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Analysis of M-polynomial and NM – polynomial Graphs in Topographies using Fuzzy Mathematical Modeling

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Objective: Molecular topology, chemical-based graph theory, and mathematical chemistry all depend on the study of topological criteria because these metrics capture the structural, chemical, and physical properties of molecules. However, there is a clear challenge in characterising non-isomorphic graphs that have the same topological measure value. Numerous areas of chemistry benefit from the application of algebraic graph theory. It is a strong theoretical method for predicting either the common and unusual properties of molecules because it clarifies how the many orientations of macromolecules and crystals impact their structure and behaviour.
Methods : In this study, we first calculate the M and NM polynomials of the graph and then recover some degree-based and neighbourhood degree sum based indices. In addition, a few outcomes are shown graphically for contrast.
Findings : First Zagreb Index (U_1), Second Zagreb Index (U_2), Redefined third Zagreb Index (U_3), Y-Tally (U_y), Forgotten topological Index (U_f), Second modified Zagreb Index (U_m), Symmetric division deg Index (U_d), Harmonic Index (U_h), Inverse sum indeg Index (U_i), and Augmented Zagreb Index (U_a) are among the topographies of the Graph that this work aims to forecast and analyse using fuzzy mathematical modelling.
Novelty: This research used ANOVA one-way classification to show that the graph's various topographies are the same.
Keywords: Molecular topology, mathematical chemistry.

1. Introduction

Mathematical modeling is the process of using mathematics to describe, assess, and predict events that occur in the real world. Statistical methods are applied in statistical graph theory to analyze these graphs' properties and behaviors. Graph structure is one of these techniques; it involves analyzing the organizational structure of the network and can involve metrics like the clustering coefficient, average path length, and degree distribution. Statistical graph theory is widely applied in disciplines like machine learning, biology, epidemiology, and sociology where understanding the system under study requires an understanding of its networks and relationships.

A topological Tally is usually defined by some graph invariant, like the number of vertex positions, boundaries, level cycle, matching number, etc.In mathematical chemical phenomena, pharmaceutical graph theory, quantum topology, and bioinformatics, a topological Tally is a type of structural classifier that is calculated using the molecular structure of a chemical component.

Chemists often evaluate the topological coefficients of the molecular graph in order to statistically determine the chemical or physical nature of a molecule. The converse issue of topographies has been offered by experts. Given an Tally value, the goal is to build substances with that Tally value; it is not necessary to produce all isomorphic graphs. Readers looking for more information on the subject might consult. As the area developed, various scholars tried to classify objects based on isomorphism using a combination of topographies [1-3]. The main problem with isomorphism-based segmentation is that it can result in several non-isomorphic graphs having similar topographies; this problem gets worse with the number of graph's poles rises.

In the past ten years, a significant amount of research articles on polynomials and topographies have been published.For information on different topographies and how to apply them,see[4,7,8,9]. Additionally, graph polynomials concerning [5]The Hosoya polynomial is the most well-known complex that is required to compute distance-based Tallyes of the topology of graphs, such as the hyperbolic Wiener Tally [5] and Wiener Tally [10]. The M polynomial [6] is an algebraic polynomial that was first introduced in 2015 and is useful for calculating several degree-based topographies. Different approaches to solving the issue using mathematical modelling have been addressed by Mohan Kumar et al. [13, 14]. Recently Abdu Q. S. Alameri O Ejima , Dankan V. Gowda et.al [15, 16, 17]discussed topographies types in graphs and their applications. Across the present research we compare between topographies based on neighborhood degree.

2. Basic Definition

2.1 Fuzzy Set

Let $\widetilde{A}$be the subset of X where, X is the universe of objects then the characteristic function by $\mu_{\widetilde{A}}(x) = \begin{cases} 1 & \text{if } x \in \widetilde{A} \\ 0 & \text{if} x \notin \widetilde{A} \end{cases}$

The fuzzy set $\widetilde{A}$is the function $\mu_{\widetilde{A}}$: X → [0, 1], $\mu_{\widetilde{A}}$ is called the membership function which is a value on the unit interval that measures the degree to each $x \in \widetilde{A}$

2.2 Fuzzy number

A Fuzzy set defined on universal of real numbers R is said to be a fuzzy number has the following characteristics:

(i). $\widetilde{A}$ is convex,

$$\mu_{\widetilde{A}}(\beta a + (1-\beta)b\beta) \geq \text{minimum}\left(\mu_{\widetilde{A}}(a), \mu_{\widetilde{A}}(b)\right) \forall\, a, b \in R \text{ and } 0 \leq \beta \leq 1$$

(ii). $\widetilde{A}$ is normal, (i.e.) the membership function of $\widetilde{A}$has at least one element $x \in X$ whose Membership value is unity.

