_2. If $p+q \ge 1$ then $\Delta = \chi_\alpha(G_1) - \chi_\alpha(G_2) > 0$.*

Proof. The idea of the proof is similar to that of Lemma 3.2.2. Using similar notations we get $\Delta = (p+4)^\alpha - 4^\alpha + (q+4)^\alpha - 4^\alpha + 2(r+6)^\alpha - 4(p+q+r+6)^\alpha + (p+r+6)^\alpha + (q+r+6)^\alpha + p(p+3)^\alpha + q(q+3)^\alpha + r(r+5)^\alpha - (p+q+r)(p+q+r+5)^\alpha$. Similarly, $f(x) = (x+4)^\alpha + x(x+3)^\alpha + (x+r+6)^\alpha - 4(x+q+r+6)^\alpha - (x+q+r)(x+q+r+5)^\alpha$ and $f'(x) = \alpha(x+4)^{\alpha-1} + \alpha(x+r+6)^{\alpha-1} - 4\alpha(x+q+r+6)^{\alpha-1} + (x(\alpha+1)+3)(x+3)^{\alpha-1} - (x(\alpha+1)+q(\alpha+1)+r(\alpha+1)+5)(x+q+r+5)^{\alpha-1}$. By denoting $q+r=y$, we deduce that the partial derivative of $f'(x)$ relatively to $y \geq 0$ is greater than $-\alpha(x+y+5)^{\alpha-2}((x+y)(\alpha+1)+4\alpha+6) > 0$. Hence the smallest value of $f'(x)$ is reached for $q=r=0$ and this is

$$\alpha(x+4)^{\alpha-1} - 3\alpha(x+6)^{\alpha-1} + (x(\alpha+1)+3)(x+3)^{\alpha-1} - (x(\alpha+1)+5)(x+5)^{\alpha-1},$$

which equals the derivative of the function $(x+4)^\alpha - 3(x+6)^\alpha + x(x+3)^\alpha - x(x+5)^\alpha$. By Lemma 2.3 this derivative is strictly positive for $x \geq 0$, thus giving $f'(x) > 0$ for $x \geq 0$. By the symmetry of Δ in p and q it follows that Δ is strictly increasing in both $p \geq 0$ and $q \geq 0$, the minimum value being reached for $p=q=0$, hence $\Delta \geq 0$. Since $p+q \geq 1$ it follows that $\Delta > 0$. □

Lemmas 3.2.4 and 3.2.5 imply that in the set $\mathcal{B}(n)$ the unique graph having minimum general sum-connectivity index consists of two triangles having a common vertex and $n-5$ pendent vertices adjacent to the vertex of degree four of this graph. It can be obtained from the n-vertex star $K_{1,n-1}$ by adding a matching consisting of two edges having no common extremity ($2K_2$) and will be denoted by $K_{1,n-1} \oplus 2K_2$. Figure 3.2 is an example of a graph in $\mathcal{B}(13)$ having minimal general sum-connectivity index.

As above, we deduce the following consequence:

Corollary 3.2.6. *For every natural numbers p, q, r, s, t and $-1 \leq \alpha < 0$ the following inequality holds:*

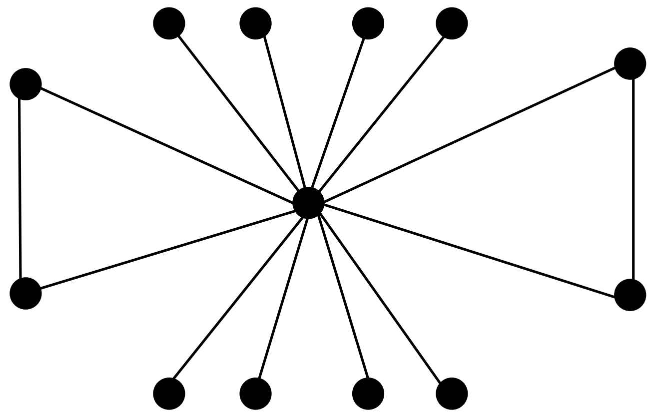

Figure 3.2: Graph having minimal general sum-connectivity index in $\mathcal{B}(13)$

$(p+q+4)^\alpha+(s+t+4)^\alpha+(p+r+6)^\alpha+(q+r+6)^\alpha+(r+s+6)^\alpha+(r+t+6)^\alpha+p(p+3)^\alpha+q(q+3)^\alpha+s(s+3)^\alpha+t(t+3)^\alpha+r(r+5)^\alpha-4(p+q+r+s+t+6)^\alpha-(p+q+r+s+t)(p+q+r+s+t+5)^\alpha \geq 2\cdot 4^\alpha$. *Equality is reached only for* $p=q=s=t=0$.

Proof. Consider a graph in $\mathcal{B}(n)$ having p,q,r,s,t pendent vertices adjacent to vertices A,B,C,D and E, respectively and swap all pendent vertices to be adjacent to C. □

Theorem 3.2.7. *For* $-1 \leq \alpha < 0$ *in the set of connected bicyclic graphs of order* $n \geq 4$ *the minimum general sum-connectivity index is reached only by the graph* $K_{1,n-1} \oplus P_3$ *consisting of two triangles with a common edge and* $n-4$ *pendent vertices adjacent to a vertex of degree three of this graph.*

Proof. Let G be a connected bicyclic graph of order n having minimum $\chi_\alpha(G)$. By successively deleting pendent edges of G we get: a) two vertex disjoint cycles joined by a path of length $l \geq 1$, or b) two cycles having a common vertex, or c) two cycles having a common path of length $r \geq 1$. This graph in either case a)$-$c) will be called the skeleton of G and denoted $S(G)$, G consisting of this skeleton and some vertex disjoint subtrees having each a common vertex with $S(G)$. These subtrees must be stars since otherwise by repeated application of t_1-transform $\chi_\alpha(G)$ will strictly decrease, contradicting the hypothesis. Now if $G \notin \mathcal{A}(n) \cup \mathcal{B}(n)$ then by the same transform $\chi_\alpha(G)$ can strictly decrease. This can be seen using Lemmas 3.1.1 and 3.1.2. It follows that $G \in \mathcal{A}(n) \cup \mathcal{B}(n)$. By the previous lemmas G is one of the graphs $K_{1,n-1} \oplus P_3$ or $K_{1,n-1} \oplus 2K_2$. It remains to compare the general sum-connectivity index for these two graphs for every $n \geq 5$. We obtain

$$\Delta = \chi_\alpha(K_{1,n-1} \oplus 2K_2) - \chi_\alpha(K_{1,n-1} \oplus P_3) = 2(4^\alpha - 5^\alpha) + 2(n+1)^\alpha - n^\alpha - (n+2)^\alpha.$$

Let $f(x) = 2(x+1)^\alpha - x^\alpha - (x+2)^\alpha$. We have $f'(x) = \alpha(2(x+1)^{\alpha-1} - x^{\alpha-1} - (x+2)^{\alpha-1}) > 0$ since function $x^{\alpha-1}$ being strictly convex, by Jensen's inequality the coefficient of α is negative. $f(x)$ being strictly increasing, it follows that $f(x) \geq f(5) = 2 \cdot 6^\alpha - 5^\alpha - 7^\alpha$ and $\Delta \geq 2 \cdot 4^\alpha - 3 \cdot 5^\alpha + 2 \cdot 6^\alpha - 7^\alpha > 5^\alpha - 7^\alpha > 0$, since $4^\alpha + 6^\alpha > 2 \cdot 5^\alpha$, again by Jensen' s inequality. □

Remark. The harmonic index of G, denoted $H(G)$ is equal to $2\chi_{-1}(G)$. In [67] it was shown that $K_{1,n-1} \oplus P_3$ is the unique graph minimizing the harmonic index in the class of connected bicyclic graphs of order $n \geq 4$. This graph has also several extremal properties. In the class of connected bicyclic graphs of order $n \geq 4$ it is the unique graph which has: maximum general sum-connectivity index for $\alpha \geq 1$ [48], maximum first and second Zagreb index [8], maximum Merrifield-Simmons index [10] and minimum Hosoya index [9]. Moreover, it is one of two graphs maximizing the Harary index [59].

