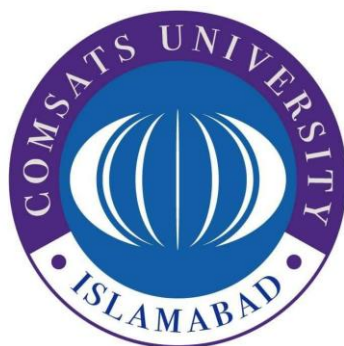


Degree-Distance Base Topological Indices from Some Graphs Operations



By

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CIIT/SP17-RMT-002/LHR

MS

In

Mathematics

COMSATS University Islamabad

Lahore Campus

Fall, 2018



COMSATS University Islamabad

Degree-Distance Base Topological Indices from Some Graphs Operations

A Thesis Presented to

COMSATS University Islamabad,

In partial fulfillment

of the requirement for the degree of

MS (Mathematics)

By

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A Post Graduate Thesis submitted to the Department of Mathematics as partial fulfillment of the requirement for the award of Degree of MS Mathematics.

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Declaration

I **Aqib Ali** registration number **CIIT/SP17-RMT-002/LHR** hereby declare that I have produced the work presented in this thesis, during the scheduled period of study. I also declare that I have not taken any material from any source except referred to wherever due, that amount of plagiarism is within acceptable range. If a violation of HEC rules on research has occurred in this thesis, I shall be liable to punishable action under the plagiarism rules of the HEC.

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It is certified that **Aqib Ali (CIIT/SP17-RMT-002/LHR)** has carried out all the work related to this report under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus and the work fulfills the requirement for award of MS Mathematics.

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DEDICATED

To

My Family

ACKNOWLEDGEMENTS

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Aqib Ali

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ABSTRACT

Degree-Distance Base Topological Indices from Some Graphs Operations

In this thesis, firstly we find the degree based topological indices and M -polynomial for line graph of t -subdivided graphs of probabilistic neural networks $L[PNN(q, c^*, c)]$ for $t \geq 1$. We also find the fourth and fifth version of atomic bond connectivity ABC_4 , ABC_5 index and fourth and fifth version of geometric-arithmetic GA_4 , GA_5 index of line graph of 1-subdivided graphs of probabilistic neural networks $L[PNN(q, c^*, c)]$. Secondly, we find the degree based topological indices and M -polynomial for line graph of m -subdivided graphs for the chain of Bismuth Tri-Iodide $L[m - Bil_3]$ for $m \geq 3$. Lastly, we find the first and third zagreb eccentric index and M -polynomial of sierpinski networks $S(n, k)$.

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Chapter 1

Introduction

The solution to seven bridges problem of Knigsberg by Leonhard Paul Euler was the beginning of graph theory in 1736. He proved that this walk is not possible in one time. Graph theory has tremendous applications in various fields of everyday sciences. Computer scientists use graphs to highlight the complicated networking of communication, computational devices, data organization and the flow of computation. Branch of graph theory that discusses chemical structures of molecules is known as chemical graph theory by which problems of chemistry can be dealt by using set theory and combinatorics as well. The main purpose of this theory is to clarify molecular characteristics of chemicals like isomers etc.

1.0.1 Graph

A graph G is an ordered pair of set of nodes known as vertices $V(G)$ and set of lines known as edges $E(G)$; each edge connects two vertices. In the following graph, if vertex set of a graph $V(G) = \{v_1, v_2, v_3, v_4, v_5\}$ then $|V(G)|$ represents the order of graph and if edge set of the graph $E(G) = \{e_1, e_2, \dots, e_{10}\}$ then $|E(G)|$ is termed as size of the graph.

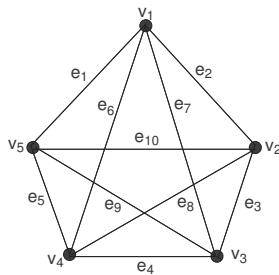


Figure 1.1: The Graph G

1.0.2 Subgraph

A subgraph (H) is a graph originates from graph (G) in which every vertex $V(H)$ and edge $E(H)$ belongs to $V(G)$ and $E(G)$ respectively.

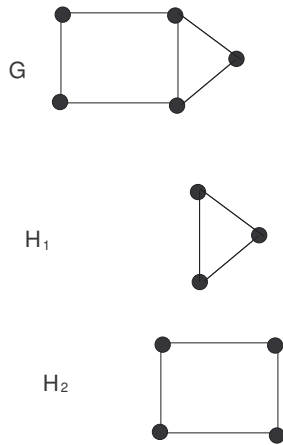


Figure 1.2: The Subgraphs H_1 and H_2 of graph G

1.0.3 Degree

The number of edges incident on a vertex is called degree of a vertex and denoted by $\deg_G(v)$. In the following graph all vertices have degree 4.

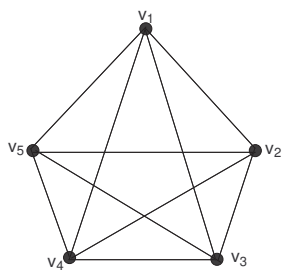


Figure 1.3

1.0.4 Distance

The distance $d(u, v)$ is the length of shortest path between vertices u and v .

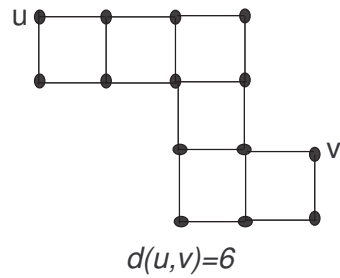


Figure 1.4: Distance of a vertex

1.0.5 Neighbourhood of a vertex

The graph neighbourhood of a vertex in a graph is the set of all the vertices adjacent to it. In the following graph neighbourhood of a vertex is $\delta(v) = 10$

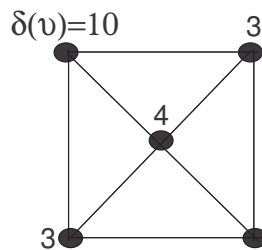


Figure 1.5: Neighborhood of a vertex

1.0.6 Cycle

A simple cycle is closed walk without repetition in vertices and edges having same starting and ending point. Cycle on n vertices is symbolized as C_n .

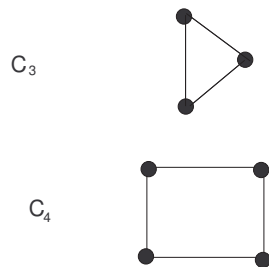


Figure 1.6: Cycle

1.0.7 Isolated vertex

An isolated vertex is known as vertex of that graph which is not the end point of any edge.

1.0.8 Adjacent vertices

If two vertices connected by an edge is known as neighbors or adjacent vertices.

1.0.9 Even vertex

Any vertex having even degree is known as even vertex.

1.0.10 Odd vertex

Any vertex having odd degree is named as odd vertex.

1.0.11 Loop

A loop is an edge with two coincident vertices.

1.0.12 Line graph

Let G be a simple graph. The line graph of G is obtained when edges of G is transformed into vertices and two vertices in $L(G)$ are connected if and only if the adjacent edges in G have an end in common.

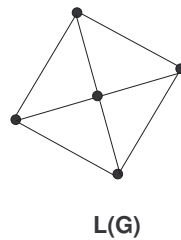
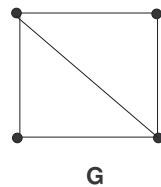


Figure 1.7: Line graph of G

1.0.13 Complete graph

A complete graph is a graph in which each pair of different vertices is joined by an edge of graph.

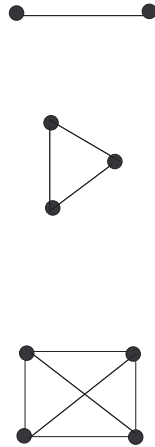


Figure 1.8: Complete Graphs K_2 , K_3 , K_4

1.0.14 Acyclic

A graph is acyclic if there is no cycle in it.

1.0.15 Connected Graph

An undirected graph is said to be connected when there is a path between every pair of vertices.

1.0.16 Tree graph

An acyclic connected graph is called tree graph. In this graph, if we take $|V| = m$ in tree then $|E| = m - 1$ and there is only one track between every two vertices.

1.0.17 Bipartite Graph

A bipartite graph $G(Y, Z, E)$ is a graph that has two set of vertices Y , Z and there will be edges between two vertices of Y and Z . No edge exists between vertices of Y and vertices of Z itself.

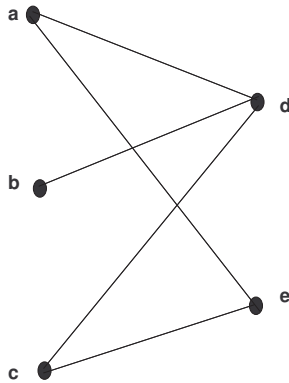


Figure 1.9: Bipartite Graph

1.0.18 Complete Bipartite Graph

A graph is called a complete bipartite graph in which all vertices of Y will be connected with all the vertices of Z . It is symbolized by $K_{n,m}$.

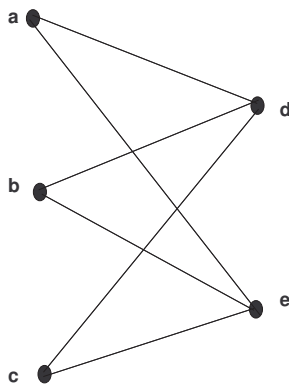


Figure 1.10: Complete Bipartite Graph $K_{2,3}$

1.0.19 Walk

Walk is a sequential path from starting vertex to end vertex, where number of vertices covered during this path is called length of walk.

1.0.20 Path

A path in a diagram is a limited or unbounded grouping of edges which interface a succession of vertices which, are on the whole particular from each other.

1.0.21 Eccentricity

The eccentricity of a vertex u_1 is the maximum of distances of u_1 from elements of $V(G)$ i.e, $ecc(v) = \max\{d(u_1, v) : v \in V(G)\}$. The $ecc(u_1)$ will be ∞ if u_1 belongs to the disconnected graph. In the following graph eccentricity of v is 7 and symbolically it is $\xi(v) = 7$.

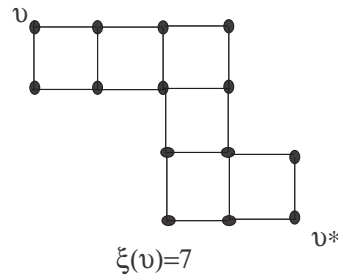


Figure 1.11: $\xi(v) = 7$

1.0.22 Subdivision of Graph

A subdivision of a graph G is a graph obtained by adding vertices in each edge set of a graph G . It is denoted by $S(G)$.

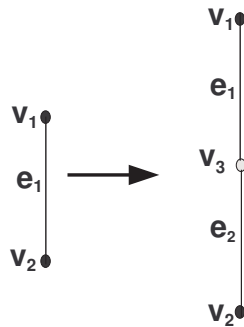


Figure 1.12: Subdivision of Graph

1.1 Topological Indices of Graph

"A topological index of a graph is actual number identified with the graph; it doesn't rely upon pictorial representation or labeling of a graph. The descriptors of molecular structure (can be called topological indices) are used for pharmacologic, biological modeling physicochemical, toxicological and other properties of chemical compounds in theoretical chemistry [11]. There exist several kinds of topological indices.

Topological index is categorized in three aspects."

