Topological Indices of Chemical Graphs

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CIIT/SP14-BSMATH-002/LHR

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Topological Indices of Chemical Graphs

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DEDICATION

To

My family and my teachers

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Abstract

Topological indices are real numerical parameters of a molecular structural networks and structural networks. These networks are characterize its topology and graph invariant. The molecular networks plays a vital role in QSAR \QSPR study, phisco-chemical properties and topological indices like Randic, atom-bond connectivity(ABC) and geometric-arithmetic(GA) are used to diagnose the bioactivity of chemical compounds. Actually these topological indices is designed by transforming a chemical structure into a numeric number. In the area of research graph theory has been found to be very useful.

In this thesis, we will compute the degree based topological indices the so-called general Randic index $R_\gamma(G)$ for $\gamma = \{1, \frac{1}{2}, -1, -\frac{1}{2}\}$,atom bond connectivity(ABC), geometric-arithmetic(GA), first Zagreb, second Zagreb, second modified Zagreb, third zagreb, hyper Zagreb and augmented zagreb topological indices for subdivision of different kinds of networks like sierpinksi s(n,k) networks as well as molecular structural networks. This study will give us a very interesting and different results by using new topological index that is first Zagreb, second Zagreb, second modified Zagreb, third zagreb, hyper Zagreb and augmented zagreb topological indices.

Chapter 1

Introduction

The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in QSPR/QSAR study. In the last few years, the number of proposed molecular descriptors is rapidly growing due to the chemical significance of these descriptors. These descriptors correlate certain chemical and physical properties of chemical compounds. A close correlation of Randic index to the boiling point and Kovats constants has been found. A good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes is provided by the atom-bond connectivity (ABC) index. For certain physico-chemical properties like boiling point, Entropy, Enthalpy of vaporization, Standard enthalpy of vaporization, Enthalpy of formation and Acentric factor, the predictive power of geometric-arithmetic (GA) index is better than predictive power of the Randic connectivity index [8]. Topological characterization of chemical structures allows the classification of molecules and modelling unknown structures with desired properties. Molecules and molecular compounds are often modeled by molecular graphs. A model that is used to characterize a chemical compound is called chemical graph. A molecular graph is a representation of the structural formula of a chemical

compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. The combination of chemistry, mathematics and information science which studies QSAR/QSPR relationships is known as cheminformatics. Many chemical and physical properties of the chemical compounds can be found with the help of QSAR /QSPR models. The topological indices such as Wiener index, Szeged index, Randic index, Zagreb indices and ABC index are used to correlate different chemical and physical properties like the boiling point, molecular weight, vapour pressure, -electrom energy etc. A molecular graph can be described by different ways such as, a drawing, a polynomial, a sequence of numbers, a matrix or by a derived number called a topological index . A topological index is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under the graph automorphism. To establish a correlation model between the structures of chemical compounds and the coressponding chemical and physical properties it is required to numerically code the structures of chemical compounds. hence in the QSAR/QSPR studied the task is to transfer the graph into numerical format. for this purpose there are many techniques in which the popular one is topological indices. In more precise way, a topological index Top(G) of a graph, is a number such that, if H is isomorphic to G, then Top(H) = Top(G). The concept of topological indices came from Wiener [30] while he was working on boiling point of paraffin, named this index as path number. Later on, the path number was renamed as Wiener index [7]. There are three major classes of topological indices which are distance based topological indices, degree based topological indices and counting related. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in

theoretical chemistry

In Chapter 2, we discuss the fundamental concept, definitions, notations and terminologies that will be used in which and strong the concept about graph theory.

In Chapter 3, we have some basic introduction about topological indices, terminologies and some formulas that will be used in our research work.

In Chapter 4, In this section, we have described the applications and find out the results for subdivision of molecular structural networks.

In Chapter 5, For further study in this area, we give conclusion and some open problems.

In Chapter 6, Bibliography

Chapter 2

Basic Concepts

2.1 Introduction

In this chapter, there are presented here some notations, basic concepts and terminologies about graph theory. Their importance to provide strong and enough powerful concept that is based on the present study.

2.2 Basic Definitions

2.2.1 Preliminaries

2.2.2 Graphs

The ordered pair of $(V(G), E(G))$ any graph G which disjoint from $V(G)$, where non empty set of vertices $V(G)$ and set of edges $E(G)$. $V(G)$ represents vertices set and E(G) represents edges set. Explicitly, Finitely graphs are considered only, i.e, V and E are finite always. $V = V(G)$ represents the vertex set and $E = E(G)$ represents the edge set of any graph of G. Any vertices g and h join with an *edge* that is $\{g, h\}$ and represented by gh. Hence, gh and hg represents exactly the same edge; The end vertices of this edge are g and h vertices