(iii). $\mu_{\widetilde{A}}$ is continuous except at a finite number of points in its domain.

2.3 Definition

Let V (G) = {a_i, d_i, $1 \leq i \leq 2n - 2$, b_i, $1 \leq i \leq n - 1$, c_i, $1 \leq i \leq n$} be the vertex set and

E(G) = {e_i, f_i, $1 \leq i \leq 2n - 2$, g_i, $1 \leq i \leq n - 1$, h_i, $1 \leq i \leq 2n$} be the edge set of G respectively.

That is there are 6n + 3 vertices and 7n + 2 edges in the graph G

2.4. Example

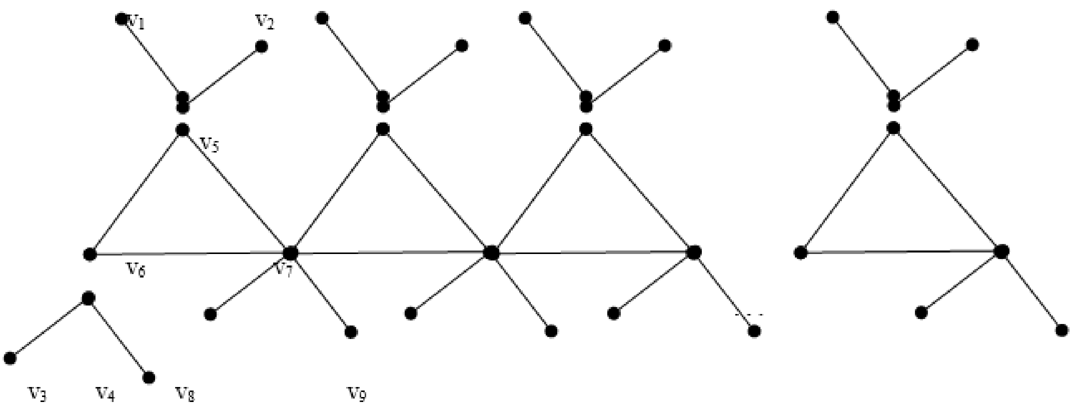

Figure 2.1 Graph G

2.5 Definition

Let V(H) = {a_i, d_i, $1 \leq i \leq 2n$, b_i, c_i, $1 \leq i \leq n$} be the vertex set of H and E(H) = {e_i, i_i, $1 \leq i \leq 2n$, f_i, h_i, $1 \leq i \leq n - 1$, f_i, $1 \leq i \leq n - 1$} be the edge set of H respectively.

That is there are 6n + 6 vertices and 7n + 5 edges in the graph H

2.6 Example

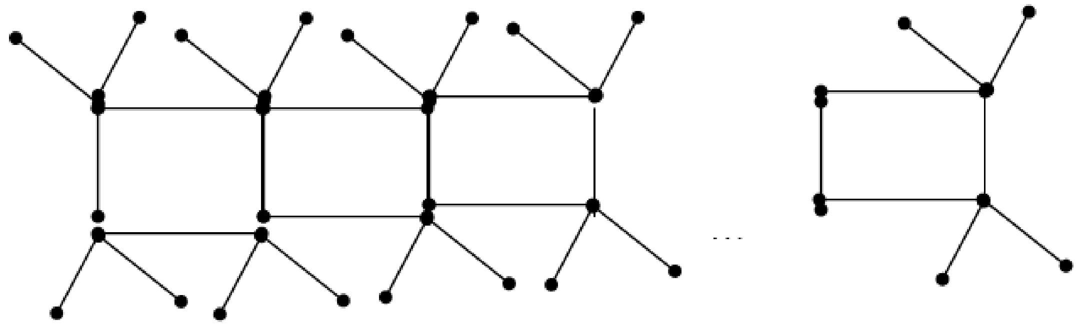

Figure 2.2 Graph H

2.7 Definition

The extent relying topological metrics, for example, can be rapidly triggered from a computational expression associated to the pharmaceutical visualisations called the M-polynomial. The topographies are vital in determining the physique- pharmaceutical characteristics of chemical graphs. If G has become a graph , then M- Polynomial of G is defined as