1. Distance based.
2. Degree based.
3. Spectrum based.

1.1.1 Degree based topological indices

Some familiar Degree based topological indices are written bellow:

- Atom-bond Connectivity (ABC) index
- Geometric-arithmetic (GA) index
- Randic (R_γ) index
- Zagreb (M) index
- Augmented Zegreb (AZI) index
- Harmonic (H) index
- Sum-connectivity (SCI) index

Atom-bond connectivity index

"According to Estrada et al. [5] a notable Atomic bound connectivity index usually depends on degree of graph G , known as $ABC(G)$. The ABC index can be mentioned

as”

$$ABC(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d_{\alpha} + d_{\beta} - 2}{d_{\alpha}d_{\beta}}}$$

Randic index

”Randic index is named after a mathematician Milan Randic who derived it, in 1975. Afterwards, it is known as generalized Randic index due to its differentiation for some real numeral α . In chemoinformatics Randic index consists a large number of applications, such as to discover organic compounds.

Randic index is symbolized as” $R_{-\frac{1}{2}}(G)$. The Randic index elaborated as:

$$R_{-\frac{1}{2}}(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{\sqrt{\deg(\alpha)\deg(\beta)}}$$

The general Randic index $R_{\alpha}(G)$ is defined as:

$$R_{\alpha}(G) = \sum_{\alpha\beta \in E(G)} (\deg(\alpha)\deg(\beta))^{\alpha}$$

For $\alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}$

In [17] Imran et al. recently computed topological descriptors of certain interconnection linkages. They found various indices for butterfly, benes network system, silicates and discover outcomes of generalized Randic index $R_{\alpha}(G)$.

Zagreb index

”Trinajstić and Gutman presented Zagreb index. Balaban et al. categorized zagreb index into two types, M_1 denotes first zagreb index and defines as”

$$M_1(G) = \sum_{\alpha\beta \in E(G)} [\deg(\alpha) + \deg(\beta)]$$

while M_2 represents second zagreb index written as

$$M_2(G) = \sum_{\alpha\beta \in E(G)} [deg(\alpha)deg(\beta)].$$

”In [27], Siddiqui et al. at Zagreb indices, Zagreb polynomials, first numerous Zagreb index, second various Zagreb index and hyper Zegren index for some dendrimers and nanostars.”

”Ghorbani et al. [10] in 2010, presented the fourth form of ABC index, which depends on nieghbourhood degree of graph, which is formulated as”

$$ABC_4(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{S_\alpha + S_\beta - 2}{S_\alpha S_\beta}}$$

Imran et al. [17] calculated ABC_4 of silicates, honeycomb, and hexagonal networks.

Augmented Zagreb index

”Furtula et al. [8] by the accomplishment of the ABC index, set forward its altered adaptation, that they named augmented Zagreb index. It is characterized as”

$$AZI(G) = \sum_{\alpha\beta \in E(G)} \left(\frac{d_\alpha(G)d_\beta(G)}{d_\alpha(G)d_\beta(G) - 2} \right)^3$$

Geometric-arithmetic index

”Vukicevic et al. put forward Geometric-arithmetic denoted as GA index of any graph G , whose mathematical form is

$$GA(G) = \sum_{\alpha\beta \in E(G)} \frac{2(\sqrt{d_\alpha(G)d_\beta(G)})}{(d_\alpha(G) + d_\beta(G))}$$

In 2011, fifth form of GA index symbolized as GA_5 is presented by Graovac et al. it defined as”

$$GA_5(G) = \sum_{\alpha\beta \in E(G)} \frac{2(\sqrt{S_\alpha(G)S_\beta(G)})}{(S_\alpha(G) + S_\beta(G))}$$

In [18], Bokhary and Imran worked on GA_5 for some categorizes of dendrimers and formulate them.

Nadeem et al. computed GA_5 of wheel, ladder and line graph of tadpole by subdividing them in [27].

Harmonic index

Zhang put forward the concept of harmonic index as:

$$H(G) = \sum_{\alpha\beta \in E(G)} \frac{2}{d_\alpha(G) + d_\beta(G)}$$

Sum-connectivity Index

sum connectivity index is presented by Zhou and Trinajstić

$$SCI(G) = \sum_{\alpha\beta \in E(G)} \frac{1}{d_\alpha(G) + d_\beta(G)}$$

1.2 M-polynomial

”The M -polynomial of G is defined as

$$M(G, x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j$$

where $\delta = \min\{d_v : v \in V(G)\}$, $\Delta = \max\{d_v : v \in V(G)\}$, and $m_{ij}(G)$ the number of edges $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$ ”

1.2.1 First zagreb index

”The First zagreb index narrated as”

$$M_1(G_n^m) = \sum_{vu \in E(G)} (d_v)^2$$

1.2.2 Second zagreb index

”The Second zagreb index described as”

$$M_2(G_n^m) = \sum_{vu \in E(G)} d_v d_u$$

1.2.3 Second modified zagreb index

”The Second modified zagreb index described as”

$$mM_2(G_n^m) = \sum_{vu \in E(G)} \frac{1}{d_v d_u}$$

1.2.4 General Randic Index

”The GRI known as General Randic Index of G stated as”

$$\sum_{vu \in E(G)} (d_v d_u)^\alpha$$

where α is an arbitrary real number see [24]

1.2.5 Symmetric Division Index

”The SDI known as Symmetric Division Index described as”

$$SDI(G_n^m) = \sum_{vu \in E(G)} \left\{ \frac{\min(d_v, d_u)}{\max(d_v, d_u)} + \frac{\max(d_v, d_u)}{\min(d_v, d_u)} \right\}$$

1.2.6 Harmonic Index

”The HI known as Harmonic Index $H(G)$ is another variant of Randic index stated as”

$$H(G_n^m) = \sum_{vu \in E(G)} \frac{2}{d_v + d_u} [33, 34]$$

1.2.7 Inverse sum topological index

”The inverse sum topological index ISI stated as”

$$ISI(G_n^m) = \sum_{vu \in E(G)} \frac{d_v d_u}{d_v + d_u}$$

1.2.8 Augmented Zagreb Index

”The AZI known as Augmented Zagreb Index of G stated as”

$$AZI(G_\alpha^\beta) = \sum_{vu \in E(G)} \left\{ \frac{d_v d_u}{d_v + d_u - 2} \right\}^3$$

”Derivation of some degree-based topological indices from M-polynomial”

Topological Index	Derived form $M(G_\alpha^\beta, \alpha, \beta)$
First zagreb	$(D_\alpha + D_\beta)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Second zagreb	$(D_\alpha D_\beta)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Second Modified zagreb	$(S_\alpha S_\beta)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
General Randic (GR) $m \in N$	$(D_\alpha^m D_\beta^m)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
General Randic (GR) $m \in N$	$(S_\alpha^m S_\beta^m)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Symmetric Division Index (SDI)	$(D_\alpha S_\beta + D_\beta S_\alpha)[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Harmonic Index (HI)	$2S_\alpha J[M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Inverse Sum Index (ISI)	$S_\alpha J D_\alpha D_\beta [M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$
Augmented Zagreb Index (AZI)	$S_\alpha^3 Q_{-2} J D_\alpha^3 D_\beta^3 [M(G_\alpha^\beta, \alpha, \beta)]_{\beta=\alpha=1}$

Where $D_\alpha f = \alpha \frac{\partial(f(\alpha,\beta))}{\partial \alpha}$, $D_\beta f = \beta \frac{\partial(f(\alpha,\beta))}{\partial \beta}$, $S_\alpha = \int_0^\alpha \frac{f(\beta,t)}{t} dt$, $S_\beta = \int_0^\beta \frac{f(\alpha,t)}{t} dt$,

1.2.9 Distance based topological indices

”The separation between the vertices of G is described as, the distance between two vertices α^* and β^* of graph G length of the is equivalent to the length of the most restricted way interfacing and indicated as $d(\alpha^*, \beta^* | G)$. The historical backdrop of distance based topological indices climb down to 1947, when Wiener figured the boiling points of alkanes, he utilized the distance in the sub-atomic charts of alkanes. This exploration of topological index is called wiener list that moved toward becoming most well known sub-atomic structure descriptors. We portray some distance based topological indices”.

- Wiener (W) index
- Wiener polarity (W_P) index
- Hyper Wiener (WW) index
- Terminal Wiener (TW) index
- Electric Connectivity (ξ) index
- Schultz (MTI) index
- Gutman (Gut) index

1.2.10 Eccentricity based topological indices

”Eccentricity is of any vertex α is the longest path number among any of other vertex in G . One of the mist famous topological index based on eccentricity is New Atomoc

bound connectivity index ABC_5 is defined as:

$$ABC_5(G) = \sum_{u,v \in E(G)} \sqrt{\frac{ecu(u) + ecu(v) - 2}{ecu(u)ecu(v)}}$$

Another one is eccentric connectivity index depends on eccentricity and degree of that vertex as”

$$\xi^c(G) = \sum_{\alpha \in V} ecc_G(\alpha) deg_G(\alpha)$$

1.3 Literature Review

”Randi’c index and Zagreb indices [23] are illustration of topological indices based on degree [24] for aspect on Randi’c index. In 1975, Milan Randi’c comprehended leading degree based topological index [28]. Gutman et al. introduced second geometric-arithmetic index [7]. Ghorbani et al. [10] elaborated the second atomic-bond connectivity index of chemical compounds. Estrada et al. [5] introduced degree based topological index which is known as the atomic bond connectivity index (ABC). ABC index turned out to be a practical device to demonstrate the thermodynamic possessions of molecular compounds. Imran et al. recently computed topological descriptors of certain interconnection linkages. They found various indices for butterfly, benes network system and silicates. Bokhary et al. [18] studied these indices for dendrimers. Nadeem et al. utilized several indices for line graph (in which edges transformed vertices and vice versa) of 2D lattice, nano tubes and nanotaurus in [26, 27]. The eccentric connectivity index for star, bipartite graph, path, cycle, lollipop, broom and volcano graph was piled up in [4, 25]. Hayat generalized $(ABC)_4$ and $(GA)_5$ index of nancones CNC; With respect to $(GA)_5$ he also generalized the features of K-regular graphs; Hayat estimated the ABC and GA index of networks of chains of silicates and oxides. By using the concept of subdivision (a graph attained by substituting edges of graphs

by P_2 . Young Hao et al. describes the (GA) index of nanotubes Graovac et al. studies the 5th member of the class of GA index.

The distance base topological invariants are extensively used to describe the structure of molecular graph and relationship between particles [15]. Wiener [33] utilized the distances in the molecular graphs of alkanes to analyze the boiling points. Gao et al. [9] defined distance-based topological indices and polynomials of friendship graphs. Moreover, distance-based topological indices which are launched are the vertex-Szeged index [12, 20] edge-Wiener index [22, 29] the edge-Szeged index [14] the PI index [21] etc. For the part of distance-sum-based molecular descriptors in a drug discovery process we illustrate [32] and the references in that. Jamil [19] studied some distance based topological indices for general double graphs He calculated the Harary index, Wiener index, additively weighted Harary index, multiplicative weighted Harary index (ECI) and total (EI) of $D[G]$, where $D[G]$ is the double graph of G . He verified the results for S_m , P_m , K_m and C_m be the star, path, complete and cyclic graph respectively with m vertices. The eccentricity connectivity index (ECI) of a graph G was characterized by Doli [4]. Distance base index specified by eccentric atom-bond connectivity index was defined by Farahani [6]. Madan et al. [32] introduced the (ECI) of the molecular graph G , denoted as $\zeta(G)$. Lokesh et al. [30] studied the (ECI) of the subdivision graph of wheel graphs, tadpole graphs, complete graphs. Hua and Das [16] considered the relationship between the Zagreb indices and (ECI). De [2] generalized expressions for the (ECI) and its polynomial of the thorn graphs. Rao and Lakshmi [31] yielded explicit formulas for (ECI) of phenylenic nanotubes.”

