

T. R.  
VAN YÜZÜNCÜ YIL UNIVERSITY  
INSTITUTE OF NATURAL AND APPLIED SCIENCES  
DEPARTMENT OF MATHEMATICS

**ON RELATION BETWEEN ZAGREB INDICES AND STRATIFIED  
DOMINATION NUMBER**

M.Sc. THESIS

PREPARED BY: Abdalla Khdir Abdalla MANGURI  
SUPERVISOR: Assist. Prof. Dr. Mehmet Şerif ALDEMİR

VAN-2018



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## ACCEPTANCE and APPROVAL PAGE

This thesis entitled "ON RELATION BETWEEN ZAGREB INDICES AND STRATIFIED DOMINATION NUMBER" presented by Abdalla Khdir Abdalla MANGURI under supervision of Assist. Prof. Dr. Mehmet Şerif ALDEMİR in the department of Mathematics has been accepted as a M.Sc thesis according to Legislations of Graduate Higher Education on 30/03/2018 with unanimity of votes members of jury.

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Prof. Dr. Mustafa ŞERİF  
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All the information's presented in the thesis were obtained according to the frame of ethical behavior and academic rules. And also, all kinds of statement and source information that does not belong to me in this work prepared in accordance with the rules of thesis were cited to the source of information absolutely.



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Abdalla Khdir Abdalla MANGURI





## ABSTRACT

### ON RELATION BETWEEN ZAGREB INDICES AND STRATIFIED DOMINATION NUMBERS

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M.Sc. Thesis, Mathematics Science  
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This master thesis study, which is consists of four chapter, was presented some last studies about the Zagreb indices and domination parameter numbers. Zagreb indices are the most important things in a graph theory and used indices in mathematical chemistry. The relations between Zagreb indices and the other graph invariants have been studied for forty years. But the relationships between Zagreb indices and the domination type parameters have been studied very recently. In this paper we characterize maximum trees with a known as stratified domination number and we firstly compute the eccentric connectivity indices for the generalized Petersen graphs.

**Keywords:** Domination number, Eccentric connectivity index, Generalized Petersen Graphs, Stratified domination, Zagreb indices.



## ÖZET

### ZAGREB İNDEKSLERİ İLE PARÇALANIŞLI BASKINLIK SAYILARI ARASINDAKİ İLİŞKİLER

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Dört bölümden oluşan bu tez çalışmasında Zagreb İndeksleri ve Baskınlık sayıları arasındaki bazı ilişkiler sunulmuştur. Zagreb İndeksleri, matematiksel kimyada en önemli olan ve en çok kullanılan indekslerdir. Zagreb indeksleriyle, diğer graf değişmezleri arasındaki ilişkiler kırk yıldır çalışılmaktadır. Fakat Zagreb indekslerinin baskınlık sayıları ile olan ilişkisi son zamanlarda çalışılmaya başlanmıştır. Bu çalışma da Zagreb indekslerini, parçalanışlı baskınlık sayılarına göre maksimum yapan ağaç grafları karakterize edilerek, en uzak bağlantılılık indekslerinin genelleştirilmiş Petersen grafları için değerleri hesaplanmıştır.

**Anahtar kelimeler:** Baskınlık sayısı, En Uzak Bağlıntılılık İndeksi, Genelleştirilmiş Petersen Graf, Parçalanışlı Baskınlık, Zagreb İndeksleri.



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2018

Abdalla Khdir Abdalla MANGURI



## CONTENTS

|   | <b>Pages</b> |
|---|--------------|
| ABSTRACT .....  | i            |
| ÖZET .....  | iii          |
| ACKNOWLEDGMENT .....  | v            |
| CONTENTS .....  | vii          |
| LIST OF TABLES.....   | ix           |
| LIST OF THE FIGURES .....   | xi           |
| SYMBOLS AND ABBREVIATIONS .....   | xiii         |
| 1. INTRODUCTION .....   | 1            |
| 1.1. Connection Dominating Set and Applications.....                          | 3            |
| 1.2. Bipartite Graph and Set Covering Problem .....                           | 4            |
| 1.3. Some Definitions.....  | 6            |
| 2. LITERATURE REVIEW .....  | 9            |
| 3. FIRST ZAGREB INDICES.....  | 13           |
| 3.1. Comparing First Zagreb Index and the Maximum degree of Trees.....        | 15           |
| 3.2. Second Zagreb Indices .....  | 16           |
| 3.3. Comparing the Second Zagreb Index and Co-index of Trees.....             | 16           |
| 3.4. On the Relation between First Zagreb Index and Second Zagreb Index ..... | 18           |
| 4. ECCENTRIC CONNECTIVITY INDICES OF GENERALIZED PETERSEN<br>GRAPHS.....      | 29           |
| 5. CONCLUSION .....   | 37           |
| REFERENCES .....  | 39           |
| EXTENDED TURKISH SUMMARY .....  | 43           |
| CURRICULUM VITAE.....   | 49           |





## LIST OF TABLES

| Tables   | Pages |
|--|-------|
| 3.1. Show the degree for $T_n, \gamma_{F_3}$ ..... | 21    |
| 3.2. Parameter $\gamma_{F_i}(G)$ .....             | 27    |





## LIST OF THE FIGURES

| Figures   | pages |
|---|-------|
| Figure 1.1. Two Dominating Sets in a Graph G.....   | 2     |
| Figure 1.2. Completed and Empty Graph.....  | 3     |
| Figure 1.3. Connected Dominating Set .....  | 4     |
| Figure 1.4. Connected Dominating Set .....  | 4     |
| Figure 1.5. Bipartite Graph $G = (V, E)$ .....  | 5     |
| Figure 1.6. Bipartite Graph .....   | 5     |
| Figure 1.7. Undirected Graph.....   | 6     |
| Figure 1.8. Undirected Graph Edge adjacency.....  | 7     |
| Figure 1.9. The Graph G for the Example 1.3.2.....  | 7     |
| Figure 3.1. First Zagreb Indices.....   | 13    |
| Figure 3.2. The Trees forming the class $T^*(9) = \{T(9,3,3)$ (right), $T(9,2,5)$ (left) $\}$ . ..... | 14    |
| Figure 3.3. Second Zagreb Indices .....   | 16    |
| Figure 3.4. Non-Star Trees with a Stratified Domination Number .....                                  | 20    |
| Figure 3.5. Stratified Domination of $T_{n,F_3}$ with the Maximum First Zagreb Indices .....          | 21    |
| Figure 3.6. Stratified Domination Graph $T_{15,10}$ .....   | 21    |
| Figure 3.7. $F_3$ -domination in a Non-Star Tree.....   | 22    |
| Figure 3.8. An example of Stratified Domination of a Tree.....  | 23    |
| Figure 3.9. Stratified Domination Number.....   | 25    |
| Figure 3.10. Stratified Domination Graph $T_{12,10}$ .....  | 25    |
| Figure 3.11. Stratified Domination Graph $T_{24,16}$ .....  | 27    |

| <b>Figures</b>   | <b>pages</b> |
|--|--------------|
| Figure 3.12. The five 2-Stratified domination graphs ..... | 27           |
| Figure 4.1. Eccentricity Graph .....                       | 34           |
| Figure 4.2. Generalized Petersen Graph (8, 2) .....        | 35           |
| Figure 4.3. Generalized Petersen Graph (8, 3) .....        | 36           |



## SYMBOLS AND ABBREVIATIONS

Some symbols and abbreviations used in this study are presented below, along with descriptions.

| <b>Symbols</b>                     | <b>Description</b>                 |
|------------------------------------|------------------------------------|
| $\mathbf{A} = \mathbf{a}_{i,j}$    | Adjacency Matrices of a graph G    |
| $\mathbf{u}, \mathbf{v}$           | Vertices of a graph G              |
| $\mathbf{e}$                       | Edge of a graph G                  |
| $\mathbf{E}(\mathbf{G})$           | The Set of edges of a graph G      |
| $\mathbf{M}_1(\mathbf{G})$         | First Zagreb indices               |
| $\mathbf{M}_2(\mathbf{G})$         | Second Zagreb indices              |
| $\acute{\mathbf{M}}_1(\mathbf{G})$ | First Zagreb co-index              |
| $\acute{\mathbf{M}}_2(\mathbf{G})$ | Second Zagreb co-index             |
| $\mathbf{d}(\mathbf{u})$           | Degree of vertex u                 |
| $\mathbf{d}(\mathbf{v})$           | Degree of vertex v                 |
| $\boldsymbol{\gamma}(\mathbf{G})$  | Domination number of a graph (G)   |
| $\boldsymbol{\gamma}_t$            | Total Domination Number            |
| $\boldsymbol{\gamma}_r$            | Restrained Domination Number       |
| $\boldsymbol{\gamma}_{tr}$         | Total Restrained Domination Number |
| $\boldsymbol{\gamma}_k$            | K-Domination Number                |
| $\boldsymbol{\gamma}_{F_3}$        | Stratified Domination Number       |
| $\mathbf{T}$                       | Tree                               |
| $\mathbf{Diam}(\mathbf{t})$        | Diameter of tree (t)               |

| <b>Abbreviation</b> | <b>Description</b>                        |
|---------------------|---|
| <b>TDN</b>          | Total Domination Number                   |
| <b>TDS</b>          | Total Domination Set                      |
| <b>RDS</b>          | Restrained Domination Set                 |
| <b>TRDS</b>         | Total Restrained Domination Set           |
| <b>QSPR</b>         | Quantitative-Structure Property Relations |
| <b>CDS</b>          | Connected Dominating Set                  |
| <b>ECI</b>          | Eccentric Connectivity Index              |
| <b>CEI</b>          | Connective Eccentric Index                |
| <b>GPG</b>          | Generalized Petersen Graph                |

## 1. INTRODUCTION

A graph is a ordered pair such that  $G = (V, E)$ , the set of  $V$  is a limited arrangement of vertices and the arrangement of  $E$  is a set component of elements. Set of  $E$  consists of the two component subsets of  $V$ . In this examination we are researching just finite graphs without directed and self-loops or several edges (Diestel, 2000). Let graph  $G = (V, E)$  be a graph. The vertices of the graph  $G$  are denoting by  $n$ , and for each vertex of  $u$  and  $v$ , the graph  $G$  has an edges denoted by  $uv$ , linking the vertices of  $u$  and  $v$ . The term  $d(u)$  denotes the number of degree of edges which is incident to the vertex  $u$ . In chemistry many molecules have been presented by it's a graph. Numbers which are obtained from the molecular graphs of molecules are called topological indices. Some topological indices show an important role in chemistry and pharmacology, etc. topological indices may group into two classes: degree version topological indices and distance version topological indices. The First Zagreb Index  $M_1(G)$ , Second Zagreb Index  $M_2(G)$  are illustrated as follows:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 \quad (1.1)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \quad (1.2)$$

(Gutman and Trinajstić, 1972).

The two oldest of topological indices are famous as Zagreb indices, that defined by Gutman and Trinajstić in 1972. The authors observed the dependence of full  $\pi$ -electron energy on some octanes. The graph  $G$  is known as a stratified graphs if  $V(G)$  is partitioned in some subsets. The fixed partition  $V(G)$  with the graph  $G$  consist of only two subsets such that the graph  $V(G) = \{V_1, V_2\}$ , then graph  $(G)$  is named as a 2-stratified graph. In a 2-stratified graph, we accept that the one class is colored blue and the other class is colored red. Let graph  $G = (V, E)$  be a simple graph with the edge set  $E$  and vertex set  $V$ , and let  $S \subseteq V$ . The set  $S$  is named as a (DS) dominating set if each vertex in  $V - S$  is adjacent to at

least one vertex of  $S$ . The set  $S$  is known as the (TDS) Total dominating set if all vertex in  $V$  is adjacent to at least one vertex of  $S$ , and  $S$  is called as (RDS) Restrained dominating set if all vertex in  $V - S$  is adjacent to a vertex in  $S$  and to a vertex in  $V - S$ . If  $S$  is simultaneously a (TDS) Total Domination Set and a (RDS) Restrained Domination Set, then  $S$  is a (TRDS) Total Restrained Dominating Set of a graph  $G$ . The set is named  $S$  as a  $k$ -dominating set if all vertex in  $V - S$  is adjacent at least  $k$  vertices in  $S$ . Number of his domination of a graph  $G$ , represented by  $\gamma(G)$ , is equal to the smallest cardinality of the dominating set. A dominating set of the graph  $G$  of cardinality  $\gamma(G)$  is called a  $\gamma(G)$  - set. The (TDS) total domination number, (RDS) restrained domination number, (TRDS) total restrained domination number and  $k$ -domination number of the graph  $G$  by  $\gamma_t(G)$ ,  $\gamma_r(G)$ ,  $\gamma_{tr}(G)$  and  $\gamma_k(G)$ , respectively (Chartrand et al., 1995).

Domination Number of a graph  $G$  as vertex a recollection that a neighbor of  $v$  is a vertex together to  $v$  in a graph  $G$ . Also, the district  $N(v)$  of  $v$  is the set of nationals of  $v$  a vertex  $v$  in a graph  $G$  is said to dominate it self and every of it is national, that is,  $v$  dominates the vertices in it is closed district  $N(v)$ , then,  $v$  dominates  $1 + \deg v$  vertices of a graph  $G$ , for example a set  $S$  of vertices of graph  $G$  is set of dominating of graph  $G$  if each of  $G$  is dominated as vertex by specific vertex in  $S$  (Teresa et al., 2009).