2.2.3 Simple or strict Graph

Except loops and multi edges graphs are known as *simple or strict graphs.* If V(G) and E(G) are finite then a graph G is *finite* and V(G) and E(G) are infinite then G is infinite graph. A strict or simple, finite and undirected graph is shown in the following figure. $V(G) = \{g_1, g_2, g_3, g_4, g_5\}$ and $E(G) = \{g_1g_2, g_2g_3, g_3g_4, g_4g_5, g_1g_5, g_2g_5\}$

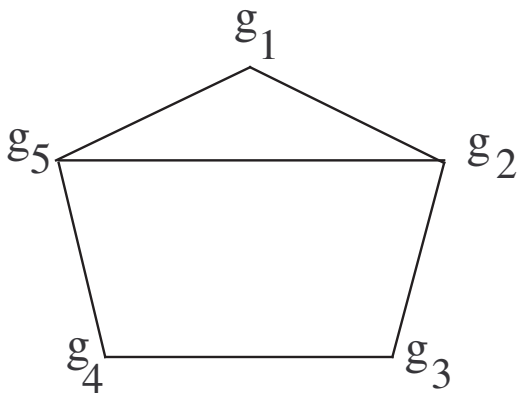

Figure 2.1: simple or strict Graph

Cardinality of $V(G)$ is called order of G_i and cardinality of $E(G)$ is called size of G of any graph of G, symbolized as $k(G)$ and $l(G)$ or simply k and l respectively. If $e = ij \in E(G)$, then i, j are adjacent vertices. Symbolically, its representation is $i \sim j$. If they have a common end vertex, two distinct edges g and h are said to be adjacent. The number of vertices that are adjacent to vertex g is called the*degree* of a vertex g. It is symbolized as $d_g(G)$ or simply d_g.

Maximum degree of a vertex(node) of G is known as degree of G.

The *isolated vertex* is a vertex which have **zero** degree. The *end or pendent vertex* is

that vertex which have **one** degree. An edge is said to be pendent if one of its vertex is pendent.

2.2.4 Sub-Graphs

A **sub-graph** U is a graph of G if $V(U) \subseteq V(G)$ and $E(U) \subseteq E(G)$, where $V(G)$ and $E(G)$ vertex and edges sets of any graph of G. In other words if every vertex of U belongs to $V(G)$ and every edge of U belongs to $E(G)$.

Itself every graph G is sub-graph U. Deleting the vertex(node) or edge of G, we get a sub-graph of a graph G. If order of G and U is same then U is a sub-graph of G and U is called **spanning sub-graph** of G.

If for every $gh \in V(U)$ and $gh \in E(G)$, then $gh \in E(U)$, is known as a **induced sub-graph** of U of G.

2.2.5 Multi graph

Multiple edges are two or more edges that connect the same two vertices. A loop is an edge (directed or undirected) that connects a vertex to itself; it may be permitted or not, according to the application. In this context, an edge with two different ends is called a link.

A multi graph, as opposed to a simple graph, is an undirected graph in which multiple edges (and sometimes loops) are allowed.

Where graphs are defined so as to disallow both multiple edges and loops, a multi graph is often defined to mean a graph which can have both multiple edges and loops, although many use the term pseudograph for this meaning. Where graphs are defined so as to allow both multiple edges and loops, a multi graph is often defined to mean a graph without loops.

2.2.6 Cyclic Graph

Let $e_i = u_i u_{i+1}$ be edges of G where $i \in [1, t]$, the sequence K of edges such that $K = e_1 e_2 ... e_t$ are called *walk* of length $t - 1$, if every two edges are adjacent in K.

If all edges of K are distinct then walk is known as a *trail*. A walk $K = e_1 e_2 ... e_t (e_i = u_i u_{i+1})$ is called a *path* if all vertices of K is distinct. If starting and ending point of a path is same then it is said to be closed path or said to be cycle.

A *cyclic graph* if it contains a cycle of any graph of G. A cycle of n vertices(nodes) is symbolized as C_n.

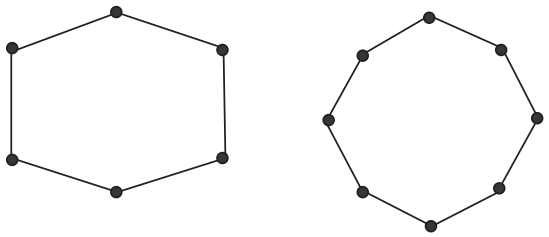

Figure 2.2: Cyclic graph C_6 and C_8

2.2.7 Size of ghraph

The size of a graph is. E. , its number of edges. The degree or valency of a vertex is the number of edges that connect to it, where an edge that connects to the vertex at both ends (a loop) is counted twice.