Chapter 2

Topological Indices from Some Graphs Operations

2.1 Probabilistic Neural Networks $PNN(q, c^*, c)$

"A Probabilistic neural network $PNN(q, c^*, c)$ is a feedforward neural network, which is widely used in classification and pattern recognition problem. It always move in one direction it never goes backward. A feedforward neural network is an artificial neural networks wherein connections between the nodes do not form a cycle. An artificial neural network is an interconnected group of nodes, similar to the vast network of neurons in a brain. In this section we find out the atomic-bound connectivity (ABC) index, geometric arithmetic (GA) index for line graph of t -subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$ for $t \geq 1$. We also find fourth version of atomic bound connectivity (ABC_4) index and the fifth version of geometric-arithmetic (GA_5) index for line graph of 1-subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$. We also calculate eccentric version of atomic bound connectivity ABC_5 index and eccentric version of geometric-arithmetic $GA_4(G)$ index for line graph of 1-subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$. Furthermore, we formulate first zagreb index, second zagreb index and modified zagreb index for line graph of 1-subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$."

In Fig. 2.1, a probabilistic neural networks $PNN(q, c^*, c)$ shown for $q = 3$, $c^* = 2$, $c = 2$

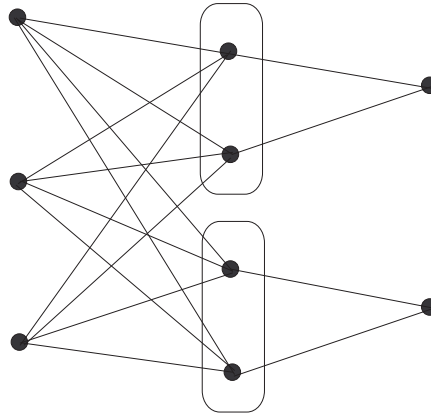


Figure 2.1: probabilistic neural networks $PNN(3, 2, 2)$

In Fig. 2.2, a line graph of 1-subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$ shown for $q = 3, c^* = 2, c = 2$

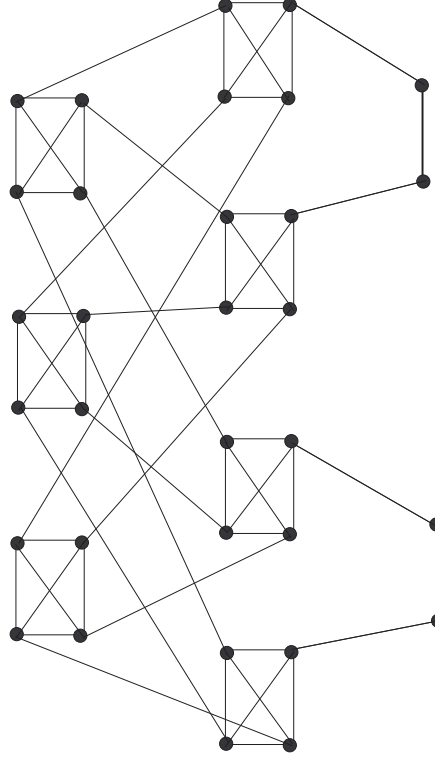


Figure 2.2: Line graph of 1-subdivided probabilistic neural networks $L[PNN(3, 2, 2)]$

Theorem 2.1.1. *Let G be a line graph of 1-subdivided probabilistic neural networks then atomic bound connectivity index of G is given as*

$$\begin{aligned}
 ABC(G) = & \frac{q(cc^* - 1)\sqrt{(cc^* - 1)}}{2} + \frac{qcc^*\sqrt{q}}{\sqrt{2}} + \frac{c^*(c - 1)\sqrt{(c - 1)}}{\sqrt{2}} + \frac{qcc^*\sqrt{cc^* + q - 1}}{\sqrt{cc^*(q + 1)}} \\
 & + \frac{cc^*\sqrt{c + q - 1}}{\sqrt{c(q + 1)}}.
 \end{aligned}$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line

graph of 1-subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^*-1)qcc^*}{2}$
$(q+1, q+1)$	$\frac{qcc^*(q+1)}{2}$
(c, c)	$\frac{cc^*(c-1)}{2}$
$(cc^*, q+1)$	qcc^*
$(q+1, c)$	cc^*

Now we find the atomic bound connectivity index of line graph of 1 subdivided probabilistic neural networks. Then according to formula of atomic bound connectivity index

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

Now,

$$\begin{aligned}
ABC(G) &= \frac{qcc^*(cc^*-1)}{2} \frac{\sqrt{cc^*+cc^*-2}}{(cc^*)^2} + \frac{qcc^*(q+1)}{2} \frac{\sqrt{(q+1)+(q+1)-2}}{(q+1)^2} \\
&+ \frac{cc^*(c-1)}{2} \frac{\sqrt{c+c-2}}{c^2} + \frac{qcc^*\sqrt{cc^*+q+1-2}}{cc^*(q+1)} + \frac{cc^*(q+1+c-2)}{c(q+1)} \\
&= \frac{q(cc^*-1)\sqrt{(cc^*-1)}}{2} + \frac{qcc^*\sqrt{q}}{\sqrt{2}} + \frac{c^*(c-1)\sqrt{(c-1)}}{\sqrt{2}} + \frac{qcc^*\sqrt{cc^*+q-1}}{\sqrt{cc^*(q+1)}} \\
&+ \frac{cc^*\sqrt{c+q-1}}{\sqrt{c(q+1)}} \quad \square
\end{aligned}$$

Verification.

Step 1. If $L[PNN(3, 2, 2)]$ be a graph have following edge types according to degree $(4, 4)$, $(2, 4)$ and $(2, 2)$ having accounts 54, 4 and 2 respectively. Then according to formula

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$\begin{aligned}
ABC[PNN(3,2,2)] &= 54\sqrt{\frac{4+4-2}{(4)(4)}} + 2\sqrt{\frac{2+2-2}{(2)(2)}} + 4\sqrt{\frac{4+2-2}{(4)(2)}} \\
&= 54\frac{\sqrt{6}}{4} + \frac{2}{\sqrt{2}} + 4\sqrt{\frac{1}{2}} \\
&= \frac{27}{2}\sqrt{6} + \sqrt{2} + 2\sqrt{2}.
\end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 32, then according to theorem 2.1.1 Atomic bound connectivity index of $PNN(3,2,2)$ is

$$\begin{aligned}
ABC[PNN(3,2,2)] &= \frac{3(3)}{2}\sqrt{2(3)} + \frac{12}{2}\sqrt{2(3)} + \frac{2}{2}\sqrt{2} + 12\sqrt{\frac{4+2}{4(4)}} + 4\sqrt{\frac{3+1}{2(4)}} \\
&= \frac{9}{2}\sqrt{6} + 6\sqrt{6} + \sqrt{2} + 3\sqrt{6} + 4\sqrt{\frac{1}{2}} \\
&= \frac{27}{2}\sqrt{6} + \sqrt{2} + 2\sqrt{2}.
\end{aligned}$$

So, we can find Atomic bound connectivity index of any graph of the form $L[PNN(q, c^*, c)]$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.2. Let G be a line graph of 2-subdivided probabilistic neural networks then ABC atomic bound connectivity index of G is given as

$$ABC(G) = q(cc^* - 1)\sqrt{\frac{cc^* - 1}{2}} + c^*(c - 1)\sqrt{\frac{c - 1}{2}} + \frac{2cc^*}{\sqrt{2}}\left[\frac{q\sqrt{q}}{2} + q + 1\right]$$

Proof.

Let G be line graph of 2-subdivided Probabilistic neural networks in which there are

three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph of 2-subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^*-1)qcc^*}{2}$
$(q+1, q+1)$	$\frac{qcc^*(q+1)}{2}$
(c, c)	$\frac{cc^*(c-1)}{2}$
$(cc^*, 2)$	qcc^*
$(2, q+1)$	$qcc^* + cc^*$
$(2, c)$	cc^*

Now we find the atomic bound connectivity index of line graph of 2-subdivided probabilistic neural networks. Then according to formula of atomic bound connectivity index

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

Now,

$$\begin{aligned}
ABC(G) &= \frac{qcc^*(cc^*-1)}{2} \frac{\sqrt{cc^*+cc^*-2}}{(cc^*)^2} + \frac{qcc^*(q+1)}{2} \frac{\sqrt{(q+1)+(q+1)-2}}{(q+1)^2} \\
&+ \frac{cc^*(c-1)}{2} \frac{\sqrt{c+c-2}}{c^2} + \frac{qcc^*\sqrt{cc^*+2-2}}{2cc^*} + (qcc^*+cc^*) \sqrt{\frac{(q+1)+2-2}{2(q+1)}} \\
&+ cc^* \sqrt{\frac{c+2-2}{2c}} \\
&= q(cc^*-1) \sqrt{\frac{cc^*-1}{2}} + c^*(c-1) \sqrt{\frac{c-1}{2}} + \frac{2cc^*}{\sqrt{2}} \left[\frac{q\sqrt{q}}{2} + q+1 \right] \quad \square
\end{aligned}$$

Verification.

Step 1. If $PNN(3,2,2)$ be a graph have following edge types according to degree $(4,4)$, $(2,2)$ and $(4,2)$ having accounts 42, 6 and 28 respectively. Then according to

formula

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$\begin{aligned} ABC[PNN(3,2,2)] &= 42\sqrt{\frac{4+4-2}{(4)(4)}} + 6\sqrt{\frac{2+2-2}{(2)(2)}} + 28\sqrt{\frac{4+2-2}{(4)(2)}} \\ &= \frac{42}{4}\sqrt{6} + \frac{6}{\sqrt{2}} + \frac{28}{\sqrt{2}} \\ &= \frac{21}{2}\sqrt{6} + \frac{34}{\sqrt{2}}. \end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 48, then according to theorem 2.1.2 Atomic bound connectivity index of $PNN(3,2,2)$ is

$$\begin{aligned} ABC[PNN(3,2,2)] &= 3(4-1)\sqrt{\frac{4-1}{2}} + 2(2-1)\sqrt{\frac{2-1}{2}} + \frac{2(4)}{\sqrt{2}}\left[\frac{3\sqrt{3}}{2} + 3 + 1\right] \\ &= 9\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{2}} + 12\sqrt{\frac{3}{2}} + \frac{32}{\sqrt{2}} \\ &= 21\sqrt{\frac{3}{2}} + \frac{34}{\sqrt{2}} \\ &= \frac{21}{2}\sqrt{6} + \frac{34}{\sqrt{2}} \end{aligned}$$

So, we can find Atomic bound connectivity index of any graph of the form $L[PNN(q, c^*, c)]$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.3. Let G be a line graph for t -subdivided probabilistic neural networks for $t \geq 3$ then atomic bound connectivity (ABC) index of G is given as

$$ABC(G) = q(cc^* - 1)\sqrt{\frac{cc^* - 1}{2}} + c^*(c - 1)\sqrt{\frac{c - 1}{2}} + \frac{2cc^*}{\sqrt{2}}\left[\frac{q\sqrt{q}}{2} + q + 1 + \frac{(q + 1)(t - 2)}{2}\right]$$

Proof.