Finally, we propose the following conjecture:

Conjecture 3.2.1. For $-1 \leq \alpha < 0$, among the connected graphs of order n and cyclomatic number equal to γ ($\gamma \geq 1$), the graph obtained from γ triangles having a common edge and $n - \gamma - 2$ pendent vertices adjacent to a vertex of maximum degree of this graph, has the minimum general sum-connectivity index.

Note that the conjecture is true for $\gamma = 1$ [11] and $\gamma = 2$ by Theorem 3.2.7 and the extremal graph for $\gamma = 0$ is $K_{1,n-1}$ [64]. For $\gamma = 1$ the graph $K_{1,n-1} \oplus K_2$ also minimizes Randić index for $-1 \le \alpha < 0$ [33].

Chapter 4

Extremal First and Second Zagreb Indices of k-Apex Trees

In this chapter we shall deduce upper and lower bounds of $M_1(G)$ and an upper bound of $M_2(G)$ in k-apex trees. The corresponding extremal k-apex trees are also characterized in each case.

Apex trees and k-apex trees were introduced in [58] under the name quasi-tree graphs and k-generalized quasi-tree graphs, respectively. Recently in [61] Kinkar Ch. Das et al. determined upper and lower bounds on weighted Harary indices for apex trees and k-apex trees.

For any $n \geq 3$ and $k \geq 1$, let

(a) $T(n)$ denote the set of all non-trivial apex trees of order n.

(b) $T_k(n)$ denote the set of all $k-$apex trees of order n.

Note that $T_1(n) = T(n)$.

We need the following upper bounds on Zagreb indices:

Lemma 4.0.1. [7, 8] If T is a tree of order n, then

(a) $M_1(T) \leq n(n-1)$

(b) $M_2(T) \leq (n-1)^2$

and in both cases equality holds if and only if $T = S_n$, the star graph of order n.

The following Lemma easily follows from definitions.

Lemma 4.0.2. If $u, v \in V(G)$ are not adjacent, then
(a) $M_1(G + uv) > M_1(G)$
(b) $M_2(G + uv) > M_2(G)$.

Lemma 4.0.3. If $G \in T(n)$, $M_1(G)$ and $M_2(G)$ are as large as possible and x is an apex vertex of G, then:
(a) $\delta G = 2$; (b) $d(x) = n - 1$.

Proof. (a) Suppose that $\delta G = 1$ and $y \in V(G)$ is a pendent vertex, then $xy \notin E(G)$ and $G + xy \in T(n)$. By Lemma 4.0.2, $M_1(G + xy) > M_1(G)$, which contradicts our hypothesis. Now we will show that $\delta G \leq 2$. Suppose that all vertices have degree greater or equal to three. Now for any vertex $v \in G$, each vertex in $G - v$ has degree greater or equal to two, which implies that $G - v$ is not a tree for any $v \in V(G)$. Hence $\delta G = 2$. The conclusion similarly holds for $M_2(G)$.

(b) Let $G \in T(n)$, $M_1(G)$ is as large as possible and x be an apex vertex of G. Suppose to the contrary that $d(x) < n - 1$; then there is a vertex $y \in V(G)$ such that $xy \notin E(G)$. Now $G + xy$ is also in $T(n)$ and $M_1(G + xy) > M_1(G)$, a contradiction, hence $d(x) = n - 1$. The conclusion similarly holds for $M_2(G)$. □

4.1 Extremal k-Apex Trees for $M_1(G)$

In this section we will find upper and lower bounds of $M_1(G)$ for k-apex trees.

Lemma 4.1.1. [31] For any two vertex-disjoint graphs G and H, we have:

$$\begin{aligned} M_1(G+H) = {} & M_1(G) + M_1(H) + |V(G)|\left(|V(G+H)| - |V(G)|\right)^2 \\ & + |V(H)|\left(|V(G+H)| - |V(H)|\right)^2 \\ & + 4|E(G)|\left(|V(G+H)| - |V(G)|\right) \\ & + 4|E(H)|\left(|V(G+H)| - |V(H)|\right). \end{aligned}$$

Theorem 4.1.1. *If $G \in T(n)$ and $n \geq 5$, then*

$$M_1(G) \leq 2n^2 - 6$$

and equality holds if and only if $G = K_1 + S_{n-1}$.

Proof. If $G \in T(n)$ and $M_1(G)$ is as large as possible, then by Lemma 4.0.3 we have $G = K_1 + T_{n-1}$, where T_{n-1} is a tree of order $n-1$, therefore by using Lemma 4.1.1, we obtain

$$\begin{aligned} M_1(G) =& M_1\left(K_1 + T_{n-1}\right) \\ =& M_1\left(K_1\right) + M_1\left(T_{n-1}\right) + \left|V\left(K_1\right)\right|\left(\left|V\left(K_1 + T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right)^2 \\ &+ |V(T_{n-1})|(|V(K_1 + T_{n-1})| - |V(T_{n-1})|)^2 \\ &+ 4|E(K_1)|(|V(K_1 + T_{n-1})| - |V(K_1)|) \\ &+ 4|E(T_{n-1})|(|V(K_1 + T_{n-1})| - |V(T_{n-1})|). \end{aligned}$$

Using Lemma 4.0.1 yields

$$\begin{aligned} M_1(G) \leq& \left(n-1\right)\left(n-2\right) + \left(n-1\right)^2 + \left(n-1\right)\left(n-\left(n-1\right)\right)^2 \\ &+ 4\left(n-2\right)\left(n-\left(n-1\right)\right) \\ =& 2n^2 - 6. \end{aligned}$$

Lemma 4.0.1 guaranties that equality holds if and only if $G = K_1 + S_{n-1}$. □

Theorem 4.1.2. *If $k \geq 2$, $n \geq 5$ and $G \in T_k(n)$, then*

$$M_1(G) \leq (k+1)(n-1)^2 + (n-k-1)(k+1)^2$$

and equality holds if and only if $G = K_k + S_{n-k}$.