2.2.8 Directed graph

A directed graph or digraph is a graph in which edges have orientations. It is written as an ordered pair $G = (V, A)$ (sometimes $G = (V, E)$) with

V a set whose elements are called vertices, nodes, or points; A a set of ordered pairs of vertices, called arrows, directed edges (sometimes simply edges with the corresponding set named E instead of A), directed arcs, or directed lines. An arrow (x, y) is considered to be directed from x to y; y is called the head and x is called the tail of the arrow; y is said to be a direct successor of x and x is said to be a direct predecessor of y. If a path leads from x to y, then y is said to be a successor of x and reachable from x, and x is said to be a predecessor of y. The arrow (y, x) is called the inverted arrow of (x, y).

A directed graph G is called symmetric if, for every arrow in G, the corresponding inverted arrow also belongs to G. A symmetric loop less directed graph G = (V, A) is equivalent to a simple undirected graph G = (V, E), where the pairs of inverse arrows in A correspond one-to-one with the edges in E; thus the number of edges in G is $|E| = |A|/2$, that is half the number of arrows in G.

2.2.9 Undirected graph

An undirected graph is a graph in which edges have no orientation. The edge (x, y) is identical to the edge (y, x), i.e., they are not ordered pairs, but sets x, y (or 2-multi sets) of vertices. The maximum number of edges in an undirected graph without a loop is $n(n1)/2$.

2.2.10 Operations on Graphs

Let G_1 and G_2 be a **union of graphs**. If two graphs $G_1 = (g_1, h_1)$ and $G_2 = (g_2, h_2)$ consisting a vertex set $g_1 \cup g2$ and edge set $h_1 \cup h_2$ then $G_1 \cup G_2$.

Let G_1 and G_2 be a **join of graphs**. If two graphs G_1 and G_2 are join $G_1 + G_2$, consisting a vertex$g_1 \cup g_2$ and edge $H(G_1 + G_2) = \{gh|g \in V(G_1), h \in V(G_2)\}$ sets.

2.2.11 Sub-divided Graphs

Inserting a new two degree vertex of G in each edge then we obtained a sub-divided graph $G^{\star}$ of a graph $G = (G(G), H(G))$ is known as sub-divided graphs, Where $G(G)$ and H(G) symbolized the vertex and edge of any graph of G. After subdivision inserting a new node in edge of G is shown in below figure 2.3. We can Easily differentiate between normal and subdivided graph of G.

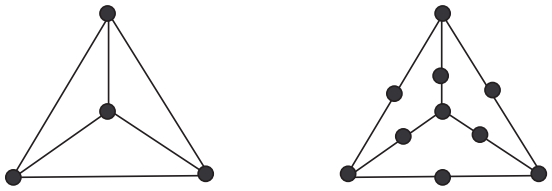

Figure 2.3: A normal and subdivide representation of graph G

2.2.12 Molecular or Chemical Graphs

A graph(or molecular network) of G is called molecular or chemical graph if vertices(nodes) represents carbon atoms and edges of G represents bonds(covalent bond) between corresponding carbon atoms of an organic molecule. The molecules or chemical compounds are modeled as under

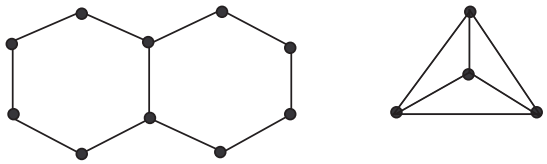

Figure 2.4: Molecular or Chemical graphs of honeycomb and silicate structure

Chapter 3

Degree Based Topological Indices

Topological index or *Molecular descriptor* is obtained by transforming the chemical information into a numerical number. Topological index is a molecular graphics invariant which is the correlation with the physico-chemical properties of a molecular graphical numbers. There are three important types of topological indices like Distance based topological index,Degree based topological index and Counting related polynomials index of the graphs. Among these classifications degree based topological indices have major importance and perform an extraordinary work in a graphs of chemicals. In the short way, a topological index Top(G) of a graph, is a number of property that for every graph U isomorphic to G, $Top(U) = Top(G)$. The idea of topological indices delivered by Wiener [25] during the working on paraffin's boiling points, introduce that index as a *path number*, after called it *wiener index*.

In 1947, Harry Wiener [25] introduced the *wiener index*. His success based on it, chemical graphs have many other topological indices consist of information of molecular branching [24].

Definition 3.0.1. The *wiener's index* is defined as

$$W(G) = \frac{1}{2}\sum_{(g,h)} d(g,h)$$

where (g,h) is the distance between two points write in ordered pair of (nodes)vertices of G and the length is $d(g,h)$ of a g-h i.e *geodesic*. *Geodesic* is a shortest distance between two points.

After Wiener's work index another, a freshly introduction of *Szeged index* [14], which is same kind of winner's denoted by S_z is a newly introduced in graph invariant, this index having a lots of applications in chemistry. This formula is a Cartesian product of graphs is obtained and some other composite graphs are considered. A basic mathematical properties of *Szeged index* S_z were established [3-5,14] and a certain types of chemical applications were reported in mentioned references [15,19].

