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COMPUTING CERTAIN TOPOLOGICAL INDICES OF THE LINE GRAPH OF OCTAGONAL NETWORK

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Abstract

A topological index is a molecular index that converts molecular structures into specific real values. Chemical graph theory relies heavily on topological indices to build quantitative structure activity correlations in which attributes of molecules can be connected to their chemical structures. Chemical graph theory should be seen not only as equivalent to other fields of theoretical chemistry, but also as complementary and important for a deeper knowledge of the nature of chemical structure and helpful in modelling the networks. The main goal of this research work is to construct the line graph of octagonal network, then computing topological indices for the line graph of octagonal network which based on the degree of vertices and neighborhood degree of vertices. After that, we give graphically representation of the computed topological indices.

Keywords: degree-based topological indices; line graph; octagonal network.

1. Introduction and Preliminaries

A fundamental and dynamic technique for constructing and modelling a graph or network is graph theory. A number of topological indices are based on factors like degree, distance, eccentricity, etc. The topological indices basically link the corresponding synthetic and atomic structure to certain physiochemical characteristics and bioactivity. The study of graphs using chemistry attracts a lot of researchers globally because of its enormous applications [1].

Topological indices or descriptors have gained some prominence in recent years, because they are simple to create and may be completed quickly. Typically, we are interested in estimating the structural features to develop quantitative structure-activity connections by utilizing methods from graph theory. Let G be a connected graph with a vertex set V(G) and an edge set E(G). Any connected graph without multiple edges or loops is referred to as a simple graph [6]. The degree of vertex x is the number of edges incident with x, which is denoted by d_x. For more detailed study, we recommend the following articles [2-5, 15-30].

In this research work, we calculate some degree-based indices (shown in Tabel 1) and some neighborhood degree based topological indices (shown in Tabel 2) of line graph of octagonal network. Octagonal network represented by (O_n^m), where m rows and n columns as

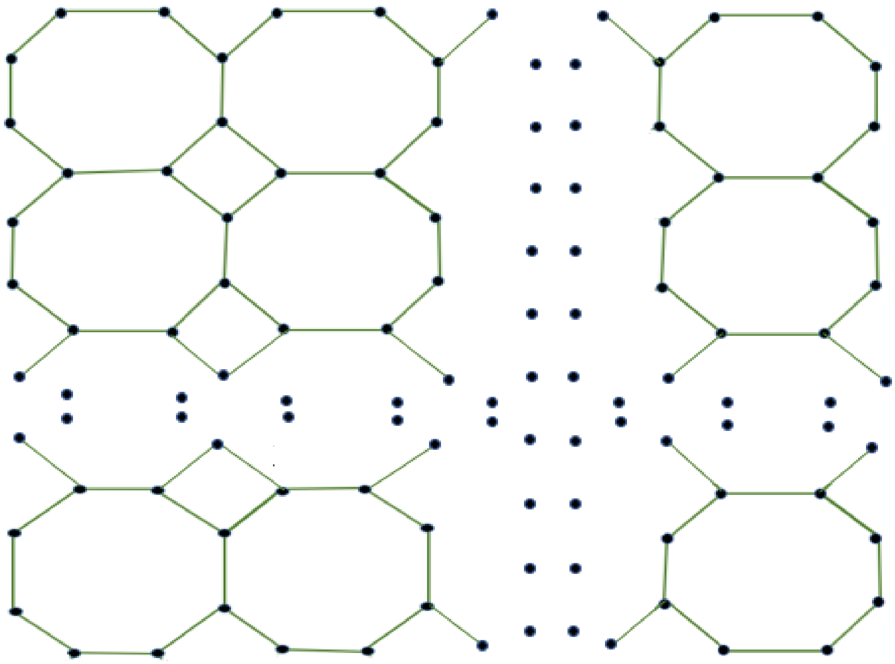

Figure 1: Octagonal network O_n^m.

shown in Figure 1. $((4m+2)n+2m)$ is the number of vertices and $((6m+1)n+m)$ is the number of edges in the octagonal network. The line graph denoted by $L(G)$ is the graph derived from G, the edges in G are changed by vertices in $L(G)$ and two vertices in $L(G)$ are linked whenever the corresponding edges in G are adjacent [7]. Figure 2 shows the line graph of octagonal network $\left(L(O_2^2)\right)$.