Proof. We will prove it by induction on k. We have already proved this property for $k = 1$ in Theorem 4.1.1. Now suppose that the result is true for $(k-1)$-apex trees. Let $G \in T_k(n)$ has the maximum $M_1(G)$. Let $V_k \subset V(G)$ be the set of k-apex vertices. As $M_1(G+uv) > M_1(G)$ for any $uv \notin E(G)$ this implies that V_k forms a complete graph and for any $u \in V_k$, $d(u) = n-1$. So the number m of edges of the graph G is

$$\begin{aligned} m &= \binom{k}{2} + k(n-k) + n - k - 1 \\ &= \frac{k(k+1)}{2} + (k+1)(n-k-1). \end{aligned} \tag{4.1.1}$$

Let $x \in V_k$ and $V_{k-1} = V_k - x$. Note that $d(x) = n-1$, $G-x$ is a $(k-1)-$apex tree and

$$\begin{aligned} M_1(G-x) &= \sum_{v\in V(G-x)} (d_G(v)-1)^2 \\ &= \sum_{v\in V(G-x)} d_G^2(v) - 2\sum_{v\in V(G-x)} d_G(v) + \sum_{v\in V(G-x)} 1 \\ &= \sum_{v\in V(G)} d_G^2(v) - 2\sum_{v\in V(G)} d_G(v) + (n-1) - (n-1)^2 + 2(n-1) \\ &= M_1(G) - 4m - n^2 + 5n - 4 \end{aligned}$$

$$M_1(G) = M_1(G-x) + 4m + n^2 - 5n + 4.$$

By equation (4.1.1) we have

$$M_1(G) = M_1(G-x) + 4\left(\frac{k(k+1)}{2} + (k+1)(n-k-1)\right) + n^2 - 5n + 4.$$

As we have supposed that the result is true for $(k-1)$-apex trees, we deduce

$$\begin{aligned} M_1(G) \leq & k(n-2)^2 + (n-k-1)k^2 + 4\left(\frac{k(k+1)}{2} + (k+1)(n-k-1)\right) \\ & + n^2 - 5n + 4 \\ = & (k+1)(n-1)^2 + (n-k-1)(k+1)^2. \end{aligned}$$

Equality holds if and only if $G = K_k + S_{n-k}$. □

Theorem 4.1.3. *If $G \in T_k(n)$, $k \geq 1$ and $n \geq 3k$, then*

$$M_1(G) \geq 4n + 10k - 10$$

and equality holds if and only if G has $n - 2k + 2$ vertices of degree 2 and $2k - 2$ vertices of degree 3.

Proof. By definition of a k-apex tree, there exists a subset X of $V(G)$ of cardinality k such that $G - X$ is a tree and for any $Y \subset V(G)$ and $|Y| < k$, $G - Y$ is not a tree. It follows that $d(v) \geq 2$ for any vertex $v \in X$. If m denotes the number of edges of G, it follows that $m \geq 2k + n - k - 1 = n + k - 1$. For given natural numbers n and p, denote $f(x_1, \ldots, x_n; p) = \sum_{i=1}^{n} x_i^2$, where $\sum_{i=1}^{n} x_i = p$. If $\sum_{i=1}^{n} x_i = p$ and p is fixed, it is well known that $f(x_1, \ldots, x_n; p)$ is minimum if and only if $x_1, \ldots, x_n$ are almost equal, or $-1 \leq x_i - x_j \leq 1$ for every $i, j = 1, \ldots, n$. Denote this minimum by $f(n, p)$. It is clear that the function $f(n, p)$ is strictly increasing in p. We have $M_1(G) \geq f(n, 2m) \geq f(n, 2n + 2k - 2)$ since $m \geq n + k - 1$. Equality holds if and only if the degrees of G are almost equal and all vertices in X have the degree equal to two. Suppose that G has exactly the minimum number of edges, equal to $n + k - 1$ and denote by n_t and n_{t+1} the number of vertices of G having the degrees equal to t and $t + 1$, respectively, where $1 \leq n_t \leq n$. It follows that $n_{t+1} = n - n_t$ and $tn_t + (t + 1)(n - n_t) = 2n + 2k - 2$, or

$$(t + 1)n - n_t = 2n + 2k - 2. \tag{4.1.2}$$

If $t = 1$ then (4.1.2) becomes $2n - n_t = 2n + 2k - 2$, which is not possible since $2n - n_t \leq 2n - 1$ and $2n + 2k - 2 \geq 2n$. Also, if $t \geq 3$ we have $(t+1)n - n_t \geq 4n - n_t \geq 3n$ but $2n + 2k - 2 \leq \frac{8n}{3} - 2$ since $k \leq \frac{n}{3}$. Consequently, we have $t = 2$. From (4.1.2) we get $n_2 = n - 2k + 2$, hence the minimum of $M_1(G)$ is reached if and only if there exist $n - 2k + 2$ vertices of degree 2 and $2k - 2$ vertices of degree 3. Such a graph is illustrated in Fig. 4.1 □

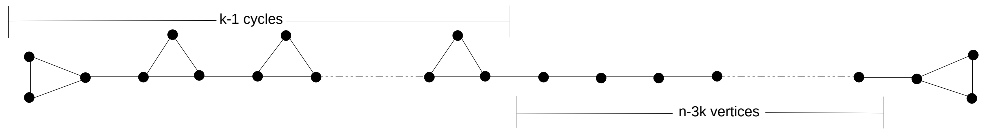

Figure 4.1: k-apex tree with almost equal degrees

4.2 Upper Bound of $M_2(G)$ for k-Apex Trees

In this section we will find a sharp upper bound of $M_2(G)$ for k-apex trees.

Lemma 4.2.1. [31] For any two vertex-disjoint graphs G and H, we have:

$$\begin{aligned}M_2(G+H) =& M_2(G) + (|V(G+H)| - |V(G)|)\,M_1(G) \\ &+ (|V(G+H)| - |V(G)|)\,|E(G)| + M_2(H) \\ &+ (|V(G+H)| - |V(H)|)\,M_1(H) \\ &+ (|V(G+H)| - |V(H)|)\,|E(H)| \\ &- \frac{1}{2}[2|E(G)| + |V(G)|(|V(G+H)| - |V(G)|)]^2 \\ &- \frac{1}{2}[2|E(H)| + |V(H)|(|V(G+H)| - |V(H)|)]^2 \\ &+ \frac{1}{2}\begin{bmatrix} 2|E(G)| + |V(G)|(|V(G+H)| - |V(G)|) \\ +2|E(H)| + |V(H)|(|V(G+H)| - |V(H)|)\end{bmatrix}^2.\end{aligned}$$

Theorem 4.2.1. *If $G \in T(n)$ and $n \geq 3$, then*

$$M_2(G) \leq (n-1)(5n-9)$$

and equality holds if and only if $G = K_1 + S_{n-1}$.

Proof. If $G \in T(n)$ and $M_2(G)$ is as large as possible then by Lemma4.0.3 $G = K_1 + T_{n-1}$, where T_{n-1} is a tree of order $n-1$. Therefore

$$M_2(G) = M_2(K_1 + T_{n-1})$$

and by using Lemma 4.2.1, we have

$$\begin{aligned}M_2(K_1+T_{n-1}) =& M_2(K_1) + \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right) M_1\left(K_1\right)\\ &+ \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right) E\left(K_1\right)\\ &+ M_2\left(T_{n-1}\right) + \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(T_{n-1}\right)\right|\right) M_1\left(T_{n-1}\right)\\ &+ \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(T_{n-1}\right)\right|\right) E\left(T_{n-1}\right)\\ &- \frac{1}{2}[2E\left(K_1\right) + \left|V\left(K_1\right)\right| \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right)]^2\\ &- \frac{1}{2}[2E\left(T_{n-1}\right) + \left|V\left(T_{n-1}\right)\right| \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(T_{n-1}\right)\right|\right)]^2\\ &+ \frac{1}{2}\begin{bmatrix} 2E\left(K_1\right) + \left|V\left(K_1\right)\right| \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right)\\ + \left|V\left(T_{n-1}\right)\right| \left(\left|V\left(K_1+T_{n-1}\right)\right| - \left|V\left(T_{n-1}\right)\right|\right)\\ + 2E\left(T_{n-1}\right)\end{bmatrix}^2\end{aligned}$$

Using Lemma 4.0.1 yields

$$M_2(G) \leq (n-1)(5n-9).$$

Lemma 4.0.1 guaranties that equality holds if and only if $G = K_1 + S_{n-1}$. □

Theorem 4.2.2. *If $k \geq 2$, $n \geq 5$ and $G \in T_k(n)$, then*

$$M_2(G) \leq \frac{(n-1)(k+1)(3nk+2n-5k-2k^2-2)}{2}$$

and equality holds if and only if $G = K_k + S_{n-k}$.