In 1972, *Zägreb* indices have been introduced by *Zägreb* Group [12]. The original *Zägreb* indices are defined as follows: $M_1 = d(j)d(j)$ vertices, $M_2 = d(j)d(k)$ edges, where $d(j)$ is the degree of vertex j and $d(j)d(k)$ is the weight of edge j k [13]. A pair of topological indices, denoted by symbols M_1 and M_2 [12]. In literature, there are different names given it, such as the *Zägreb* Group indices [6], the *Zägreb* group parameters and most knowing, the *Zägreb* indices [2]. Introduction of an important topological index by Ivan *Gutmán* and *Trinájstiċ* [12] and its representation of *Zägreb* index is $M_1(G)$ and defined as

Definition 3.0.2. The *first Zägreb index* and *second Zägreb index* are defined below as

$$M_1(G) = \sum_{gh \in E(G)} (d_g + d_h)$$

$$M_2(G) = \sum_{(g,h)} (d_g.d_h)$$

In 1975, [22] *Randić* index have been introduced this invariant by *Milan Randić*. It's an often used in chemo informatics to investigate the compounds of chemicals. The *Randić* index, also said the connectivity index of graph is defined as

Definition 3.0.3. The *Randić index* is defined as

$$R_{1/2}(G) = \sum_{(g,h)} 1/\sqrt{(d_g d_h)}$$

where d_g and d_h are the degrees of the vertices.

Later, *Böllöbás* and *Erdös* generalized it for γ, where $\gamma \in R$ and is called generalized *Randić index*[1] is defined as

$$R_\gamma(G) = \sum_{gh \in E(G)} (d_g d_h)^\gamma,$$

for $\gamma = \{-1, -1/2, 1/2, 1\}$.

In 2003, *Nikoli*$\acute{c}$ et al. developed modified form of second *Zägreb* index [21]. Modified *Zägreb* index of graph G is defined as

Definition 3.0.4. The *Modified Zägreb index* is defined as

$$SMZ(G) = \sum_{gh \in E(G)} (d_g d_h)^{-1}$$

In 1998, *Ernestö* Estrada et al.[7] proposed a new topological index, named atom-bond connectivity(ABC) index defined as

Definition 3.0.5. The atom-bond connectivity *ABC index* is defined as

$$ABC(G) = \sum_{gh \in E(G)} \sqrt{\frac{d_g + d_h - 2}{d_g d_h}}$$

In 2008, It is an excellent correlation with the heat for the formation of alkanes [7,8]. Where $E(G)$ is the edges set and d_g,d_h are the degrees of vertices g and h in G, respectively.

In 2009, D. *Vukicevíc* and B. *Furtulá* established first $C(GA)$ index in [19]. The first geometric-arithmetic (GA) index of a graph G is defined as

Definition 3.0.6. The geometric-arithmetic *GA index* is defined as

$$G(GA) = \sum_{gh \in E(G)} \frac{2\sqrt{d_g d_h}}{d_g + d_h}$$

In 2010, *Furtulá* et al. established another molecular descriptor called Augmented *Zägreb* index [9] is defined as

Definition 3.0.7. The *Augmented Zägreb index* is defined as

$$AZM(G) = \sum_{gh \in E(G)} (\frac{d_g d_h}{d_g + d_h - 2})^3$$

In 2011, after first and second *Zägreb* indices, the third *Zägreb* index is discussed in [11]. This new graph invariant is symbolized as $M_3 = M_3(G)$ and defined as

Definition 3.0.8. The *third Zägrebindex* is defined as

$$M_3(G) = \sum_{gh \in E(G)} |d(g) - d(h)|$$

In 2013, Recently [23] a new degree based topological index introduced is hyper *Zägreb* index which is defined below

Definition 3.0.9. The*hyper-Zägreb index* is defined as

$$HM(G) = \sum_{gh \in E(G)} (deg(g) + deg(h))^2$$

[16] [26-28].

In 2015, M. R. Farahani, [10] computing the hyper-*Zägreb* index of hexagonal nanotube Some new results on the hyper-*Zägreb* ,index can be found in [10].

Main Results

In this section, We discuss the general *Randić*, ABC, GA, first *zägreb*, second *zägreb*, second modified *zägreb*, third *zägreb*, hyper-*ägreb* and augmented *zägreb* indices. We compute the subdivision of different kinds of networks like sierpinski networks $S(n, 4)$ and $S(n, 5)$ etc

Chapter 4

Topological Indices on Different Networks

4.1 Topological Indices on Different Networks

4.1.1 Results for Subdivision of Sierpinski Networks

the definition of sierpinski networks $S(n,k)$ originated from the topological studies of the Lipscomb's space and sierpinski network $S(n,k)$ is isomorphic to the graph of the Tower of Hanoi with n disks. Moreover, sierpinski graphs are the first nontrivial families of graphs of fractal type for which the crossing number is known ans several metric invariants such as unique 1-perfect codes, average distance of sierpinski graphs are studied in the literature.the division of sierpinski networks $S(n,4)$ and $S(n,5)$ are depicted in fig 3.1 and fig [17].