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

Where $m_{ij}, (i, j) \geq 1$, is the number edges uv in G such that $d_G(u) = i$ and $d_G(v) = j$

3. Topographies

Let γ(u) represent a graph G's vertex u's degree. The definition of an M-polynomial of G is: = Σ {number of all edges uv such that γ(u) = i, γ(v) = j ; x^i y^j } and

Similar to neighbourhood degree sum-based indices, neighbourhood N-polynomials serve the same purpose. The neighbourhood N-polynomial approach is used to obtain several topographies for the bismuth tri-iodide chain and sheet based on the neighbourhood degree sum. Let G's degree total of all its vertices that are close to u be represented by Γ(u). The neighbourhood grade sum of u in G is denoted by Γ(u). The definition of G's neighbourhood M-polynomial is: Σ {number of all edges uv such that Γ(u) = i, Γ(v) = j ; x^i y^j }. The neighbourhood degree sum-based (N) and degree-based (M) topographies defined on the partition of edge set E(G) of a graph G can be expressed as

Table 3.1 Partition of Edge set

S.No	Degree Set	No. of Edges	S.No	Degree Set	No. of Edges
1	(4, 4)	2	4	(6, 1)	2n-2
2	(4, 6)	2	5	(6, 6)	n-2
3	(4, 1)	2n + 4	6	(6,4)	2n-2

The Segregated M- G's polynomial is outlined as

$M G (x, y) = 2x^4y^4 + 2x^4y^6 + (2n + 4)x^4y + (2n - 2)x^6y + (n - 2)x^6y^6 + (2n - 2)x^6y^4$

Table 3.2 Partition of Edge set

S.No	Degree Set	No. of Edges	S.No	Degree Set	No. of Edges
1	(4, 4)	2	4	(5, 5)	3n-5
2	(4, 1)	8	5	(5, 1)	4n-4
3	(4, 5)	4			

The Segregated M- H's polynomial is outlined as

$M H (x, y) = 2x^4y^4 + 8x^4y + 4x^4y^5 + (3n - 5)x^5y^5 + (4n - 4)x^5y$

Table 3.3 Partition of Neighborhood Edge set

S.No	Neighborhood Degree	No. of Edges	S.No	Neighborhood Degree	No. of Edges
1	(4, 14)	2n-4	6	(14, 20)	2
2	(14, 22)	2n-6	7	(12, 12)	2
3	(6, 22)	2n-6	8	(12, 20)	4
4	(22, 22)	n-4	9	(6, 20)	4
5	(20, 22)	2	10	(4, 12)	8

The neighborhood Segregated N- G's polynomial is outlined as

$N G (x, y) = (2n - 4)x^4y^{14} + (2n - 6)x^{14}y^{22} + (2n - 6)x^6y^{22} + (n - 4)x^{22}y^{22} + 2x^{20}y^{22}$
$+ 2x^{14}y^{20} + 2x^{12}y^{12} + 4x^{12}y^{20} + 4x^6y^{20} + 8x^4y^{12}$

Table 3.4 Partition of Neighborhood Edge set

S.No	Neighborhood Degree	No. of Edges
1	(4, 11)	8
2	(11, 11)	2
3	(11, 16)	4
4	(5, 16)	4n-4
5	(16, 16)	3n-5

The neighborhood Segregated N-polynomial of H is defined as, N H(x, y) = $8x^4y^{11}+2x^{11}y^{11}+4x^{11}y^{16}+(4n-4)x^5y^{16}+(3n-5)x^{16}y^{16}$