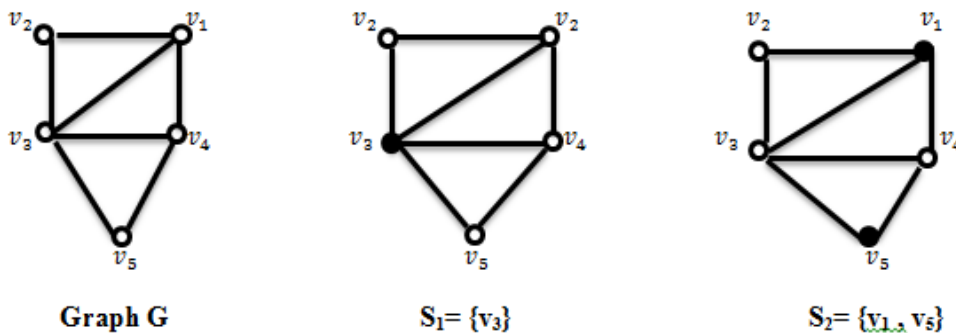


Figure 1.1. Two Dominating Sets in a Graph  $G$ .

The Domination number is definite for all graphs let  $G$  is an order graph  $n$ , then  $1 \leq \gamma(G) \leq n$ . A graph  $G$  is a graph of order  $n$ , has number of domination equal 1 if and only if  $G$  holds a degree of vertex  $v$  is  $n - 1$ , in which case of  $\{v\}$  as a minimum set of



dominating, while  $\gamma(G) = n$  if and only if  $\gamma(G) = \bar{k}n$  in which item  $v(G)$  is the single set of dominating. For example:

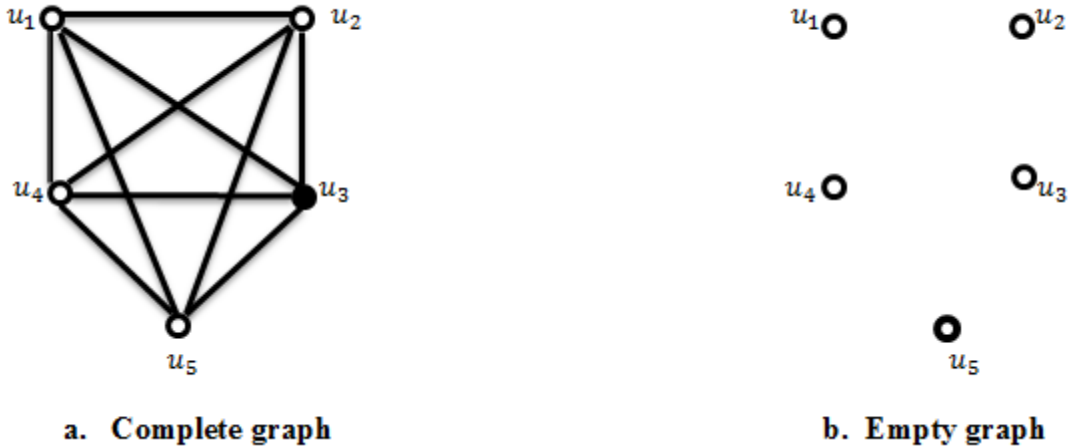


Figure 1.2. Complete and Empty graph.

$\gamma(G) = 1$  for a complete graph.  $\gamma(G) = n$  for an empty graph.

Defined by  $K_5$  but for the figure (b) is empty graph there for define by  $\bar{k}_5$ . (Diestel, 2000).

### 1.1. Connection Dominating Set and Applications

A dominating set  $D$  for the graph  $G$  which was set with all vertex of  $G$  is also in  $D$  or adjacent to some vertex in  $D$ . Domination number of the graph  $G$  denoted by the maximum size of set of the dominating of vertices in  $G$ . The dominating set problem concerns result a maximum dominating set. For example, figure 1.3, there are two red vertices  $b$  and  $c$  are clearly memberships of a dominating set as all vertex that is not in the dominating set  $\{b, c\}$ , is adjacent  $b$  or  $c$ .

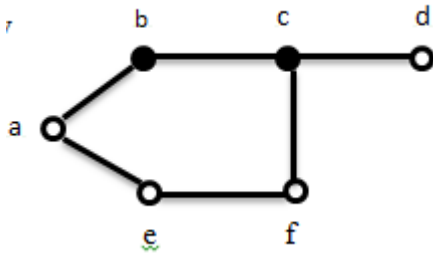


Figure 1.3. Connected Dominating set.

For this example we can change to the dominating set by convert the vertex b to a vertex e. After that we say that this graph is dominating set because all a summit in this graph is dominated by the some vertex exactly c and e. (Diestel, 2000).

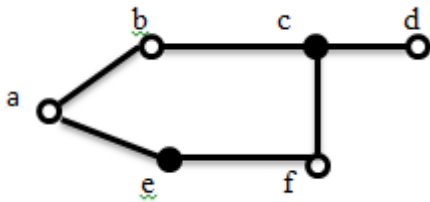


Figure 1.4. Connected Dominating set.

## 1.2. Bipartite Graph and Set Covering Problem

The connected set of dominating problem is used to find a maximum connected set of dominating, determining a maximum connected set of dominating to be known as NP-complete problems, this essentially means that these problem class of s cannot be solved quickly, some authors have suggested procedures for finding approximate maximal connected dominating set the problem for calculating a maximum connected dominating set was mapped in to a set covering problem, the set covering problem is basically a problem regarding bipartite graphs that can be specified as follows suppose that  $H$  is a bipartite graph, containing of two sets of vertex  $A$  and vertex  $B$  where edges only produce a connection between set vertex  $A$  and set vertex  $B$ , also assume that for each vertex in  $B$ , there is at least one edge connecting it to a vertex in  $A$ , the goal is to find maximal subset  $C$

of set vertex of A such that every vertex in set B is covered by some vertex in C. (Diestel, 2000).

**Example 1.2.1** graph (G) is a connected graph (v) is represented the vertex (or node) and (e) is represented the edge (or element), let A and B are copies of vertices of E, construct a bipartite graph H putting an edge between vertices v of A and vertex u of B is they are adjacent to each other. All vertices (a,b,c,d,e and f) in a graph G are represented by A, and is also all vertices (a,b,c,d,e and f) in G represented by B,

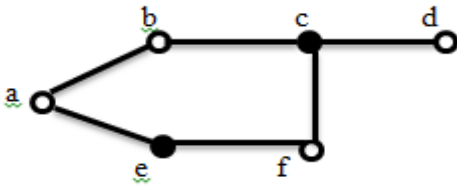


Figure 1.5. Bipartite Graph  $G = (V, E)$ .

Now we put at between vertex from A and vertex from B and they are adjacent to each other, for original graph, clearly.

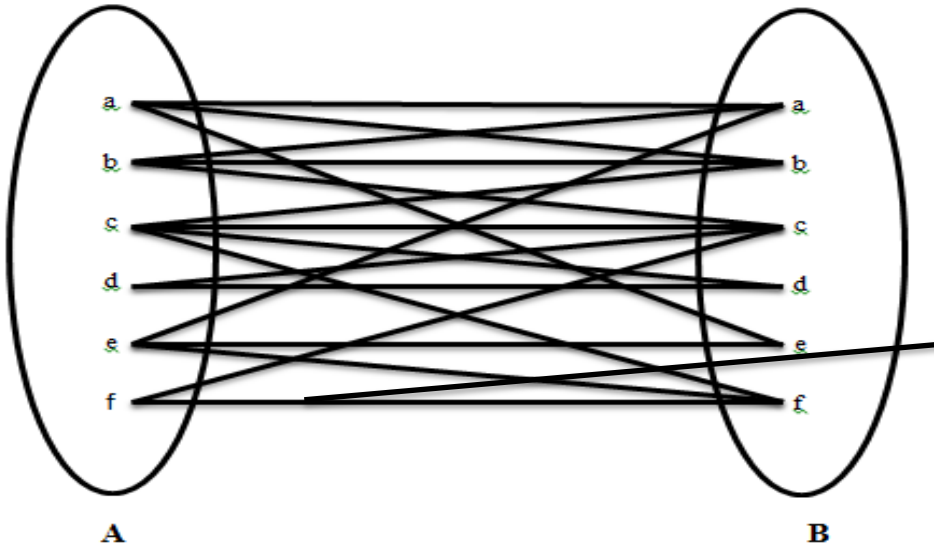


Figure 1.6. Bipartite Graph.

### 1.3. Some Definitions

Definition 1.3.1: (Undirected graph): Graph  $(G)$  is a tuple  $(V, E)$ , where finite set is signed as  $V$  of nodes called vertices, and the set of  $E$  is a finite set of edges (or elements). See figure 1.7 and undirected graph. In undirected graph edge  $e \in E$  is an unordered match  $(u,v)$  where  $u,v \in V$  but in directed graph the edge  $e$  is a requested combine  $(u,v)$  an edge  $(u,v)$  is outline from vertex  $u$  and is occurrence to vertex  $v$ . (Diestel, 2000). We show this basic facts in the below example.

**Example 1.3.1:** The set of vertex  $v = \{1,2,3,4,5\}$  In Fig 1.7 the set of edges denote by  $e = \{(1,2), (1,3), (2,3), (2,4), (3,5), (4,5)\}$

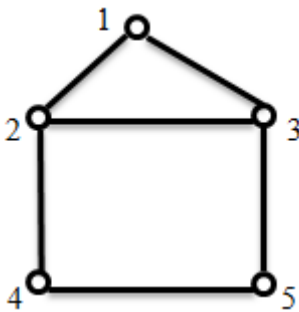


Figure 1.7. Undirected Graph.

Definition 1.3.2: (Vertex Adjacency). Let  $G = (V, E)$  as a simple graph. 2 vertices  $v_1$  and  $v_2$  are said will be adjoining if there exists an edge  $e \in E$  so  $e = (v_1, v_2)$ . A vertex  $v$  is self-contiguous if  $e = \{v\}$  is a component of  $E$  (Diestel, 2000).

Definition 1.3.3: (Edge Adjacency): Let  $G = (V, E)$  be a graph. 2 edges  $e_1$  and  $e_2$  are said to be adjoining if there exists a vertex  $v$  with the goal that  $v$  is a component of both  $e_1$  and  $e_2$  (as sets). Graph can be spoken to by the nearness network or an edge (or vertex) list. Adjacency matrices have a value  $a_{i,j}=1$  if vertex  $i$  and vertex  $j$  share an edge and  $a_{i,j} = 0$  if vertex do not share an edge (Diestel, 2000). See Fig 1.8 for the explanation.

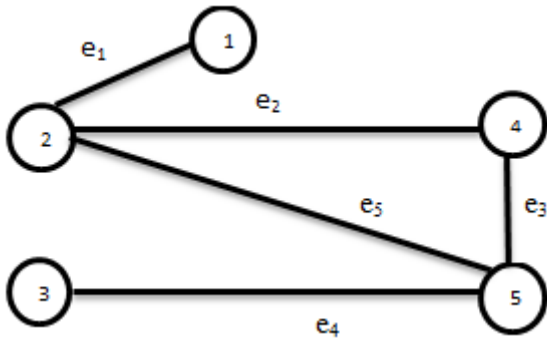


Figure 1.8. Undirected Graph Edge Adjacency.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 1 & 1 \\ 3 & 0 & 0 & 0 & 0 & 1 \\ 4 & 0 & 1 & 0 & 0 & 1 \\ 5 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}$$

An undirected graph and its adjacent matrix representation.

**Example 1.3.2.** Consider the set of vertices  $V = \{1, 2, 3, 4\}$ . The set of edges

$$E = \{(1, 2), (2, 3), (3, 4), (4, 1)\}.$$

Then the graph of  $G = (V, E)$  has 4 edges and 4 vertices. It is typically easier denoted this graphically. See Fig 1.9

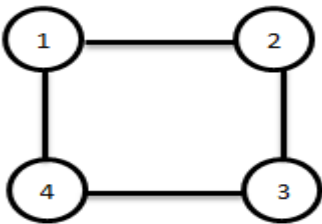


Figure 1.9. The Graph  $G$  for the example 1.3.2.

**Definition 1.3.** (Biregular graph) A graph  $G$  is said to be biregular if its vertex degrees accept precisely two distinct esteems. The edge  $E(G)$  of a diagram  $G$  is equivalent to the aggregate of the supreme estimations of the eigenvalues of  $G$ .

Definition 1.3.5: (First Zagreb co-index) Let  $G$  a chance to be a basic associated graph, at that point the First Zagreb co-index is characterized as  $\dot{M}_1(G) = \sum(d(u) + d(v))$ .

Definition 1.3.6: (Second Zagreb co-index) Let  $G$  a chance to be a basic associated graph, at that point the Second Zagreb co-index is characterized as  $\dot{M}_2(G) = \sum(d(u)d(v))$ . (Ranjini et al., 2013)

Definition 1.3.7: (Eccentricity) Let  $G$  be a connected simple graph with the vertex set  $V$  and the edge set  $E$ . The distance between two vertices  $u, v$  of  $G$ , written  $d(u, v)$ , is the length of a shortest  $u-v$  path in  $G$ . For any vertex  $v$  of  $G$ , the eccentricity of  $v$ , denoted by  $\varepsilon_v$ , is the largest distance from  $v$  to other vertices in  $G$ . (Diestel, 2000).