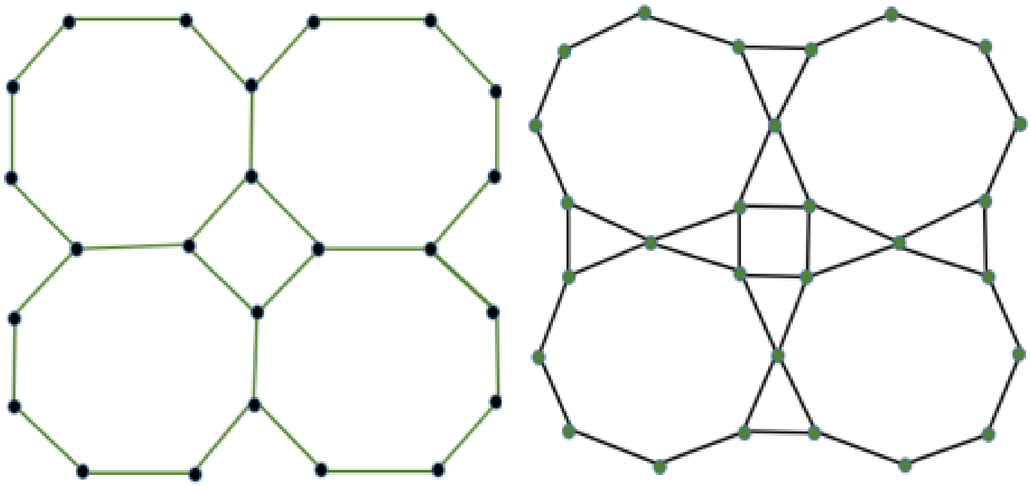

Figure 2: Octagonal network O_2^2 and its line graph.

Tabel 1: Degree-based topological indices.

S.No.	Topological Index	Symbol	Formula
1	General Randic Index [8]	$R_\alpha(L(G))$	$\sum_{xy\in E(L(G))} (d_x d_y)^\alpha$
2	First Zegreb Index [9]	$M_1(L(G))$	$\sum_{xy\in E(L(G))} (d_x + d_y)$
3	Atom Bond Connectivity Index [10]	$ABC(L(G))$	$\sum_{xy\in E(L(G))} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}$
4	Geometric Arithmetic Index [11]	$GA(L(G))$	$\sum_{xy\in E(L(G))} \frac{2\sqrt{d_x d_y}}{(d_x + d_y)}$

Tabel 2: Neighbourhood degree-based topological indices.

S.No.	Topological Index	Symbol	Formula
1	Fourth Atom Bond Connectivity Index [12]	$ABC_4(L(G))$	$\sum_{xy\in E(L(G))} \sqrt{\frac{S_x + S_y - 2}{S_x \times S_y}}$
2	Fifth Geometric Arithmetic Index [13]	$GA_5(L(G))$	$\sum_{xy\in E(L(G))} \frac{2\sqrt{S_x \times S_y}}{S_x + S_y}$
3	Fifth Arithmetic Geometric Index [13]	$AG_5(L(G))$	$\sum_{xy\in E(L(G))} \frac{S_x + S_y}{2\sqrt{S_x \times S_y}}$
4	Sanskruti Index [14]	$S(L(G))$	$\sum_{xy\in E(L(G))} \left(\frac{S_x \times S_y}{S_x + S_y - 2}\right)^3$

where,

$$S_x = \sum_{y \in N_x} d_y$$

and $N_x = \{y \in V(L(G)) | xy \in E(G)\}$.

Theorem.1: Consider the line graph of octagonal network $L(\mathrm{O}_n^m)$. Then,

1. $$R_\alpha(L(\mathrm{O}_n^m)) = \begin{cases} 192mn - 102(m+n) + 44 \ \alpha = 1 \\ 48mn - 42(m+n) + 52 + 4\sqrt{6}(n+m-2) + 8\sqrt{3}(n+m-2) \ \alpha = \frac{1}{2} \\ \frac{27mn+17(m+n)+5}{36} \ \alpha = -1 \\ 3mn + \frac{-7(m+n)+17}{3} + \left(\frac{4}{\sqrt{6}} + \frac{2}{\sqrt{3}}\right)(n+m-2) \ \alpha = -\frac{1}{2} \end{cases}$$

2. $M_1(L(\mathrm{O}_n^m)) = 96mn + 156(m+n) + 8$.