Proof. We will prove this theorem by induction on k. We have already proved this property for $k = 1$ in Theorem 4.2.1. Now suppose that the result is true for $(k-1)-$apex trees. Let $G \in T_k(n)$ has the maximum $M_2(G)$. Let $V_k \subset V(G)$ be the set of k-apex vertices. As $M_2(G+uv) \geq M_2(G)$ for any $uv \notin E(G)$ this property implies that V_k forms a complete graph and for any $u \in V_k$, $d(u) = n-1$. So the number m

of edges of graph G is

$$\begin{aligned} m &= \binom{k}{2} + k(n-k) + n - k - 1 \\ &= \frac{k(k+1)}{2} + (k+1)(n-k-1). \end{aligned} \tag{4.2.1}$$

Let $x \in V_k$ and $V_{k-1} = V_k - x$. Note that $d(x) = n-1$, $G - x$ is a $(k-1)-$apex tree and

$$\begin{aligned} M_2(G-x) = &\sum_{uv \in E(G-x)} (d_G(u)-1)(d_G(v)-1) \\ = &\sum_{uv \in E(G-x)} d_G(u)\, d_G(v) - \sum_{uv \in E(G-x)} (d_G(u) + d_G(v)) \\ &+ \sum_{uv \in E(G-x)} 1 \\ = &\sum_{uv \in E(G-x)} d_G(u)\, d_G(v) + \sum_{xu \in E(G)} (n-1)\, d_G(u) \\ &- \sum_{xu \in E(G)} (n-1)\, d_G(u) - \sum_{uv \in E(G-x)} (d_G(u) + d_G(v)) \\ &- \sum_{xu \in E(G)} ((n-1) + d_G(u)) + \sum_{xu \in E(G)} ((n-1) + d_G(u)) \\ &+ m - n + 1 \\ = &\sum_{uv \in E(G)} d_G(u) d_G(v) - \sum_{uv \in E(G)} (d_G(u) + d_G(v)) \\ &- \sum_{xu \in E(G)} (n-1) d_G(u) + \sum_{xu \in E(G)} ((n-1) + d_G(u)) + m - n + 1 \\ = &M_2(G) - M_1(G) - (n-1)(2m-n+1) + (n-1)^2 \\ &+ 2m - n + 1 + m - n + 1, \ \ or \end{aligned}$$

$$M_2(G) = M_2(G-x) + M_1(G) - 3m + 2n - 2 + (n-1)(2m-n+1) - (n-1)^2.$$

By equation (4.2.1) and Theorem 4.1.2, we have

$$\begin{aligned}M_2(G) \leq & M_2(G-x) + (k+1)(n-1)^2 + (n-k-1)(k+1)^2 \\ & - 3\left(\frac{k\,(k+1)}{2} + (k+1)\,(n-k-1)\right) + 2n - 2 \\ & + (n-1)\left(2\left(\frac{k\,(k+1)}{2} + (k+1)\,(n-k-1)\right) - n + 1\right) - (n-1)^2.\end{aligned}$$

As we have supposed that the result is true for $(k-1)$-apex trees, we get

$$\begin{aligned}M_2(G) \leq & \frac{k(n-2)\,(3(n-1)(k-1) + 2n - 2 - 5k + 5 - 2(k-1)^2 - 2)}{2} + \\ & + (k+1)(n-1)^2 + (n-k-1)(k+1)^2 - \\ & - 3\left(\frac{k\,(k+1)}{2} + (k+1)\,(n-k-1)\right) + 2n - 2 + \\ & + (n-1)\left(2\left(\frac{k\,(k+1)}{2} + (k+1)\,(n-k-1)\right) - n + 1\right) - (n-1)^2 \\ = & \frac{1}{2}\Big(5n^2k + 3n^2k^2 - 10nk^2 - 2nk^3 - 12nk + 2n^2 + 7k^2 + \\ & + 2k^3 + 7k - 4n + 2\Big) \\ = & \frac{1}{2}(nk + n - k - 1)(2n + 3nk - 5k - 2k^2 - 2) \\ = & \frac{(n-1)(k+1)(3nk + 2n - 5k - 2k^2 - 2)}{2}.\end{aligned}$$

Equality holds if and only if $G = K_k + S_{n-k}$. □

Chapter 5

Graphs with Fixed Number of Pendent Vertices and Minimal First General Zagreb Index

In this chapter we deal with the extension of our previous work [24]. We shall derive explicit expressions for minimal first general Zagreb index, which directly can be extended for $\gamma > 2$, where γ is the cyclomatic number of a graph.

Let $d(v)$ be the degree of the vertex $v \in V(G)$. If n_1 is the number of pendent vertices in a graph G of order n, then the graph is said to be an (n, n_1)-*graph*. First Zagreb index M_1 and first general Zagreb index $Z_p(G)$ for $p \in \mathbb{R}$ are defined as:

$$M_1(G) = \sum_{v \in V(G)} (d\,(v))^2,$$

$$Z_p(G) = \sum_{v \in V(G)} (d\,(v))^p.$$

Ivan Gutman in [16] found minimal $Z_p(G)$ for $p \geq 2$, G having n_1 pendent vertices and with very special number of vertices for simple connected graphs having cyclomatic number $\gamma \geq 0$. In what follows we will deduce the explicit expressions of minimal $Z_p(G)(p > 1)$ for (n, n_1)-graphs. Jamil et al. [27] have derived the explicit expressions for some other indices of the same graphs. The results obtained by us in

[24] now are special case of our new results for $p = 2$. For this we need an auxiliary result [8, 66].

5.1 An Auxiliary Lemma

Let $i_1, i_2, \ldots, i_n$ be positive integers. We say that these integers are almost equal if

$$\max\{i_1, i_2, \ldots, i_n\} - \min\{i_1, i_2, \ldots, i_n\} \leq 1.$$

Let $f(x) = x^p - (x-k)^p$, where $p > 1$, k is a positive integer and $x \geq k$. We get

$$\begin{aligned} f'(x) &= px^{p-1} - p(x-k)^{p-1} \\ f'(x) &= p\left(x^{p-1} - (x-k)^{p-1}\right) > 0 \qquad \text{for all } p > 1. \end{aligned}$$

This shows that $f(x)$ is strictly increasing for all $x \geq k$ and for all $p > 1$.

