



## FIRST AND SECOND ZAGREB COINDICES OF CERTAIN SPECIAL TYPES OF GRAPHS

A.P.Pushpalatha<sup>1</sup>, S.Suganthi<sup>2</sup>, Gowri Senthil<sup>3</sup> and M.Sivanandha Saraswathy

<sup>1</sup>Department of Mathematics, Velammal College of Engineering and Technology, Madurai, India

<sup>2</sup>Department of Mathematics, Velammal College of Engineering and Technology, Madurai, India.

<sup>3</sup>Department of Mathematics, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences, Saveetha university, Chennai, India

<sup>4</sup>Department of Mathematics, Kalasalingam Academy of Research and Education, Krishnankovil, Tamil Nadu, India.

### Abstract

Let  $G(V,E)$  be a simple, finite, connected and undirected graph. The first Zagreb index  $M_1(G)$  is equal to the sum of squares of the degrees of the  $(n)$  vertices and the second Zagreb index  $M_2(G)$  is equal to the sum of the products. The thorn graph of a Path  $P_n$ , denoted by  $T_{a,b}(P_n)$  where  $a$  and  $b$  are positive integers was introduced by Gutmann [10]. In this paper, we calculate the first Zagreb coindex of  $T_{1,1}(P_n)$  denoted by  $M_1[T_{1,1}(\overline{P_n})]$  and the second Zagreb coindex of  $T_{1,1}(P_n)$  denoted by  $M_2[T_{1,1}(\overline{P_n})]$ . Here, we also demonstrate a few characterization theorems.

**Keywords:** Zagreb index, Zagreb coindex, Thorn graph, Barbell graph

### I. Introduction

In this study, we focus on simple graphs without self loops, undirected edges, or unweighted edges. Assume that  $G$  is such a graph and that  $V(G)$  and  $E(G)$  are, respectively, its vertex and edge sets. The number of edges and vertices will be indicated by the symbols  $m = m(G)$  and  $n = n(G)$ , respectively. Additionally,  $uv$  will be used to represent the edge that connects the vertices  $u$  and  $v$  in  $G$ .

The first and second Zagreb indices are graph theoretical descriptors that provide information about the molecular structure of a chemical compound represented by a graph. They are named after the Croatian mathematician Milan Randić, who introduced these indices in the field of chemical graph theory.

In 1972's, the topological indices like Zagreb indices were developed [5,6], and for more information on their characteristics and additional sources, see [2, 4, 7, 8, 9, 14] and [11] as well as [2, 4, 7, 8, 9, 14]. The Zagreb indices were originally defined as follows;

**First Zagreb index (M1 index):** The first Zagreb index of a graph  $G$  is defined as the sum of the squared degrees of all vertices in the graph. Mathematically, it can be expressed as:

$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$ , where  $\deg(v)$  represents the degree of vertex  $v$  in the graph  $G$ . The

first Zagreb index is related to the topological connectivity and symmetry of the graph.

It has been used in various applications, including:

(I) **Estimation of physical and chemical properties of molecules:** The first Zagreb index has been correlated with various properties such as boiling point, enthalpy of vaporization, and molar refractivity of chemical compounds. It can be used as a molecular descriptor in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies.

(II) **Characterization of chemical reactivity:** The first Zagreb index has been employed to predict chemical reactivity and stability of molecules. Higher values of the index are associated with higher chemical stability and resistance to reactions.

(III) **Drug design and bioactivity prediction:** The first Zagreb index has been used in the development of computational models for drug design and prediction of biological activities. It can provide insights into the structural properties of molecules that are important for drug-target interactions.

**Second Zagreb index (M2 index):** The second Zagreb index of a graph  $G$  is defined as the sum of the products of degrees of pairs of adjacent vertices in the graph. Mathematically, it can be expressed as:  $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$ , where  $u$  and  $v$  are adjacent vertices in the graph  $G$ . The

second Zagreb index provides information about the edge connectivity of the graph. Some applications of the second Zagreb index include:

(I) **Predicting chemical reactivity:** The second Zagreb index has been used in the prediction of chemical reactivity and stability of molecules. It captures the interaction between adjacent vertices, which can be indicative of the likelihood of chemical reactions.

(II) **Network analysis:** The second Zagreb index has applications in the analysis of complex networks, such as social networks, biological networks, and communication networks. It can provide insights into the connectivity patterns and robustness of these networks.

(III) **Structure-activity relationship studies:** The second Zagreb index has been employed in the development of computational models for predicting the activity of chemical compounds. It can capture the local structural features that are important for the activity of molecules.

Both the first and second Zagreb indices are part of a larger family of graph indices that are used to quantify various properties of graphs. They are valuable tools in chemical graph theory, computational chemistry, and network analysis for understanding the structural and functional aspects of graphs and molecular systems.

The Zagreb co-indices are topological indices that provide information about the molecular structure of a chemical graph. These indices are based on the degree of vertices in the graph and are useful in various areas of chemistry and graph theory. The Zagreb co-indices are defined as follows:

$$M_1(\overline{G}) = \sum_{uv \in E(G)} [d(u) + d(v)] \quad , \quad M_2(\overline{G}) = \sum_{uv \in E(G)} [d(u)d(v)].$$

Here are some examples of Zagreb co-indices' applications in various industries:

1. **Quantitative Structure-Activity Relationship (QSAR) studies:** QSAR models seek to relate a chemical compound's structure to its biological activity or other attributes. In QSAR investigations, Zagreb co-indices can be utilized as molecular descriptors to forecast and comprehend the activity or characteristics of substances.
2. **Drug design and discovery:** Chemical graphs' Zagreb co-indices can be examined to learn more about the structural characteristics of molecules. These discoveries can be used to improve the molecular qualities of drugs, such as bioavailability, solubility, and activity.
3. **Chemical graph theory:** Zagreb co-indices aid in the study of graph theory, particularly in the examination and comparison of chemical compound structures. Based on their connectedness and degree distributions, these indexes can be used to categorize and distinguish distinct chemical graphs.
4. **Network analysis:** Atoms act as nodes in chemical graphs, and bonds act as edges in networks. These networks' connectivity patterns are revealed by Zagreb co-indices, enabling for the investigation of several network characteristics as centrality, robustness, and resilience.
5. **Mathematical chemistry:** In mathematical chemistry, where mathematical models and methods are used to understand chemical systems, Zagreb co-indices have applications. These indices can be used to create mathematical models and equations that describe the characteristics and behaviour of molecules.

It is significant to remember that the uses listed above are not all-inclusive and that Zagreb co-indices might be used in additional fields. The particular application relies on the user's situation and research preferences.