Definition 1.3.8: (Eccentric connectivity and connective eccentric index ) The eccentric connectivity index of a simple connected graph known as;

$$\varepsilon^c(G) = \sum_{v \in V} \varepsilon_v d_v.$$

And the connective oddness index of a simple connected graph known as;

$$\varepsilon^{ce}(G) = \sum_{v \in V} \frac{d_v}{\varepsilon_v}.$$

Definition 1.3.9: (Generalized Petersen Graph) The generalized Petersen graph of  $GP(n, k)$  is the graph with set of vertex  $V = U \cup W$ , where  $U = \{u_i : 0 \leq i \leq n-1\}$  and  $W = \{w_i : 0 \leq i \leq n-1\}$ , and the edge set is the form of  $E = \{u_i u_{i+1}, u_i w_i, w_i w_{i+k} : 0 \leq i \leq n-1, \text{subscripts modulo } n\}$  (Diestel, 2000)

## 2. LITERATURE REVIEW

In today's world from to basic sciences to social sciences, many problems can be represented by graph theory especially in chemistry. The theory of chemical graphs has an important place in theoretical chemistry. In the medicine and chemical experiments, the researchers found that there is a potential connection between the properties of the compounds and their sub-atomic structures. Thus, the researchers have a tendency to decide the highlights of medications by ideals of mathematical method. This is done with the help of topological indices. Topological indices have been expansively used to modeling some chemical and physical properties of molecules in physics, chemistry and pharmacological sciences. A numerical value obtained from the structure of graph is called a topological index, Wiener, 1947 and Gutman 1972, showed that topological indices could be used modeling chemical properties of octanes. (Wiener, 1947; Gutman et al., 1972).

Actually the story of topological indices has been started by Wiener and Platt in 1947. Both authors showed that the chemical properties of alkanes gave good correlation to their indices value. (Platt, 1947; Wiener, 1947). The well-known degree based Zagreb indices defined by Gutman and Trinajstić, to modeling  $\pi$ -electron energy of alternant carbons (Gutman et al., 1972). Among the all topological indices, the Zagreb indices have been used for QSPR researches more considerably than any other topological indices in chemical and mathematical literature (Gutman et al., 1972).

Up to now, studies on the Zagreb indices have focused on the relationships of the Zagreb indices to other graph invariants. The relations between Zagreb indices and domination number parameter have been recently started. As of now, all educations have been focused on the relations between domination number parameter and Zagreb indices (Das et al., 2013) Studies on the total, restrained and stratified domination numbers of the Zagreb indices have not been studied yet.

The aim of this study is to find new upper and lower bounds on Zagreb indices of trees and unicyclic graphs in terms of total, restrained and stratified domination numbers. Also, one of the aim of this study is to characterize extremal trees, chemical trees and

unicyclic graphs in respect to total, restrained and stratified domination numbers (Chartrand et al., 1995).

The mathematical possessions of Zagreb indices were been started to study for the last fifteen years. Loud bounds for the first Zagreb index of a graph were obtained by (Das, 2003). Graphs with the smallest in relation to the first Zagreb index were characterized by (Gutman, 2003). Graphs with the greatest in relation to the first Zagreb index were characterized by (Das, 2004). Upper bounds for connected graphs in Zagreb indices of were studied by (Liu and et al., 2006). Loud bounds for the unicyclic graphs of the Second Zagreb index were characterized by (Yan et al., 2006). Deng was studied the extremal bicyclic graph regarding Zagreb indices. (Deng, 2007). Hua was characterized the graphs in relation to independence number, connectivity and the first Zagreb index (Hua, 2008). , Extraordinary estimations of the total of squares of degrees of bipartite graph were studied by (Cheng et al., 2009). Sharp bounds for the bicyclic graphs in Zagreb indices with k-pendent vertices were studied by (Zhao et al., 2011). Sharp upper bounds on bicyclic graphs in Zagreb indices with a certain matching number were categorized by (Li et al., 2011). Sharp bounds on Zagreb indices of cacti with k suspended vertices were deliberate by (Li et al., 2012). Trees with permanent number of suspended vertices with minima lof the first Zagreb index were considered by (Gutman et al., 2013). The Second Zagreb Indices of the graphs of unicyclic with specified degree groupings, were studied by (Liu et al., 2014). On the minimum and maximum Zagreb indices of trees with a specified many of vertices of maximum degree were considered by (Borovicánin et al., 2015).

Results obtained in the theory of Zagreb indices are summarized in the reviews (Nikolić et al., 2003), (Gutman et al., 2004) and (Liu et al., 2011). Multiplicative versions of Zagreb indices were defined and investigated in (Eliasi et al., 2012). Finding bounds related to Zagreb indices see in (Liu et al, 2017) and references therein. Zagreb indices of graph operations see in (De, 2017) and references therein.

The relations between topological indices and domination number parameter have been recently started (Borovićánin et al., 2016) published a seminal study about Zagreb indices and domination number. The authors characterized extremal trees of Zagreb indices with respect to given domination number (Borovićánin et al., 2016). Also, Li et al



investigated the relations between Harmonic index and domination number (Li et al, 2016). Extreme values of the Zagreb index of bipartite graphs were studied by (Cheng et al, 2009) For other indistinct documentation and wording from graph hypothesis the peruses are indicated to (Cvetkovic et al., 1980).

The Zagreb indices are characterized by the accompanying equations:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad (2.1)$$

And

$$M_2(G) = \sum_{u \in V(G)} d_G(u)d_G(v) \quad (2.2)$$

Both of this indices mirror the reach out of isolating of a sub-atomic structure that is inevitably associated with those physical and chemical properties in view of the state of sub-atomic (or molecular) (Balaban et al., 1983), the main properties of  $M_1(G)$  and  $M_2(G)$  where summarized in (Nikolić et al., 2003) and the references there in, as of late, there have played out various articles studding extremal graphs that limit Zagreb indices of different diagrams (Feng et al., 2010; Wang et al., 2015; Xu et al., 2014; Liu, 2014) another diagram invariant that will be pondered in the content in Harary. It was presented in 1992 by (Mihalic et al., 1992) and is illustrated as follows:

$$H(G) = \frac{1}{2} \sum_{u=1}^n \sum_{v=1}^n \frac{1}{d(u,v)} \quad (2.3)$$

Where  $d(u, v)$  is the separation between vertex  $v$  and vertex  $u$  in a graph  $(G)$ . The book (Xu et al., 2014) and the references there in, as of late (Das et al., 2013) represented an upper bound on Harary index is terms of  $n$  and the two Zagreb indices.

$$H(G) \leq \frac{(2M_2(G)+M_1(G)+3n^2+11n-14)}{24} \quad (2.4)$$

Domination number  $\gamma(G)$  of a simple graph  $G$  is the base cardinality of a subset  $D$  of  $V(G)$  to such an extent that every vertex of  $G$  that isn't contained in  $D$  is adjoining no less than one vertex of  $D$ . A subset  $D$  is known minimum dominating set of  $G$ . The meaning of the domination number proposes that a vertex with in excess of one pendent neighbor has a place with each base commanding arrangement of a graph (Borovicainin et al., 2016).

Connection between a few topological indices and domination number of a graph  $G$  is in the focal point of intrigue and this theme is essential these days also (Borovicainin et al.,

2016). This paper is duration of these examinations. Specifically, we compute the single tree who's the First Zagreb indices and Second Zagreb indices accomplishes most extreme between a few trees with a specific stratified domination number. As an outcome, we locate the upper bound on index of Harary of trees with a specific domination number. Ultimately, trees with number of control and certain request that have insignificant first Zagreb index are considered. Number of Domination spoke to by  $T(n,\gamma)$  an arrangement of  $n$ -vertex trees whose number of control is  $\gamma$ . We will ascertain the trees from  $T(n,\gamma)$  whose first Zagreb indices and Second Zagreb indices is most extreme. Clearly,  $\gamma(T) = 1$  if and only if  $T \cong K_{1,n-1}$ . Well-known result, that each graphs of order  $n$  without any isolated vertices has number of domination at most  $\frac{n}{2}$  is given. (Fink et al., 1985). Verified that equality holds only for  $C_4$  and for any graphs of the form  $H \circ K_1$  for some  $H$ . Denote by  $T_{n,\gamma}$  the tree found from the star of  $K_{1,n-\gamma}$  by assigning a pendant edge to it is  $\gamma - 1$  pendent vertices. If  $\Delta = n - \gamma$  in a tree  $T$  of command  $n$  and domination number  $\gamma$ , then  $T = T_{n,\gamma}$ . The First Zagreb indices and tree of Second Zagreb indices a  $T_{n,\gamma}$  can be easily be deliberate as

$$M_1(T_{n,\gamma}) = (n - \gamma)(n - \gamma + 1) + 4(\gamma - 1), \quad (2.5)$$

$$M_2(T_{n,\gamma}) = 2(n - \gamma + 1)(\gamma - 1) + (n - \gamma)(n - 2\gamma - 1). \quad (2.6)$$

### 3. FIRST ZAGREB INDICES

The First Zagreb Index can be similarly determined as a total over the vertex of the graph  $G$ . and the calculation for First Zagreb Indices by the below equation. (Gutman and Trinajstić, 1972).

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 \quad (3.1)$$

**Example 3.1.** Original Zagreb indices.

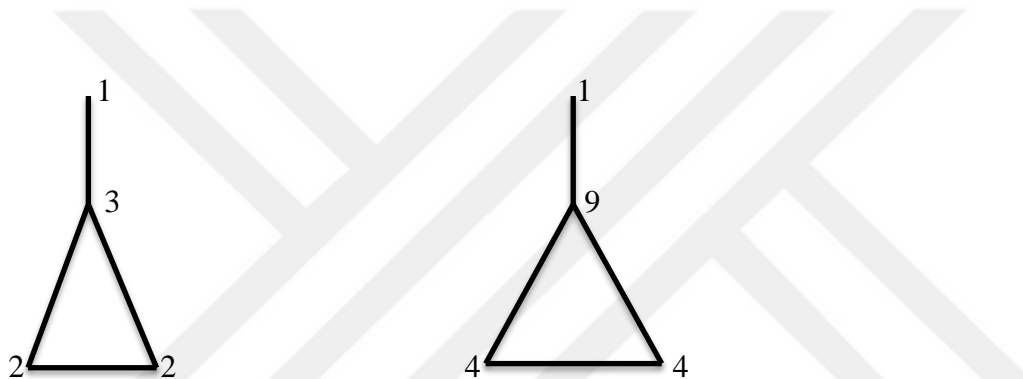


Figure 3.1. First Zagreb Indices.

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 \quad (3.2)$$

$$M_1(G) = 18$$

$d(u)$  (The degree of vertex  $u$ )

We saw that, this idea firstly in (Narumi et al., 1984) who invent what at now is called to as the Narumi Katayama index,

$$\Pi_1(G) = \prod_{u \in V(G)} d(u)^2 \quad (3.3)$$

Gutman presented the multiplicative type of the Zagreb indices (Gutman, 2011) In particular he invented that  $\Pi_1 = (NK)^2$ . Extremal graphs with regarded to the first multiplicative Zagreb Index where characterized in (Gutman et al., 2012). Eliasi et al., 2012) proposed that in the light of the identity (1), another multiplicative type of the  $M_1(G)$ , such as

$$\prod_1^*(G) = \prod_{uv \in E(G)} [d(u) + d(v)] \quad (3.4)$$

It must be straightforwardly noticed that in the all-inclusive circumstance, the indices  $\prod_1(G)$  and  $\prod_1^*(G)$ . Take different values (Eliasi et al., 2012). For example, consider the  $P_3$ , its values are 1 and 2, separately. It is clear that informal to see that if the simple graph  $G$  is fixed, then,

$$\prod_1(G) = \prod_1^*(G) \quad (3.5)$$

If the graph  $G$  does not have edge than the equation (2) is invalid. If the edge set  $E(G) = \emptyset$ , then we may, conventionally, accept that both  $\prod_1^*(G) = 0$  or better,  $\prod_1^*(G) = 1$ . For the connected the graph such problems do not occurred (Eliasi et al, 2012). Eliasi et al show that among the all connected graphs the path has the minimum value of  $\prod_1^*(G)$ . index, also Eliasi et al investigated the second minimal  $\prod_1^*(G)$ .value for the all trees with  $n \geq 7$  vertices, have the second small  $\prod_1^*(G)$  value. In the below figures which are took from the article of Eliasi denote the minimal trees with respect to  $\prod_1^*(G)$ .



Figure 3.2. The Trees forming the class  $T^*(9) = \{T(9,3,3)$  (right),  $T(9,2,5)$  (left) $\}$ .

### 3.1. Comparing First Zagreb Index and the Maximum Degree of Trees

In this section we give an important theorem which states the relationship between The First Zagreb index and the maximum degree for trees.

**Theorem 3.1:** (Das et al, 2012). Let accept that  $T$  be a tree graph with  $n$  vertices and maximum degree  $\Delta$ . Then

$$M_1(T) \leq n^2 - 3n + 2(\Delta + 1) \quad (3.6)$$

With equality number (1) holds that if and only if  $T \cong K_{1, n-1}$  or  $T \cong P_4$ .