Lemma 5.1.1. [8, 66] *For $p > 1$ the general Zagreb index $Z_p(G)$ of a graph G will be minimal if the degrees of its non-pendent vertices are almost equal.*

Proof. Let u and v be any two vertices of the graph G. Let $d(u) = a$ and $d(v) = b$, such that $a - b = 2k$ or $2k+1$, where $k \geq 1$. If G' is a graph obtained from G so that $d(u) = a - k$ and $d(v) = b + k$, whereas the degrees of all other vertices in G' are the same as in G, then

$$\begin{aligned} Z_p(G) - Z_p(G') &= a^p + b^p - [(a-k)^p + (b+k)^p] \\ &= [a^p - (a-k)^p] - [(b+k)^p - b^p]. \end{aligned}$$

As above defined $f(x)$ is a strictly increasing function and $a > b + k$, therefore

$$f(a) = a^p - (a-k)^p > f(b) = (b+k)^p - b^p$$

$$\text{this implies} \qquad Z_p(G) - Z_p(G') > 0,$$

which shows that if the degrees of u and v are not almost equal then $Z_p(G)$ cannot be minimal for $p > 1$. □

5.2 (n, n_1)-Trees With Minimal First General Zagreb Index

Theorem 5.2.1. *Let T be a tree of order n with n_1 pendent vertices. Then for any $p > 1$*

$$Z_p(T) \geqslant n_1 + \left((n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor - n_1 + 2\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 1\right)^p +$$
$$\left(n - 2 - (n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 2\right)^p.$$

Equality is attained if and only if T consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor - n_1 + 2$ vertices of degree $t = \left\lfloor\frac{n-2}{n-n_1}\right\rfloor + 1$ and $n_{t+1} = n - 2 - (n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor$ vertices of degree $t+1$.

Proof. By lemma 5.1.1 the first general Zagreb index $Z_p(T)$ will be minimum if the degrees of its non-pendent vertices are almost equal.

Suppose that the tree T has minimum first general Zagreb index when it has n_t $(0 < n_t \leq n - n_1)$ non-pendent vertices of degree t and $n_{t+1} = n - n_1 - n_t$ non-pendent vertices of degree $t+1$. Then

$$Z_p(T) = n_1 + n_t t^p + (n - n_1 - n_t)(t+1)^p. \tag{5.2.1}$$

As tree of order n has size $n-1$, it follows that

$$n_1 + t n_t + (t+1)(n - n_1 - n_t) = 2n - 2, \tag{5.2.2}$$

or

$$t(n-n_1)-n_t=n-2. \tag{5.2.3}$$

We deduce

$$t-\frac{n_t}{n-n_1}=\frac{n-2}{n-n_1}$$
$$\left\lfloor t-\frac{n_t}{n-n_1}\right\rfloor=\left\lfloor\frac{n-2}{n-n_1}\right\rfloor$$
$$t-1=\left\lfloor\frac{n-2}{n-n_1}\right\rfloor$$

$$t=\left\lfloor\frac{n-2}{n-n_1}\right\rfloor+1. \tag{5.2.4}$$

From equations (5.2.3) and (5.2.4) we get

$$(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor+n-n_1-n_t=n-2$$

$$n_t=(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor-n_1+2. \tag{5.2.5}$$

As $n_{t+1}=n-n_1-n_t$, we deduce

$$n_{t+1}=n-2-(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor.$$

From equations (5.2.3), (5.2.4) and (5.2.5) we can write:

$$Z_p(T)\geqslant n_1+\left((n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor-n_1+2\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor+1\right)^p+$$
$$\left(n-2-(n-n_1)\left\lfloor\frac{n-2}{n-n_1}\right\rfloor\right)\left(\left\lfloor\frac{n-2}{n-n_1}\right\rfloor+2\right)^p.$$

Equality is attained if and only if T consists of n_1 pendent vertices, n_t vertices of degree t and n_{t+1} vertices of degree $t+1$. □

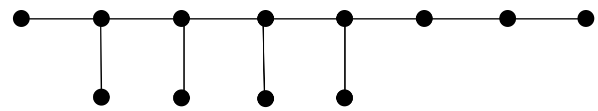

Figure 5.1: A tree having minimal first general Zagreb index

(n, n_1)-Trees with minimal first general Zagreb index of the form specified in Theorem 5.2.1 exist for any values of n and n_1 provided $n > n_1 \geq 2$. Figure 5.1 is an example of a tree of order 12 with 6 pendent vertices having minimal first general Zagreb index.

5.3 Unicyclic and Bicyclic (n, n_1)-Graphs with Minimal First General Zagreb Index

For $\gamma > 0$ the considerations are fully analogous although instead of equation (5.2.2) one has to use

$$n_1 + tn_t + (t+1)(n - n_1 - n_t) = 2(n - 1 + \gamma).$$

Without proof we state the results for $\gamma = 1$ and $\gamma = 2$.

Theorem 5.3.1. *Let U be a unicyclic graph of order n with n_1 pendent vertices. Then for any $p > 1$,*

$$Z_p(U) \geqslant n_1 + \left((n - n_1)\left\lfloor \frac{n}{n - n_1} \right\rfloor - n_1\right)\left(\left\lfloor \frac{n}{n - n_1} \right\rfloor + 1\right)^p + \left(n - (n - n_1)\left\lfloor \frac{n}{n - n_1} \right\rfloor\right)\left(\left\lfloor \frac{n}{n - n_1} \right\rfloor + 2\right)^p.$$

Equality is attained if and only if U consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor - n_1$ vertices of degree $t = \left\lfloor \frac{n}{n-n_1} \right\rfloor + 1$ and $n_{t+1} = n - (n - n_1)\left\lfloor \frac{n}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Unicyclic (n, n_1)-graphs with minimal first general Zagreb index of the form specified in Theorem 5.3.1, exist for any values of n and n_1, provided $n \geq 3$ and $n_1 \geq 0$. Figure 5.2 is an example of a unicyclic graph of order 13 with 8 pendent vertices having minimal first general Zagreb index.

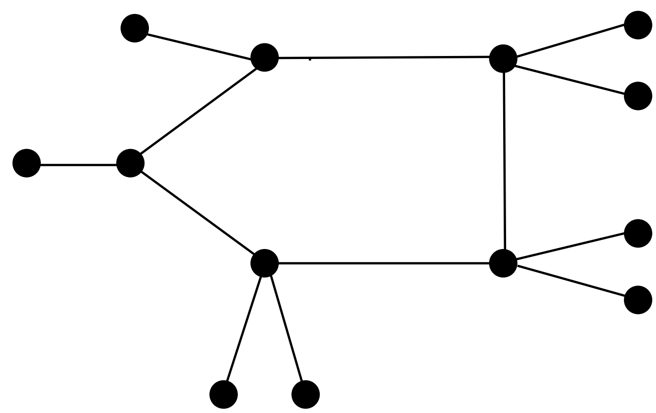

Figure 5.2: A unicyclic graph having minimal first general Zagreb index

Theorem 5.3.2. *Let B be a bicyclic graph of order n with n_1 pendent vertices. Then for any $p > 1$,*

$$Z_p(B) \geqslant n_1 + \left((n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor - n_1 - 2\right)\left(\left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 1\right)^p + \left(n + 2 - (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor\right)\left(\left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 2\right)^p .$$

Equality is attained if and only if B consists of n_1 pendent vertices, $n_t = (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor - n_1 - 2$ vertices of degree $t = \left\lfloor \frac{n+2}{n-n_1} \right\rfloor + 1$ and $n_{t+1} = n + 2 - (n - n_1)\left\lfloor \frac{n+2}{n-n_1} \right\rfloor$ vertices of degree $t + 1$.