**The first Zagreb coindex** of a graph  $G$  is defined as  $M_1(\overline{G}) = \sum_{uv \in E(G)} [d(u) + d(v)]$ ,

and **the second Zagreb coindex** of a graph  $G$  is defined as  $M_2(\overline{G}) = \sum_{uv \in E(G)} [d(u)d(v)]$ .

The features of the two Zagreb indices, which are among the earliest molecular structure descriptors, have been thoroughly studied. Recently, the idea of Zagreb coindices was advanced, garnering the interest of many mathematical chemistry researchers. Recently, there was some in-depth research done on the Zagreb coindices in [11] & [13]

**The relation between Zagreb indices and coindices:**

**Theorem 1** [13]. Let  $G$  be a graph with  $n$  vertices and  $m$  edges. Then

$$M_1(\overline{G}) = M_1(G) + n(n-1)^2 - 4m(n-1)$$

$$\overline{M}_1(G) = 2m(n-1) - M_1(G)$$

$$\overline{M}_1(\overline{G}) = 2m(n-1) - M_1(G)$$

For any simple graph  $G$ ,  $\overline{M}_1(G) = \overline{M}_1(\overline{G})$

**Theorem 2** [13]. Let  $G$  be any graph with  $n$  vertices and  $n$  edges. Then  $M_1(G) = M_1(\overline{G})$  holds if

and only if  $\frac{1}{2} \binom{n}{2}$

**Theorem 3**[13] Let  $G$  be a graph with  $n$  vertices and  $m$  edges. Then

$$M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{2n-3}{2}M_1(G) - M_2(G)$$

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

$$\overline{M}_2(\overline{G}) = m(n-1)^2 - (n-1)M_1(G) + M_2(G).$$

The aim of this paper is to establish the first and second Zagreb coindices of Thorn graph of a Path  $P_n$ .

### Basic characteristics of Zagreb coindices

**Proposition 1** [1] Let  $G$  be a simple graph on  $n$  vertices and  $m$  edges. Then

$$M_1(\overline{G}) = M_1(G) + 2(n-1)(\overline{m} - m).$$

**Proposition 2** [1] Let  $G$  be a simple graph on  $n$  vertices and  $m$  edges. Then

$$\overline{M}_1(G) = 2m(m-1) - M_1(G)$$

**Proposition 3** [1] Let  $G$  be a simple graph on  $n$  vertices and  $m$  edges. Then

$$\overline{M}_1(G) = \overline{M}_1(\overline{G}).$$

**Proposition 4** [1] Let  $G$  be a simple graph on  $n$  vertices and  $m$  edges. Then

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

**Proposition 5** [1] Let  $G$  be a simple graph on  $n$  vertices and  $m$  edges. Then

$$\overline{M}_2(G) = M_2(\overline{G}) - (n-1)M_1(\overline{G}) + \overline{m}(n-1)^2$$

**Proposition 6**[1]  $\overline{M}_1(K_n) = \overline{M}_1(\overline{K}_n) = 0$ ,  $\overline{M}_2(K_n) = \overline{M}_2(\overline{K}_n) = 0$ .

**Proposition 7**[1]  $\overline{M}_1(P_n) = 2(n-1)^2$ ;  $\overline{M}_2(P_n) = 2n^2 - 10n + 13$ ;  $\overline{M}_1(C_n) = \overline{M}_2(C_n) = 2n(n-3)$ .

## II. Literature survey

### Definition of Thorn graph of a Path 2.1 [8,16]

Let  $a, b$  be any two positive integers not necessarily  $a = b$ . Let  $P_n$  ( $n \geq 3$ ) be a path on  $n$ -vertices namely  $v_1, v_2, \dots, v_n$ . The Thorn graph of  $P_n$  is denoted by  $T_{a,b}(P_n)$  by attaching  $a d_i + b$ , number of pendant vertices with each vertex of  $P_n$ , where  $d_i$  is the degree of vertex  $v_i$ ,  $1 \leq i \leq n$ .

**Result**[16]

The number of vertices, edges, and the positive constant terms a and b have been used to generate an expression for the first and second Zagreb indices value of the path's thorn graph.

1. First Zagreb index of  $T_{a,b}(P_n)$  is derived as

$$M_1(T_{a,b}(P_n)) = (4n - 6)a^2 + (4n - 4)ab + nb^2 + a(10n - 14) + b(5n - 4) + (4n - 6), n \geq 3$$

2. Second Zagreb index of  $T_{a,b}(P_n)$  is given by

$$M_2(T_{a,b}(P_n)) = (8n - 14)a^2 + (8n - 10)ab + b^2(2n - 1) + a(12n - 22) + b(6n - 8) + (4n - 8), n \geq 3$$

**Definition of Barbell graph 2.2 [16]**

The  $n$  – Barbell graph is a simple graph obtained by connecting two copies of a complete graph  $K_n$  by a bridge and it is denoted by  $B(K_n, K_n), n \geq 3$ . It has  $2n$  vertices and  $n^2 - n + 1$  number of edges.  $(2n - 2)$  Vertices are of degree  $n - 1$  and two vertices are of degree  $n$ .

For a Barbell graph  $B(K_n, K_n)$ ,  $M_1[B(K_n, K_n)] = 2(n - 1)[n^2 - n + 1] + 2n$ , and

$$M_2[B(K_n, K_n)] = (n - 1)^2 [n^2 - n + 2] + n^2, n \geq 3.$$

**III. Main Result**

The first Zagreb coindex of a graph  $G$  is defined as  $M_1(\overline{G}) = \sum_{uv \in E(G)} [d(u) + d(v)]$ ,

and the second Zagreb coindex of a graph  $G$  is defined as  $M_2(\overline{G}) = \sum_{uv \in E(G)} [d(u)d(v)]$ .

The two new invariants were formally proposed with the intention of strengthening this paper.

**Theorem 3.1**

Let  $T_{1,1}(\overline{P_n})$  be the complement of  $T_{1,1}(P_n)$ . The first Zagreb coindex of  $T_{1,1}(\overline{P_n})$

$$M_1[T_{1,1}(\overline{P_n})] = 64n^3 - 192n^2 + 208n - 88, n \geq 3$$

Proof:

Let  $u_1, u_2, u_3, \dots, u_n$  be the vertices of  $P_n$ . Let  $u'_1, u''_1, \dots, u_1^{a+b}$  are the pendant vertices attached with  $u_1$ . Let  $u'_2, u''_2, \dots, u_2^{2a+b}$  are the pendant vertices attached with  $u_2$ . Let  $u'_{n-1}, u''_{n-1}, \dots, u_{n-1}^{2a+b}$  are the pendant vertices attached with  $u_{n-1}$  and let  $u'_n, u''_n, \dots, u_n^{a+b}$  are the pendant vertices attached with  $u_n$  respectively. The resultant graph is  $T_{1,1}(P_n)$

$T_{1,1}(\overline{P_n})$  is the complement of  $T_{1,1}(P_n)$ . In  $T_{1,1}(P_n)$  there are  $(4n-2)$ - vertices,  $(4n-3)$ - edges and  $(3n-2)$ -pendant vertices. The following is the adjacent vertices of all the vertices in each vertex in  $T_{1,1}(P_n)$  and  $T_{1,1}(\overline{P_n})$ .