3. $ABC(L(\mathrm{O}_n^m)) = \frac{4(m+n-2)}{3} + \frac{2\sqrt{5}(n+m-2)}{\sqrt{3}} + \frac{4(n+m)+6\sqrt{3}(mn-m-n+1)}{\sqrt{2}}$.

4. $GA(L(\mathrm{O}_n^m)) = 2(6mn - 5(m+n) + 8) + (n+m-2)\left(\frac{8\sqrt{6}}{5} + \frac{16\sqrt{3}}{7}\right)$.

5. $ABC_4(\ L(\mathrm{O}_n^m)) = \sqrt{\frac{7}{20}}(8) + \frac{8}{9}(n+m-2) + \frac{\sqrt{30}}{4}(mn-n-m+1) + 8\sqrt{\frac{1}{15}}(n+m-2)$

$$+\frac{2\sqrt{6}}{3}(n+m-2) + 2\sqrt{2}(mn-n-m+1).$$

6. $GA_5(\ L(\mathrm{O}_n^m)) = \frac{32\sqrt{5}}{9} + \frac{12\sqrt{5}}{7}(n+m-2) + \frac{24\sqrt{14}}{23}(n+m-2) + \frac{32\sqrt{14}}{15}(mn$

$$-n-m+1+(4mn-2n-2m).$$

7. $AG_5(\ L(\mathrm{O}_n^m)) = \frac{18}{\sqrt{5}} + \frac{28}{\sqrt{45}}(n+m-2) + \frac{46}{\sqrt{126}}(n+m-2) + \frac{15\sqrt{14}}{7}(mn-n-m+)$

$$+2(2mn-n-m).$$

8. $S(\ L(\mathrm{O}_n^m)) = 6581.5mn - 5247.1n - 5247.1m + 4099.2$

Proof. Let $(L(\mathrm{O}_n^m))$ be the line graph of octagonal network. Since $E(G) = V(L(G))$, so total number of vertices in $(L(\mathrm{O}_n^m))$ is $((4m+2)n+2m)$. In $(L(\mathrm{O}_n^m))$, we have $(2n+2m+4)$ vertices of degree 2, $(4n+4m-8)$ vertices of degree 3 and $(6mn-5n-5m+4)$ vertices of degree 4.

Now by using handshaking lemma, we can calculate the total number of edges in $(L(\mathrm{O}_n^m))$, i.e.,

$$2(2n+2m+4) + 3(4n+4m-8) + 4(6mn-5n-5m+4 = 2|E(L(G))|$$

$$12mn - 2n - 2m = E(L(G))$$

There are five types of edges in $(L(\mathrm{O}_n^m))$ based on degrees of end vertices of each edge. Table 3 shows such edge partition of $(L(\mathrm{O}_n^m))$.

Table 3. Edge partition of line graph of octagonal network $(L(O_n^m))$.

(d_x, d_y) where $xy \in E(L(G))$	Number of edges
(2,2)	8
(2,3)	$4n + 4m - 8$
(3,3)	$2m + 2n - 4$
(3,4)	$4n + 4m - 8$
(4,4)	$12mn - 12n - 12m + 12$

1. For $\alpha = 1$, we apply the formula of $R_\alpha(L(G))$, i.e.,

$$R_1(L(G)) = \sum_{xy\in E(L(G))} (d_x \times d_y)$$

By using Table 3, we get

$$R_1(L(O_n^m)) = 8(2\times 2) + (4n + 4m - 8)(2\times 3) + (2m + 2n - 4)(3\times 3) + (4n + 4m - 8)(3\times 4) + (12mn - 12n - 12m + 12)(4\times 4).$$

$$R_1(L(O_n^m)) = 44 - 102n - 102m + 192mn.$$

$$R_1(L(O_n^m)) = 192mn - 102(m + n) + 44.$$

For $\alpha = \frac{1}{2}$, we apply the formula of $R_\alpha(L(G))$, i.e.,

$$R_{\frac{1}{2}}(L(G)) = \sum_{xy\in E(L(G))} \sqrt{(d_x \times d_y)}.$$

By using edge partition given in Table 3, we get

$$R_{\frac{1}{2}}(L(O_n^m)) = 8(\sqrt{2\times 2}) + (4n + 4m - 8)(\sqrt{2\times 3}) + (2m + 2n - 4)(\sqrt{3\times 3}) + (4n + 4m - 8)(\sqrt{3\times 4}) + (12mn - 12n - 12m + 12)(\sqrt{4\times 4}).$$

$$R_{\frac{1}{2}}(L(O_n^m)) = 48mn - 42(n + m) + 52 + 4\sqrt{6}(n + m - 2) + 8\sqrt{3}(n + m - 2).$$