Bicyclic (n, n_1)-graphs with minimal first general Zagreb index of the form specified in Theorem 5.3.2, exist for any values of n and n_1, provided $n \geq 4$ and $n_1 \geq 0$. Figure 5.3 is an example of a bicyclic graph of order 13 with 8 pendent vertices having minimal first general Zagreb index.

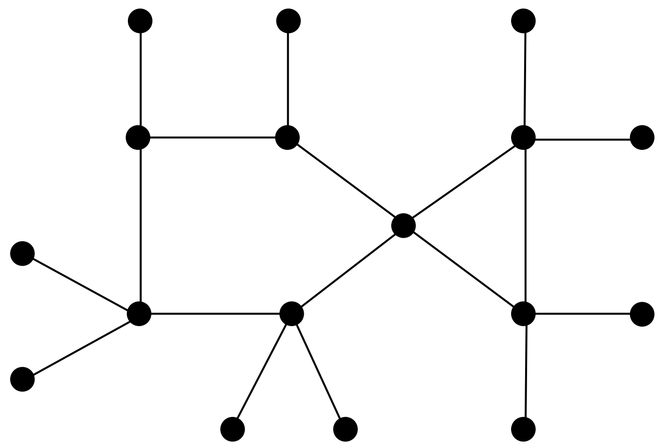

Figure 5.3: A bicyclic graph having minimal first general Zagreb index

Also for any value of γ greater than 2, structural characterizations of γ-cyclic (n, n_1)-graphs with minimal first general Zagreb index can be achieved in a fully analogous manner.

Chapter 6

Extremal Degree-Product Indices of Graphs with Fixed Number of Pendent Vertices and Cyclomatic Number

In this chapter, we compute the extremal $NK(G)$, $\prod_1(G)$ and $\prod_2(G)$ for the graphs with given order, number of pendent vertices and cyclomatic number.

In [24], I. Gutman et al. computed the minimal first Zagreb index of graphs with fixed number of pendent vertices. In this chapter we determine the extremal values of the Narumi-Katayama, first Zagreb and second Zagreb indices of connected (n, n_1)-graphs with fixed cyclomatic number and show that these bounds are tight [27].

6.1 Extremal (n, n_1)-Graphs Relatively to Narumi-Katayama Index

We need the following well-known property.

Lemma 6.1.1. Let $n, r, x_1, x_2, \dots, x_n$ be positive integers such that $x_i \geq r$ and

$$\sum_{i=1}^{n} x_i = a \geq rn.$$

Then $\prod_{i=1}^{n} x_i$ is minimum if and only if there exists an index i, $1 \leq i \leq n$ such that $x_i = a-(n-1)r$ and $x_j = r$ for every $j \neq i$ and it is maximum if and only if $x_1, \dots, x_n$ are almost equal, i.e., $\max\{x_1, \dots, x_n\} - \min\{x_1, \dots, x_n\} \leq 1$.

Since in a connected graph a non-pendent vertex has at least degree 2 and $NK(G) = \prod_{x \in V(G), d(x) \geq 2} d(x)$, by Lemma 6.1.1 we have the following consequence:

Corollary 6.1.1. *If G is a connected graph of order n and size m with n_1 pendent vertices $(n > n_1)$ then*

$$NK\left(G\right) \geq 2^{n-n_1-1}\left(2m - 2n + n_1 + 2\right).$$

This bound is achieved if G has one vertex of degree $2m - 2n + n_1 + 2$ and all other non-pendent vertices are of degree 2.

Let G be a connected (n, n_1)-graph with cyclomatic number γ. If $\gamma = 0$ then G is a tree and $2 \leq n_1 \leq n-1$. Otherwise we suppose that $0 \leq n_1 \leq n-1$. We define the auxiliary quantities t, n_t and n_{t+1} as:

$$t = \left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 1, \qquad n_t = (n - n_1)\left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor - n_1 - 2(\gamma - 1)$$

$$n_{t+1} = n - (n - n_1)\left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 2(\gamma - 1).$$

Recall that $\lfloor x \rfloor$ is the greatest integer that is not greater then x.

Theorem 6.1.1. *Let G be a connected (n, n_1)-graph with cyclomatic number γ. Then*

$$2^{n-n_1-1}(2\gamma + n_1) \leq NK\left(G\right) \leq \left(\left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 1\right)^{n_t} \left(\left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 2\right)^{n_{t+1}}.$$

(a) For trees ($\gamma = 0$) both lower and upper bounds are reached.

(b) For $\gamma \geq 1$ lower bound can be attained for $n \geq 2\gamma + 1 + n_1$ and upper bound for $n \geq 3\gamma + n_1$.

Proof. Lower bound. A graph with n vertices and cyclomatic number γ has size $m = n + \gamma - 1$, so by Corollary 6.1.1, we have

$$NK(G) \geq 2^{n-n_1-1}(2\gamma + n_1).$$

To see that this bound can be reached for $\gamma = 0$ consider a path with $n - n_1 + 1$ vertices and add $n_1 - 1$ pendent vertices, all adjacent to a unique end vertex of this path.

For $\gamma > 0$ take γ cycles, having together $n - n_1$ vertices and a unique common vertex. Then all n_1 remaining vertices are joined each by an edge to this common vertex. It follows that $n \geq 2\gamma + 1 + n_1$, and equality holds when all γ cycles have a length equal to 3. Figures 6.1, 6.3 and 6.5 illustrate graphs having minimum NK index for $n = 22, n_1 = 13$ and $\gamma = 0, 1, 2$ respectively.

Upper bound. By Lemma **??** $NK(G)$ will be maximum if G has n_t $(0 < n_t \leq n - n_1)$ non-pendent vertices of degree t and $n_{t+1} = n - n_1 - n_t$ non-pendent vertices of degree $t + 1$, then

$$NK\,(G) \leq t^{n_t}(t+1)^{n_{t+1}}. \tag{6.1.1}$$

As a graph of order n with cyclomatic number γ has size $n + \gamma - 1$, we can write:

$$n_1 + tn_t + (t+1)(n - n_1 - n_t) = 2(n + \gamma - 1), \tag{6.1.2}$$

which yields

$$t(n - n_1) - n_t = n + 2(\gamma - 1), \tag{6.1.3}$$

or

$$t - \frac{n_t}{n - n_1} = \frac{n + 2(\gamma - 1)}{n - n_1}.$$

Taking integer parts,

$$\left\lfloor t - \frac{n_t}{n-n_1} \right\rfloor = \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor.$$

Since t is a positive integer, we obtain

$$t-1 = \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor,$$

or

$$t = \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 1. \tag{6.1.4}$$

From equations (6.1.3) and (6.1.4),

$$(n-n_1) \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + n - n_1 - n_t = n + 2(\gamma-1),$$

which gives

$$n_t = (n-n_1) \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor - n_1 - 2(\gamma-1).$$

As $n_{t+1} = n - n_1 - n_t$, we get:

$$n_{t+1} = n + 2(\gamma-1) - (n-n_1) \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor.$$

From equations (6.1.1) and (6.1.4) we deduce:

$$NK\,(G) \leq \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 1 \right)^{n_t} \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 2 \right)^{n_{t+1}},$$

as required.