**Proof:** If  $T = K_{1, n-1}$ , then  $M_1(T) = n^2 - 3n + 2(\Delta + 1) = n(n - 1)$ , the equality holds in (1). If  $T = P_n$ , then  $M_1(T) = 4n - 6 < n^2 - 3n + 2(\Delta + 1)$  for  $n > 4$  and  $M_1(T) = 4n - 6 = n^2 - 3n + 2(\Delta + 1)$  for  $n = 4$ . Das et al, assume that  $T \neq K_{1, n-1}, P_n$ , that is,  $3 \leq \Delta \leq n - 2$ . For this situation we need to demonstrate that the imbalance in (1) is strict. Allow  $v_i$  to be the most extraordinary degree vertex of degree  $\Delta$  in  $T$ . Also let  $v_k$  be a vertex of degree one, nearby vertex  $v_j$  of the degree  $d_j \neq \Delta$  in  $T$ . We change  $T$  into another tree  $T^*$  by erasing the edge  $v_k v_j$ , and joining the vertices  $v_i$  and  $v_k$  by an edge. Let the new degree sequence be  $\langle d_1^*, d_2^*, \dots, d_n^* \rangle$ . Therefore  $d_t^* = d_t$  for  $t \neq i, j$  where as  $d_i^* = \Delta + 1$  and  $d_j^* = d_j - 1$ . Thus

$$M_1(T) - M_1(T^*) = \Delta^2 + d_j^2 - (\Delta + 1)^2 - (d_j - 1)^2 = -2(\Delta - d_j + 1) \leq -2$$

because  $\Delta - d_j \geq 0$ . Therefore we have  $M_1(T) \leq M_1(T^*) - 2$ , with equality holding if and only if  $\Delta = d_j$ .

By the above portrayed development we have expanded the estimation of  $M_1(T)$ . If  $T^*$  is the star, then  $T \cong S_{n, n-1}$ ,  $\Delta = n - 2$  and hence  $M_1(S_{n, n-1}) = n^2 - 3n + 6 < n^2 - n - 2$ , as  $n > 4$  ( $T \neq K_{1, n-1}, P_n$ ). Otherwise, the construction is continued as follows. If one pendent vertex was chosen, which is not adjacent to  $v_i$ , from  $T^*$ . Rehashing the above system adequate number of times, touched base at a tree in which the vertex  $v_i$  is of degree  $n - 1$ , i. e.,  $K_{1, n-1}$ . Thus

$$M_1(T) \leq M_1(T^*) - 2 < M_1(T^*) - 4 < \dots < M_1(K_{1, n-1}) - 2(n - \Delta - 1) = n^2 - 3n + 2(\Delta + 1)$$

That is,  $M_1(T) < n^2 - 3n + 2(\Delta+1)$ .

□.

### 3.2. Second Zagreb Indices

The Second Zagreb Index can similarly be characterized as a whole finished the all edges of the graph (G) and the calculation for Second Zagreb Indices by the below equation. (Gutman and Trinajstić, 1972).



Figure 3.3. Second Zagreb Indices.

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \quad (3.7)$$

$$\Pi_2 = \Pi_2(G) = \prod_{u,v \in E(G)} d(u) d(v) \quad (3.8)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \quad (3.9)$$

$$M_2(G) = 19$$

$d(u)d(v) \in E(G)$  (the degree of edge)

### 3.3. Comparing the Second Zagreb Index and Co-index of Trees

The First Zagreb Index of ( $M_1(G)$ ) and the Second Zagreb Index of ( $M_2(G)$ ), as well as First Zagreb co-index of  $\acute{M}_1(G)$ , the Second Zagreb co-indices  $\acute{M}_2(G)$ , and the relation between this two type of Zagreb indices and co-index of trees are observed. An upper bound on the  $M_1(T)$  and the lower bound on the  $2M_2(T) + \frac{1}{2}M_1(T)$  of trees acquired, in relations of the number of vertices ( $n$ ) and maximum degree ( $\Delta$ ).

**Lemma 3.3.1.** (Das et al., 2012) if  $G$  be a simple graph with edges denoted by  $m$  and vertices denoted by  $n$ . Then,

$$\acute{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G) \quad (3.10)$$

For the Path  $P_n$  ( $n \geq 5$ ),

$$\acute{M}_2(P_n) = 2n^2 - 10n + 13 > 4n - 8 = M_2(P_n).$$

Note that  $\Delta(P_n) = 2$ . For trees with  $\Delta$ -values greater than 2 we have.

**Theorem 3.3.2.** (Das et al., 2012) if the  $T$  be tree of command  $n$  with maximum degree  $\Delta$ .

If

$$\Delta \geq 1.5 + \sqrt{\frac{4}{5}n^2 - \frac{28}{5}n + \frac{173}{20}} \quad (3.11)$$

Then

$$\acute{M}_2(G) \leq M_2(G).$$

**Proof:** From Lemma 3.3.1,

$$\begin{aligned} \acute{M}_2(G) - M_2(G) &= 2(n-1)^2 - 2M_2(G) - \frac{1}{2}M_1(T) \\ &\leq 2n^2 - 2n + 2 - \left(\frac{5}{2}\Delta^2 - \frac{15}{2} + 10n - 14\right) \\ &= 2n^2 - 14n - \left(\frac{5}{2}\Delta^2 + \frac{15}{2} + 16\right) \leq 0 \end{aligned}$$

As

$$\Delta \geq 1.5 + \sqrt{\frac{4}{5}n^2 - \frac{28}{5}n + \frac{173}{20}}.$$

In the accompanying two outcomes, we give upper limits on the first and second Zagreb files of trees in wording of  $n$ .

### 3.4. On the Relation between the First Zagreb Index and Second Zagreb Index

The Zagreb indices of the simple connected graphs were defined as over forty years ago by Gutman and Trinajstić, (Gutman et al., 1972). In mathematical and chemical literature, the Zagreb indices and related parameters of graphs has been studied abundantly. Liu and You, getting the several original inequalities established among the First Zagreb Index and Second Zagreb Index. (Liu et al., 2011).

The  $M_1(G)$ , represented to as the summation of the degrees of all vertices power two, and Second Zagreb index (or list) of the simple connected graph  $G$ ,  $M_2(G)$  is represented as the summation of the multiplicative of the degrees of all edges. (Reti, 2012).

The difference between the First and Second Zagreb Index started by (Hansen et al., 2007). Hansen and Vukičević conjectured that

$$\frac{M_1}{n} \leq \frac{M_2}{m} \quad (3.12)$$

And this inequality named as Zagreb indices inequality by Gutman et al. (Gutman et al., 2011). Its shown that this inequality holds for sub division graphs, biregular graphs and triregular graphs. The equality version of the Zagreb inequality

$$\frac{M_1}{n} = \frac{M_2}{m} \quad (3.13)$$

Has been investigated by (Hansen et al., 2007). They showed that this equality holds for regular graphs. Reti investigated some graph classes which are satisfying this equality (Reti, 2012). Das and Gutman, has proved that there is no simple connected triregular graph which are fulfill the Zagreb records balance. Additionally they displayed that if a graph  $G$  with most extreme degree for achieves the Zagreb indices equality. For the case the graphs with maximum degree five do not hold the Zagreb indices equality. (Das et al., 2004). In the same article, the authors proved that,

$$M_1 + 2M_2 \leq 4m^2 \quad (3.14)$$

With correspondence holds for if and only if  $G$  is the basic simple graph on number of  $n$  vertices. Moreover some authors presented that for a graph  $G$ ;

$$M_2 \leq 2m^2 - (n - 1)m\delta + \frac{1}{2}(\delta - 1)M_1 \quad (3.15)$$

With equality if  $G$  is a star graph or regular graph. (Das et al., 2004).



And now we give the below proposition which states that relationship between maximum degree, size,  $M_1$ ,  $M_2$ .

**Proposition 3.4.1.** (Reti, 2012) Let  $G$  be is a connected graph then

$$M_1 \geq \frac{M_2}{\Delta} + \delta m \quad (3.16)$$

With equality holds for if  $G$  is regular.

**Proposition 3.4.2.** (Reti, 2012) Let  $G$  be is a simple connected graph then

$$M_1 \leq \frac{M_2}{\delta} + \delta m \quad (3.17)$$

And

$$M_1 \leq \frac{M_2}{\Delta} + \Delta m \quad (3.18)$$

In two cases, the equalities satisfies if and only if,  $G$  is a connected biregular graph or regular graph.

**Corollary 3.4.3.** (Reti, 2012). Since  $\delta \leq [d] = 2 \frac{m}{n} \leq \Delta$ , from (3.16) we have

$$M_1 \leq \frac{M_2}{\delta} + [d]m = \frac{M_2}{\delta} + \frac{m^2}{n} \quad (3.19)$$

Similarly, from (3.17) we have

$$M_1 \leq \frac{M_2}{[d]} + \Delta m = \frac{nM_2}{2m} + \Delta m. \quad (3.20)$$

It is clear that this equality satisfies for fixed graphs.

**Corollary 3.4.4.** (Reti, 2012). Using (3.16) and (3.17) one obtains directly,

$$M_1 \leq \frac{1}{2} \left\{ M_2 \left( \frac{1}{\Delta} + \frac{1}{\delta} \right) + m(\Delta + \delta) \right\} = \frac{\Delta + \delta}{2} \left\{ \frac{M_2}{\Delta \delta} + m \right\} \quad (3.21)$$

and

$$M_1 \leq \sqrt{\left( \frac{M_2}{\delta} + \delta m \right) \left( \frac{M_2}{\Delta} + \Delta m \right)} \quad (3.22)$$

From the prior consideration it illustrated that equality satisfies in (3.16) and (3.17) not a lone for the regular graphs but also for simple associated biregular graphs.

On the most extreme Zagreb indices of non-star trees with a Stratified Domination number denote by  $\mathcal{T}(n, \gamma_{F_3})$  a set of n-vertex non-star trees whose (stratified)  $F_3$ -domination number is  $\gamma_{F_3}$ . We will decide trees from  $\mathcal{T}(n, \gamma_{F_3})$  whose Zagreb indices are maximum. Obviously,  $\gamma_{F_3}(T) = 2$  if and only if diameter (T) is tree (i.e T is a double star) see the below Example:

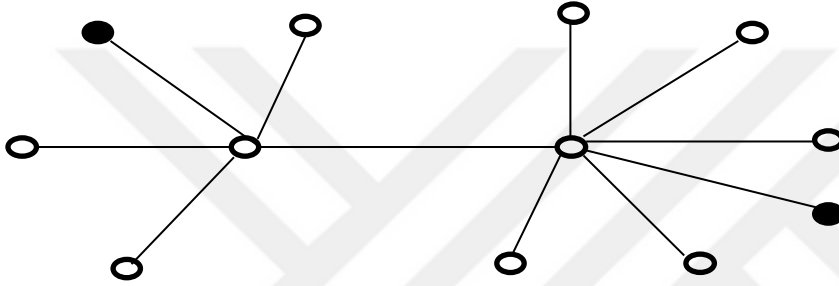


Figure 3.4. Non-Star Trees with a Stratified Domination Number.

If the randomly chosen both leaves from different stars is colored blue, the  $F_3$ -dominating of the tree T is two. (Teresa et al., 2009). Showed that all connected graph  $(G \cong K_{1,n})$  of instruction  $n \geq 3$ ,  $\gamma_{F_3}(G) \leq 2n/3$ .

Let  $T_{1,\gamma_{F_3}}$  denotes the non-star tree acquired from the separate union of a star  $K_{1,n-\gamma_{F_3}}$  and sub divided star  $K^*_{1,n-\gamma-1}$  by connection a leaf of the star to the central vertex of the sectioned star.

If  $\Delta = n - \gamma_{F_3}$  in a tree T of request n and domination number denoted by  $\gamma$ , at that point  $T \cong T_{n,F_3}$ .

The first indices of a tree  $T_{n,\gamma_{F_3}}$  can be calculated as (Fink et al., 1985).

**Proposition 3.4.5:**

$$M_1(T_{n,\gamma}) = 2(n - \gamma)^2 + 6(n - \gamma) - 2 \quad (3.23)$$

For  $n=9$ ,  $\gamma=4$ , the tree  $T_{n,F_3}$  are illustrated below.

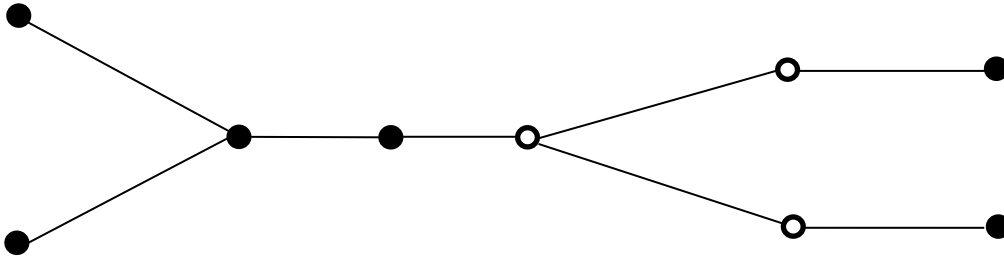


Figure 3.5. Stratified Domination of  $T_{n,F_3}$  with the maximum the First Zagreb Index.