Let G be line graph for t -subdivided Probabilistic neural networks for $t \geq 3$ in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph for t -subdivided probabilistic neural networks for $t \geq 3$ w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^* - 1)qcc^*}{2}$
$(q + 1, q + 1)$	$\frac{qcc^*(q + 1)}{2}$
(c, c)	$\frac{cc^*(c - 1)}{2}$
$(cc^*, 2)$	qcc^*
$(2, q + 1)$	$qcc^* + cc^*$
$(2, c)$	cc^*
$(2, 2)$	$cc^*(q + 1)(t - 2)$

Now we find the atomic bound connectivity index of line graph for t -subdivided probabilistic neural networks for $t \geq 3$. Then according to formula of atomic bound connectivity index

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

Now,

$$\begin{aligned}
ABC(G) &= \frac{qcc^*(cc^*-1)}{2} \frac{\sqrt{cc^*+cc^*-2}}{(cc^*)^2} + \frac{qcc^*(q+1)}{2} \frac{\sqrt{(q+1)+(q+1)-2}}{(q+1)^2} \\
&+ \frac{cc^*(c-1)}{2} \frac{\sqrt{c+c-2}}{c^2} + \frac{qcc^*\sqrt{cc^*+2-2}}{2cc^*} + (qcc^*+cc^*)\sqrt{\frac{(q+1)+2-2}{2(q+1)}} \\
&+ cc^*\sqrt{\frac{c+2-2}{2c}} + cc^*(q+1)(t-2)\sqrt{\frac{2+2-2}{2(2)}} \\
&= q(cc^*-1)\sqrt{\frac{cc^*-1}{2}} + c^*(c-1)\sqrt{\frac{c-1}{2}} + \frac{2cc^*}{\sqrt{2}}\left[\frac{q\sqrt{q}}{2} + q+1 + \frac{(q+1)(t-2)}{2}\right] \quad \square
\end{aligned}$$

Verification.

Step 1. If $L[PNN(3,2,2)]$ be a graph have following edge types according to degree $(4,4)$, $(2,2)$ and $(4,2)$ having accounts 42, 22 and 28 respectively. Then according to formula

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$\begin{aligned}
ABC[PNN(3,2,2)] &= 42\sqrt{\frac{4+4-2}{(4)(4)}} + 22\sqrt{\frac{2+2-2}{(2)(2)}} + 28\sqrt{\frac{4+2-2}{(4)(2)}} \\
&= \frac{42}{4}\sqrt{6} + \frac{22}{\sqrt{2}} + \frac{28}{\sqrt{2}} \\
&= \frac{21}{2}\sqrt{6} + \frac{50}{\sqrt{2}}.
\end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 64, then according to theorem 2.1.3 Atomic bound connectivity index of $PNN(3,2,2)$ is

$$\begin{aligned}
ABC[PNN(3,2,2)] &= 3(4-1)\sqrt{\frac{4-1}{2}} + 2(2-1)\sqrt{\frac{2-1}{2}} + \frac{2(4)}{\sqrt{2}}\left[\frac{3\sqrt{3}}{2} + 3 + 1 + \frac{(3+1)(1)}{2}\right] \\
&= 9\sqrt{\frac{3}{2}} + \frac{2}{\sqrt{2}} + 12\sqrt{\frac{3}{2}} + \frac{48}{\sqrt{2}} \\
&= 21\sqrt{\frac{3}{2}} + \frac{50}{\sqrt{2}} \\
&= \frac{21}{2}\sqrt{6} + \frac{50}{\sqrt{2}}
\end{aligned}$$

So, we can find Atomic bound connectivity index of any graph of the form $L[PNN(q, c^*, c)]$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.4. *Let G be a line graph of 1-subdivided probabilistic neural networks then geometric-arithmetic index of G is given as*

$$L[GA(G)] = \frac{qcc^*}{2}[(cc^* + q) + \frac{4\sqrt{cc^*(q+1)}}{cc^* + q + 1}] + \frac{cc^*}{2}[(c-1) + \frac{4\sqrt{c(q+1)}}{c + q + 1}]$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph of 1-subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^*-1)qcc^*}{2}$
$(q+1, q+1)$	$\frac{qcc^*(q+1)}{2}$
(c, c)	$\frac{cc^*(c-1)}{2}$
$(cc^*, q+1)$	qcc^*
$(q+1, c)$	cc^*

Now we find the geometric-arithmetic index of line graph of 1 subdivided probabilistic neural networks. Then according to formula of geometric-arithmetic index

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Now,

$$\begin{aligned}
L[GA(G)] &= \frac{qcc^*(cc^*-1)}{2} \frac{2\sqrt{(cc^*)^2}}{2cc^*} + \frac{qcc^*(q+1)}{2} \frac{\sqrt{(q+1)^2}}{2(q+1)} \\
&+ \frac{cc^*(c-1)}{2} \frac{2\sqrt{c^2}}{2c} + \frac{2qcc^*\sqrt{cc^*(q+1)}}{(cc^*+q+1)} + \frac{2cc^*\sqrt{c(q+1)}}{(c+q+1)} \\
&= \frac{qcc^*}{2} [(cc^*+q) + \frac{4\sqrt{cc^*(q+1)}}{cc^*+q+1} + \frac{cc^*}{2} [(c-1) + \frac{4\sqrt{c(q+1)}}{c+q+1}] \quad \square
\end{aligned}$$

Verification.

Step 1. If $PNN(3,2,2)$ be a graph have following edge types according to degree $(4,4)$, $(2,2)$ and $(4,2)$ having accounts 54, 2 and 4 respectively. Then according to formula

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$\begin{aligned}
GA(L[PNN(3,2,2)]) &= 54 \frac{2\sqrt{4(4)}}{4+4} + 2 \frac{2\sqrt{2(2)}}{2+2} + 4 \frac{2\sqrt{4(2)}}{4+2} \\
&= \frac{8(54)}{8} + \frac{16\sqrt{2}}{6} + \frac{8}{4} \\
&= 56 + \frac{8\sqrt{2}}{3}.
\end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 32, then according to theorem 2.1.4 geometric-arithmetic index of $PNN(3,2,2)$ is

$$\begin{aligned}
GA(L[PNN(3,2,2)]) &= \frac{12}{2} [7 + \frac{4\sqrt{4(4)}}{4+3+1}] + \frac{4}{2} [(2-1) + \frac{4\sqrt{2(3+1)}}{2+3+1}] \\
&= 6[7 + \frac{16}{8}] + \frac{4}{2} [1 + \frac{8\sqrt{2}}{6}] \\
&= 56 + \frac{8\sqrt{2}}{3}
\end{aligned}$$

So, we can find geometric-arithmetic index of any graph of the form $PNN(q, c^*, c)$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.5. Let G be a line graph for 2-subdivided probabilistic neural networks then geometric-arithmetic index of G is given as

$$L[GA(G)] = \frac{qcc^*}{2} [cc^* + q + 4\sqrt{2}(\frac{\sqrt{cc^*}}{cc^*+2} + \frac{\sqrt{q+1}}{q+3})] + cc^* [\frac{c-1}{2} + 2\sqrt{2}(\frac{\sqrt{q+1}}{q+3} + \frac{\sqrt{c}}{c+2})]$$

Proof.

Let G be line graph for 2-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line

graph for 2-subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^*-1)qcc^*}{2}$
$(q+1, q+1)$	$\frac{qcc^*(q+1)}{2}$
(c, c)	$\frac{cc^*(c-1)}{2}$
$(cc^*, 2)$	qcc^*
$(2, q+1)$	$qcc^* + cc^*$
$(2, c)$	cc^*

Now we find the geometric-arithmetic index of line graph for 2-subdivided probabilistic neural networks. Then according to formula of geometric-arithmetic index

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Now,

$$\begin{aligned}
L[GA(G)] &= \frac{qcc^*(cc^*-1)}{2} \frac{2\sqrt{(cc^*)^2}}{2cc^*} + \frac{qcc^*(q+1)}{2} \frac{2\sqrt{(q+1)^2}}{2(q+1)} + \frac{cc^*(c-1)}{2} \frac{2\sqrt{c^2}}{2c} \\
&+ \frac{2qcc^*\sqrt{2cc^*}}{(cc^*+2)} + 2(cc^*+qcc^*) \frac{\sqrt{2(q+1)}}{2+q+1} + 2cc^* \frac{\sqrt{2c}}{c+2} \\
&= \frac{qcc^*}{2} [cc^*+q+4\sqrt{2}(\frac{\sqrt{cc^*}}{cc^*+2} + \frac{\sqrt{q+1}}{q+3})] + cc^*[\frac{c-1}{2} + 2\sqrt{2}(\frac{\sqrt{q+1}}{q+3} + \frac{\sqrt{c}}{c+2})] \quad \square
\end{aligned}$$

Verification.

Step 1. If $PNN(3,2,2)$ be a graph have following edge types according to degree $(4,4)$, $(2,2)$ and $(4,2)$ having accounts 42, 6 and 28 respectively. Then according to formula

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$\begin{aligned}
GA[PNN(3,2,2)] &= \frac{42(2)\sqrt{4(4)}}{4+4} + \frac{6(2)\sqrt{2(2)}}{2+2} + \frac{28(2)\sqrt{2(4)}}{2+4} \\
&= 42 + 6 + \frac{112\sqrt{2}}{6} \\
&= 48 + \frac{56\sqrt{2}}{3}
\end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 48, then according to theorem 2.1.5 geometric-arithmetic index of $PNN(3,2,2)$ is

$$\begin{aligned}
GA[PNN(3,2,2)] &= \frac{12}{2} [4 + 3 + 4\sqrt{2}(\frac{\sqrt{4}}{6} + \frac{\sqrt{4}}{6})] + 4[\frac{2-1}{2} + 2\sqrt{2}(\frac{\sqrt{3+1}}{3+3} + \frac{\sqrt{2}}{2+2})] \\
&= 42 + 24\sqrt{2}(\frac{4}{6}) + 4[\frac{1}{2} + \frac{2\sqrt{2}}{3} + \frac{4}{4}] \\
&= 48 + \frac{56\sqrt{2}}{3}
\end{aligned}$$

So, we can find geometric-arithmetic index of any graph of the form $PNN(q, c^*, c)$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.6. Let G be a line graph for t -subdivided probabilistic neural networks for $t \geq 3$ then geometric-arithmetic (GA) index of G is given as

$$\begin{aligned}
L[GA(G)] &= \frac{qcc^*}{2} [cc^* + q + 4\sqrt{2}(\frac{\sqrt{cc^*}}{cc^*+2} + \frac{\sqrt{q+1}}{q+3}) + cc^*[\frac{c-1}{2} + (q+1)(t-2) \\
&\quad + 2\sqrt{2}(\frac{\sqrt{q+1}}{q+3} + \frac{\sqrt{c}}{c+2})]
\end{aligned}$$

Proof.