Table 3.4 Representations of Topographies

S.No	Name of the Indices	Formula
1	First Zagreb Index (U_1)	$(\Gamma(u))+(\Gamma(v))$
2	Second Zagreb Index (U_2)	$(\Gamma(u)).(\Gamma(v))$
3	Redefined third Zagreb Index (U_3)	$(\Gamma(u)).(\Gamma(v))(\Gamma(u))+(\Gamma(v))$
4	Y- Index (Z_y)	$(\Gamma(u))^3+(\Gamma(v))^3$
5	Forgotten topological Index (Z_f)	$(\Gamma(u))^2+(\Gamma(v))^2$
6	Second modified Zagreb Index (U_m)	$\frac{1}{\Gamma(u).\Gamma(v)}$
7	Symmetric division deg Index (U_d)	$\frac{\Gamma(u)^2+\Gamma(v)^2}{\Gamma(u).\Gamma(v)}$
8	Harmonic Index (Z_h)	$\frac{2}{\Gamma(u)+\Gamma(v)}$
9	Inverse sum indeg Index (U_i)	$\frac{\Gamma(u).\Gamma(v)}{\Gamma(u)+\Gamma(v)}$

3.2 Induction 1

If G is a mathematical structure with 7n+2 edges and 6n+3 vertices, then the fuzzy topographies as follows.

First Zagreb Tally (Z_1)

= [(-1.6+44.8n) + r(-0.4+11.2n), (-2.6+72.8n)+r(0.6 -16.8n)]

Second Zagreb Tally (Z_2)

= [(-28.8+135.2n)+r(-7.2-31.2n), (-46.8+135.2n)+r(10.8-31.2n)]

Redefined third Zagreb Tally (Z_3)

= [(-489.6+1346.8n)+r(-122.4-310.8n), (-795.6+1346.8n)+r(183.6-310.8n)]

Y- Tally (Z_y)

= [(-625.6+2022.8n)+r(-156.4-466.8n), (-1016.6+2022.8n)+r(234.6 -466.8n)]

Forgotten topological Tally (Z_f)

= [(-68.8+369.2n)+r(-17.2-85.2n), (-111.8+369.2)+r(25.8-85.2n)]

Second modified Zagreb Tally (Z_m)

= [(0.588888889+1.227777778n)+r(0.147222222-0.283333333n), (0.956944444+1.227777778n)+r(-0.220833333-0.283333333n)]

Symmetric division deg Tally (Z_d)

= [(3.733333333+35.31666667n)+r(0.933333333-8.15n), (6.066666667 +35.31666667n)+r(-1.4-8.15n)]

Harmonic Tally (Z_h)

= [(0.956190476+2.51952381n)+r(0.239047619-0.581428571n), (1.553809524 + (2.51952381 n)+r(-0.358571429-0.581428571n)]

Inverse sum indeg Tally (Z_i)

= [(-0.411428571+14.44857143n)+r(-0.102857143-3.334285714n), (-0.668571429+14.44857143n)+r(0.154285714-3.334285714n)]

3.3 Induction 2

If G is a mathematical structure with 7n+2 edges and 6n+3 vertices the fuzzy neigbourhood topographies as follows.

Neighborhood First Zagreb Index (z_1)

= [(-57.6+166.4n)+r(-14.4+41.6n), (-93.6+270.4n)+r(21.6-62.4n)]

Neighborhood Second Zagreb Index (z_2)

= [(-998.4+1918.8n)+r(-249.6-442.8n), (-1622.4+1918.8n)+r(374.4 -442.8n)]

Neighborhood Redefined third Zagreb Index (z_3)

= [(-52531.2+68744n)+r(-13132.8-15864n), (-85363.2+68744n) +r(19699.2-15864n)]

Neighborhood Y- Index (z_y)

= [(-72115.2+98051.2n)+r(-18028.8-22627.2n), (-117187.2+98051.2n) +r(27043.2-22627.2n)]

Neighborhood Forgotten topological Index (z_f)

= [(-2547.2+4929.6n)+r(-636.8-1137.6n), (-4139.2+ 4929.6n)+r(955.2-1137.6n)]

Neighborhood Second modified Zagreb Index (Z_m)

= [(0.078092614+0.07725305n)+r(0.019523154-0.017827627n), (0.126900498 +0.07725305n)+r(-0.02928473-0.017827627n)]

Neighborhood Symmetric division deg Index (z_d)

= [(2.012813853+28.42554113n)+r(0.503203463-6.55974026n), (3.270822511 + 28.42554113n)+r(-0.754805195-6.55974026n)

Neighborhood Harmonic Index (z_h)

= [(0.439261392+0.678138528n)+r(0.109815348-0.156493506), (0.713799762 +0.678138528n)+r(-0.164723022-0.156493506n)]

Neighborhood Inverse sum indeg Index (z_i)

= [(-11.34318753+56.89047619n)+r(-2.835796883-13.12857143n), (-18.43267974 +56.89047619n)+r(4.253695324-13.12857143n)]

3.4 Induction 3

If G is a mathematical structure with 6n + 6 edges and 7n + 5 vertices then the fuzzy topographies as follows.