The degree of the  $T_{n,\gamma_{F_3}}$  are classified by in table 3.1

Table 3.1. Show the degree for  $T_{n,\gamma_{F_3}}$

| Degree             | Number             |
|--------------------|--------------------|
| 1                  | $\gamma_{F_3} - 2$ |
| 2                  | $n - \gamma$       |
| $n - \gamma_{F_3}$ | 2                  |

And now, we begin to compute  $M_1(T_{n,\gamma_{F_3}})$ . From definition of the first Zagreb index;

$$M_1(T_{n,\gamma_{F_3}}) = \sum_{v \in T_{n,\gamma_{F_3}}} deg(v)^2 = (\gamma_{F_3} - 2) \cdot 1^2 + (n - \gamma) \cdot 4 + (n - \gamma_{F_3})^2 \cdot 2$$

$$= \gamma - 2 + 4(n - \gamma) + 2(n - \gamma)^2 = 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2$$

□

**Example 3.4.1:**

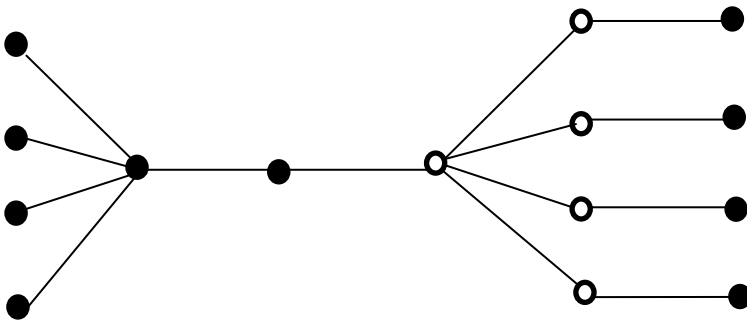


Figure 3.6. Stratified Domination Graph  $T_{15,10}$ .

The  $T_{15}$  has the maximum First Zagreb Indices  $M_1(G)$  among the all 15-vertex trees with maximum  $\gamma_{F_3}$ .

For any non-star tree with  $n \geq 7$  vertices  $n - \gamma \geq 3$ .

Henning and Maritz proved the following facts. (Henning et al., 2004)

- If diameter (T) = 3 then  $\gamma_{F_3}(T) = 2$  those  $n - \gamma > 3$
- If diameter (T) = 4 then  $\gamma_{F_3}(T) \leq \frac{n+1}{2}$  those  $n - \gamma \geq \frac{n-1}{2} \geq 3$
- If diameter (T) = 5 then  $\gamma_{F_3}(T) = \frac{2n}{3}$  those  $\gamma_{F_3}(T) = \frac{2n}{3}$  if  $T \cong \mathcal{T}$  then  $n - \gamma > 3$  for  $T \cong \mathcal{T}_2$  on  $n - \gamma > 3$  ( $T \cong \mathcal{T}_2, k \geq 3$ ) and  $\gamma_{F_3}(T) < \frac{2n}{3}$ .  
Thus  $n - \gamma \geq \frac{n}{3}$ ,  $n - \gamma \geq 3$  since  $n$  and  $\gamma$  must be integers.
- If diameter (T)  $\geq 6$  then  $\gamma_{F_3}(T) < \frac{2n}{3}$ . those  $n - \gamma \geq \frac{n}{3} \geq 3$

By the above facts (if  $T \cong \mathcal{T}$  has order  $n$ , then  $diam(T) = 5$  and  $\gamma_{F_3}(T) = \frac{2n}{3}$ . Additional, all vertex of  $T$  goes to same  $\gamma_{F_3}$ -set of  $T$ ).

Equality holds for the trees  $T \cong \mathcal{T}_{n, \gamma_{F_3}}$ .

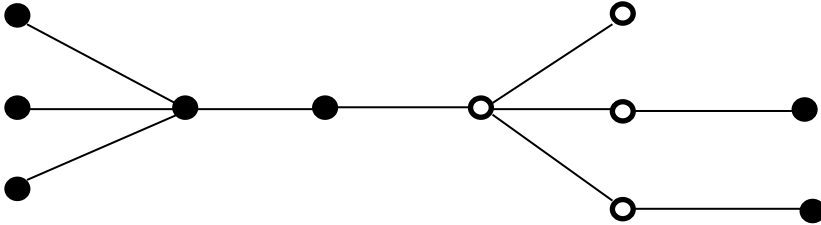


Figure 3.7.  $F_3$ -domination in a Non-Star Tree.

In the above both equalities hold if and only if a pendent vertex of the sub divided star. Of  $\mathcal{T}_{n, \gamma_{F_3}}$ .

**Theorem 3.4.6:** Let tree T be a non-star tree with Stratified Domination Number  $\gamma$ , then

$$M_1(T) \leq 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 \quad (3.24)$$

The equality holds if and only if  $T \cong T_{n, \gamma}$ .

Before the proof we provide the below example about the theorem.

**Example 3.4.2:** For  $n = 4, T \cong P_4, \gamma_{F_3} = 2$  and  $M_1(P_4) = 6$

$$6 \leq 2(4 - 2)^2 + 4 \cdot (4 - 2) + 2 - 2$$

$$6 \leq 16$$

The inequality in (3.24) is strict.

For  $n = 5, T \cong P_5$ ,  $T$  is isomorphic to a double star ( $\Delta_5$ ).

If  $T \cong P_5$ , then  $M_1(P_5) = 14$  and  $\gamma_F = 3$

Then;

$$14 \leq 2(5 - 3)^2 + 4 \cdot (5 - 3) + 3 - 2$$

$$14 \leq 17$$

The inequality in (3.24) is strict.

If  $T \cong \Delta_5$  then  $M_1(\Delta_5) = 16$  and  $\gamma_F = 2$ . Then;

$$16 \leq 2(5 - 2)^2 + 4 \cdot (5 - 2) + 2 - 2$$

$$16 \leq 30$$

The inequality in (3.24) is strict.

For  $n = 6$ .

If  $T \cong P_6$ , or ( $T \cong T_1$ ) or

$M_1(P_6) = 18$  and  $\gamma_F = 4$ .

Then;

$$18 \leq 2(6 - 4)^2 + 4 \cdot (6 - 4) + 4 - 2$$

$$18 \leq 18$$

The equality in holds in (3.24).

If  $T \cong P_6$ , then these two possibilities of the choice of  $T$ . The first is  $T$  is double star. In this case  $T$  must be the following trees  $T_1, T_2$ .

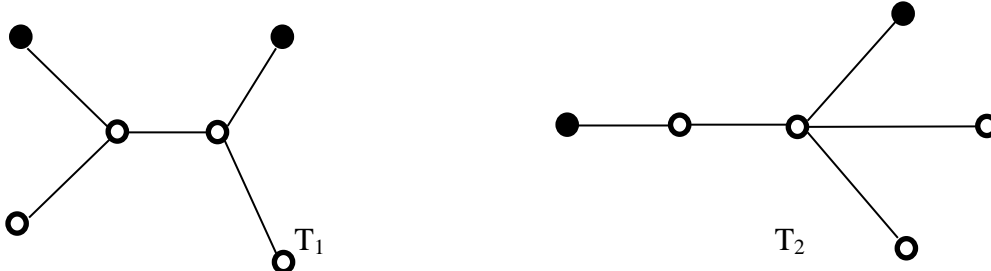


Figure 3.8. An example of Stratified Domination of a Tree.

For  $T_1$ ,  $M_1(T_1) = 22$  and  $\gamma(T_1) = 2$ .

Then: From the inequality of (3.23) we can write that,

$$\begin{aligned} M_1(T_1) &< 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 \\ 22 &< 2 \cdot 4^2 + 4 \cdot 4 + 0 \\ 22 &< 48 \end{aligned}$$

The inequality in (3.24) is strict

For  $T_2$ ,  $M_1(T_2) = 24$ , and  $\gamma(T_2) = 2$ .

Then; From the inequality of \* we can write that,

$$\begin{aligned} M_1(T_2) &< 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 \\ 24 &< 2 \cdot 4^2 + 4 \cdot 4 + 0 \\ 24 &< 48 \end{aligned}$$

The inequality in (3.24) is strict.

The second choice of T is that T is isomorphic to a branch  $S_{5,2}$ . For  $S_{5,2}$ ,  $M_1(S_{5,2}) = 20$  and  $\gamma(S_{5,2}) = 3$ . Then from the inequality of star, we can write that

$$\begin{aligned} M_1(S_{5,2}) &< 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 \\ 20 &< 2 \cdot 3^2 + 4 \cdot 3 + 1 \\ 20 &< 31 \end{aligned}$$

The inequality in (3.24) is strict.

And now, we give proof of the Theorem 3.4.6 for that  $n \geq 7$  and  $\Delta \geq 3$ .

**Proof of the theorem 3.4.6:** Let  $P_{d+1}: V_1 V_2 \dots \dots V_{d+1}$  be a longest path in T, (d is a diameter of T) and let  $\Delta$  be a minimum  $F_3$  stratified dominating set of T. Then  $|\Delta| = \gamma_F$  and both vertices  $V_1$  and  $V_{d+1}$  are pendent.

Relucca proved that  $\Delta \leq n - \gamma$ . We can prove that theorem by introduction on n.

For every non-star tree with  $4 \leq n \leq 6$ , this is trivial statement of the theorem holds.

Expect that, the theorem holds for a possible integer n and prove that the report holds for true when n replace by n+1.

There are two possible cases.

**Case1:**  $\gamma_{F_3}(T - \{V_1\}) = \gamma_{F_3}(T)$ . From the induction hypothesis,

$$\begin{aligned} M_1(T) &= M_1(T - \{V_1\}) + 2 \deg(V_2) \leq 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 + 2 \deg(V_2) \\ &= 2(n - \gamma + 1)^2 + 4(n - \gamma) + \gamma - 2 + 2(\deg(V_2) - 2(n - \gamma) + 3) \end{aligned}$$

Since  $\deg(V_2) \leq \Delta \leq n - \gamma \leq 2(n - \gamma + 1)^2 + 4(n - \gamma) + \gamma - 2$ .

**Case 2:** Suppose next that  $\gamma_{F_3}(T - \{V_1\}) = \gamma_{F_3}(T) - 1$ .

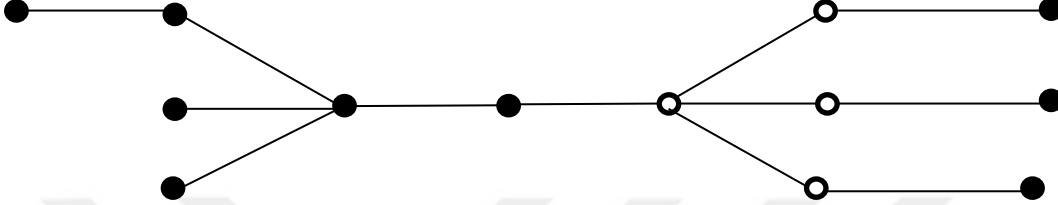


Figure 3.9. Stratified Domination Number.

At that point, by the meaning of stratified domination number it must be  $d(v_2) = 2$ ,  $d(v_2) = \Delta$ ,  $d(v_2)$  is diametrical path by the induction hypothesis,

$$\begin{aligned} M_1(T) &= M_1(T - \{V_1\}) + 2 \deg(V_2) \leq 2(n - \gamma)^2 + 4(n - \gamma) + \gamma - 2 + 2 \deg(V_2) \\ &= 2(n - \gamma + 1)^2 + 4(n - \gamma + 1) + \gamma - 2 + 2 \deg(V_2) - 2(2n - 2\gamma + 1). \end{aligned}$$

**Proposition 3.4.7:** Let  $T \in T_{n,\gamma}$  be a tree then

$$M_2(T) = 3(n - \gamma)^2 + 5(n - \gamma) - 2 \quad (3.25)$$

**Proof:** Observe that from the Figure 3.10.

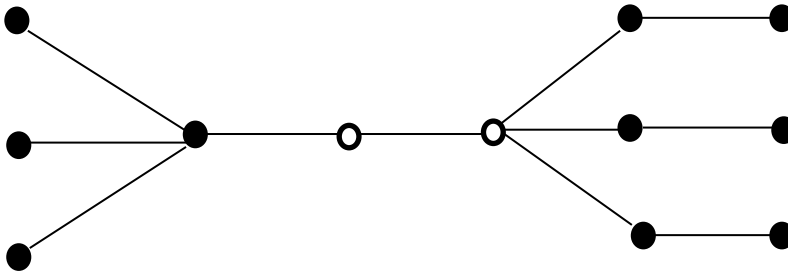


Figure 3.10. Stratified Domination Graph  $T_{12,10}$ .

Figure 3.10, there are three types of edge. The first type edges with its end vertices consist of the degree 1 and the degree 2. And the number of the first type of edges is  $\Delta - 1$ .

The second type of edges which its end vertices consist of the degree 1 and degree  $\Delta$ . And the number of the second type of edges is  $\Delta - 1$ . And the third type edges which its end

vertices consist of the degree 2 and the degree  $\Delta$ . And the number of the third type of is  $\Delta + 2$ .

Hence

$$\begin{aligned} M_2(T) &= (\Delta - 1) \cdot 2 \cdot 1 + (\Delta - 1)(\Delta \cdot 1) + (\Delta + 2)2\Delta \\ &= (2\Delta - 2) + \Delta^2 - \Delta + 2\Delta^2 + 4\Delta = 3\Delta^2 + 5\Delta - 2 \end{aligned}$$

Since  $\Delta = n - \gamma$

We can rewrite the last equality as  $3(n - \gamma)^2 + 5(n - \gamma) - 2$ .

**Theorem 3.4.8:**

$$M_2(T) \leq 3(n - \gamma)^2 + 5(n - \gamma) - 2 \quad (3.26)$$

the equality holds if  $T \cong T_{n,\gamma}$ .