Points in $T_{1,1}(\overline{P_n})$	Adjacent points in $T_{1,1}(P_n)$	Adjacent points in $T_{1,1}(\overline{P_n})$	Degree of the point in $T_{1,1}(\overline{P_n})$

$u_1$	$u_2, u_1', u_1''$	$u_3, u_4, \dots, u_{n-1}, u_n, u_2', u_2'', u_2''', \dots, u_n', u_n''$	4n-6
$u_2$	$u_1, u_3, u_2', u_2'', u_2'''$	$u_4, u_5, \dots, u_{n-1}, u_n, u_1', u_1'', u_1''', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n', u_n''$	4n-8
$u_3$	$u_2, u_4, u_3', u_3'', u_3'''$	$u_1, u_5, u_6, \dots, u_{n-1}, u_n, u_4', u_4'', u_4''', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n', u_n''$	4n-8
.	.	.	
.	.	.	
.	.	.	
$u_{n-1}$	$u_{n-2}, u_n, u_{n-1}', u_{n-1}'', u_{n-1}'''$	$u_1, u_2, \dots, u_{n-3}, u_1', u_1'', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n', u_n''$	4n-8
$u_n$	$u_{n-1}, u_n', u_n''$	$u_1, u_2, \dots, u_{n-2}, u_1', u_1'', u_2', u_2'', u_2''', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n', u_n''$	4n-6
$u_1'$	$u_1$	$u_1'', u_2', u_2'', u_2''', \dots, u_{n-1}', u_{n-1}'', u_n', u_n''$	4n-4
$u_1''$	$u_1$	$u_1', u_2', u_2'', u_2''', \dots, u_{n-1}', u_{n-1}'', u_n', u_n''$	4n-4
.	.	.	
.	.	.	
.	.	.	
$u_n'$	$u_n$	$u_1', u_1'', u_2', u_2'', u_2''', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n'$	4n-4
$u_n''$	$u_n$	$u_1', u_1'', u_2', u_2'', u_2''', \dots, u_{n-1}', u_{n-1}'', u_{n-1}''', u_n'$	4n-4
Total			$16n^2 - 28n + 12$

$T_{1,1}(\overline{P_n})$  has  $(4n-2)$ - vertices. Since  $\sum_{uv \in E(T_{1,1}(\overline{P_n}))} \deg(v) = 2$  times of the number of edges in  $T_{1,1}(\overline{P_n})$ ,  $8n^2 - 14n + 6$ , number of edges in  $T_{1,1}(\overline{P_n})$ .

### Calculation of finding the first Zagreb coindex of $T_{1,1}(\overline{P_n})$

In  $T_{1,1}(\overline{P_n})$ , The vertex  $u_1$  is adjacent to  $u_3, u_4, \dots, u_{n-1}, u_n, u_2', u_2'', u_2''', \dots, u_n', u_n''$ .

The edge contribution to  $u_1$ , the first Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned}
 & [d(u_1) + d(u_3)] + [d(u_1) + d(u_4)] + \dots + [d(u_1) + d(u_n)] + [d(u_1') + d(u_2)] + [d(u_1') + d(u_3)] + \dots + [d(u_1') + d(u_n)] \\
 & \quad + [d(u_1'') + d(u_2)] + [d(u_1'') + d(u_3)] + \dots + [d(u_1'') + d(u_n)] + [d(u_1) + d(u_2')] + [d(u_1) + d(u_2'')] + [d(u_1) + d(u_2''')] + \dots \\
 & \quad + [d(u_1) + d(u_n')] + [d(u_1) + d(u_n'')] \\
 & = [(4n-6) + (4n-8)] + [(4n-6) + (4n-8)] + \dots + [(4n-6) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] \\
 & \quad + \dots + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-6)] \\
 & \quad + [(4n-8) + (4n-4)] + [(4n-8) + (4n-4)] + \dots + [(4n-8) + (4n-4)] + [(4n-8) + (4n-4)] \\
 & = [(8n-14)] + [(8n-14)] + \dots + [(8n-12)] + [(8n-12)] + [(8n-12)] + \dots + [(8n-10)] + [(8n-12)] + [(8n-12)] + \dots + [(8n-10)] \\
 & \quad + [(8n-12)] + [(8n-12)] + \dots + [(8n-12)] + [(8n-12)] \\
 & = (8n-14)(n-3) + (8n-12)(2n-3) + (8n-10)(3n-2)
 \end{aligned}$$

The edge contribution to  $u_2$ , the first Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned}
 & [d(u_2) + d(u_4)] + [d(u_2) + d(u_5)] + \dots + [d(u_2) + d(u_n)] + [d(u'_2) + d(u_3)] + [d(u'_2) + d(u_4)] + \dots + [d(u'_2) + d(u_n)] \\
 & + [d(u''_2) + d(u_3)] + [d(u''_2) + d(u_4)] + \dots + [d(u''_2) + d(u_n)] + [d(u'''_2) + d(u_3)] + [d(u'''_2) + d(u_4)] + \dots + [d(u'''_2) + d(u_n)] + \\
 & \quad [d(u'_3) + d(u_2)] + [d(u''_3) + d(u_2)] + [d(u'''_3) + d(u_2)] + \dots + [d(u'_n) + d(u_2)] + [d(u''_n) + d(u_2)] \\
 = & [(4n-8) + (4n-8)] + [(4n-8) + (4n-8)] + \dots + [(4n-8) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \dots + \\
 & [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] \\
 & + [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \\
 & \quad [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] \\
 = & [8n-16] + [8n-16] + \dots + [8n-16] + [8n-12] + [8n-12] + \dots + [8n-10] \\
 & + [8n-12] + [8n-12] + \dots + [8n-12] + [8n-12] + [8n-12] + \dots + [8n-10] + [8n-12] + [8n-12] + \\
 & \quad [8n-12] + \dots + [8n-12] + [8n-12] \\
 = & (8n-16)(n-4) + (8n-14) + (8n-12)(3n-9) + 3(8n-14) + (8n-12)(3n-9) + 2(8n-14) \\
 = & (8n-16)(n-4) + 4(8n-14) + (8n-12)(6n-16)
 \end{aligned}$$