For $\alpha = -1$, we apply the formula of $R_\alpha(L(G))$, i.e.,

$$R_{-1}(L(G)) = \sum_{xy\in E(L(G))} \frac{1}{(d_x \times d_y)}$$

$$R_{-1}(L(O_n^m)) = 8\frac{1}{(2\times 2)} + (4n + 4m - 8)\frac{1}{(2\times 3)} + (2m + 2n - 4)\frac{1}{(3\times 3)} + (4n + 4m - 8)\frac{1}{(3\times 4)} + (12mn - 12m - 12n + 12)\frac{1}{(4\times 4)}.$$

$$R_{-1}(L(O_n^m)) = \frac{5}{36} + \frac{17}{36}n + \frac{17}{36}m + \frac{3}{4}mn.$$

$$R_{-1}\big(L(\mathrm{O}_n^m)\big) = \frac{27mn + 17(m+n) + 5}{36}.$$

For $\alpha = -\frac{1}{2}$, we apply the formula of $R_\alpha(L(G))$, i.e.,

$$R_{-\frac{1}{2}}(L(G)) = \sum_{xy \in E(L(G))} \frac{1}{\sqrt{(d_x \times d_y)}}$$

$$R_{-\frac{1}{2}}\big(L(\mathrm{O}_n^m)\big) = 8\frac{1}{\sqrt{2\times 2}} + (4n+4m-8)\frac{1}{\sqrt{2\times 3}} + (2m+2n-4)\frac{1}{\sqrt{3\times 3}} + (4n+4m-8)\frac{1}{\sqrt{3\times 4}} + (12mn-12m-12n+12)\frac{1}{\sqrt{4\times 4}}.$$

$$R_{-\frac{1}{2}}\big(L(\mathrm{O}_n^m)\big) = 3mn + \frac{-7(m+n)+17}{3} + \left(\frac{4}{\sqrt{6}} + \frac{2}{\sqrt{3}}\right)(n+m-2).$$

2. By using Table 3, we can easily prove the first Zagreb index, i.e.,

$$M_1(L(G)) = \sum_{xy \in E(L(G))} (d_x + d_y)$$

$$M_1\big(L(\mathrm{O}_n^m)\big) = 8(2+2) + (4n+4m-8)(2+3) + (2m+2n-4)(3+3) + (4n+4m-8)(3+4) + (12mn-12n-12m+12)(4+4).$$

$$M_1(L(\mathrm{O}_n^m)) = 96mn + 156(m+n) + 8$$

3. By using Table 3, we can easily prove the ABC index, i.e.,

$$ABC(L(G)) = \sum_{xy \in E(L(G))} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}.$$

$$ABC\big(L(\mathrm{O}_n^m)\big) = 8\sqrt{\frac{2+2-2}{2\times 2}} + (4n+4m-8)\sqrt{\frac{2+3-2}{2\times 3}} + (2m+2n-4)\sqrt{\frac{3+3-2}{3\times 3}} + (4n+4m-8)\sqrt{\frac{3+4-2}{3\times 4}} + (12mn-12m-12n+12)\sqrt{\frac{4+4-2}{4\times 4}}.$$

$$ABC\big(L(\mathrm{O}_n^m)\big) = \frac{(4n+4m)}{2} + \frac{4m+4n-8}{3} + \frac{\sqrt{5}(4n+4m-8}{\sqrt{12}} + \frac{\sqrt{3}(12mn-12m-12n+12}{\sqrt{8}}.$$

$$ABC\big(L(\mathrm{O}_n^m)\big) = \frac{4(m+n-2)}{3} + \frac{2\sqrt{5}(n+m-2)}{\sqrt{3}} + \frac{4(n+m) + 6\sqrt{3}(mn-m-n+1)}{\sqrt{2}}.$$