Let G be line graph for t -subdivided probabilistic neural networks for $t \geq 3$ in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of t -subdivided probabilistic neural networks for $t \geq 3$ w.r.t. degrees and there count are

Type of edges	Count
(cc^*, cc^*)	$\frac{(cc^*-1)qcc^*}{2}$
$(q+1, q+1)$	$\frac{qcc^*(q+1)}{2}$
(c, c)	$\frac{cc^*(c-1)}{2}$
$(cc^*, 2)$	qcc^*
$(2, q+1)$	$qcc^* + cc^*$
$(2, c)$	cc^*
$(2, 2)$	$cc^*(q+1)(t-2)$

Now we find the geometric-arithmetic index of t -subdivided probabilistic neural networks for $t \geq 3$. Then according to formula of geometric-arithmetic index

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Now,

$$\begin{aligned}
L[GA(G)] &= \frac{qcc^*(cc^*-1)}{2} \frac{2\sqrt{(cc^*)^2}}{2cc^*} + \frac{qcc^*(q+1)}{2} \frac{2\sqrt{(q+1)^2}}{2(q+1)} + \frac{cc^*(c-1)}{2} \frac{2\sqrt{c^2}}{2c} \\
&+ \frac{2qcc^*\sqrt{2cc^*}}{(cc^*+2)} + 2(cc^* + qcc^*) \frac{\sqrt{2(q+1)}}{2+q+1} + 2cc^* \frac{\sqrt{2c}}{c+2} + 2cc^*(q+1)(t-2) \frac{\sqrt{2(2)}}{2+2} \\
&= \frac{qcc^*}{2} [cc^* + q + 4\sqrt{2}(\frac{\sqrt{cc^*}}{cc^*+2} + \frac{\sqrt{q+1}}{q+3})] + cc^*[\frac{c-1}{2} + (q+1)(t-2) \\
&+ 2\sqrt{2}(\frac{\sqrt{q+1}}{q+3} + \frac{\sqrt{c}}{c+2})] \quad \square
\end{aligned}$$

Verification.

Step 1. If $PNN(3,2,2)$ be a graph have following edge types according to degree $(4,4)$, $(2,2)$ and $(4,2)$ having accounts 42, 22 and 28 respectively. Then according to formula

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$\begin{aligned} GA[PNN(3,2,2)] &= \frac{42(2)\sqrt{4(4)}}{4+4} + \frac{22(2)\sqrt{2(2)}}{2+2} + \frac{28(2)\sqrt{2(4)}}{2+4} \\ &= 42 + 22 + \frac{112\sqrt{2}}{6} \\ &= 64 + \frac{56\sqrt{2}}{3} \end{aligned}$$

Step 2. If $PNN(3,2,2)$ be a graph having order 64, then according to theorem 2.1.6 geometric-arithmetic index of $PNN(3,2,2)$ is

$$\begin{aligned} GA[PNN(3,2,2)] &= \frac{12}{2} [4 + 3 + 4\sqrt{2}(\frac{\sqrt{4}}{6} + \frac{\sqrt{4}}{6})] + 4[\frac{2-1}{2} + (3+1) + 2\sqrt{2}(\frac{\sqrt{3+1}}{3+3} + \frac{\sqrt{2}}{2+2})] \\ &= 42 + 24\sqrt{2}(\frac{4}{6}) + 4[\frac{1}{2} + 4 + \frac{2\sqrt{2}}{3} + \frac{4}{4}] \\ &= 64 + \frac{56\sqrt{2}}{3} \end{aligned}$$

So, we can find geometric-arithmetic index of any graph of the form $PNN(q, c^*, c)$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.1.7. Let G be a line graph of 1-subdivided probabilistic neural networks then the fourth version of atomic bound connectivity ABC_4 index of G is given as

$$\begin{aligned}
ABC_4(G) = & qcc^* \left[\frac{(cc^* - 1)}{\sqrt{2}} \frac{\sqrt{(cc^*)^2 + q - 1}}{cc^*(cc^* - 1) + q + 1} + \frac{(q - 1)}{\sqrt{2}} \left(\frac{\sqrt{q^2 + q + cc^* - 1}}{q(q + 1) + cc^*} \right) \right. \\
& + \frac{\sqrt{2q^2 + 2q + cc^* + c - 2}}{\sqrt{(q(q + 1) + cc^*)(q(q + 1) + c)}} + \left. \frac{\sqrt{(cc^*)^2 + q^2 + 2q - 1}}{(cc^*(cc^* - 1) + q + 1)(q(q + 1) + cc^*)} \right] \\
& + cc^* \left[\frac{c - 1}{\sqrt{2}} \frac{\sqrt{c^2 - c + q}}{c(c - 1) + q + 1} + \frac{\sqrt{q^2 + c^2 + 2q - 1}}{\sqrt{(q^2 + q + c)(c^2 - c + q + 1)}} \right]
\end{aligned}$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph of 1-subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
$cc^*(cc^* - 1) + q + 1, cc^*(cc^* - 1) + q + 1$	$\frac{(cc^* - 1)qcc^*}{2}$
$q(q + 1) + cc^*, q(q + 1) + cc^*$	$\frac{qcc^*(q + 1) - 2qcc^*}{2}$
$q(q + 1) + cc^*, q(q + 1) + c$	qcc^*
$c(c - 1) + q + 1, c(c - 1) + q + 1$	$\frac{(c - 1)cc^*}{2}$
$cc^*(cc^* - 1) + q + 1, q(q + 1) + cc^*$	qcc^*
$q(q + 1) + c, c(c - 1) + q + 1$	cc^*

Now we find the fourth version of atomic bound connectivity ABC_4 index of the line graph for 1-subdivided probabilistic neural networks. Then according to formula of atomic bound connectivity ABC_4 index

$$ABC_4(G) = \sum_{u,v \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

Now,

$$\begin{aligned}
ABC_4(G) &= \frac{qcc^*(cc^*-1)}{2} \frac{\sqrt{2[cc^*(cc^*-1)+q+1]-2}}{\sqrt{[cc^*(cc^*-1)+q+1]^2}} + \frac{qcc^*(q+1)-2qcc^*}{2} \frac{\sqrt{2[q(q+1)+cc^*]-2}}{\sqrt{[q(q+1)+cc^*]^2}} \\
&+ qcc^* \frac{\sqrt{q(q+1+cc^*+q(q+1)+c-2)}}{\sqrt{[q(q+1)+cc^*][q(q+1)+c]}} + \frac{cc^*(c-1)}{2} \frac{\sqrt{2[c(c-1)+q+1]-2}}{\sqrt{[c(c-1)+q+1]^2}} \\
&+ qcc^* \frac{\sqrt{[cc^*(cc^*-1)+q+1]+[q(q+1+cc^*)]-2}}{\sqrt{[cc^*(cc^*-1)+q+1][q(q+1)+cc^*]}} \\
&+ cc^* \frac{\sqrt{q(q+1)+c+c(c-1)+(q+1)-2}}{\sqrt{[q(q+1)+c][c(c-1)+q+1]}} \\
&= qcc^* \left[\frac{(cc^*-1)}{\sqrt{2}} \frac{\sqrt{(cc^*)^2+q-1}}{cc^*(cc^*-1)+q+1} + \frac{(q-1)}{\sqrt{2}} \left(\frac{\sqrt{q^2+q+cc^*-1}}{q(q+1)+cc^*} \right) \right. \\
&+ \left. \frac{\sqrt{2q^2+2q+cc^*+c-2}}{\sqrt{(q(q+1)+cc^*)(q(q+1)+c)}} + \frac{\sqrt{(cc^*)^2+q^2+2q-1}}{(cc^*(cc^*-1)+q+1)(q(q+1)+cc^*)} \right] \\
&+ cc^* \left[\frac{c-1}{\sqrt{2}} \frac{\sqrt{c^2-c+q}}{c(c-1)+q+1} + \frac{\sqrt{q^2+c^2+2q-1}}{\sqrt{(q^2+q+c)(c^2-c+q+1)}} \right] \quad \square
\end{aligned}$$

Theorem 2.1.8. *Let G be a line graph of 1-subdivided probabilistic neural networks then fifth version of geometric-arithmetic GA_5 index of G is given as*

$$\begin{aligned}
GA_5(G) &= qcc^* \left[\frac{(cc^*-1)}{2} - \frac{1-(cc^*)^2}{2[(cc^*)^2+q]} + \frac{q-1}{4} + \frac{(q^2+q+cc^*)(q^2+q+c)}{2q(q+1)+c(cc^*+1)} \right. \\
&+ \left. \frac{[(cc^*)^2-cc^*+q+1][(q^2+q+cc^*)]}{[(cc^*)^2(q+1)^2]} + cc^* \left[\frac{c-1}{4} + \frac{(q^2+q+c)(c^2-c+q+1)}{(q^2+c^2+2q+1)} \right] \right]
\end{aligned}$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph for $t = 1$ -subdivided probabilistic neural networks w.r.t. degrees and there count are

Type of edges	Count
$cc^*(cc^* - 1) + q + 1, cc^*(cc^* - 1) + q + 1$	$\frac{(cc^* - 1)qcc^*}{2}$
$q(q + 1) + cc^*, q(q + 1) + cc^*$	$\frac{qcc^*(q + 1) - 2qcc^*}{2}$
$q(q + 1) + cc^*, q(q + 1) + c$	qcc^*
$c(c - 1) + q + 1, c(c - 1) + q + 1$	$\frac{(c - 1)cc^*}{2}$
$cc^*(cc^* - 1) + q + 1, q(q + 1) + cc^*$	qcc^*
$q(q + 1) + c, c(c - 1) + q + 1$	cc^*

Now we find the fifth version of geometric-arithmetic GA_5 index of line graph of 1-subdivided probabilistic neural networks. Then according to formula of fifth version of geometric-arithmetic GA_5 index

$$GA_5(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

Now,

$$\begin{aligned}
GA_5(G) &= qcc^*(cc^* - 1) \left[\frac{cc^*(cc^* - 1) + q + 1}{2(cc^*)^2 + 2q} \right] + \frac{qcc^*(q + 1) - 2qcc^*}{2} \left[\frac{q(q + 1) + cc^*}{2[q(q + 1) + cc^*]} \right] \\
&+ qcc^* \left[\frac{[q(q + 1) + cc^*][q(q + 1) + c]}{q(q + 1) + cc^* + q(q + 1) + c} \right] + \frac{cc^*(c - 1)}{2} \left[\frac{c(c - 1) + q + 1}{2[c(c - 1) + q + 1]} \right] \\
&+ qcc^* \left[\frac{[cc^*(cc^* - 1) + q + 1][q(q + 1) + cc^*]}{[cc^*(cc^* - 1) + q + 1][q(q + 1) + cc^*]} \right] + cc^* \left[\frac{[q(q + 1) + c][c(c - 1) + q + 1]}{(q + 1)q + c + c(c - 1) + (q + 1)} \right] \\
&= qcc^* \left[\frac{(cc^* - 1)}{2} - \frac{1 - (cc^*)^2}{2[(cc^*)^2 + q]} + \frac{q - 1}{4} + \frac{(q^2 + q + cc^*)(q^2 + q + c)}{2q(q + 1) + c(c^* + 1)} \right. \\
&+ \left. \frac{[(cc^*)^2 - cc^* + q + 1][(q^2 + q + cc^*)]}{[(cc^*)^2((q + 1)^2)]} \right] + cc^* \left[\frac{c - 1}{4} + \frac{(q^2 + q + c)(c^2 - c + q + 1)}{(q^2 + c^2 + 2q + 1)} \right] \quad \square
\end{aligned}$$

Theorem 2.1.9. Let G be a line graph of 1-subdivided probabilistic neural networks then the eccentric version of atomic bound connectivity ABC_5 index of G is given as

$$ABC_5(G) = qcc^* \left(\frac{16 + 8\sqrt{5} - 6\sqrt{6}}{48} \right) + cc^* \left(\frac{8\sqrt{5} - 6\sqrt{6}}{48} \right) + \frac{\sqrt{6}c^2(c^*)^2q}{8} + \frac{\sqrt{6}c^2c^*}{8} + \frac{cq^2c^*}{3}$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are three layers called input, hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph for 1-subdivided probabilistic neural networks w.r.t. degrees and there count are

type of edges	count
$(4, 4)$	$\frac{cc^*}{2}[q(cc^* - 1) + (c - 1)]$
$(3, 4)$	$cc^*(q + 1)$
$(3, 3)$	$\frac{qcc^*(q+1)}{2}$