The edge contribution to  $u_3$ , the first Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned}
 & [d(u_3) + d(u_5)] + [d(u_3) + d(u_6)] + \dots + [d(u_3) + d(u_n)] + [d(u'_3) + d(u_4)] + [d(u'_3) + d(u_5)] + \dots + [d(u'_3) + d(u_n)] \\
 & + [d(u''_3) + d(u_4)] + [d(u''_3) + d(u_5)] + \dots + [d(u''_3) + d(u_n)] + [d(u'''_3) + d(u_4)] + [d(u'''_3) + d(u_5)] + \dots + [d(u'''_3) + d(u_n)] + \\
 & \quad [d(u'_4) + d(u_3)] + [d(u''_4) + d(u_3)] + [d(u'''_4) + d(u_3)] + \dots + [d(u'_n) + d(u_3)] + [d(u''_n) + d(u_3)] \\
 = & [(4n-8) + (4n-8)] + [(4n-8) + (4n-8)] + \dots + [(4n-8) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \dots + \\
 & [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] \\
 & + [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \\
 & \quad [(4n-4) + (4n-8)] + \dots + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] \\
 = & [8n-16] + [8n-16] + \dots + [8n-14] + [8n-12] + [8n-12] + \dots + [8n-10] + [8n-12] + [8n-12] + \dots + [8n-10] + [8n-12] \\
 & + [8n-12] + \dots + [8n-10] + [8n-12] + [8n-12] + [8n-12] + \dots + [8n-12] + [8n-12] \\
 = & (8n-16)(n-5) + (8n-14) + (8n-12)(3n-12) + 3(8n-10) + (8n-12)(3n-12) + 2(8n-12)
 \end{aligned}$$

We follow the same procedure for the vertices  $u_4, u_5, \dots, u_{n-4}$ .

Similarly, The edge contribution to  $u_{n-3}$ , the first Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows;

$$\begin{aligned}
 & [d(u_{n-3}) + d(u_{n-1})] + [d(u_{n-3}) + d(u_n)] + [d(u'_{n-3}) + d(u_{n-2})] + [d(u'_{n-3}) + d(u_{n-1})] + [d(u'_{n-3}) + d(u_n)] + [d(u''_{n-3}) + d(u_{n-2})] + \\
 & \quad [d(u''_{n-3}) + d(u_{n-1})] + [d(u''_{n-3}) + d(u_n)] + [d(u'''_{n-3}) + d(u_{n-2})] + [d(u'''_{n-3}) + d(u_{n-1})] + [d(u'''_{n-3}) + d(u_n)] \\
 & + [d(u'_{n-2}) + d(u_{n-3})] + [d(u''_{n-2}) + d(u_{n-3})] + [d(u'''_{n-2}) + d(u_{n-3})] + [d(u'_{n-1}) + d(u_{n-3})] + [d(u''_{n-1}) + d(u_{n-3})] + \\
 & \quad [d(u'''_{n-1}) + d(u_{n-3})] + [d(u'_n) + d(u_{n-3})] + [d(u''_n) + d(u_{n-3})] \\
 = & [(4n-8) + (4n-8)] + [(4n-8) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + \\
 & [(4n-4) + (4n-8)] + [(4n-4) + (4n-6)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-6)] \\
 & + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + \\
 & \quad [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] + [(4n-4) + (4n-8)] \\
 = & [8n-16] + [8n-14] + [8n-12] + [8n-12] + [8n-10] + [8n-12] + [8n-12] + [8n-10] + [8n-12] \\
 & + [8n-12] + [8n-10] + [8n-12] + [8n-12] + [8n-12] + [8n-12] + [8n-12] + \\
 & \quad [8n-12] + [8n-12] + [8n-12] \\
 = & [8n-16] + [8n-16] + \dots + [8n-14] + [8n-12] + [8n-12] + \dots + [8n-10] + [8n-12] + [8n-12] + \dots + [8n-10] + [8n-12] \\
 & + [8n-12] + \dots + [8n-10] + [8n-12] + [8n-12] + [8n-12] + \dots + [8n-12] + [8n-12] \\
 = & 1.(8n-16) + (8n-14) + 3.2.(8n-12) + 3.(8n-10) + 3.2.(8n-12) + 2(8n-12).
 \end{aligned}$$

Also, The edge contribution to  $u_{n-2}$ , the first Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} & [d(u_{n-2}) + d(u_n)] + [d(u'_{n-2}) + d(u_{n-1})] + [d(u'_{n-2}) + d(u_n)] + [d(u''_{n-2}) + d(u_{n-1})] + \\ & [d(u''_{n-2}) + d(u_n)] + [d(u'''_{n-2}) + d(u_{n-1})] + [d(u'''_{n-2}) + d(u_n)] + [d(u'_{n-1}) + d(u_{n-2})] + \\ & [d(u''_{n-1}) + d(u_{n-2})] + [d(u'''_{n-1}) + d(u_{n-2})] + [d(u'_n) + d(u_{n-2})] + [d(u''_n) + d(u_{n-2})] \\ & = (8n - 14) + 3.1.(8n - 12) + 3.(8n - 10) + 3.(8n - 12) + 2.(8n - 12). \end{aligned}$$

The edge contribution to  $u_{n-1}$ , the first Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} & [d(u'_{n-1}) + d(u_n)] + [d(u''_{n-1}) + d(u_n)] + [d(u'''_{n-1}) + d(u_n)] + [d(u'_n) + d(u_{n-1})] + [d(u''_n) + d(u_{n-1})] \\ & = 3(8n - 10) + 2(8n - 12). \end{aligned}$$

Since  $u_n$  is the end vertex of the path in  $T_{1,1}(\overline{P_n})$ , already all the contribution of edges are counted with respect to the vertex  $u_n$ . Therefore the contribution of the edges **with respect to**  $u_n$  which is zero in  $T_{1,1}(\overline{P_n})$ .

Also, **a)** The sum of the contribution of the edges **with respect to**  $u_1$  and  $u_2$ , the first Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is given by,

$$\begin{aligned} M_1[T_{1,1}(\overline{P_n})]_{u_1} + M_1[T_{1,1}(\overline{P_n})]_{u_2} &= (n - 4)(8n - 16) + (8n - 14)(n - 3 + 1) + \\ & (8n - 12)(1 + 2n - 4 + 3n - 9 + 3n - 9 + 2) + (8n - 10)(2 + 3n - 6 + 2 + 3) \\ &= (n - 4)(8n - 16) + (n - 2)(8n - 14) + (8n - 19)(8n - 12) + (8n - 10)(3n + 1) \\ &= 104n^2 - 348n + 310 \end{aligned}$$