**Proof:** For  $\Delta = 2$ , the equality is satisfied.

For  $\Delta \geq 3$ , we illustrated the inequality by generation on  $n$ .

Let diametrical path of the  $T$  is  $P_{d+1}: V_1 V_2 \dots V_{d+1}$  of length  $d$ ,  $d$  is a diameter of Tree  $T$ .

The vertex  $V_2$  is adjacent to  $V_1$ . We denote  $S(v_2)$  the sum of neighboring vertices of  $V_2$ .

Then

$$\begin{aligned} S(v_2) &= \sum_{v \in V(T)} d(v) - d(V_2) - \sum_{vv_2 \notin V(T)} d(u) \leq 2(n - 1) - d(V_2) - (n - 1 - d(V_2)) \\ &= (n - 1) \end{aligned}$$

Notice that  $S(v_2) = (n - 1)$  when all vertices not adjacent to  $V_2$  are pendent. There are two possible cases.

**Case1:**  $\gamma_F(T - (V_1)) = \gamma(T)$

$$\begin{aligned} M_2(T) &= M_2(T) \setminus \{V_1\} + S(V_2) + d(V_2) - 1 \\ &\leq 3(n - \gamma - 1)^2 + 5(n - \gamma - 1) - 2 + n - 1 + d(V_2) - 1 \\ &\leq 3(n - \gamma)^2 + 5(n - \gamma) - 2 \end{aligned}$$

Since  $d(V_2) \leq \Delta \leq (n - \gamma)$ . Accordingly the inequality holds by mathematical induction.

The equality holds for if  $d(V_2) = n - \gamma$  the vertices not contiguous to  $V_2$  are pendent i.e.

$T \cong T_{n,\gamma}$ .

**Case2:**  $\gamma_F(T - (V_1)) = \gamma(T) - 1$

In this case  $d(V_2)$  must be equal two. By the mathematical induction and faucet that

$S(v_2) = 1 + d(V_3)$ . We have



$$M_2(T) = M_2(T)\{V_1\} + S(V_3) \leq 3(n - \gamma - 1)^2 + 5(n - \gamma - 1) - 2 + n - 1 + d(V_3) + 2$$

$$\leq 3(n - \gamma)^2 + 5(n - \gamma) - 2$$

Since  $d(V_3) \leq n \leq (n - \gamma)$ . Clearly the equality holds  $T \cong T_{n,\gamma}$ .

**Example 3.4.3:**

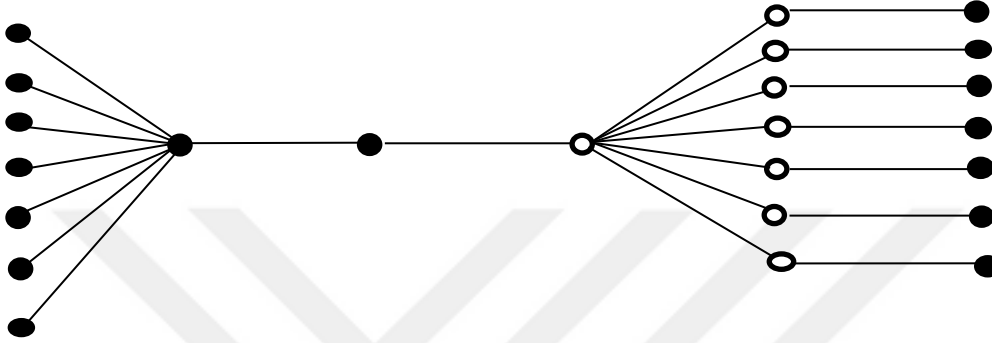


Figure 3.11. Stratified Domination Graph  $T_{24,16}$ .

The  $T_{24}$  has the maximum Second Zagreb Indices  $M_2(G)$  among the all 24-vertex trees with maximum  $\gamma_{F_3}$

**Theorem 3.4.9:** (Chartrand et al, 1997). If the  $G$  is a simple graph of connected order at least 3 and then for  $i \in \{1,2,4,5\}$ , the parameter  $\gamma_{F_i}(G)$  is illustrated in table 3.2:

Table 3.2. Parameter  $\gamma_{F_i}(G)$

| i                 | 1             | 2           | 4             | 5             |
|-------------------|---------------|-------------|---------------|---------------|
| $\gamma_{F_i}(G)$ | $\gamma_t(G)$ | $\gamma(G)$ | $\gamma_r(G)$ | $\gamma_2(G)$ |

Where  $\gamma_t(G)$  means the total number,  $\gamma_r(G)$  denote the restrained domination number and  $\gamma_2(G)$  denote the 2-domination number.

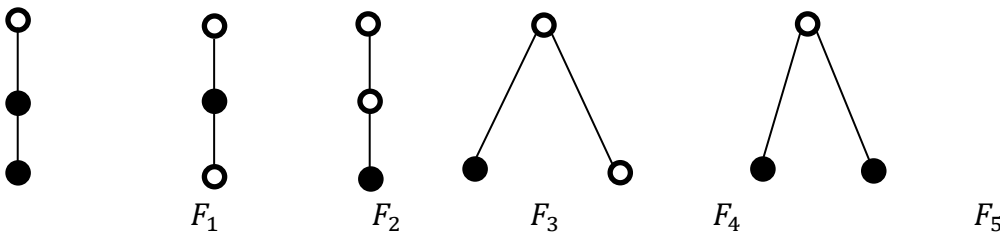


Figure 3.12. The five 2-stratified domination graphs.

The parameter  $\gamma_{F_3}(G)$  appears to be new.  $k$ -step domination is different from  $F_3$ -domination. For the set  $S \subseteq V$  is called that a  $k$ -step set of domination if for all vertex  $u \in V - S$ , there always exist a path graph of length  $k$  from the vertex  $u$  to some other vertex in  $S$ . The minimum order of any  $k$ -step dominating set of the graph  $G$  gives the  $k$ -step domination number. The difference in  $F_3$ -domination and 2-step domination is explained as follows: in  $F_3$ -domination all the blue vertices must lie in a blue vertex-blue vertex-red vertex path (of length two) to some the other red vertices. Because of this fact we clearly state that all 2-step dominating set is a stratified dominating set, but the contrary not need hold. For example let us look to star graph. The stratified domination number of a star with  $n$  vertices is equal to  $n$  but the  $k$ -step domination star number equals two. Henning and Maritz studied the  $F_3$ -dominating number of trees and proved the following fact.

**Proposition 3.4.10:** (Henning and Maritz, 2006). For  $n \geq \gamma_{F_3}$

$$(P_n) = \left\lfloor \frac{n+7}{3} \right\rfloor + \left\lfloor \frac{n}{3} \right\rfloor - \left\lfloor \frac{n}{3} \right\rfloor \quad (3.27)$$

#### 4. ECCENTRIC CONNECTIVITY INDICES OF GENERALIZED PETERSEN GRAPHS

Chemical graph theory has an important effect to develop new drugs in medicine and pharmacology by using topological indices. For convenience we use the abbreviations ECI and CEI for the Eccentric connectivity index and connective eccentricity index, respectively ECI and CEI are among these classes of indices. Sharma et al. (1997) introduced the ECI, for a graph, for the development of some new drugs. Sardana and Madan (2001). GUPTA, (2002). Wang, (2015) Investigated extremal trees of the ECI. Venkatakrisnan et al. (2015) computed the ECI of generalized thorn graphs. Das and Arani and Das (2015). compared between the Szeged index and the ECI. Ashrafi et al. (2011) computed the exact value of the ECI of nanotubes and nanotori. Morgan et al. (2014), investigated the extremal regular graphs with respect to the ECI. Doslić and Saheli. (2014) studied the ECI of composite graphs. Zhang et al. (2014) characterized maximal graphs respect to ECI. Dankelmann et al. (2014) studied the relation between Wiener index and ECI. Eskender and Vumar (2013) computed the exact value of ECI and eccentric distance sum of some graph operations. Hua and Das (2014) studied the relationship between the ECI and Zagreb indices. Zhang et al. (2012) investigated the minimal ECI of graphs. For more explanation discussion we refer the reader to Morgan et al. (2013) and references therein.

Gupta et al. (2000) introduced connective eccentricity index when considering the antihypertensive action of derivatives of N-benzyl imidazole. Yu and Feng (2013) derived upper or lower bounds for the CEI in terms of various graph invariants such as the minimum degree, maximum degree, vertex connectivity, radius, independence number etc. Moreover, the authors in Yu and Feng (2013) investigated the maximal and the minimal values of CEI between all  $n$ -vertex graphs with stable number of pendent vertices, characterized the extremal graphs and considered the cactus on vertices of  $n$  with  $k$  cycles having the maximal CEI. Yu et al. (2014) considered the connective eccentricity index of trees and unicyclic graphs with given asotti diameter. Xu et al. (2015) investigated some

extremal results on connective eccentricity index. For more explanation discussion we mention the interested reader to Li and Zhao (2016) and references therein.

Computing some graph invariants of generalized Petersen graphs have been well studied in graph theory. For coloring of generalized Petersen graphs see in Zhu et al. (2016) and references therein. For computing domination number of generalized Petersen graphs see in Wang et al. (2015) and references therein. For computing labeling of generalized Petersen graphs see in Benini and Pasotti. (2015) and references therein. For computing decycling number of generalized Petersen graphs see in Gao et al. (2015) and references therein. And for computing connectivity of generalized Petersen graphs see in Ferrero and Hanusch (2014) and references therein.

There is not any study related to computing topological index of generalized Petersen graphs in the literature for the time being. The aim of this chapter is to compute the eccentric connectivity and the connective eccentricity indices of generalized Petersen graphs.

Firstly we compute the eccentricities of the vertices  $U$  and  $W$  of  $GP(n,1)$  and  $GP(n,2)$  and secondly, we compute the eccentric connectivity index and the connective eccentricity index of  $GP(n,1)$  and  $GP(n,2)$ .

**Proposition 4.1.** The eccentricity of a vertex  $u_i$  of  $U$  in  $GP(n,1)$  is

$$\varepsilon_{u_i} = \left\lceil \frac{n+1}{2} \right\rceil \quad (4.1)$$

**Proof.** Notice that the generalized Petersen graph  $GP(n,1)$  consists of two  $n$ -vertex cycles in which corresponding vertices of  $U$  and  $W$  say  $u_i$  and  $w_i$  are adjacent to each other.

And we know that the eccentricity of a vertex of a  $n$ -vertex cycle equals  $\left\lceil \frac{n}{2} \right\rceil$ . Therefore

from this point of view we can say that the eccentric vertex of a vertex from  $U$  lies in the

set  $W$ . Let  $u_i \in U$ . Then the path  $u_i w_i w_{i+1} w_{i+2} \dots w_{i+\lfloor \frac{n}{2} \rfloor - 1} w_{i+\lfloor \frac{n}{2} \rfloor}$  or  $u_i u_{i+1} u_{i+2} \dots u_{i+\lfloor \frac{n}{2} \rfloor - 1} u_{i+\lfloor \frac{n}{2} \rfloor} w_{i+\lfloor \frac{n}{2} \rfloor}$

is the eccentric path of  $u_i$ . Thus  $\varepsilon_{u_i} = 1 + \left\lceil \frac{n}{2} \right\rceil = \left\lceil \frac{n+1}{2} \right\rceil$ . From symmetry all the

eccentricities of the vertices of  $U$  equals the same value. Therefore the proof is completed.

**Proposition 4.2.** *The eccentricity of a vertex  $w_i$  of  $W$  in  $GP(n,1)$  is*

$$\varepsilon_{w_i} = \left\lceil \frac{n+1}{2} \right\rceil \quad (4.2)$$

**Proof.** Let  $w_i \in V$ . From the same arguments of the proof of the Proposition 4.1. we get the eccentric paths of  $w_i$ ,  $w_i u_i u_{i+1} u_{i+2} \dots u_{i+\lfloor \frac{n}{2} \rfloor - 1} u_{i+\lfloor \frac{n}{2} \rfloor}$  or  $w_i w_{i+1} w_{i+2} \dots w_{i+\lfloor \frac{n}{2} \rfloor - 1} w_{i+\lfloor \frac{n}{2} \rfloor} u_{i+\lfloor \frac{n}{2} \rfloor}$ . Thus

$\varepsilon_{w_i} = 1 + \left\lfloor \frac{n}{2} \right\rfloor = \left\lceil \frac{n+1}{2} \right\rceil$ . From symmetry, all the eccentricities of the vertices of  $W$  equal the same value. Therefore the proof is completed.

**Proposition 4.3.** *Let  $n \geq 3$  be odd integer. The eccentricity of a vertex  $u_i$  of  $U$  in  $GP(n,2)$*

$$\text{is } \varepsilon_{u_i} = \left\lfloor \frac{n}{2} \right\rfloor \quad (4.3)$$

**Proof.** Let  $u_i$  be a vertex of  $U$ . Then the paths  $u_i u_{i+1} \dots u_{i+\lfloor \frac{n}{2} \rfloor}$  and  $u_i w_i w_{i+2} \dots w_{i+\lfloor \frac{n}{2} \rfloor} u_{i+\lfloor \frac{n}{2} \rfloor}$  are the eccentric paths of the vertex  $u_i$ . Then the eccentricity of  $u_i$  is  $\left\lfloor \frac{n}{2} \right\rfloor$ . From the symmetry all

the eccentricities of the vertices of  $U$  are  $\left\lfloor \frac{n}{2} \right\rfloor$ .