Now we find the the eccentric version of atomic bound connectivity ABC_5 index of line graph of 1-subdivided probabilistic neural networks. Then according to formula of the eccentric version of atomic bound connectivity ABC_5 index

$$ABC_5(G) = \sum_{u,v \in E(G)} \sqrt{\frac{e_u + e_v - 2}{e_u e_v}}$$

Now,

$$\begin{aligned}
 ABC_5(G) &= \frac{cc^*}{2}[q(cc^* - 1) + c - 1] \sqrt{\frac{4+4-2}{4(4)}} + cc^*(q+1) \sqrt{\frac{3+4-2}{3(4)}} + \frac{qcc^*(q+1)}{2} \sqrt{\frac{3+3-2}{3(3)}} \\
 &= qcc^* \left(\frac{16+8\sqrt{5}-6\sqrt{6}}{48} \right) + cc^* \left(\frac{8\sqrt{5}-6\sqrt{6}}{48} \right) + \frac{\sqrt{6}c^2(c^*)^2q}{8} + \frac{\sqrt{6}c^2c^*}{8} + \frac{cq^2c^*}{3} \quad \square
 \end{aligned}$$

Theorem 2.1.10. *Let G be a line graph of 1-subdivided probabilistic neural networks then eccentric version of geometric-arithmetic $GA_4(G)$ index of G is given as*

$$GA_4(G) = \frac{c^2q(c^*)^2}{2} + \frac{c^2c^*}{2} + cc^* \left(\frac{4\sqrt{3}}{7} - \frac{1}{2} \right) + \frac{4\sqrt{3}qcc^*}{7} + \frac{cq^2c^*}{2}$$

Proof.

Let G be line graph of 1-subdivided Probabilistic neural networks in which there are

three layers called input ,hidden and output layers having q nodes, c^* classes in which each class contain c nodes. The following table shows the partition of edges of line graph for 1-subdivided probabilistic neural networks w.r.t. degrees and there count are

type of edges	count
$(4, 4)$	$\frac{cc^*}{2}[q(cc^* - 1) + (c - 1)]$
$(3, 4)$	$cc^*(q + 1)$
$(3, 3)$	$\frac{qcc^*(q+1)}{2}$

Now we find the eccentric version of geometric-arithmetic GA_4 of this graph. Then according to formula of eccentric version of geometric-arithmetic GA_4 index

$$GA_4(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{e_u e_v}}{e_u + e_v}$$

Now,

$$\begin{aligned} GA_4(G) &= \frac{cc^*}{2}[q(cc^* - 1) + c - 1] \frac{2\sqrt{16}}{8} + cc^*(q + 1) \frac{2\sqrt{12}}{7} + \frac{qcc^*(q + 1)}{2} \frac{2\sqrt{9}}{6} \\ &= \frac{c^2 q (c^*)^2}{2} + \frac{c^2 c^*}{2} + cc^* \left(\frac{4\sqrt{3}}{7} - \frac{1}{2} \right) + \frac{4\sqrt{3} q cc^*}{7} + \frac{cq^2 c^*}{2} \quad \square \end{aligned}$$

Theorem 2.1.11. *Let G be generalized M -polynomial of line graph for 1-subdivided Probabilistic neural networks. Then*

$$M_1(P, x, y) = cc^*[c^2 q (c^*)^2 + 4q^2 + 3q + c^2 + 1]$$

Proof.

Let $P(x, y)$ be the M -polynomial of $PNN(x, y)$. Then

$$(Dx + Dy)[M(I_{x,y})]_{y=x=1}$$

$$Dy = y \frac{\partial M}{\partial y}$$

$$\begin{aligned} Dy &= y \left[\frac{c^2 q (c^*)^2 (cc^* - 1)}{2} x^{cc^*} y^{cc^* - 1} + \frac{qcc^*(q+1)^2}{2} x^{q+1} y^q + \frac{c^* c^2 (c-1)}{2} x^c y^{c-1} \right. \\ &\quad \left. + qcc^*(q+1) x^{cc^*} y^q + c^* x^{q+1} y^{c-1} \right] \end{aligned}$$

$$Dy = \frac{c^2 q (c^*)^2 (cc^* - 1)}{2} x^{cc^*} y^{cc^*} + \frac{qcc^*(q+1)^2}{2} x^{q+1} y^{q+1} + \frac{c^* c^2 (c-1)}{2} x^c y^c$$

$$\begin{aligned}
& + qcc^*(q+1)x^{cc^*}y^{q+1} + c^*c^2x^{q+1}y^c \\
Dx &= x \frac{\partial M}{\partial x} \\
Dx &= x \left[\frac{c^2q(c^*)^2(cc^*-1)}{2} x^{cc^*-1}y^{cc^*} + \frac{qcc^*(q+1)^2}{2} x^qy^{q+1} + \frac{c^2(c^*)(c-1)}{2} x^{c-1}y^c \right. \\
& \left. + c^2q(c^*)^2x^{cc^*-1}y^{q+1} + cc^*(q+1)x^qy^c \right] \\
Dx &= \frac{c^2q(c^*)^2(cc^*-1)}{2} x^{cc^*}y^{cc^*} + \frac{qcc^*(q+1)^2}{2} x^{q+1}y^{q+1} + \frac{c^2(c^*)(c-1)}{2} x^cy^c \\
& + c^2q(c^*)^2x^{cc^*}y^{q+1} + cc^*(q+1)x^{q+1}y^c \\
(Dx + Dy) &= c^2q(c^*)^2(cc^*-1)x^{cc^*}y^{cc^*} + qcc^*(q+1)^2x^{q+1}y^{q+1} + c^2(c^*)(c-1)x^cy^c \\
& + qcc^*(cc^* + q + 1)x^{cc^*}y^{q+1} + cc^*(c + q + 1)x^{q+1}y^c \\
(Dx + Dy)_{x=y=1} &= cc^*[c^2q(c^*)^2 + 4q^2 + 3q + c^2 + 1] \quad \square
\end{aligned}$$

Theorem 2.1.12.

$$M_1(P, x, y) = \frac{mnk}{2} [(mk+1)^3 + (n+1)^3 - 4m^2k^2 - mk + 2mnk + 2m] + m^2k \left[\frac{m^2}{2} - \frac{m}{2} - 1 \right]$$

Proof.

Let $P(x, y)$ be the M-polynomial of $PNN(x, y)$. Then

$$\begin{aligned}
& (DxDy)[M(P, x, y)]_{x=y=1} \\
Dy &= \frac{m^2nk^2(mk-1)}{2} x^{mk}y^{mk} + \frac{mnk(n+1)^2}{2} x^{n+1}y^{n+1} + \frac{m^2k(m-1)}{2} x^my^m \\
& + mnk(n+1)x^{mk}y^{n+1} + m^2kx^{n+1}y^m \\
DxDy &= x \left[\frac{m^3nk^3(mk-1)}{2} x^{mk-1}y^{mk} + \frac{mnk(n+1)^3}{2} x^ny^{n+1} + \frac{m^3k(m-1)}{2} x^{m-1}y^m \right. \\
& \left. + m^2nk^2x^{mk-1}y^{n+1} + m^2k(n+1)x^ny^m \right] \\
DxDy &= \frac{m^3nk^3(mk-1)}{2} x^{mk}y^{mk} + \frac{mnk(n+1)^3}{2} x^{n+1}y^{n+1} + \frac{m^3k(m-1)}{2} x^my^m \\
& + m^2nk^2x^{mk}y^{n+1} + m^2k(n+1)x^{n+1}y^m \\
(DxDy)_{x=y=1} &= \frac{mnk}{2} [(mk+1)^3 + (n+1)^3 - 4m^2k^2 - mk + 2mnk + 2m] + m^2k \left[\frac{m^2}{2} - \frac{m}{2} - 1 \right]
\end{aligned}$$

Theorem 2.1.13. Let G be generalized M-polynomial of line graph for 1-subdivided Probabilistic neural networks. Then

$$M_2(PNN) = \frac{mk-1}{2m^3k^2} + \frac{mk}{2n(n+1)} + \frac{k(m-1)}{2m^3} + \frac{mk}{n(n+1)^2} + \frac{k}{m^3}$$

Proof.

$$(SxSy)[M(P,x,y)]_{x=y=1}$$

$$Sy = \frac{mk-1}{2m}x^{mk}y^{mk} + \frac{mk}{2}x^{n+1}y^{n+1} + \frac{k(m-1)}{2m}x^my^m + \frac{mk}{n+1}x^{mk}y^{n+1} + \frac{k}{m}x^{n+1}y^m$$

$$SxSy = \frac{mk-1}{2m^3k^2}x^{mk}y^{mk} + \frac{mk}{2n(n+1)}x^{n+1}y^{n+1} + \frac{k(m-1)}{2m^3}x^my^m + \frac{mk}{n(n+1)^2}y^{mk}x^{n+1} +$$

$$\frac{k}{m^3}x^my^{n+1}$$

$$(SxSy)_{x=y=1} = \frac{mk-1}{2m^3k^2} + \frac{mk}{2n(n+1)} + \frac{k(m-1)}{2m^3} + \frac{mk}{n(n+1)^2} + \frac{k}{m^3} \quad \square$$

2.2 The chain of Bismuth Tri-Iodide ($m - Bil_3$)

"Bismuth Tri-Iodide $m - Bil_3$ is the inorganic compound with the formula Bil_3 . Bismuth Tri-Iodide is gray-black solid that is the product of the reaction of bismuth and iodine." In Fig. 2.3, The chain of bismuth tri-iodide shown for $m = 3$

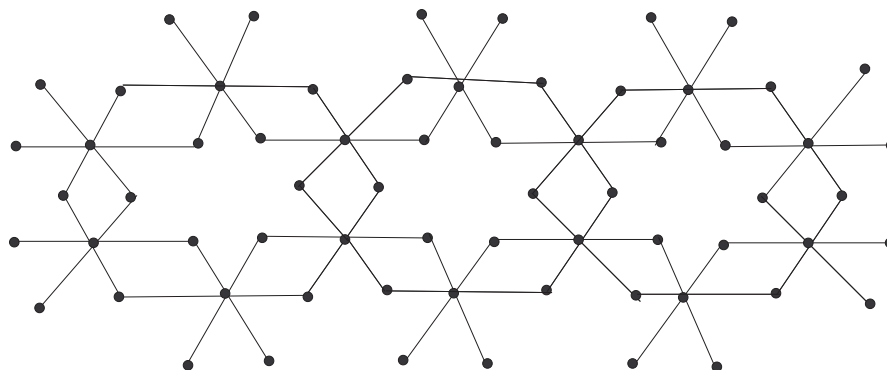


Figure 2.3: $3 - Bil_3$

In Fig. 2.4, a line graph of m -subdivided bismuth tri-iodide $m - Bil_3$ shown for $m = 3$

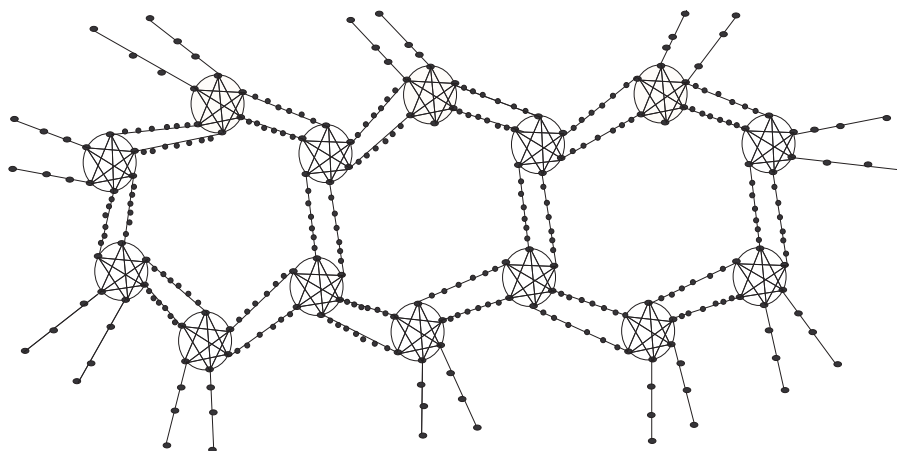


Figure 2.4: $L[3 - Bil_3]$

Theorem 2.2.1. Let G be a line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ then the atomic-bond connectivity (ABC) index of G is given as

$$ABC(G) = 12\sqrt{2}m^2 + (10\sqrt{10} + 11\sqrt{2})m + (5\sqrt{10} + \sqrt{2})$$

Proof.