**b)** The sum of the contribution of the edges **with respect to**  $u_3, \dots, u_{n-3}$ , the first Zagreb index of  $T_{1,1}(\overline{P_n})$  is given by,

$$\begin{aligned} & M_1[T_{1,1}(\overline{P_n})]_{u_3} + M_1[T_{1,1}(\overline{P_n})]_{u_4} + \dots + M_1[T_{1,1}(\overline{P_n})]_{u_{n-3}} \\ &= (8n - 16)[(n - 5) + \dots + 2 + 1] + (n - 5)(8n - 14) + 3(8n - 12)[(n - 4) + \dots + 3 + 2] + \\ & 3(n - 5)(8n - 10) + 3(8n - 12)[(n - 4) + \dots + 3 + 2] + 2(n - 5)(8n - 12) \\ &= (8n - 16) \left[ \frac{(n - 5)(n - 4)}{2} \right] + (n - 5)(8n - 14) + 3.2(8n - 12) \left[ \frac{(n - 4)(n - 3)}{2} - 1 \right] + 3(n - 5)(8n - 10) \\ &= 28n^3 - 200n^2 + 436n - 180. \end{aligned}$$

**c)** The sum of the contribution of the edges **with respect to**  $u_{n-2}, u_{n-1}$  and  $u_n$ , the first Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is given by,

$$\begin{aligned} & M_1[T_{1,1}(\overline{P_n})]_{u_{n-2}} + M_1[T_{1,1}(\overline{P_n})]_{u_{n-1}} + M_1[T_{1,1}(\overline{P_n})]_{u_n} \\ &= (8n - 14) + (8n - 12)(3 + 3 + 2 + 2) + (8n - 10)(3 + 3) = 136n - 194. \end{aligned}$$

**d)** The pendant vertices in  $T_{1,1}(\overline{P_n})$ ,  $u'_1, u''_1, \dots, u'_n, u''_n$  are adjacent to the other all remaining pendant vertices in  $T_{1,1}(\overline{P_n})$ . Hence the total contribution of all the pendant vertices are given below:

$$\frac{(3n - 3)(3n - 2)}{2} \times [(4n - 4) + (4n - 4)] = 12(n^2 - 2n + 1)(3n - 2) = 36n^3 - 96n^2 + 84n - 24$$

Hence the total contribution of all the edges connected with the vertices  $u_1, u_2, \dots, u_n$  (except the pendant edges) is nothing but the sum of **a**, **b** and **c** is equal to  $28n^3 - 96n^2 + 124n - 64$ .



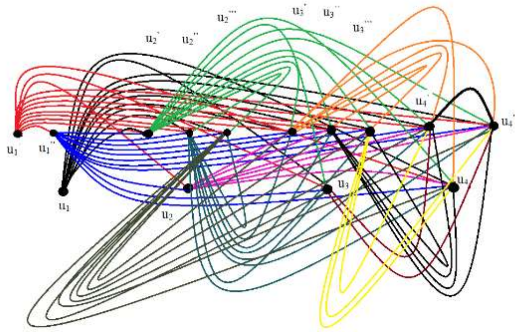
Additionally if we consider (d), we have

$$M_1[T_{1,1}(\overline{P_n})] = (36n^3 - 96n^2 + 84n - 24) + (28n^3 - 96n^2 + 124n - 64)$$

$$M_1[T_{1,1}(\overline{P_4})] = 64n^3 - 192n^2 + 208n - 88, n \geq 3.$$

**Example3.2 :** Let  $n = 4$

$$M_1[T_{1,1}(\overline{P_4})]:$$



$$M_1[T_{1,1}(\overline{P_n})] = 64n^3 - 192n^2 + 208n - 88$$

$$M_1[T_{1,1}(\overline{P_4})] = 64(4^3) - 192(4^2) + 208(4) - 88 = 1768$$

By using a manual calculation, we have:

	$u_1$	$u_2$	$u_3$	$u_4$	$u_1'$	$u_1''$	$u_2'$	$u_2''$	$u_2'''$	$u_3'$	$u_3''$	$u_3'''$	$u_4'$	$u_4''$	$M_1[T_{1,1}(\overline{P_4})]$
$u_1$			18	20			22	22	22	22	22	22	22	22	214
$u_2$				18						20	20	20	20	20	118
$u_3$													20	20	40
$u_4$															
$u_1'$		20	20	22		24	24	24	24	24	24	24	24	24	278
$u_1''$		20	20	22			24	24	24	24	24	24	24	24	254
$u_2'$			20	22				24	24	24	24	24	24	24	210
$u_2''$			20	22					24	24	24	24	24	24	186
$u_2'''$			20	22						24	24	24	24	24	162
$u_3'$				22							24	24	24	24	118
$u_3''$				22								24	24	24	94
$u_3'''$				22									24	24	70
$u_4'$														24	24
$u_4''$															24
$u_4'''$															
															1768

When we calculated the topological index  $M_1[T_{1,1}(\overline{P_4})]$  both manually and mathematically, it yields the same results.

**Calculation of finding the second Zagreb indices of  $T_{1,1}(\overline{P_n})$**

**Theorem3.3:**

The Second Zagrebcoindex of  $T_{1,1}(\overline{P_n})$  is

$$M_2[T_{1,1}(\overline{P_n})] = 128n^4 - 544n^3 + 936n^2 - 808n + 308, n \geq 3.$$

Proof:

In  $T_{1,1}(\overline{P_n})$ , The vertex  $u_1$  is adjacent to  $u_3, u_4, \dots, u_{n-1}, u_n, u'_2, u''_2, u'''_2, \dots, u'_n, u''_n$ .

The edge contribution to  $u_1$ , the second Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} &= [(4n-6)(4n-8)] + [(4n-6)(4n-8)] + \dots + [(4n-6)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] \\ &\quad + \dots + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-6)] \\ &\quad + [(4n-8)(4n-4)] + [(4n-8)(4n-4)] + \dots + [(4n-8)(4n-4)] + [(4n-8)(4n-4)] \\ &= (n-3)(4n-6)(4n-8) + (4n-6)^2 + 2(n-2)(4n-4)(4n-8) + (3n-3)(4n-6)(4n-4) \end{aligned}$$

The edge contribution to  $u_2$ , the second Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} &[d(u_2)d(u_4)] + [d(u_2)d(u_5)] + \dots + [d(u_2)d(u_n)] + [d(u'_2)d(u_3)] + [d(u'_2)d(u_4)] + \dots + [d(u'_2)d(u_n)] \\ &\quad + [d(u''_2)d(u_3)] + [d(u''_2)d(u_4)] + \dots + [d(u''_2)d(u_n)] + [d(u'''_2)d(u_3)] + [d(u'''_2)d(u_4)] + \dots + [d(u'''_2)d(u_n)] + \\ &\quad [d(u'_3)d(u_2)] + [d(u'_3)d(u_2)] + [d(u'_3)d(u_2)] + \dots + [d(u'_n)d(u_2)] + [d(u'_n)d(u_2)] \\ &= [(4n-8)(4n-8)] + [(4n-8)(4n-8)] + \dots + [(4n-8)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \dots + \\ &\quad [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] \\ &\quad + [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \\ &\quad [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] \\ &= (4n-8)^2(n-4) + (4n-8)(4n-6) + (4n-4)(4n-8)(6n-16) + 3(4n-6)(4n-4) \end{aligned}$$