For $\gamma = 0$ the upper bound can be reached. To see this consider a path P_{n-n_1} with $n - n_1$ vertices. Now add the remaining n_1 pendent vertices using the following algorithm: join each new vertex sequentially, to a vertex of P_{n-n_1}, having minimum degree. Initially, all vertices have degrees 1 and 2 and after that we obtain, by construction, a tree with n_1 pendent vertices and non-pendent vertices having almost equal degrees.

For $\gamma > 0$ take γ vertex disjoint cycles containing together $n - n_1$ vertices and joined by edges, such that by contracting each cycle to a vertex yields a path with γ vertices. Then join each new vertex sequentially, to a vertex on the cycles, having minimum degree. Initially all degrees are 2 and 3 and after that we obtain, by construction, almost equal degrees for non-pendent vertices. We have $n \geq 3\gamma + n_1$, and equality holds when all vertex disjoint cycles have a length equal to 3. Figures 6.2, 6.4 and 6.6 illustrate graphs having maximum NK index for $n = 22, n_1 = 13$ and $\gamma = 0, 1, 2$ respectively. □

6.2 Extremal (n, n_1)-Graphs Relatively to Multiplicative Zagreb Indices

Since $\prod_1(G) = NK(G)^2$, Theorem 6.1.1 implies the following corollary.

Corollary 6.2.1. *Let G be a connected (n, n_1)-graph with cyclomatic number γ. Then*

$$4^{n-n_1-1}(2\gamma+n_1)^2 \leq \prod\nolimits_1(G) \leq \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 1\right)^{2n_t} \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 2\right)^{2n_{t+1}}.$$

(a) For trees ($\gamma = 0$) both lower and upper bounds are reached.
(b) For $\gamma \geq 1$ lower bound can be attained for $n \geq 2\gamma + 1 + n_1$ and upper bound for $n \geq 3\gamma + n_1$.

Some extremal properties of the second multiplicative Zagreb index in some families of graphs are deduced below. First we need the following property:

Lemma 6.2.1. Function $\varphi(x) = \frac{x^x}{(x-1)^{x-1}}$ is increasing for $x \geq 2$.

Proof. We get

$$\varphi'(x) = \frac{x^x(x-1)^{x-1}(\ln x - \ln(x-1))}{(x-1)^{2(x-1)}} > 0,$$

therefore φ is increasing for $x \geq 2$. □

Let Γ_{n,n_1} be the family of connected graphs with order n and n_1 pendent vertices. We define a family of trees of order n with n_1 pendent vertices, denoted $\mathcal{T}^*_{n,n_1}$ as the set of trees of order n consisting of n_1 paths having a common end vertex. Note that $\mathcal{T}^*_{n,2} = \{P_n\}$.

Theorem 6.2.1. *Let T be a tree in Γ_{n,n_1}, where $n > n_1 \geq 2$, then*

$$\prod\nolimits_2(T) \leq n_1^{n_1}4^{n-n_1-1}$$

and the equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$.

Proof. We shall prove this result by induction on $n + n_1$. Let $f(n, n_1) = n_1^{n_1}4^{n-n_1-1}$. If $n_1 = 2$ and $n > n_1$, then $T \cong P_n$ and by direct calculation $\prod_2(P_n) = 4^{n-2}$ and this equals $f(n, 2)$, hence the property is verified.

Let $n_1 \geq 3$ and suppose that the result is true for any tree of order n' with n'_1 pendent vertices such that $7 \leq n' + n'_1 < n + n_1$. Let T be a tree in Γ_{n,n_1} and x be a pendent vertex of T. If $xy \in E(T)$, suppose that $d(y) = a$. We shall consider two cases: 1) $a = 2$ and 2) $a \geq 3$.

1) In this case $T - x$ has order $n - 1$ and n_1 pendent vertices, hence $\prod_2(T) = 2^2\prod_2(T - x)$ and by the induction hypothesis $\prod_2(T - x) \leq f(n - 1, n_1)$ and the equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1}$. It follows that $\prod_2(T) \leq f(n, n_1)$ and the equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$.

2) $T - x$ having order $n - 1$ and $n_1 - 1$ pendent vertices, we have

$$\prod\nolimits_2(T) = \frac{a^a}{(a-1)^{a-1}}\prod\nolimits_2(T - x).$$

By our supposition of induction,

$$\prod\nolimits_2 (T) \leq \frac{a^a}{(a-1)^{a-1}} f(n-1, n_1-1).$$

Equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1-1}$. The last inequality may be written

$$\prod\nolimits_2 (T) \leq \frac{a^a}{(a-1)^{a-1}} \frac{(n_1-1)^{n_1-1}}{n_1^{n_1}} f(n, n_1).$$

By Lemma 6.2.1, $\varphi(x)$ is an increasing function, so $\frac{a^a}{(a-1)^{a-1}}$ is maximum for maximum value of a and in the set of trees with n_1 pendent vertices the maximum degree of a vertex is n_1, so

$$\prod\nolimits_2 (T) \leq f(n, n_1).$$

Equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$ since $d(y) = n_1$ only if x is adjacent to the unique vertex in $T - x$ of degree $n_1 - 1$. □

We define a family of unicyclic graphs of order n with n_1 pendent vertices, denoted $\mathcal{U}^*_{n,n_1}$, as the set of unicyclic graphs of order n consisting of a cycle C_p ($p \geq 3$) and n_1 paths having a common end vertex which lies on C_p.

Theorem 6.2.2. *Let U be a unicyclic graph in Γ_{n,n_1} such that $n > n_1 \geq 0$, then*

$$\prod\nolimits_2 (U) \leq (n_1+2)^{n_1+2} 4^{n-n_1-1}$$

and the equality holds if and only if $U \in \mathcal{U}^*_{n,n_1}$.

Proof. We shall prove this result also by induction on $n+n_1$. Let $g(n, n_1) = (n_1+2)^{n_1+2}4^{n-n_1-1}$. If $n_1 = 0$, then $U \cong C_n$ and by direct calculations $\prod_2 (C_n) = 4^n = g(n, 0)$. Let $n_1 \geq 1$ and suppose that the result is true for any unicyclic graph of order n' with n'_1 pendent vertices, such that $4 \leq n' + n'_1 < n + n_1$. As before, let U be a unicyclic graph in Γ_{n,n_1} and x a pendent vertex of U. If y is adjacent to x in U, let $d(y) = a$. We shall consider two cases: 1) $a = 2$ and 2) $a \geq 3$.

1) In this case $U - x$ is unicyclic, has order $n - 1$ and n_1 pendent vertices, hence

$\prod_2(U) = 2^2 \prod_2(U-x)$ and by the induction hypothesis $\prod_2(U-x) \leq g(n-1, n_1)$ and the equality holds if and only if $U - x \in \mathfrak{U}^*_{n-1,n_1}$. It follows that $\prod_2(U) \leq g(n, n_1)$ and the equality holds if and only if $U \in \mathfrak{U}^*_{n,n_1}$.