In this thesis, we compute the subdivided sierpinski networks $S(n,4)$ and $S(n,5)$

4.1.2 Results for Subdivision of sierpinski Network $G = S(n, 4)$

using general *Randić* $R_\alpha(G)$ for $\gamma = \{-1, -\frac{1}{2}, \frac{1}{2}, 1\}$, ABC, GA, first *Zägreb*, second *Zägreb*, second modified *Zägreb*, third *Zägreb* and hyper-*Zägreb* and augmented *Zägreb* indices for $S(n, 4)$.

In the subdivided sierpinski network $S(n, 4)$, the number of edges are

$$16(4^n + 1) + 12$$

. There are three types of degree based edges that is 2,3 and 4.The following table 4.1 give us two types of edges,

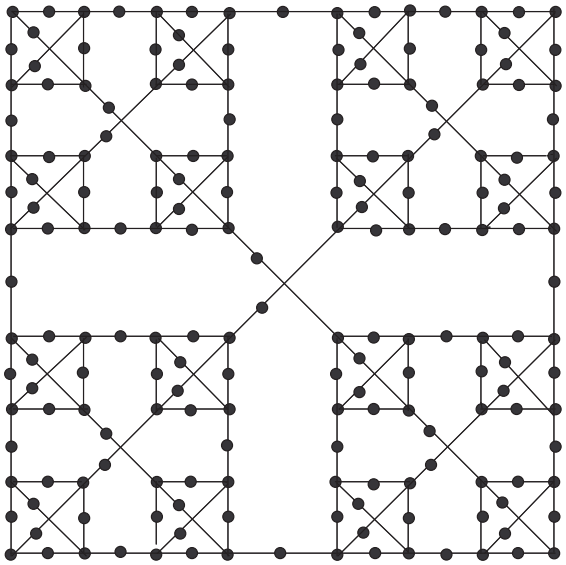

Figure 4.1: The subdivided sierpinski network $S(n, 4)$

Theorem 4.1.1. *For Subdivided Sierpinski network $S(n, 4)$, then general Randić index is equal to*

Table 4.1: Edge partitioned of a graph G based on degree sum of end vertices of each edge.

(d_g, d_h),where $gh \in E(G)$	No. of E(G)
$(2,3)$	12
$(2,4)$	$16(4^n-1)$

$$R_\gamma S(n,4) = \begin{cases} 72 + 128(4^n-1), & for \ \ \gamma = 1 \\ 12(\sqrt{6}) + 32(4^n-1)(\sqrt{2}), & for \ \ \gamma = \frac{1}{2} \\ 2\sqrt{6} + 4(4^n-1)(\sqrt{2}), & for \ \ \gamma = -\frac{1}{2} \\ 2(4^n), & for \ \ \gamma = -1 \end{cases}$$

Proof. Let G be a subdivided sierpniski network $S(n,4)$ of n dimension, we have $|E(2,4)| = 16(4^n-1)$ and $|E(2,3)| = 12$ respectively.

Section 1. $\gamma = -1$

application of *Randić* index $R_\gamma(G)$ for $\gamma = -1$

$$R_{-1}(G) = \sum_{gh \in E(G)} \frac{1}{d_g.d_h}$$

Using the above table, we know

$R_{-1}(G) = \frac{16(4^n-1)}{2.4} + \frac{12}{2.3}$

by doing some calculation, we get

$R_{-1}(G)$=$2(4^n)$

Section 2. $\gamma = -\frac{1}{2}$

Now, application of *Randić* index $R_\alpha(G)$ for $\gamma = -\frac{1}{2}$

$$R_{-\frac{1}{2}}(G) = \sum_{gh \in E(G)} \frac{1}{\sqrt{(d_g)(d_h)}}$$

Using the above table, we know

$$R_{-\frac{1}{2}}(G) = \frac{12}{\sqrt{(2)(3)}} + \frac{16(4^n - 1)}{\sqrt{(2)(4)}}$$

by doing some calculation, we get

$R_{-\frac{1}{2}}$=$2(\sqrt{6}) + 4(4^n - 1)(\sqrt{2})$

Section 3. $\gamma = \frac{1}{2}$

Now, application of *Randić* index $R_\alpha(G)$ for $\gamma = \frac{1}{2}$

$$R_{\frac{1}{2}} = \sum_{gh \in E(G)} \sqrt{d_g.d_h}$$

$R_{\frac{1}{2}}(G) = 12(\sqrt{2.3}) + (16(4^n - 1))(\sqrt{2.4})$

by doing some calculation, we get

$R_{\frac{1}{2}}$= $12(\sqrt{6}) + 32(4^n - 1)(\sqrt{2})$

Section 4. $\gamma = 1$

Now, application of *Randić* index $R_\gamma(G)$ for $\gamma = 1$

$$R_1(G) = \sum_{gh \in E(G)} (d_g.d_h)$$

$R_1(G)$ =$12(2.3) + 16(4^n - 1)(2.4)$

by doing some calculation, we get

R_1= $72 + 128(4^n - 1)$.