**Proposition 4.4.** Let  $n \geq 6$  be even integer. The eccentricity of a vertex  $u_i$  of  $U$  in

$$GP(n,2) \text{ is } \varepsilon_{u_i} = \left\lfloor \frac{n}{2} \right\rfloor$$

(4.4)

**Proof.** Let  $u_i$  be a vertex of  $U$ . Then the paths  $u_i u_{i+1} \dots u_{i+\lfloor \frac{n}{2} \rfloor}$  and  $u_i u_{i+1} w_{i+1} w_{i+3} \dots w_{i+\lfloor \frac{n}{2} \rfloor} u_{i+\lfloor \frac{n}{2} \rfloor}$

are the eccentric paths of the vertex  $u_i$ . Then the eccentricity of  $u_i$  is  $\left\lfloor \frac{n}{2} \right\rfloor$ . From the

symmetry all the eccentricities of the vertices of  $U$  are  $\left\lfloor \frac{n}{2} \right\rfloor$ .

**Proposition 4.5.** Let  $n \geq 3$  be odd integer. The eccentricity of a vertex  $w_i$  of  $W$  in  $GP(n,2)$

$$is \ \varepsilon_{w_i} = \left\lfloor \frac{n}{2} \right\rfloor \quad (4.5)$$

**Proof.** Let  $w_i \in V$ . The path  $w_i u_i u_{i+1} u_{i+2} \dots u_{i+\lfloor \frac{n}{2} \rfloor - 1} u_{i+\lfloor \frac{n}{2} \rfloor}$  is not the eccentric path of  $w_i$ .

Because the path  $w_i w_{i+2} \dots w_{i+\lfloor \frac{n}{2} \rfloor} u_{i+\lfloor \frac{n}{2} \rfloor}$  is shorter. Then the eccentricity of  $w_i$  is  $\left\lfloor \frac{n}{2} \right\rfloor$ . From

the symmetry all the eccentricities of the vertices of  $W$  are  $\left\lfloor \frac{n}{2} \right\rfloor$ .

**Proposition 4.6.** Let  $n \geq 6$  be even integer. The eccentricity of a vertex  $w_i$  of  $W$  in

$$GP(n,2) \text{ is } \varepsilon_{w_i} = \left\lfloor \frac{n}{2} \right\rfloor \quad (4.6)$$

**Proof.** Let  $w_i \in V$ . The path  $w_i u_i u_{i+1} u_{i+2} \dots u_{i+\lfloor \frac{n}{2} \rfloor - 1} u_{i+\lfloor \frac{n}{2} \rfloor} w_{i+\lfloor \frac{n}{2} \rfloor}$  is not the eccentric path of  $w_i$ .

Because the path  $w_i u_i u_{i+1} u_{i+2} w_{i+2} \dots w_{i+\lfloor \frac{n}{2} \rfloor}$  is shorter. Then the eccentricity of  $w_i$  is  $\left\lfloor \frac{n}{2} \right\rfloor$ . From

the symmetry all the eccentricities of the vertices of  $W$  are  $\left\lfloor \frac{n}{2} \right\rfloor$ .

**Theorem 4.7.** The eccentric connectivity index of  $GP(n, 1)$  is

$$\varepsilon^c(GP(n,1)) = 6n \left\lfloor \frac{n+1}{2} \right\rfloor. \quad (4.7)$$

**Proof.** From the definition of the eccentric connectivity index, we can directly write;

$$\varepsilon^c(G) = \varepsilon^c(GP(n,1)) = \sum_{v \in V} \varepsilon_v d_v.$$

Since the all generalized Petersen graphs are 3-regular, then we get;

$$\varepsilon^c(GP(n,1)) = \sum_{v \in V} \varepsilon_v d_v = 3 \sum_{v \in V} \varepsilon_v.$$

We know that  $\varepsilon_v = \left\lceil \frac{n+1}{2} \right\rceil$  for every vertex of  $v \in V$  from Proposition 4.1 and Proposition 4.2. And we know that the generalized Petersen graphs have  $2n$  vertices from the definition of the generalized Petersen graphs. Then, we can get;

$$\varepsilon^c(GP(n,1)) = 3 \sum_{v \in V} \varepsilon_v = 3.2n \left\lceil \frac{n+1}{2} \right\rceil = 6n \left\lceil \frac{n+1}{2} \right\rceil.$$

**Theorem 4.8.** The eccentric connectivity index of  $GP(n, 2)$  is

$$\varepsilon^c(GP(n,2)) = 6n \left\lfloor \frac{n}{2} \right\rfloor. \quad (4.8)$$

**Proof.** From the same facts stated in the proof of Theorem 4.7. We can write;

$$\varepsilon^c(GP(n,2)) = \sum_{v \in V} \varepsilon_v d_v = 3 \sum_{v \in V} \varepsilon_v.$$

We know that  $\varepsilon_v = \left\lfloor \frac{n}{2} \right\rfloor$  from the Proposition 4.3, Proposition 4.4, Proposition 4.5 and Proposition 4.6. Then, we can get;

$$\varepsilon^c(GP(n,2)) = 3 \sum_{v \in V} \varepsilon_v = 6n \left\lfloor \frac{n}{2} \right\rfloor.$$

**Theorem 4.9.** The connective eccentricity index of  $GP(n,1)$  is

$$\varepsilon^{ce}(GP(n,1)) = \frac{6n}{\left\lceil \frac{n+1}{2} \right\rceil}. \quad (4.9)$$

**Proof.** We can directly write  $\varepsilon^{ce}(GP(n,1)) = \sum_{v \in V} \frac{d_v}{\varepsilon_v}$ . From the above arguments in

Theorem 4.5 and the definition of the connective eccentricity index, we get that;

$$\varepsilon^{ce}(G) = \varepsilon^{ce}(GP(n,1)) = \sum_{v \in V} \frac{d_v}{\varepsilon_v} = 3.2n \cdot \frac{1}{\left\lceil \frac{n+1}{2} \right\rceil} = \frac{6n}{\left\lceil \frac{n+1}{2} \right\rceil}.$$

**Theorem 4.10.** The connective eccentricity index of  $GP(n,2)$  is

$$\varepsilon^{ce}(GP(n,2)) = \frac{6n}{\left\lfloor \frac{n}{2} \right\rfloor}. \quad (4.10)$$

**Proof.** We can directly write  $\varepsilon^{ce}(GP(n,1)) = \sum_{v \in V} \frac{d_v}{\varepsilon_v}$ . From the above arguments in

Theorem 4.6 and the definition of the connective eccentricity index, we get that;

$$\varepsilon^{ce}(G) = \varepsilon^{ce}(GP(n,2)) = \sum_{v \in V} \frac{d_v}{\varepsilon_v} = 3.2n \cdot \frac{1}{\left\lfloor \frac{n}{2} \right\rfloor} = \frac{6n}{\left\lfloor \frac{n}{2} \right\rfloor}.$$

**Example 4.1:** Consider the Eccentricity vertex  $u$  for the below Graph.

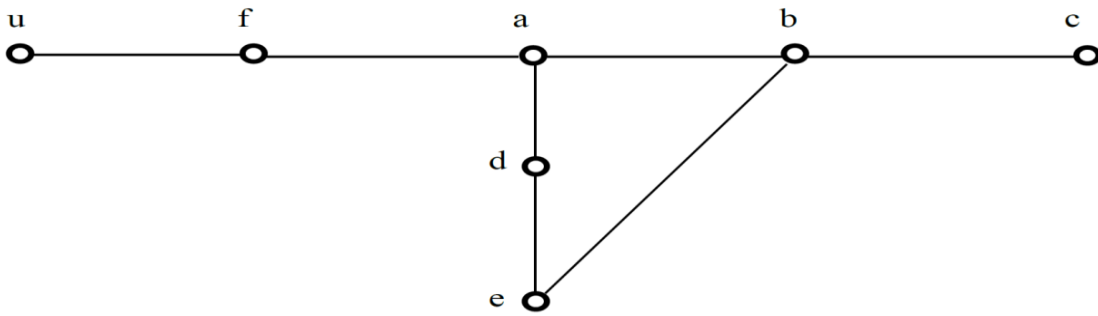


Figure 4.1. Eccentricity graph.

Eccentricity for a vertex  $u \in G$  the  $\text{ecc}(u)$  is denoted by  $\varepsilon(u)$ ,  $\text{ecc}(u) = \max \{d(u,v) \mid v \in G\}$

Is the furthest distance between  $u$  and any vertex for example  $e$ .

$$d(u,f) = 1, \quad d(u,a) = 2, \quad d(u,b) = 3, \quad d(u,c) = 4, \quad d(u,d) = 3, \quad d(u,e) = 4, \\ \text{ecc}(u) = 4$$

In the same way we get:

$$\text{ecc}(f) = 3, \text{ecc}(a) = 2, \text{ecc}(b) = 3, \text{ecc}(c) = 4, \text{ecc}(d) = 3 \text{ and } \text{ecc}(e) = 4$$

For the above graph we can calculate the eccentricity connective index by below equation:

$$ECI(G) = \sum_{u \in V} \text{deg}(u) \cdot \text{ecc}(u) \quad (4.11)$$

$$ECI = 1.4 + 2.3 + 3.3 + 1.4 + 2.3 + 2.4 = 37$$

And for calculating connective eccentricity index CEI, we can calculate by below equation:

$$CEI(G) = \sum_{u \in V} \frac{\text{deg}(u)}{\text{ecc}(u)} \quad (4.12)$$

$$CEI = \frac{1}{4} + \frac{2}{3} + \frac{3}{3} + \frac{1}{4} + \frac{2}{3} + \frac{2}{4} = \frac{10}{3}$$



**Example 4.2:** Draw the Generalized Petersen Graph,  $G(8, 2)$

In the generalized Petersen graph we have two vertex sets for example  $U$  and  $W$ ,  $U = (u_1, u_2, \dots, u_8)$  and  $w = (w_1, w_2, \dots, w_8)$ , every time the set  $U$  represent a cycle and corresponding vertices between  $U$  and  $W$  are adjacent each other and the other edges of consists of  $w_i w_{i+2}$

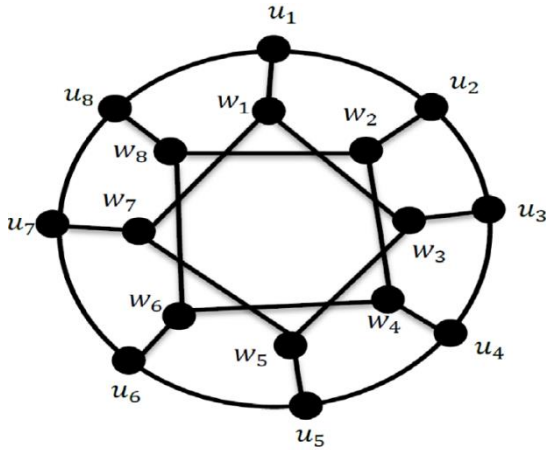


Figure 4.2. Generalized Petersen Graph (8, 2).

**Example 4.3:** Draw the Generalized Petersen Graph,  $G(8, 3)$

In the generalized Petersen graph we have two vertex sets for example  $U$  and  $W$ ,  $U = (u_1, u_2, \dots, u_8)$  and  $w = (w_1, w_2, \dots, w_8)$ , every time the set  $U$  represent a cycle and corresponding vertices between  $U$  and  $W$  are adjacent each other and the other edges of consist of  $w_i w_{i+3}$ .

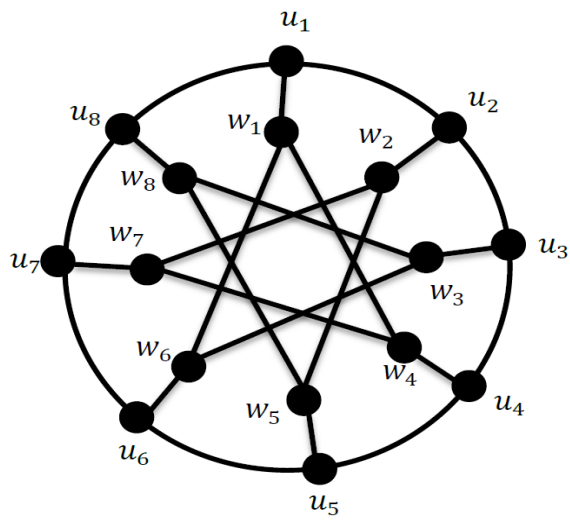


Figure 4.3. Generalized Petersen Graph  $(8, 3)$ .

## 5. CONCLUSION

Graph theory has become an important discipline in its own right because of its applications to computer science, communication networks, and combinatorial optimization through the design of efficient algorithms. It has seen increasing interactions with other areas of Mathematics. We know there are many interactions between the theories of a graph and other branches of mathematics,

Firstly, a graph is an order pair of a non-empty set of objects called vertices along with an unordered pair of distinct vertices (or peaks) called edges. In this thesis, we investigate the relationship between Zagreb indices and stratified domination number of trees.

We focused on the relationship between Zagreb indices and domination number exactly stratified domination number. In chapter one, necessary definitions and theorems related to graph theory are given. Basic facts and theorems about Zagreb indices are given in chapter two.

Also we computed the eccentric connectivity indices for the generalized Petersen Graphs in chapter three.

The literature review of the Zagreb indices and domination number are given in chapter four. The relationship between Zagreb indices and stratified domination number of trees are given.

We give two novel theorems which characterize maximum trees with a given stratified domination number.