The edge contribution to  $u_3$ , the second Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} &[d(u_3)d(u_5)] + [d(u_3)d(u_6)] + \dots + [d(u_3)d(u_n)] + [d(u'_3)d(u_4)] + [d(u'_3)d(u_5)] + \dots + [d(u'_3)d(u_n)] \\ &\quad + [d(u''_3)d(u_4)] + [d(u''_3)d(u_5)] + \dots + [d(u''_3)d(u_n)] + [d(u'''_3)d(u_4)] + [d(u'''_3)d(u_5)] + \dots + [d(u'''_3)d(u_n)] + \\ &\quad [d(u'_4)d(u_3)] + [d(u'_4)d(u_3)] + [d(u'_4)d(u_3)] + \dots + [d(u'_n)d(u_3)] + [d(u'_n)d(u_3)] \\ &= [(4n-8)(4n-8)] + [(4n-8)(4n-8)] + \dots + [(4n-8)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \dots + \\ &\quad [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] \\ &\quad + [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \\ &\quad [(4n-4)(4n-8)] + \dots + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] \\ &= (4n-8)(4n-8)(n-5) + (4n-8)(4n-6) + 3(n-4)(4n-4)(4n-8) + 3(4n-4)(4n-6) \\ &\quad + 3(n-4)(4n-4)(4n-8) + 2(4n-4)(4n-8) \end{aligned}$$

We follow the same procedure for the vertices  $u_4, u_5, \dots, u_{n-4}$ .

Similarly, The edge contribution to  $u_{n-3}$ , the second Zagreb coindex of  $T_{1,1}(\overline{P_n})$  is as follows:

$$\begin{aligned} &[d(u_{n-3})d(u_{n-1})] + [d(u_{n-3})d(u_n)] + [d(u'_{n-3})d(u_{n-2})] + [d(u'_{n-3})d(u_{n-1})] + [d(u'_{n-3})d(u_n)] + [d(u''_{n-3})d(u_{n-2})] + \\ &\quad [d(u''_{n-3})d(u_{n-1})] + [d(u''_{n-3})d(u_n)] + [d(u'''_{n-3})d(u_{n-2})] + [d(u'''_{n-3})d(u_{n-1})] + [d(u'''_{n-3})d(u_n)] + \\ &\quad + [d(u'_{n-2})d(u_{n-3})] + [d(u'_{n-2})d(u_{n-3})] + [d(u'_{n-2})d(u_{n-3})] + [d(u'_{n-1})d(u_{n-3})] + [d(u'_{n-1})d(u_{n-3})] + \\ &\quad [d(u''_{n-1})d(u_{n-3})] + [d(u''_{n-1})d(u_{n-3})] + [d(u''_{n-1})d(u_{n-3})] \\ &= [(4n-8)(4n-8)] + [(4n-8)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + \\ &\quad [(4n-4)(4n-8)] + [(4n-4)(4n-6)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-6)] \\ &\quad + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + \\ &\quad [(4n-4)(4n-8)] + [(4n-4)(4n-8)] + [(4n-4)(4n-8)] \\ &= (4n-8)(4n-8) + (4n-8)(4n-6) + 3.2(4n-4)(4n-8) + 3(4n-4)(4n-6) \\ &\quad + 3.2(4n-4)(4n-8) + 2(4n-4)(4n-8) \end{aligned}$$

Also, The edge contribution to  $u_{n-2}$ , the second Zagreb coindex of  $T_{1,1}(\overline{P}_n)$  is as follows:

$$\begin{aligned} & [d(u_{n-2})d(u_n)] + [d(u'_{n-2})d(u_{n-1})] + [d(u'_{n-2})d(u_n)] + [d(u''_{n-2})d(u_{n-1})] + [d(u''_{n-2})d(u_n)] + [d(u'''_{n-2})d(u_{n-1})] \\ & + [d(u'''_{n-2})d(u_n)] + [d(u'_{n-1})d(u_{n-2})] + [d(u''_{n-1})d(u_{n-2})] + [d(u'''_{n-1})d(u_{n-2})] + \\ & [d(u'_n)d(u_{n-2})] + [d(u''_n)d(u_{n-2})] \end{aligned}$$

$$= (4n-8)(4n-6) + 3(4n-4)(4n-8) + 3(8n-10) + 3(4n-8)(4n-6) + 3(4n-4)(4n-8) + 2(4n-4)(4n-8)$$

The The edge contribution to  $u_{n-1}$ , the second Zagreb coindex of  $T_{1,1}(\overline{P}_n)$  is as follows:

$$\begin{aligned} & [d(u'_{n-1})d(u_n)] + [d(u''_{n-1})d(u_n)] + [d(u'''_{n-1})d(u_n)] + [d(u'_n)d(u_{n-1})] + [d(u''_n)d(u_{n-1})] \\ & = 3(4n-4)(4n-6) + 2(4n-4)(4n-8) \end{aligned}$$

Since  $u_n$  is the end vertex of the path in  $T_{1,1}(\overline{P}_n)$ , already all the contribution of edges are counted with respect to the vertex  $u_n$ . Therefore the contribution of the edges with respect to  $u_n$  is zero in  $T_{1,1}(\overline{P}_n)$ .

Also,

- a) The sum of the contribution of the edges with respect to  $u_1$  and  $u_2$ , the second Zagreb coindex of  $T_{1,1}(\overline{P}_n)$  is given by,

$$M_2[T_{1,1}(\overline{P}_n)]_{u_1} + M_2[T_{1,1}(\overline{P}_n)]_{u_2} = 208n^3 - 1008n^2 + 1680n - 932$$