Neighborhood First Zagreb Index (z_1)

= [(14.4+43.2n)+r(3.6+10.8n), (23.4+70.2n)+r(-5.4-16.2n)]

Neighborhood Second Zagreb Index (z_2)

= [(-0.8+123.5n)+r(-0.2-28.5n), (-1.3+123.5n)+r(0.3 -28.5n)]

Neighborhood Redefined third Zagreb Index (z_3)

= [(-187.2+1131n)+r(-46.8-261n), (-304.2+1131n)+r(70.2-261n)]

Neighborhood Y- Index (z_y)

= [(8+330.2n)+r(2-76.2n), (13+330.2n)+r(-3 -76.2n)]

Neighborhood Forgotten topological Index (z_f)

= [(-177.6+1630.2n)+r(-44.4-376.2n), (-288.6+1630.2n)+r(66.6-376.2n)]

Neighborhood Second modified Zagreb Index (Z_m)

= [(1.06+1.196n)+r(0.265-0.276n), (1.7225+ 1.196n)+r(-0.3975-0.276n)]

Neighborhood Symmetric division deg Index (z_d)

= [(12.32+34.84n)+r(3.08-8.04n), (20.02+34.84n)+r(-4.62-8.04n)]

Neighborhood Harmonic Index (z_h)

= [(1.804444+2.513333n)+r(0.451111-0.58n), (2.932222+2.513333n) +r(-0.67667-0.58n)]

Neighborhood Inverse sum indeg Index (z_i)

= [(2.764444+14.08333n)+r(0.691111-3.25n), (4.492222+14.08333)+r(-1.03667-3.25n)]

3.5 Hypothesis 4

If G is a mathematical structure with 6n + 6 edges and 7n + 5 vertices then neighborhoods of topographies as follows.

Neighborhood First Zagreb Index (z_1)

= [(22.4+144n)+r(5.6+36n), (36.4+234n)+r(-8.4-54n)]

Neighborhood Second Zagreb Index (z_2)

= [(-241.6+1414.4n)+r(-60.4-326.4n), (-392.6+1414.4n)+r(90.6-326.4n)]

Neighborhood Redefined third Zagreb Index (z_3)

= [(-14454.4+40684.8n)+r(-3613.6-9388.8n), (-23488.4+40684.8)
+r(5420.4-9388.8n)]

Neighborhood Y- Index (z_y)

= [(-476.8+3458n)+r(-119.2-798n), (-774.8+3458n)+r(178.8-798n)]

Neighborhood Forgotten topological Index (z_f)

= [(-15721.6+53898n)+r(-3930.4-12438n), (-25547.6+53898n)

+r(5895.6-12438n)]

Neighborhood Second modified Zagreb Index (Z_m)

= [(0.121235 +0.080234n)+r(0.030309 -0.01852n), (0.197006+0.080234)

+r(-0.04546-0.01852n)]

Neighborhood Symmetric division deg Index (z_d)

= [(10.74182+26.065n)+r(2.685455-6.015n), (17.45545+26.065n)

+r(-4.02818-6.015n)]

Neighborhood Harmonic Index (z_h)

= [(0.681063+0.738988n)+r(0.170266-0.17054n), (1.106727+0.738988n)

+r(-0.2554-0.17054n)]

Neighborhood Inverse sum indeg Index (z_i)

= [(4.242116+51.00952n)+r(1.060529 -11.7714n), (6.893439+51.00952n)

+r(-1.59079-11.7714n)]

4. Mathematical modeling of G and H

In practice of utilizing mathematics to represent, evaluate, and forecast real-world occurrences is known as mathematical modeling. In statistical graph theory, statistical techniques are used to examine the characteristics and behaviors of these graphs. These techniques include graph structure, which entails examining the network's organizational structure and etc.,