Theorem 4.1.2. *For subdivided sierpinski network $S(n, 4)$, the first Zägreb index is equal to*

$M_1(G) = 60 + 96(4^n - 1)$

Proof. Let G be the subdivided sierpinski network $S(n, 4)$. Using above table, we get

$$M_1(G) = \sum_{gh \in E(G)} (d_g + d_h)$$

$M_1(G) = 12(2 + 3) + 16(4^n - 1)(2 + 4)$

by doing some calculations, we get

$M_1(G) = 60 + 96(4^n - 1)$

Corollary 4.1.3. *For $\gamma = 1$ is called a second Zägreb index in a general Randić index for any graph of G.*

$$M_2(G) = \sum_{gh \in E(G)} (d_g.d_h)$$

Corollary 4.1.4. *For $\gamma = -1$ is the second modified Zägreb index in a general Randić index for any graph of G.*

$$SMZ(G) = \sum_{gh \in E(G)} \frac{1}{d_g d_h}$$

Theorem 4.1.5. *For subdivided sierpinski network $S(n,4)$, the third Zägreb index is equal to*

$M_3(G) = 12 + 32(4^n - 1)$.

Proof.Let G be a subdivided sierpinski network $S(n,4)$. Using above table, we know

$$M_3(G) = \sum_{gh \in E(G)} |d_g - d_h|$$

$M_3(G) = 12|2-3| + 16(4^n - 1)|2-4|$

by doing some calculations, we get

$M_3(G) = 12 + 32(54n - 1)$.

Theorem 4.1.6. *For subdivided sierpinski network $S(n,4)$, the hyper Zägreb index is equal to*

$HM(G) = 300 + 576(4^n - 1)$

Proof. Let G be the subdivided sierpinski network $S(n,4)$. Using above table, we know

$$HM(G) = \sum_{gh \in E(G)} (d_g + d_h)^2$$

$HM(G) = 12(2+3)^2 + 16(4^n - 1)(2+4)^2$

by doing some calculations, we get

$HM(G) = 300 + 576(4^n - 1)$

Theorem 4.1.7. *For $S(n,4)$, the Augmented Zagreb index is equal to*

$AMZ(G) = 96 + 128(4^n - 1)$

Proof. Let G be the subdivided sierpinski network $S(n,4)$. Using above table, we know

$$AMZ(G) = \sum_{gh \in E(G)} (\frac{d_g d_h}{d_g + d_h - 2})^3$$

$AMZ(G) = 12(\frac{2.3}{2+3-2})^3 + 16(4^n - 1)(\frac{2.4}{2+4-2})^3$

by doing some calculations, we get

$AMZ(G) = 96 + 128(4^n - 1)$

Theorem 4.1.8. *For subdivided sierpinski network $S(n,4)$, the ABC index is equal to*

$ABC(G) = 6\sqrt{2} + 8(4^n - 1)(\sqrt{2})$.

Proof. Let G be the subdivided sierpinski network $S(n,4)$. Using above table table, we know

$$ABC(G) = \sum_{gh \in E(G)} \sqrt{\frac{d_g + d_h - 2}{d_g d_h}}$$

$ABC(G) = 12(\sqrt{\frac{2+3-2}{2.3}}) + 16(4^n - 1)(\sqrt{\frac{2+4-2}{2.4}})$

by doing some calculations, we get

$ABC(G) = 6(\sqrt{2}) + 8(4^n - 1)(\sqrt{2})$.

Theorem 4.1.9. *For subdivided sierpinski network $S(n, 4)$, the GA index is equal to* $GA(G) = 4\sqrt{6} + \frac{(\sqrt{2})(32)(4^n-1)}{3}$.

proof. Let G be the subdivided sierpinski network $S(n, 4)$. Using above table, we know

$$GA(G) = \sum_{gh \in E(G)} \frac{2\sqrt{d_g d_h}}{(d_g + d_h)}$$

$GA(G) = 12(\frac{2\sqrt{2.3}}{2+3}) + 16(4^n - 1)(\frac{2\sqrt{2.4}}{2+4})$

by doing some calculations, we get

$GA(G) == 4(\sqrt{6}) + \frac{32(\sqrt{2})(4^n-1)}{3}$.