Let G be line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$. The following table shows the partition of edges of line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ w.r.t. degrees and there count are

type of edges	count
(6,6)	$30(2m+1)$
(2,6)	$12(2m+1)$
(2,2)	$24m^2 - 6m - 18$
(1,2)	$4m+8$

Now we find the atomic-bond connectivity (ABC) index of this graph. Then according to formula of atomic-bond connectivity (ABC) index

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

Now,

$$\begin{aligned}
ABC(G) &= 30(2m+1) \sqrt{\frac{6+6-2}{6(6)}} + 12(2m+1) \sqrt{\frac{6+2-2}{6(2)}} + (24m^2 - 6m - 18) \sqrt{\frac{2+2-2}{2(2)}} \\
&\quad + (4m+8) \sqrt{\frac{2+1-2}{2(1)}} \\
&= 12\sqrt{2}m^2 + (10\sqrt{10} + 11\sqrt{2})m + (5\sqrt{10} + \sqrt{2}) \quad \square
\end{aligned}$$

Verification.

Step 1. If G be a line graph of $m \geq 3$ -subdivided Bismuth Tri-Iodide $m - Bil_3$ graph have following edge types according to degree bases (6,6), (2,6), (2,2) and (1,2)

having accounts 210, 84, 180 and 20 respectively. Then according to formula

$$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$\begin{aligned} ABC[3 - Bil_3] &= 210\sqrt{\frac{6+6-2}{6(6)}} + 84\sqrt{\frac{6+2-2}{6(2)}} + 180\sqrt{\frac{2+2-2}{2(2)}} + 20\sqrt{\frac{2+1-2}{2(1)}} \\ &= \frac{210}{6}\sqrt{10} + \frac{84}{2}\sqrt{2} + \frac{180}{2}\sqrt{2} + 20\frac{1}{\sqrt{2}} \\ &= 35\sqrt{10} + 142\sqrt{2} \end{aligned}$$

Step 2. If G be a line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ having order 336, then according to theorem 2.2.1 Atomic bound connectivity index of $1 - Bil_3$ is

$$\begin{aligned} ABC[3 - Bil_3] &= (12\sqrt{2})9 + (10\sqrt{10} + 11\sqrt{2})3 + (5\sqrt{10} + 2) \\ &= 108\sqrt{2} + 30\sqrt{10} + 33\sqrt{2} + 5\sqrt{10} + \sqrt{2} \\ &= 35\sqrt{10} + 142\sqrt{2} \end{aligned}$$

So, we can find Atomic bound connectivity index of any graph of the form $m - Bil_3$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.2.2. Let G be a line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ then the geometric-arithmetic (GA) index of G is given as

$$GA(G) = 24m^2 + (54 + 12\sqrt{3} + \frac{8}{3}\sqrt{2})m + (12 + 6\sqrt{3} + \frac{16}{3}\sqrt{2})$$

Proof.

Let G be line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ in which there are following types of edges are found.

type of edges	count
(6, 6)	$30(2m + 1)$
(2, 6)	$12(2m + 1)$
(2, 2)	$24m^2 - 6m - 18$
(1, 2)	$4m + 8$

Now we find the geometric-arithmetic (GA) index of this graph. Then according to formula of geometric-arithmetic (GA) index

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Now,

$$\begin{aligned}
GA(G) &= 30(2m + 1) \frac{2\sqrt{6(6)}}{6 + 6} + 12(2m + 1) \frac{2\sqrt{6(2)}}{6 + 2} + (24m^2 - 6m - 18) \frac{2\sqrt{2(2)}}{2 + 2} \\
&+ (4m + 8) \frac{2\sqrt{2(1)}}{2 + 1} \\
&= 24m^2 + (54 + 12\sqrt{3} + \frac{8}{3}\sqrt{2})m + (12 + 6\sqrt{3} + \frac{16}{3}\sqrt{2}) \quad \square
\end{aligned}$$

Verification.

Step 1. If G be a line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ have following edge types according to degree bases (6,6), (2,6), (2,2) and (1,2)

having accounts 210, 84, 180 and 20 respectively. Then according to formula

$$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$\begin{aligned} GA[3 - Bil_3] &= 210 \frac{2\sqrt{6(6)}}{6+6} + 84 \frac{2\sqrt{6(2)}}{6+2} + 180 \frac{2\sqrt{2(2)}}{2+2} + 20 \frac{2\sqrt{2(1)}}{2+1} + \\ &= 210 + 42\sqrt{3} + 180 + \frac{40}{3}\sqrt{2} \\ &= 390 + 42\sqrt{3} + \frac{40}{3}\sqrt{2} \end{aligned}$$

Step 2. If G be a line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ having order 336, then according to theorem 2.2.2 of geometric-arithmetic index of $3 - Bil_3$ is

$$\begin{aligned} GA[3 - Bil_3] &= 24(3)^2 + (54 + 12\sqrt{3} + \frac{8\sqrt{2}}{3})3 + (12 + 6\sqrt{3} + \frac{16\sqrt{2}}{3}) \\ &= 390 + 42\sqrt{3} + (8 + \frac{16}{3})\sqrt{2} \\ &= 390 + 42\sqrt{3} + \frac{40\sqrt{2}}{3} \end{aligned}$$

So, we can find geometric-arithmetic index of any graph of the form of line graph of m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$ by using their orders instead of degree.

Step 1 and 2 validates our result.

Theorem 2.2.3. Let G be generalized M -polynomial of line graph for m -subdivided

Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$. Then

$$M_1(m - Bil_3) = 4[24m^2 + 225m + 102]$$

Proof.

Let $m - Bil_3(x, y)$ be the M-polynomial of $m - Bil_3$. Then

$$(Dx + Dy)[M(m - Bil_3(x, y))]_{y=x=1}$$

$$Dy = y \frac{\partial M}{\partial y}$$

$$Dy = y[180(2m+1)x^6y^5 + 72(2m+1)x^2y^5 + 12(4m^2 - m - 3)x^2y + 8(m+2)xy]$$

$$Dy = 180x^6y^6(2m+1) + 72x^2y^6(2m+1) + 12x^2y^2(4m^2 - m - 3) + 8xy^2(m+2)$$

$$Dx = x \frac{\partial M}{\partial x}$$

$$Dx = x[180(2m+1)x^5y^6 + 24(2m+1)xy^6 + 12(4m^2 - m - 3)xy^2 + 8(m+2)y^2]$$

$$Dx = 180x^6y^6(2m+1) + 24x^2y^6(2m+1) + 12x^2y^2(4m^2 - m - 3) + 4xy^2(m+2)$$

$$(Dx + Dy) = 360x^6y^6(2m+1) + 96x^2y^6(2m+1) + 24x^2y^2(4m^2 - m - 3) + 12xy^2(m+2)$$

$$(Dx + Dy)_{x=y=1} = 4[24m^2 + 225m + 102] \quad \square$$

Theorem 2.2.4. *Let G be generalized M-polynomial of line graph for m -subdivided Bismuth Tri-Iodide $m - Bil_3$ for $m \geq 3$. Then*

$$M_1(m - Bil_3) = 16[6m^2 + 152m + 73]$$

Proof.

Let $m - Bil_3(x, y)$ be the M-polynomial of $m - Bil_3(x, y)$. Then

$$(DxDy)[M(I, x, y)]_{x=y=1}$$

$$Dy = 180x^6y^6(2m+1) + 72x^2y^6(2m+1) + 12x^2y^2(4m^2 - m - 3) + 8xy^2(m+2)$$

$$DxDy = x[1080x^5y^6(2m+1) + 144xy^6(2m+1) + 24xy^2(4m^2 - m - 3) + 8y^2(m+2)]$$

$$DxDy = 1080x^6y^6(2m+1) + 144x^2y^6(2m+1) + 24x^2y^2(4m^2 - m - 3) + 8xy^2(m+2)$$

$$(DxDy)_{x=y=1} = 16[6m^2 + 152m + 73] \quad \square$$

2.3 Sierpinski Networks $S(n, k)$

"Sierpinski networks $S(n, k)$ is isomorphic to the graphs of Tower of Hanoi with n disks." In Fig. 2.3, The chain of bismuth tri-iodide shown for $m = 3$

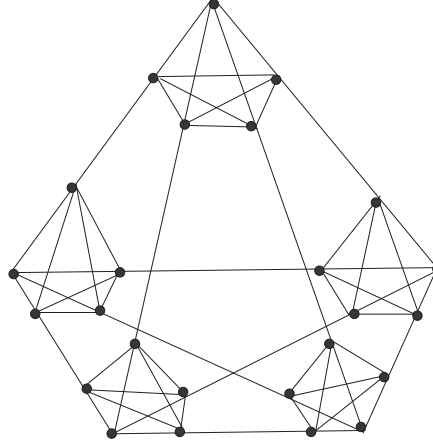


Figure 2.5: Sierpinski Networks $S(2, 5)$

Theorem 2.3.1. *Let G be a graph of sierpinski networks $S(n, k)$; then First Zagreb eccentric index of G is given as*

$$M_1^*(G) = (k^{n+1} - k)(2^{n-1})$$

Proof.

Let G be sierpinski network $S(n, k)$. Then following table shows the partition of edges of sierpinski network w.r.t. eccentric and there count are

Type of edges	Count
$(2^{n-1}, 2^{n-1})$	$\frac{k^{n+1}-k}{2}$

Now we find the First Zagreb eccentric index of sierpinski networks $S(n, k)$. Then

according to formula of First Zagreb eccentric index

$$M_1^*(G) = \sum_{u,v \in E(G)} [\varepsilon(u) + \varepsilon(v)],$$

Now,

$$\begin{aligned} M_1^*(G) &= \frac{k^{n+1} - k}{2} (2^{n-1} + 2^{n-1}) \\ &= \frac{k^{n+1} - k}{2} 2(2^{n-1}) \\ &= (k^{n+1} - k)(2^{n-1}) \quad \square \end{aligned}$$

Verification.