Table 4.1.1 t Test for Topographies of G and H

	M	N
Mean	857.730467	26801.73445
Variance	1926093.79	2598489570
Observations	9	9
Degrees of Freedom	8	
Calculated t	-1.52628934	
P(T <= t) (One –tail)	0.08272614	
t Critical one-tail	1.85954803	
P(T<=t) two-tail	0.16545227	
t Critical two-tail	2.30600413	

Therefore, the non-zero explanation H0 is accepted with the aid of the t-test result. Finally, draw the conclusion that the neighbourhood degree-based topographies of G and H and the degree-based morphological indices of G and H do not differ significantly. In other words, the different topographies for the graphs G and H correspond to the same phenomenon. This indicates that the results and characterisation provided by these two degree-based and neighborhood-based indices are comparable.

Table 4.2 F Test for Topographies of G and H

F-Test Two-Sample for Variances	Segregated Topographies	Neighborhood Segregated Topographies
Mean	857.7304674	26801.73445
Variance	1926093.786	2598489570
Degrees of freedom	8	8
F	0.000741236	
P(F<=f) one-tail	0.000000000011	
F Critical one-tail	0.290858219	

Thus, with help of F-test result, the null hypothesis H_0 is also accepted.

Table 4.3 Descriptive Statistics for G and H

Segregated Topographies		Neighborhood Segregated Topographies	
Mean	857.7304674	Mean	26801.73445
Standard Error	462.6126033	Standard Error	16991.794
Median	166	Median	552
Standard Deviation	1387.83781	Standard Deviation	50975.382
Sample Variance	1926093.786	Sample Variance	2598489570
Kurtosis	2.180676471	Kurtosis	1.973611916
Skewness	1.766365485	Skewness	1.798314829
Range	3882.430556	Range	136127.7241
Confidence Level (95.0%)	1066.786575	Confidence Level (95.0%)	39183.1472

Table 4.3 One Way ANOVA test for Segregated Tally of G and H

Clusters	Count	Sum	Average	Variance		
Segregated Tally of G	9	7719.57	857.73	1926094		
Segregated Tally of H	9	7295.9	810.655	1622764		
ANOVA						
Origin of Differencing	SS	df	MS	F	P-value	F crit
ReCluster	9972.39602	1	9972.4	0.00562	0.94117	4.494
Gaining Cluster	28390862.8	16	1774429			
Total	28400835.1	17				

Thus, with help of ANOVA one-way classification result, the null hypothesis H_0 is also accepted.

Table 4.4 One Way ANOVA test for Neighborhood Segregated Tally of G and H

Clusters	Sample size	$\sum x$	Mean	Var(x)		
Neigbourhood of G	9	241216	26801.7345	2598489570		
Neigbourhood of H	9	191661	21295.7208	1587337116		
ANOVA						
Origin of Differencing	Sum of Square	Degrees of Freedom	Mean sum of Square	F	P-value	F crit
ReCluster	136422836.3	1	136422836	0.065183223	0.80174	4.494
Gaining Cluster	33486613485	16	2092913343			
Total	33623036322	17				

Thus, with help of ANOVA one-way classification result, the null hypothesis H_0 is also accepted.