4.1.3 Results for Subdivision of sierpinski Network $G = S(n, 5)$

using general *Randić* $R_\alpha(G)$ for $\gamma = \{-1, -\frac{1}{2}, \frac{1}{2}, 1\}$, ABC, GA, first *Zägreb*, second *Zägreb*, second modified *Zägreb*, third *Zägreb* and hyper-*Zägreb* and augmented *Zägreb* indices for $S(n, 5)$.

In the subdivide sierpinski network $S(n, 5)$, the number of edges are $5(5^n - 1)$.

There are two types of degree based edges that is 2, 4and 5.The following table 4.2 give us one types of edges.

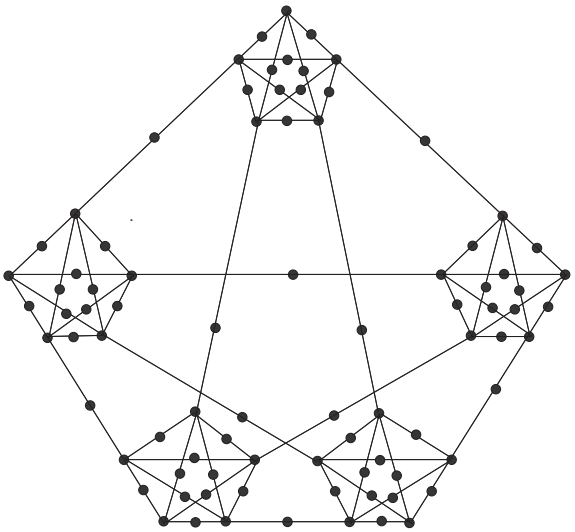

Figure 4.2: The subdivided sierpinski network $S(n, 5)$

Table 4.2: Edge partitioned of a graph G based on degree sum of end vertices of each edge.

(d_g, d_h),where $gh \in E(G)$	No. of E(G)
$(2, 4)$	20
$(2, 5)$	$25(5^n - 1)$

Theorem 4.1.10. *For Subdivided Sierpinski network $S(n, 5)$, then general Randić index is equal to*

$$R_\gamma SN(n,5) = \begin{cases} \frac{5(5^n)}{2}, & for\ \ \gamma = -1 \\ \frac{25(5^n-1)}{\sqrt{10}} + \frac{10}{\sqrt{2}}, & for\ \ \gamma = -\frac{1}{2} \\ 25\sqrt{10}(5^n-1) + 40\sqrt{2}, & for\ \ \gamma = \frac{1}{2} \\ 250(5^n) - 90, & for\ \ \gamma = 1 \end{cases}$$

proof. Let G be a subdivided sierpniski network $S(n,5)$ of n dimension, we have $|E(2,4)| = 20$ and $|E(2,5)| = 25(5^n - 1)$ respectively.

Section 1. $\gamma = -1$

application of *Randić* index $R_\gamma(G)$ for $\gamma = -1$

$$R_{-1}(G) = \sum_{gh \in E(G)} \frac{1}{d_g d_h}$$

Using the above table, we know

$R_{-1}(G) = \frac{20}{2.4} + \frac{25(5^n-1)}{2.5}$

by doing some calculation, we get

$R_{-1}(G) = \frac{5(5^n)}{2}$

Section 2. $\gamma = -\frac{1}{2}$

Now, application of *Randić* index $R_\alpha(G)$ for $\gamma = -\frac{1}{2}$

$$R_{-\frac{1}{2}} = \sum_{gh \in E(G)} \frac{1}{\sqrt{(d_g)(d_h)}}$$

$R_{-\frac{1}{2}} = \frac{20}{\sqrt{2.4}} + \frac{25(5^n-1)}{\sqrt{2.5}}$

by doing some calculation, we get

$R_{-\frac{1}{2}}=\frac{25(5^n-1)}{\sqrt{10}}+\frac{10}{\sqrt{2}}$

Section 3. $\gamma=\frac{1}{2}$

Now, application of *Randić* index $R_\alpha(G)$ for $\gamma=\frac{1}{2}$

$$R_{\frac{1}{2}}=\sum_{gh\in E(G)}\sqrt{d_g.d_h}$$

$R_{\frac{1}{2}}(G)=20\sqrt{2.4}+25\sqrt{2.5}(5^n-1)$

by doing some calculation, we get

$R_{\frac{1}{2}}=25\sqrt{10}(5^n-1)+40\sqrt{2}$

Section 4. $\gamma=1$

Now, application of *Randić* index $R_\gamma(G)$ for $\gamma=1$

$$R_1(G)=\sum_{gh\in E(G)}(d_g.d_h)$$

$R_1(G)$ =$20(2.4)+25(5^n-1)(2.5)$

by doing some calculation, we get

$R_1=250(5^n)-90.$

Theorem 4.1.11. *For subdivided sierpinski network $S(n,5)$, the first Zägreb index is equal to*