- b) The sum of the contribution of the edges with respect to  $u_3, \dots, u_{n-3}$ , the second Zagreb coindex of  $T_{1,1}(\overline{P}_n)$  is given by,,

$$\begin{aligned} & M_2[T_{1,1}(\overline{P}_n)]_{u_3} + M_2[T_{1,1}(\overline{P}_n)]_{u_4} + \dots + M_2[T_{1,1}(\overline{P}_n)]_{u_{n-3}} \\ & = (4n-8)(4n-8)[(n-5) + \dots + 2 + 1] + (n-5)(4n-8)(4n-6) + 3(4n-4)(4n-8)[(n-4) + \dots + 3 + 2] + \\ & 3(n-5)(4n-4)(4n-6) + 3(4n-4)(4n-8)[(n-4) + \dots + 3 + 2] + 2(n-5)(4n-4)(4n-8) \\ & = (4n-8)^2 \left[ \frac{(n-5)(n-4)}{2} \right] + (n-5)[(4n-8)(4n-6) + 3(4n-4)(4n-6) + 2(4n-4)(4n-8)] \\ & \quad + 3.2(4n-4)(4n-8) \left[ \frac{(n-4)(n-3)}{2} - 1 \right] \end{aligned}$$

$$= 56n^4 - 488n^3 + 1312n^2 - 1496n + 680.$$

- c) The sum of the contribution of the edges with respect to  $u_{n-2}, u_{n-1}$  and  $u_n$ , the second Zagreb coindex of  $T_{1,1}(\overline{P}_n)$  is given by,

$$\begin{aligned} & M_2[T_{1,1}(\overline{P}_n)]_{u_{n-2}} + M_2[T_{1,1}(\overline{P}_n)]_{u_{n-1}} + M_2[T_{1,1}(\overline{P}_n)]_{u_n} \\ & = (4n-8)(4n-6) + (4n-8)(4n-4)(3+3+2+2) + (4n-6)(4n-4)(3+3) \\ & = 272n^2 - 776n + 512 \end{aligned}$$

- d) The pendant vertices in  $T_{1,1}(\overline{P}_n)$ ,  $u'_1, u''_1, \dots, u'_n, u''_n$  are adjacent to the remaining all other pendant vertices in  $T_{1,1}(\overline{P}_n)$ . Hence the total contribution of all the pendant vertices are given below:

$$\frac{(3n-3)(3n-2)}{2} \times [(4n-4)(4n-4)] = 72n^4 - 264n^3 + 360n^2 - 216n + 48$$

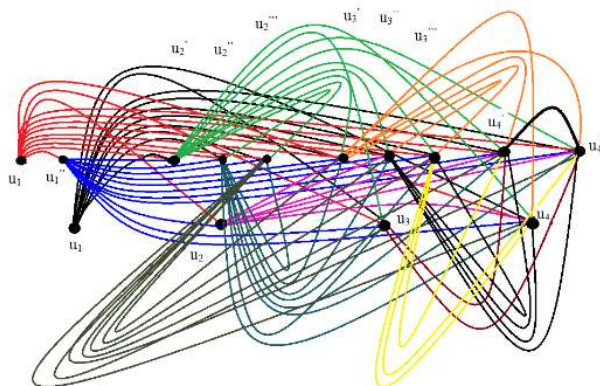
Hence the total contribution of all the edges connected with the vertices  $u_1, u_2, \dots, u_n$  (except the pendant edges) is nothing but the sum of **a**, **b** and **c** is  $= 56n^4 - 280n^3 + 576n^2 - 592n + 260$ .

Additionally if we consider **(d)**, we have

$$M_2[T_{1,1}(\overline{P_n})] = (56n^4 - 280n^3 + 576n^2 - 592n + 260) + (72n^4 - 264n^3 + 360n^2 - 216n + 48)$$

$$M_2[T_{1,1}(\overline{P_4})] = 128n^4 - 544n^3 + 936n^2 - 808n + 308, n \geq 3.$$

**3.4 Example:** Let  $n = 4$



$$M_2[T_{1,1}(\overline{P_4})]:$$

$$M_2[T_{1,1}(\overline{P_n})] = 128n^4 - 544n^3 + 936n^2 - 808n + 308$$

$$M_2[T_{1,1}(\overline{P_4})] = 128(4)^4 - 544(4)^3 + 936(4)^2 - 808(4) + 308 = 10,004$$

By using a manual calculation, we have:

	$u_1$	$u_2$	$u_3$	$u_4$	$u_1'$	$u_1''$	$u_2'$	$u_2''$	$u_2'''$	$u_3'$	$u_3''$	$u_3'''$	$u_4'$	$u_4''$	$M_2[T_{1,1}(\overline{P_4})]$
$u_1$			80	100			120	120	120	120	120	120	120	120	1140
$u_2$			80							96	96	96	96	96	560
$u_3$													96	96	192
$u_4$															
$u_1'$		96	96	120		144	144	144	144	144	144	144	144	144	1608
$u_1''$		96	96	120			144	144	144	144	144	144	144	144	1464
$u_2'$			96	120				144	144	144	144	144	144	144	1224
$u_2''$			96	120					144	144	144	144	144	144	1080
$u_2'''$			96	120						144	144	144	144	144	936
$u_3'$				120							144	144	144	144	696
$u_3''$				120								144	144	144	552
$u_3'''$				120									144	144	408
$u_4'$														144	144
$u_4''$															
															10004

When we calculated the topological index  $M_2[T_{1,1}(\overline{P_4})]$  both manually and mathematically, it yields the same results.

#### IV. Calculation of $M_1[T_{1,1}(\overline{P_4})]$ , $M_2[T_{1,1}(\overline{P_4})]$ through Program in C

Let us find the values of first and second Zagreb coindices of  $T_{1,1}(\overline{P_4})$  using C program.

```

#include<stdio.h>
#include<conio.h>
main()
{
int pd[100],tpd[100],i,j,n,a,b,tn[100];
int tnv,t,tet,tnpvt;
int M1Tab,M2Tab;
int M1TabCPn,M2TabCPn;
int dcpv,u1,u2,u3,u4;
int m1cdu1,m1cdu2,m1cdu3,m1cdu4,m1cdpv;
int m2cdu1,m2cdu2,m2cdu3,m2cdu4,m2cdpv;
clrscr();
printf("enter the path vertices \n");
scanf("%d",&n);
pd[0]=1;
pd[n-1]=1;
for(i=1;i<n-1;i++)
{
pd[i]=2;
}
for(i=0;i<n;i++)
{
if(i<n-1)
{
printf("%d---",pd[i]);
}
else
{
printf("%d",pd[i]);
}
}
printf("\nEnter the value of two variables a and b should be greater 0\n");
scanf("%d%d",&a,&b);
i=0;
tn[i]=a+b;
tn[n-1]=a+b;
for(i=1;i<n-1;i++)
{
tn[i]=2*a+b;
}
printf("\nTHORN Graph is as follows\n");
printf("=====\n");