Step 1. If $S(n, k)$ be a graph have following edge type according to eccentricities $(3, 3)$ having accounts 60. Then according to formula

$$M_1^*(G) = \sum_{u,v \in E(G)} [\varepsilon(u) + \varepsilon(v)]$$

$$\begin{aligned} M_1^*[S(n, k)] &= 60(3 + 3) \\ &= 360 \end{aligned}$$

Step 2. If $S(n, k)$ be a graph having order 25, then according to theorem 2.3.1 First Zagreb eccentric index of $S(n, k)$ is

$$\begin{aligned}
M_1^*[S(n, k)] &= (5^{2+1} - 5)(2^2 - 1) \\
&= (125 - 5)(3) \\
&= 360
\end{aligned}$$

So, we can find First Zagreb eccentric index of any graph of the form $S(n, k)$ by using their orders instead of eccentricities.

Step 1 and 2 validates our result.

Theorem 2.3.2. *Let G be a graph of sierpinski networks $S(n, k)$; then Third Zagreb eccentric index of G is given as*

$$M_1^*(G) = \left(\frac{k^{n+1} - k}{2}\right)(2^n - 1)^2$$

Proof.

Let G be sierpinski network $S(n, k)$. Then following table shows the partition of edges of sierpinski network w.r.t. eccentric and there count are

Type of edges	Count
$(2^{n-1}, 2^{n-1})$	$\frac{k^{n+1} - k}{2}$

Now we find the Third Zagreb eccentric index of sierpinski networks $S(n, k)$. Then according to formula of Third Zagreb eccentric index

$$M_2^*(G) = \sum_{u, v \in E(G)} \varepsilon(u)\varepsilon(v)$$

Now,

$$\begin{aligned}
M_2^*(G) &= \frac{k^{n+1} - k}{2} (2^{n-1})(2^{n-1}) \\
&= \left(\frac{k^{n+1} - k}{2}\right) (2^n - 1)^2 \quad \square
\end{aligned}$$

Verification.

Step 1. If $S(n, k)$ be a graph have following edge type according to eccentricities $(3, 3)$ having accounts 60. Then according to formula

$$M_2^*(G) = \sum_{u, v \in E(G)} [\varepsilon(u) + \varepsilon(v)]$$

$$\begin{aligned}
M_1^*[S(n, k)] &= 60(3)(3) \\
&= 540
\end{aligned}$$

Step 2. If $S(n, k)$ be a graph having order 25, then according to theorem 2.3.2 Third Zagreb eccentric index of $S(n, k)$ is

$$\begin{aligned}
M_2^*[S(n, k)] &= \left(\frac{5^3 - 5}{2}\right) (2^2 - 1)^2 \\
&= \left(\frac{120}{2}\right) (9) \\
&= 540
\end{aligned}$$

So, we can find Third Zagreb eccentric index of any graph of the form $S(n, k)$ by using their orders instead of eccentricities.

Step 1 and 2 validates our result.

Theorem 2.3.3. Let $S(n, k)$ be generalized sierpinski networks. Then

$$M_1[S(n, k)] = k^2 \left[2 + \frac{k^n - 5}{2} \right] + k \left[2(k - 1) + \left(\frac{k^{n+1} - 5k}{2} \right) \right]$$

Proof.

Let $S(n, k)[x, y]$ be the M-polynomial of $S(n, k)$. Then

$$(Dx + Dy)[M(S(n, k)(x, y))]|_{y=x=1}$$

$$Dy = y \frac{\partial M}{\partial y}$$

$$Dy = y \left[2k(k - 1)x^k y^{k-2} + \frac{k(k^{n+1} - 5k)}{2} x^k y^{k-1} \right]$$

$$Dy = kx^k y^k \left[2(k - 1)y^{-1} + \frac{(k^{n+1} - 5k)}{2} \right]$$

$$Dx = x \frac{\partial M}{\partial x}$$

$$Dx = x \left[2k^2 x^{k-1} y^{k-1} + k \left(\frac{k^{n+1} - 5k}{2} \right) x^{k-1} y^k \right]$$

$$Dx = k^2 x^k y^k \left[2y^{-1} + \frac{k^n - 5}{2} \right]$$

$$(Dx + Dy) = k^2 x^k y^k \left[2y^{-1} + \frac{k^n - 5}{2} \right] + kx^k y^k \left[2(k - 1)y^{-1} + \frac{(k^{n+1} - 5k)}{2} \right]$$

$$(Dx + Dy)_{x=y=1} = k^2 \left[2 + \frac{k^n - 5}{2} \right] + k \left[2(k - 1) + \frac{(k^{n+1} - 5k)}{2} \right] \quad \square$$

Theorem 2.3.4. Let $S(n, k)$ be generalized sierpinski networks. Then

$$M_1[S(n, k)] = k^2 \left[2y^{-1}(k - 1) + \frac{(k^{n+1} - 5k)}{2} \right]$$

Proof.

Let $S(n, k)[x, y]$ be the M-polynomial of $S(n, k)$. Then

$$(DxDy)[M(I, x, y)]|_{x=y=1}$$

$$Dy = kx^k y^k \left[2(k - 1)y^{-1} + \frac{(k^{n+1} - 5k)}{2} \right]$$

$$DxDy = x \left[kx^{k-1} y^k \left[2(k - 1)y^{-1} + \frac{(k^{n+1} - 5k)}{2} \right] \right]$$

$$DxDy = kx^k y^k \left[2(k - 1)y^{-1} + \frac{(k^{n+1} - 5k)}{2} \right]$$

$$(DxDy)_{x=y=1} = k^2 \left[2y^{-1}(k - 1) + \frac{(k^{n+1} - 5k)}{2} \right] \quad \square$$

Chapter 3

Conclusions

Conclusions

In this thesis, we have calculated the degree based topological indices and M -polynomial for line graph of t -subdivided graphs of probabilistic neural network $L[PNN - (q, c^*, c)]$ for $t \geq 1$ and also for line graph of m -subdivided graphs of Bismuth Tri-Iodide $L[m - Bil_3]$ for $m \geq 3$. We calculated the eccentric version of atomic bond connectivity ABC_5 index and eccentric version of geometric-arithmetic $GA_4(G)$ index for line graph of 1-subdivided probabilistic neural networks $L[PNN(q, c^*, c)]$. We also found the neighbourhood degree based topological indices for line graph of 1-subdivided graphs of probabilistic neural networks $L[PNN(q, c^*, c)]$. We formulated first and third Zagreb eccentric index and M -polynomial of sierpinski networks $S(n, k)$.

Chapter 4

References

- [1] Y. Alizadeh, A. Iranmanesh, T. Doslic, Additively weighted Harary index of some composite graphs, *Discrete Math.*, 313:1 (2013) 26-34.
- [2] N. De, On eccentric connectivity index and polynomial of thorn graph, *Applied Mathematics*, vol. 3, no. 8, pp. 931-934, 2012.
- [3] M. V. Diudea, Indices of reciprocal properties or Harary indices, *J. Chem. Inf. Comput. Sci.*, 37 (1997), 292-299.
- [4] T. Doli, M. Saheli, D. Vukievi, Eccentric connectivity index: extremal graphs and values, *Iran. J. Math. Chem.* 1 (2) (2010) 45-56.
- [5] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, An atom-bond connectivity index, modeling the enthalpy of formation of alkanes. *Indian J. Chem.* 37A (1998) 849-855.
- [6] M. R. Farahani, Eccentricity version of Atom-Bond connectivity index of Benzenoid Family ABC5(Hk), *World Appl. Sci. J.* 21 (2013) 1260-1265.
- [7] G. Fath-Tabar, B. Furtula, I. Gutman, A new geometric-arithmetic index, *J. Math. Chem.* 47 (2010) 477-486.
- [8] B. Furtula, I. Gutman, M. Dehmer, on structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.* 219 (2013) 8973-8978.
- [9] W. Gao, Mohammad Reza Farahani, Muhammad Imran and M. R. Rajesh Kanna *Springer Plus* (2016) 5:1563.
- [10] M. Ghorbani, M. A. Hosseinzadeh, Computing index of nano star dendrimers, *Opto-electron. Adv. Mater-Rapid Comm.* 4(9) (2010) 1419-1422.
- [11] Gutman, I., O.E. Polansky, "Mathematical Concepts in Organic Chemistry", Springer-Verlag, Berlin, 1986.

- [12] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* 34 (1994) 1087-1089.
- [13] I. Gutman, Degree based topological indices, *Croat. Chem. Acta.* 86(4) (2013) 351-361.
- [14] I. Gutman, A.R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* 81 (2008) 277-281.
- [15] I. Gutman, B. Furtula, *Distance in Molecular Graphs-Applications*, Univ. Kragujevac, Kragujevac (2012).
- [16] H. Hua and K. C. Das, The relationship between the eccentric connectivity index and Zagreb indices, *Discrete Applied Mathematics*, vol. 161, no. 16-17, pp. 2480-2491, 2013.
- [17] M. Imran, S. Hayat, M. Y. H. Malik, On topological indices of certain interconnection networks, *Appl. Math. Comp.* 244 (2014) 936-951.
- [18] M. Imran, S. A. Bokhary, S. Manzoor, On molecular topological properties of dendrimers, *Can. J. Chem.* 94(2) (2016) 120-125.
- [19] M. K. Jamil, Distance-Based Topological Indices and Double Graph, *Iranian J. Math. Chem.* 8(1) (2017) 83-91.
- [20] P.V. Khadikar, N.V. Deshpande, P.P. Kale, A. Dobrynin, I. Gutman, The Szeged index and an analogy with the Wiener index, *J. Chem. Inf. Comput. Sci.* 35(1995)547-550.
- [21] P.V. Khadikar, S. Karmarkar, V.K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* 41 (2001) 934-949.
- [22] D.J. Klein, I. Lukovits, I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* 35 (1995)50-52.

- [23] X. Li, Y. Shi, L. Wang, An updated survey on the indices: B.F. I. Gutman (Ed.), Recent Results in the Theory of Randić Index, University of Kragujevac and Faculty of Science Kragujevac, (2008) 9-47.
- [24] X. Li, Y. Shi, A survey on the Randić index, MATCH Commun. Math. Comput. Chem. 59(1) (2008) 127-156.
- [25] M. J. Morgan, S. Mukwembi, H.C. Swart, On the eccentric connectivity index of a graph, Discrete Math. 311 (2011) 1229-1234.
- [26] M. F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures, Appl. Math. Comput. 273 (2016) 125-130.
- [27] M. F. Nadeem, S. Zafar, Z. Zahid, Certain topological indices of the line graph of subdivision graphs, Appl. Math. Comput. 271 (2015) 790-794.
- [28] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975) 6609-6615.
- [29] M. Randić, Novel molecular descriptor for structure-property studies, Chem. Phys. Lett. 211 (1993) 478-483.
- [30] P. S. Ranjini and V. Lokesh, Eccentric connectivity index, hyper and reverse-wiener indices of the subdivision graph, General Mathematics Notes, vol. 2, pp. 34-46, 2011.
- [31] N. P. Rao and K. L. Lakshmi, Eccentric connectivity index of V-Phenylenic nanotubes, Digest J. Nanomaterials and Biostructures, vol. 6, no. 1, pp. 81-87, 2010.
- [32] A.K. Madan, D. Rohit, Role of distance-sum-based molecular descriptors in drug discovery process, in: I. Gutman, B. Furtula (Eds.), Distance in Molecular Graphs Applications, Univ. Kragujevac, Kragujevac. (2012) 225-252.

- [33] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17-20.