2) $U - x$ having order $n-1$ and $n_1 - 1$ pendent vertices, we get

$$\prod\nolimits_2 (U) = \frac{a^a}{(a-1)^{a-1}} \prod\nolimits_2 (U-x).$$

By induction hypothesis,

$$\prod\nolimits_2 (U) \leq \frac{a^a}{(a-1)^{a-1}} g\,(n-1, n_1-1),$$

and equality holds if and only if $U \in \mathfrak{U}^*_{n-1,n_1-1}$. We deduce

$$\prod\nolimits_2 (U) \leq \frac{a^a}{(a-1)^{a-1}} \frac{(n_1+1)^{n_1+1}}{(n_1+2)^{n_1+2}} g\,(n, n_1).$$

By Lemma 6.2.1, $\varphi(x)$ is strictly increasing in a and in the set of unicyclic graphs with n_1 pendent vertices the maximum degree of a vertex is $n_1 + 2$, so

$$\prod\nolimits_2 (U) \leq g\,(n, n_1).$$

Equality holds if and only if $U \in \mathfrak{U}^*_{n,n_1}$ since $d(y) = n_1 + 2$ only if x is adjacent to the unique vertex in $U - x$ of degree $n_1 + 1$, which is common to the cycle and $n_1 - 1$ pendent paths. □

In a similar way we can generalize this result for a given cyclomatic number $\gamma \geq 2$ for every $n \geq 3\gamma + n_1$ as follows: Let $G_{n,n_1,\gamma}$ be the set of connected graphs of order n, having n_1 pendent vertices and cyclomatic number γ, consisting of γ cycles having a common vertex w and n_1 paths having an end vertex w. If G is a connected graph of order n, having n_1 pendent vertices and cyclomatic number γ, then

$$\prod\nolimits_2 (G) \leq (n_1 + 2\gamma)^{n_1+2\gamma} 4^{n-n_1-1}$$

and the equality holds if and only if $G \in G_{n,n_1,\gamma}$.

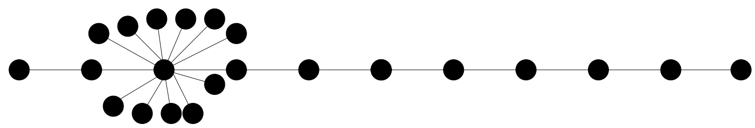

Figure 6.1: Tree with $n = 22$ and $n_1 = 13$ having minimal NK index.

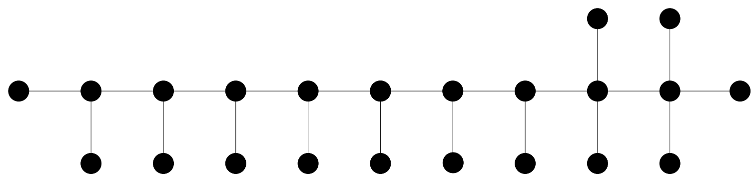

Figure 6.2: Tree with $n = 22$ and $n_1 = 13$ having maximal NK index.

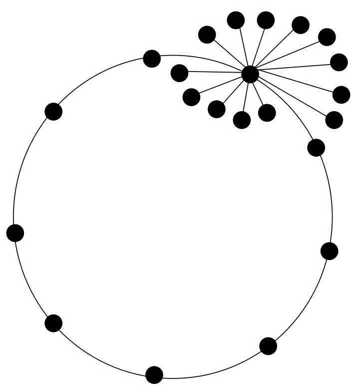

Figure 6.3: Unicyclic graph with $n = 22$ and $n_1 = 13$ having minimal NK index.

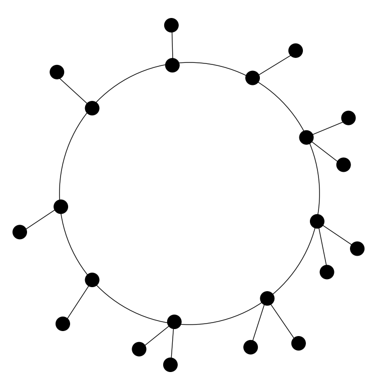

Figure 6.4: Unicyclic graph with $n = 22$ and $n_1 = 13$ having maximal NK index.

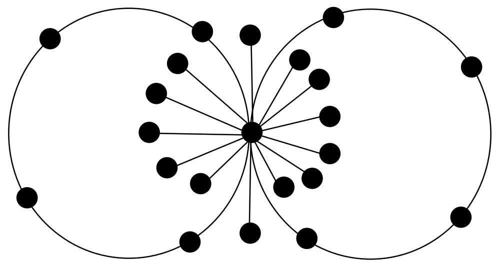

Figure 6.5: Bicyclic graph with $n = 22$ and $n_1 = 13$ having minimal NK index.

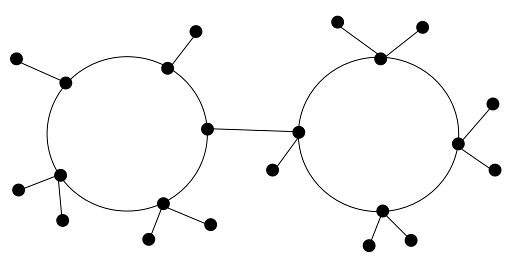

Figure 6.6: Bicyclic graph with $n = 22$ and $n_1 = 13$ having maximal NK index.

Chapter 7

Concluding Remarks and Possible Directions for Future Work

In chapter 3, using a graph transformation and several inequalities, we showed that in the class of n-vertex connected bicyclic graphs G with $n \geq 4$, the graph consisting of two triangles having a common edge and $n-4$ pendent vertices adjacent to the same vertex of degree three of this graph is the unique graph minimizing the general sum-connectivity index for $-1 \leq \alpha < 0$ [2]. For possible future work, we propose the following conjecture:

Conjecture 7.0.1. For $-1 \leq \alpha < 0$, among the connected graphs of order n and cyclomatic number equal to γ ($\gamma \geq 1$), the graph obtained from γ triangles having a common edge and $n-\gamma-2$ pendent vertices adjacent to a vertex of maximum degree of this graph, has the minimum general sum-connectivity index.

Note that the conjecture is true for $k = 1$ [11] and $k = 2$ by Theorem 3.2.7 and the extremal graph for $k = 0$ is $K_{1,n-1}$ [64]. For $k = 1$ the graph $K_{1,n-1} \oplus K_2$ also minimizes Randić index for $-1 \leq \alpha < 0$ [33].

In chapter 4 we deduced upper and lower bounds of $M_1(G)$ and an upper bound of $M_2(G)$ in k-apex trees. We proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 5$, the graph $K_k + S_{n-k}$ maximizes the first and second Zagreb indices. We also proved that in the class of k-apex trees ($k \geq 1$) of order $n \geq 3k$ the graph G that has $n-2k+2$ vertices of degree 2 and $2k-2$ vertices of degree 3 minimizes the first Zagreb index. It would be interesting to deduce similar results for other famous indices for example Randić index, sum-connectivity index, eccentric connectivity index etc. of k-apex trees.

In chapter 5 we dealt with the extension of our previous work [24]. We obtained explicit expressions for minimal first general Zagreb index $Z_p(G)$ for $p > 1$, which directly can be extended for $\gamma > 2$, where γ is the cyclomatic number of G. It would be interesting to get similar results for other values of p.

In chapter 6 we determined the extremal values of the Narumi-Katayama, first Zagreb and second Zagreb indices of connected (n, n_1)-graphs with fixed cyclomatic number and showed that these bounds are tight [27].

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