```

```

for(i=0;i<n;i++)
{
if(i<n-1)
{
printf("%d---",tn[i]);
}
else
{
printf("%d",tn[i]);
}
}
tnvt=2*a*(n-1)+n*(1+b);
tnet=n-1-2*a+n*(2*a+b);
tnpvt=n*(2*a+b)-2*a;
printf("\nTotal number of vertices for Thorn graph = %d", tnvt);
printf("\nTotal number of edges for Thorn graph = %d", tnet);
printf("\nTotal number of pendant vertices =%d",tnpvt);

u1=u4=a+b+1;
u2=u3=2*a+b+2;
printf("\ndegree of u1 = %d",u1);
printf("\tdegree of u2 = %d",u2);
printf("\ndegree of un-1 = %d",u3);
printf("\tdegree of un = %d",u4);

printf("\nComplement of Ta,b(Pn) as follows");
printf("\n=====");

//u1=u4=4*n-6;
//u2=u3=4*n-8;

u1=u4=(n-1)*(2*a+b+1)-(a+1);
u2=u3=(n-1)*(2*a+b+1)-2*(a+1);
printf("\ndegree of u1 = %d",u1);
printf("\tdegree of u2 = %d",u2);
//printf("\tdegree of u3 = .");
//printf("\ndegree of u4 = .");
printf("\ndegree of un-1 = %d",u3);
printf("\tdegree of un = %d",u4);
//printf("\nDegree of pendant vertices = %d",4*n-4);
dcpv=n*(2*a+b+1)-2*(a+1);
printf("\nDegree of pendant vertices = %d",dcpv);
printf("\nBy Formula for M1(T1,1(complement of Pn));
//M1TabCPn=(64*n*n*n)-(192*n*n)+208*n-88;

```

```

m1cdu1=(u1+u3)+(u1+u4)+2*(dcpv+u2)+2*(dcpv+u3)+2*(dcpv+u4)+8*(dcpv+u1);
m1cdu2=(u2+u4)+3*(dcpv+u2)+3*(dcpv+u4)+5*(dcpv+u2);
m1cdu3=3*(dcpv+u4)+2*(dcpv+u3);
m1cdu4=0;
m1cdpv=(dcpv+dcpv)*(tnpvt*(tnpvt-1)/2);
M1TabCPn=m1cdu1+m1cdu2+m1cdu3+m1cdu4+m1cdpv;

printf("\nM1T1,1CPn=%d",M1TabCPn);
printf("\nBy Formula for M2(T1,1(complement of Pn))");
//M2TabCPn=(128*n*n*n*n*n)-(544*n*n*n*n)+936*n*n*n-808*n+308;
m2cdu1=(u1*u3)+(u1*u4)+2*(dcpv*u2)+2*(dcpv*u3)+2*(dcpv*u4)+8*(dcpv*u1);
m2cdu2=(u2*u4)+3*(dcpv*u2)+3*(dcpv*u4)+5*(dcpv*u2);
m2cdu3=3*(dcpv*u4)+2*(dcpv*u3);
m2cdu4=0;
m2cdpv=(dcpv*dcpv)*(tnpvt*(tnpvt-1)/2);
M2TabCPn=m2cdu1+m2cdu2+m2cdu3+m2cdu4+m2cdpv;
printf("\nM2T1,1CPn=%d",M2TabCPn);

getch();
return(0);
}

```

**Output:**

```

enter the path vertices
4
1---2---2---1
Enter the value of two variables a and b should be greater 0
1
1

THORN Graph is as follows
=====
2---3---3---2
Total number of vertices for Thorn graph = 14
Total number of edges for Thorn graph = 13
Total number of pendant vertices =10
degree of u1 = 3      degree of u2 = 5
degree of un-1 = 5   degree of un = 3
Complement of Ta,b(Pn) as follows
=====
degree of u1 = 10     degree of u2 = 8
degree of un-1 = 8   degree of un = 10
Degree of pendant vertices = 12
By Formula for M1(T1,1(complement of Pn)
M1T1,1CPn=1768
By Formula for M2(T1,1(complement of Pn)
M2T1,1CPn=10004

```

**V. Conclusion:**

We close our discussion with the following remarks:

- (i) For  $a = b = 1$ , the complement of Thorn graph  $T_{a,b}(P_n), T_{a,b}(\overline{P_n})$ , we have computed the formula for first and second Zagreb coindices of  $T_{1,1}(\overline{P_n})$
- (ii) The first and second Zagreb coindices of the Barbell graph, as well as a few other peculiar graphs, were further scheduled to be derived.
- (iii) The obtained results are also verified and illustrated for the particular classes of graphs.
- (iv) This work can be carried out for numerous more households in numerous additional ways.

#### Reference:

- [1] Ashrafi A R, Doslic T, Hamzeh A, The Zagreb coindices of graph operations. Discrete Appl Math, 2010, 158: 1571-1578.
- [2] K. C. Das, I. Gutman, Some properties of the second Zagreb index, MATCH Commun. Math. Comput. Chem. 52 (2004) 103–112.
- [3] T. Doslic, Vertex weighted Wiener polynomials for composite graphs, Ars Math:Comtemp.1 (2008) 66 80.
- [4] B. Furtula, I. Gutman, M. Dehmer, On structure–sensitivity of degree–based topological indices, Appl. Math. Comput. 219 (2013) 8973–8978.
- [5] Gutman, B. Rušćić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, J. Chem. Phys. 62 (1975) 3399–3405.
- [6] Gutman, I; Trinajstić, N. Graph theory and molecular orbitals total  $\pi$ -electron energy of alternant hydrocarbons. Chemical physics. Letters, vol.17 no.4, pp.535-538,1972
- [7] I. Gutman, Degree–based topological indices, Croat. Chem. Acta 86 (2013) 351–361.
- [8] I. Gutman, K. C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004) 83–92.
- [9] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex–degree–based topological indices, J. Serb. Chem. Soc. 78 (2013) 805–810.
- [10] Gutman, I. Distance in thorny graph. Publ. Inst. Math Beograd 63(1998)31-36.
- [11] Ivan Gutman, Boris Furtula, Zana Kovijanic Vukicevic, Goran Popivoda. On Zagreb Indices and coindices, MATCH Commun. Math. Comput. Chem. 74 (2015) 5-16.
- [12] S. Hossein Zadeh, A. Hamzeh, A.R. Ashrafi, External properties of Zagreb coindices and degree distance of graphs, Miskole Math. Notes 11(2010) 129 138.
- [13] H.Hua, S.Zhang. Relations between Zagreb and some distance based topological indices ,MATCH Commun. Math. Chem.68 (2012)199 208.
- [14] S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta 76 (2003) 113–124.
- [15] A.P.Pusphalatha, S.Suganthi, First and Second Zagreb index of some special graphs, Quaestions Mathematica (communicated), 2023.
- [16] K.Thilagavathi and A.SangeethaDevi, Harmonious coloring  $C[B(k_n, k_n)]$  and  $C[F_{2k}]$ . Proceedings of International Conference on Mathematical and Computer Science (ICMCS 2009). Department of Mathematics Loyola College Chennai. Page no 50-52



- [17] M. Wang, H. Hua, More on Zagreb coindices of composite graphs, Int. Math. Forum7(2012) 669–673.
- [18] D.West, Introduction to Graph Theory, II edition, Prentice Hall, Upper Saddle River, NJ,2001.