$M_1(G)=175(5^n)-55$

proof. Let G be the subdivided sierpinski network $S(n,5)$. Using above table, we get

$$M_1(G) = \sum_{gh \in E(G)} (d_g + d_h)$$

$M_1(G) = 20(2+4) + 25(5^n - 1)(2+5)$

by doing some calculations, we get

$M_1(G) = 175(5^n) - 55$

Corollary 4.1.12. *For $\gamma = 1$ is called a second Zägreb index in a general Randić index for any graph of G.*

$$M_2(G) = \sum_{gh \in E(G)} (d_g.d_h)$$

Corollary 4.1.13. *For $\gamma = -1$ is the second modified Zägreb index in a general Randić index for any graph of G.*

$$SMZ(G) = \sum_{gh \in E(G)} \frac{1}{d_g d_h}$$

Theorem 4.1.14. *For subdivided sierpinski network $S(n, 5)$, the third Zägreb index is equal to*

$M_3(G) = 115 - 75(5^n)$.

proof:Let G be a subdivided sierpinski network $S(n,5)$. Using above table, we know

$$M_3(G) = \sum_{gh \in E(G)} |d_g - d_h|$$

$M_3(G) = 20|2-4| + 25(5^n - 1)|2-5|$

by doing some calculations, we get

$M_3(G) = 115 - 75(5^n)$.

Theorem 4.1.15. *For subdivided sierpinski network $S(n,5)$, the hyper Zägreb index is equal to*

$HM(G) = 1225(5^n) - 505$.

proof. Let G be the subdivided sierpinski network $S(n,5)$. Using above table, we know

$$HM(G) = \sum_{gh \in E(G)} (d_g + d_h)^2$$

$HM(G) = 20(2+4)^2 + 25(5^n - 1)(2+5)^2$

by doing some calculations, we get

$HM(G) = 1225(5^n) - 505$

Theorem 4.1.16. *For $S(n,5)$, the Augmented Zagreb index is equal to*

$AMZ(G) = 25(5^n) - 40$

Proof: Let G be the subdivided sierpinski network $S(n,5)$. Using above table, we know

$$AMZ(G) = \sum_{gh \in E(G)} (\frac{d_g d_h}{d_g + d_h - 2})^3$$

$AMZ(G) = 20(\frac{2.4}{2+4-2})^3 + 25(5^n - 1)(\frac{2.5}{2+5-2})^3$

by doing some calculations, we get

$AMZ(G) = 25(5^n) - 40$

Theorem 4.1.17. *For subdivided sierpinski network $S(n,5)$, the ABC index is equal to*

$ABC(G) = 20\sqrt{\frac{1}{2}} + 25(5^n - 1)\sqrt{\frac{1}{2}}$.

Proof: Let G be the subdivided sierpinski network $S(n,5)$. Using above table table, we know

$$ABC(G) = \sum_{gh \in E(G)} \sqrt{\frac{d_g + d_h - 2}{d_g d_h}}$$

$ABC(G) = 20\sqrt{\frac{2+4-2}{2.4}} + 25(5^n - 1)(\sqrt{\frac{2+5-2}{2.5}})$

by doing some calculations, we get

$ABC(G) = 20\sqrt{\frac{1}{2}} + 25(5^n - 1)\sqrt{\frac{1}{2}}$.

Theorem 4.1.18. *For subdivided sierpinski network $S(n,5)$, the GA index is equal to*

$GA(G) = \frac{40\sqrt{2}}{3} + 50\sqrt{10}((5^n) - \frac{1}{7})$.

proof: Let G be the subdivided sierpinski network $S(n,5)$. Using above table, we know

$$GA(G) = \sum_{gh \in E(G)} \frac{2\sqrt{d_g d_h}}{(d_g + d_h)}$$

$GA(G) = 20(\frac{2\sqrt{2.4}}{2+4}) + 25(5^n - 1)(\frac{2\sqrt{2.5}}{2+5})$

by doing some calculations, we get

$GA(G) = \frac{40\sqrt{2}}{3} + 50\sqrt{10}((5^n) - \frac{1}{7})$.

Chapter 5

conclusion and open problems

In this thesis, Topological indices which are particular based on degree like general *randić*, ABC, GA, first *zägreb*, second *zägreb*, second modified *zägreb*, third *zägreb*, hyper-*zägreb* and augmented *zägreb* indices for subdivision of different kinds of networks like sierpinski networks $S(n, 4)$ and $S(n, 5)$. The study of new design architectural structure always has a open problem of above networks and art/design sciences. Here new constructed networks of topological indices, construction of these networks, properties of good topological indices have discussed here.

In coming research papers, our interest to sketch some new graph and networks(webs) and discuss their topological indices that will be able to understand its topologies.

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