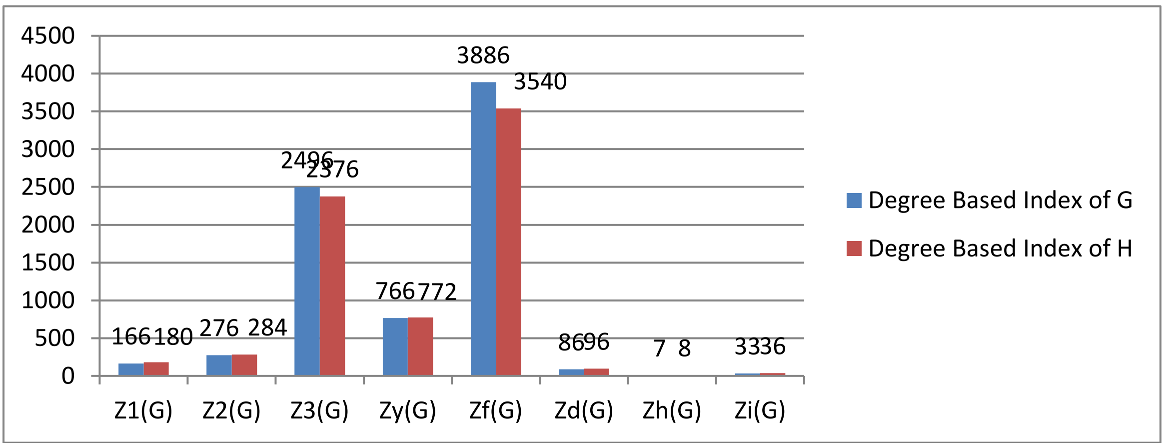

Figure 4.1-Comparison of Segregated Index of G and H

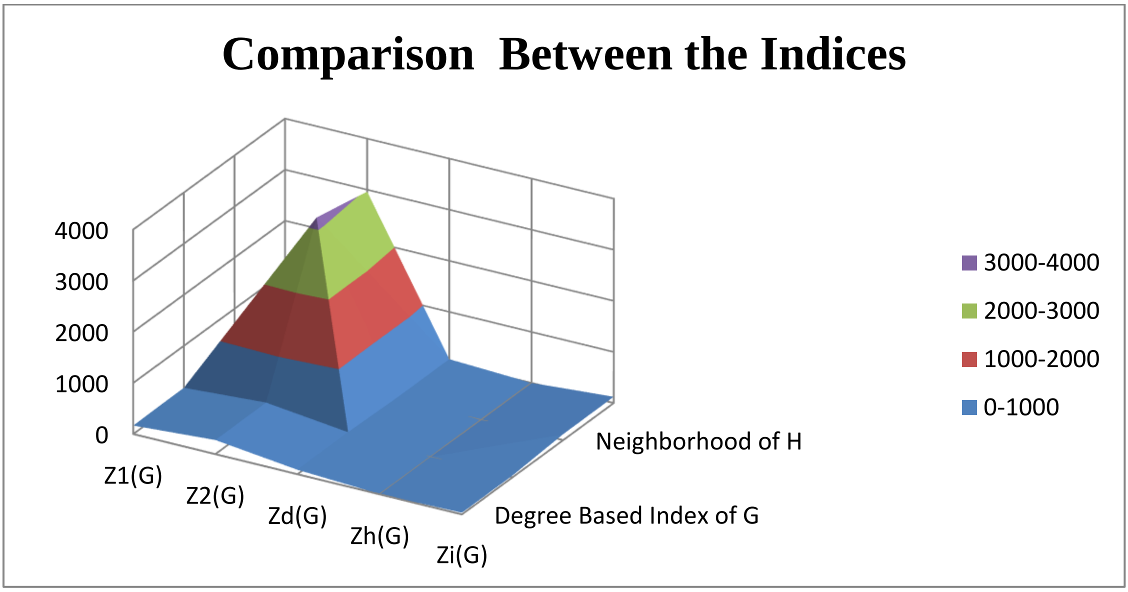

Figure 4.2- Comparison Between the Indices

4.1 Forecast Analysis

Regression lines which gives the average relation between two variables is the regression lines, the corresponding regression line is a regression equation. When X and Y are the independent and dependent variables, respectively, the econometric equation is often referred to as the estimating equation. Regression equations are used to estimate the value of the parameter that depends that corresponds to any value of the independent variable. The correlation coefficients are agnostic change of provenance but are modified by change of dimension. Currently, the formula of the regression is as follows: if H's degree-based topological tally is the dependent variable (Y), and if G's degree-based topological tally is the independent variable (X).

Degree-based tally of H (Segregated Index of G) = 27.95974 + 0.916035

Additionally, the correlation coefficient equation is if the neighbourhood degree-based conical tally of G is the independent variable (X) and the neighbourhood degree-based conical tally of H is the dependent variable (Y).

Neighborhood Index of H = 419.6908 + 0.780645 (Neighborhood tally of G)

5. Conclusion

some of the fuzzy topographies that we have obtained across the present research conclude that neighborhood Segregated topographies and Segregated topographies do not differ significantly. In other words, the phenomena represented by the different topographies for the graph is the same. This indicates that the results and characterization provided by these two degree-based indices are comparable. In future endeavors, we will incorporate this result and analyze forecasts of real-world situations.

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