Finally the thesis includes some tables and some figures on the Zagreb indices and stratified domination number of trees, and some equation for calculate the first and second Zagreb indices.

And computed some theorems and propositions about eccentric connectivity indices for the generalized Petersen Graphs.



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**APPENDIX**  
**EXTENDED TURKISH SUMMARY**  
**(GENİŞLETİLMİŞ TÜRKÇE ÖZET)**

**AMAÇ**

Uygulamalı Matematiğin bir dalı olan graf teorisi, mühendislikte, farmakolojide, kimyada ve sosyal bilimlerin bir çoğunda karşılaşılan problemlerinin modellenmesinde ve çözümlerinde gereklidir. Graf teorisinin içinde yer alan ve graf teorisinin bir alt dalı olan Kimyasal Graf Teorisi günümüzde popülerliğini giderek arttırmıştır. Bunun bir nedeni de topolojik indekslerin özellikle ilaç dizaynlarında kullanımının giderek artmasıdır.

Topolojik indeksler fizikte, kimyada ve farmakolojide, moleküllerin bazı fiziksel ve kimyasal özelliklerini modellemede yaygın olarak kullanılmaya başlanmıştır. Bir graf değişmezi olarak bir grafın resimsel görüntüsünden bağımsız olarak elde edilen bir topolojik indeks, graf yapısından elde edilen bir nümerik değerdir. Moleküllerin graflarından elde edilen topolojik indeksler bu moleküllerin fiziko-kimyasal ve biyolojik bazı özellikleri arasında bir korelasyon oluştururlar. Böylece topolojik indeksler, deney yapılmasının çok zor ve mümkün olmadığı durumlarda tahmin için önemli birer araçlardır.

Literatürde şu ana kadar yaklaşık binden fazla topolojik indeks hem kimyasal graf teorisyenleri hem de graf teorisyenleri tarafından tanımlanmıştır. Bir topolojik indeksin başka bir topolojik indeksinden daha büyük bir korelasyon vermesi onun kabul edilebilirliğini arttırmaktadır. Topolojik indeksler dört kısma ayrılırlar. Bunlar, derece temelli topolojik indeksler, uzaklık temelli indeksler, derece ve uzaklık temelli indeksler ile eşleme teorisine dayalı indekslerdir. Bu sınıflandırmaya dayalı olarak en çok bilinen ve pratikte uygulaması olan indeksler, Wiener, Zagreb, Hosoya, Estrada, En uzak bağlantılılık indeksleridir.

Topolojik indeksler üzerine yapılan çalışmalar temelde üçe ayrılırlar. Bunlardan birinci tür çalışmalar kimyasal özellikleri topolojik indeksleri kullanarak tahmin etmedir. İkinci tür çalışmalar matematiksel açıdan bu indekslerin sınırlarını bulmak için diğer graf parametreleriyle olan ilişkilerini ortaya çıkarmaktır. Üçüncü tür çalışmalar ise belli

bilgisayar ağlarında ve molekül modellerinde topolojik indekslerin değerlerini bulmaktır. Doğal olarak kimyacılar birinci tür çalışmalar ve graf teorisyenleri de ikinci ve üçüncü tür çalışmalara ağırlık vermişlerdir.

Derece temelli indekslerin en yaygın kullanılanı Zagreb indeksleridir. Literatürde Zagreb indeksiyle ilgili yakalşık ikibin beşyüz makale mevcuttur. Zagreb indekslerinin baskınlık parametreleriyele olan ilişkileri son iki yıldır araştırmacıların dikkatini çekmiştir. Şu ana kadar Zagreb indekslerinin ağaç graflarında alt ve üst sınırları adi baskınlık parametresine göre ifade edilmiştir.

Yine derece-uzaklık temelli topolojik indekslerin içinde en yaygın kullanılanı en uzak bağlantılılık indeksidir. Matematiksel açıdan şu ana kadar yapılan çalışmalar en uzak bağlantılılık indeksinin alt, üst sınırları, diğere graf değışmezleriyle olan ilişkisi ve bazı graf sınıflarındaki deęerinin hesaplanması olarak icra edilmiştir.

Genelleştirilmiş Petersen graflarında derece temelli topolojik indekslerin deęerinin hesabının, bu graf üç düzgün dereceli olduğundan bir önemi yoktur. Fakat uzaklık ve öz deęer temelindeki indekslerin genelleştirilmiş Petersen graflarındaki deęerinin hesabı hala gizemini korumaktadır. Genelleştirilmiş Petersen graflarında belli graf değışmezlerinin hesaplanması da yine araştırmacılar tarafından yğun olarak yapılmaktadır.

Aşağıda verilen literatür taramasında görüleceęi üzere Zagreb indeksleerinin parçalanışlı üstünlük sayılarına göre alt ve üst sınırlarının çalışıldığı bir çalışma henüz yapılmamıştır. Yine herhangi bir uzaklık temelli bir topolojik indeksin ve uzaklık-derece temelli bir topolojik indeksin genelleştirilmiş Petersen graflarındaki deęerlerini içeren bir çalışmada henüz yapılmamıştır.

Bu doğrultuda bu tez çalışmasında iki amaç güdülmüştür. Bunlardan birincisi, Zagreb indekslerinin parçalanışlı baskınlık sayıları kullanılarak var olan ilişkilerini ağaç graflarında alt sınırlar türünden ortaya koymaktır. İkincisi ise genelleştirilmiş Petersen graflarında en uzak bağlantılılık ve bağlantılı en uzaklık indekslerinin deęerini hesaplamaktır.

## MATERYAL METOT

Bu çalışma da konuyla direkt ilgili olan makaleler elde edilerek incelenmiştir. Nitel araştırma yöntemlerinden olan döküman analizi yöntemiyle mevcut literatür iyice taranmış ve ilgili literatürde henüz çalışılmamış yukarıda bahsedildiği üzere iki yeni konu tespit edilerek, elde edilen yeni teoremler matematiksel ispat yöntemlerinden Tümevarım yöntemiyle ispatlanmıştır.

## KAYNAK BİLDİRİŞLERİ

İlk uzaklık temeline dayalı topolojik indeks Wiener tarafından 1947 yılında alkanların bazı kimyasal özelliklerini modellemek için tanımlandı (Wiener, 1947). Wiener'den sonra yüzlerce topolojik indeks matematikçi ve kimyacılar tarafından tanımlanarak bir çok kimyasal ve matematiksel özellikleri çalışıldı. Aynı yıl, ilk derece temelli topolojik indeks Platt tarafından önerildi ve alkanların bazı fiziko-kimyasal özelliklerini modellemede kullanıldı (Platt, 1947). Bu iki çalışmadan yaklaşık 25 yıl sonra literatürde iyi bilinen Zagreb indeksleri, Gutman ve Trinajstić tarafından tanımlanarak karbonların elektron enerji seviyelerini modellemede kullanıldı (Gutman and Trinajstić, 1971). 1975 yılında, Randić, "Randić indeksi" tanımlayarak yine karbon atomlarının moleküler dallanmasını modellemede kullandı (Randić, 1975). Bütün topolojik indeksler içerisinde yukarıda bahsedilen indeksler diğer indekslere göre teorik yapı çalışmalarında kimya ve matematik literatüründe daha çok kullanılmışlardır. Zagreb indekslerle ilgili yapılan çalışmaların bir özeti için (Nikolić et al, 2003), (Gutman and Das, 2004) ve (Liu and You, 2011) çalışmalarına bakılabilir.

Topolojik indeksler ile baskınlık sayısı arasındaki ilişkileri inceleyen çalışmalar literatürde henüz başlamıştır. 2016 yılında Borovićanin ve Furtula ufuk açıcı bir çalışma yayımladılar. Yazarlar bu çalışmalarında Zagreb indeksin baskınlık sayısı ile olan ilişkisini inceleyerek Zagreb indeksin ekstremum ağaç graflarını karakterize ettiler (Borovićanin ve Furtula, 2016). Aynı zamanda Liu ve ark. Harmonik indeksle baskınlık sayısı arasındaki ilişkiyi incelediler (Li et al, 2016).

Graflarda uzaklık ve derece kavramlarını ilk kez bir araya getiren Sharma ve ark. 1997 yılında en uzaklık bağlantılık indeksini tanımlayıp bazı ilaçların dizaynında nasıl kullanıldığını gösteren çalışmalarını yayınladılar. En uzak bağlantılık indeksinin biyolojik ve farmakolojik olayları nasıl modellediğine dair (Sardana ve Madan, 2011) ve (Gupta ve ark., 2002) nin çalışmalarına bakılabilir. Ashrafi ve ark. Nanaotüpler için en uzak bağlantılık indeksini hesapladılar (Ashrafi ve ark., 2011). Zhang ve Zhou graflarda minimum en uzak bağlantılık indeksini araştırdılar (Zhang ve Zhou, 2012). Morgan ve ark., 2012 de en uzak bağlantılık indeksinin alt sınırını karakterize eden çalışmalarını yaptılar. Hua ve Das Zagreb indeksinin en uzak bağlantılık indeksiyle olan ilişkisini incelediler (Hua ve Das, 2013). Eskender ve Vumar graf işlemlerinde en uzak bağlantılık indeksinin nasıl değiştiğini araştırdılar (Eskender ve Vumar, 2013). Dankelmann ve ark., 2014 de Wiener indeksiyle en uzak bağlantılık indeksini karşılaştırdılar. Doslic ve Saheli, 2014 te bileşke graflarında en uzak bağlantılık indeksinin nasıl bir değişim gösterdiği üzerine çalışmalarını yaparak konuyla ilgili olarak bir çok eşitsizlik ifade ederek ispatladılar. Morgan ve ark., 2014 te yine en uzak bağlantılık indeksinin maksimum değerlerini ağaçgrafları, tek çevre içeren graflar , iki çevre içeren graflar ve üç çevre içeren graf sınıfları için karakterize ederek bir çok üst sınırları eşitsizlikler halinde sundular. Wang, en uzak bağlantılık indeksine göre ekstremal ağaç graflarını karakterize etti (Wang, 2015). Venkatakrisnan ve ark., 2015 te genelleştirilmiş diken graflarında en uzak bağlantılık indeksini araştırdılar.

Bağlantılı en uzaklık indeksi Yu ve Feng, 2013 tarafından tanımlanarak tek çevre içeren graflardaki değişimleri analiz edilmiştir. Yine Yu ve ark., 2014 te ağaç graflarında bağlantılı en uzaklık indeksinin değerini araştırdılar. Xu ve ark., 2015 te bağlantılı en uzaklık indeksinin ekstremal değerlerini incelediler. Li ve Zhao, 2016 da ağaç graflarında verilen değişik uzaklık parametrelerine göre bağlantılı en uzaklık indeksinin değişimini formülize ettiler.

Genelleştirilmiş Petersen grafları graf teorisinin bir alt dalı olan ağ teorisinde önemli uygulamalara sahip olan önemli bir graf sınıfını teşkil ederler. İlgili literatür incelendiğinde son yıllarda araştırmacıların daha çok genelleştirilmiş Petersen graflarında baskınlık parametrelerini araştırmaya odaklandığını göstermektedir. Ayrıca yeni ortaya atılan graf

parametreleride yine Petersen grafları için hesaplanmaktadır. Ancak topolojik indekslerin geliştirilmiş Petersen graflarındaki değerlerinin ne olacağı ile ilgili hiçbir çalışma henüz literatürde yer almamıştır.

## SONUÇ VE ÖNERİLER

Bu çalışmada ağaç graflarının Zagreb indekslerinin parçalanışlı baskınlık sayılarına göre değerlerini ifade eden iki önemli teorem ifade edilerek ispat edilmiştir. Ayrıca geliştirilmiş Petersen graflarında, en uzak bağlantılılık ve bağlantılı en uzaklık indekslerinin değerlerini ifade eden altı yeni teorem ifade edilerek ispatlanmıştır.

Diğer graf sınıfları için örneğin tek çevreli graflar, iki çevreli graflar, üç çevreli graflar, ağlar, geliştirilmiş diken grafları, benzen grafları gibi graflar içinde Zagreb indekslerinin parçalanışlı baskınlık sayılarına göre alt ve üst sınırlarının bulunması ileriki çalışmalar için yapılabilir. Ayrıca direkt çarpım, karezyen çarpım, tensör çarpımı gibi bazı graf işlemlerinde Zagreb indeksinin parçalanışlı üstünlük sayılarına göre değişiminin alt ve üst sınırlarını hesaplamak gibi daha ileri çalışmalar yapılabilir.

Genleştirilmiş Petersen graflarında topolojik indekslerin değerinin nasıl değiştiğini hesaplamak kimyasal graf teorisinin yeni bir alt alanı olarak düşünülebilir. Özellikle geliştirilmiş Petersen graflarında Estrada, Gutman, Wiener indekslerini hesaplamak ileriki çalışmalar için önem arz edebilir. Yine graf enerjisi, laplasyen graf enerjisi, eşleme enerjisi gibi yeni graf parametrelerinin geliştirilmiş Petersen graflarındaki değişimini incelemekte yine ileride araştırmacıların dikkatini çekebilir.



## **CURRICULUM VITAE**

He was born in Bastasten of Sulaymaniyah - Iraq, in 1986. He completed the primary education in Hajiawa Town and secondary education in Hajiawa. During the years of 2006-2010, He had studied in Sulaymaniyah University, the college of Science and Department of Computer. In 2010 he had graduated from here. At the September of 2014, He started his master study in Van Yuzuncu Yil University.

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