4. By using Table 3, we can easily prove the *(GA)* index, i.e.,

$$GA\big(L(G)\big) = \sum_{xy \in E(L(G))} \frac{2\sqrt{d_x d_y}}{(d_x + d_y)}.$$

$$GA\big(L(\mathrm{O}_n^m)\big) = 8\left(\frac{2\sqrt{2\times 2}}{2+2}\right) + (4n+4m-8)\left(\frac{2\sqrt{2\times 3}}{2+3}\right) + (2m+2n-4)\left(\frac{2\sqrt{3\times 3}}{3+3}\right) + (4n+4m-8)\left(\frac{2\sqrt{3\times 4}}{3+4}\right) + (12mn-12m-12n+12)\left(\frac{2\sqrt{4\times 4}}{4+4}\right).$$

$$GA\big(L(\mathrm{O}_n^m)\big) = 12mn - 10(n+m) + 16 + \frac{\sqrt{6}(8n+8m-16)}{5} + \frac{\sqrt{12}(8n+8m-16)}{7}.$$

$$GA\big(L(\mathrm{O}_n^m)\big) = 2(6mn - 5(m+n) + 8) + (n+m-2)\left(\frac{8\sqrt{6}}{5} + \frac{16\sqrt{3}}{7}\right).$$

Table 4: The (S_x, S_y)-type edge partition of the line graph of octagonal network $(L(\mathrm{O}_n^m))$.

(S_x, S_y) where $xy \in E(L(G))$	Number of edges
$(4,5)$	8
$(5,9)$	$4n+4m-8$
$(9,9)$	$2n+2m-4$
$(9,14)$	$4n+4m-8$
$(9,16)$	$8mn-8n-8m+8$
$(16,16)$	$4mn-4n-4m+4$

5. There are six types of edges in $\big(L(\mathrm{O}_n^m)\big)$ based on neighborhood degrees of end vertices of each edge. By using Table 4, we derive the expression for ABC_4 index, i.e.,

$$ABC_4(G) = \sum_{xy\in E(G)} \sqrt{\frac{S_x + S_y - 2}{S_x \times S_y}}.$$

$$ABC_4\big(L(\mathrm{O}_n^m)\big)$$

$$= \sqrt{\frac{4+5-2}{4\times 5}}(8) + \sqrt{\frac{5+9-2}{5\times 9}}(4n+4m-8)$$
$$+ \sqrt{\frac{9+9-2}{9\times 9}}(2n+2m-4)$$
$$+ \sqrt{\frac{9+14-2}{9\times 14}}(4n+4m-8) + \sqrt{\frac{14+16-2}{14\times 16}}(8mn-8n-8m+8)$$
$$+ \sqrt{\frac{16+16-2}{16\times 16}}(4mn-4n-4m+4).$$

$$ABC_4\left(L(\mathrm{O}_n^m)\right) = \sqrt{\frac{7}{20}}(8) + \sqrt{\frac{12}{45}}(4n+4m-8) + \sqrt{\frac{16}{81}}(2n+2m-4) + \sqrt{\frac{21}{126}}(4n+4m-8) + \sqrt{\frac{28}{224}}(8mn-8n-8m+8) + \sqrt{\frac{30}{256}}(4mn-4n-4m+4).$$

$$ABC_4\left(L(\mathrm{O}_n^m)\right) = \sqrt{\frac{7}{20}}(8) + \frac{8}{9}(n+m-2) + \frac{\sqrt{30}}{4}(mn-n-m+1) + 8\sqrt{\frac{1}{15}}(n+m-2) + \frac{2\sqrt{6}}{3}(n+m-2) + 2\sqrt{2}(mn-n-m+1).$$

6. By using Table 4, we can easily prove fifth geometric arithmetic index, i.e.,

$$GA_5(G) = \sum_{\mathrm{xy}\in E(G)} \frac{2\sqrt{S_x \times S_y}}{S_x + S_y}.$$

$$GA_5\left(L(\mathrm{O}_n^m)\right) = \frac{2\sqrt{4\times 5}}{4+5}(8) + \frac{2\sqrt{5\times 9}}{5+9}(4n+4m-8) + \frac{2\sqrt{9\times 9}}{9+9}(2n+2m-4) + \frac{2\sqrt{9\times 14}}{9+14}(4n+4m-8) + \frac{2\sqrt{14\times 16}}{14+16}(8mn-8n-8m+8) + \frac{2\sqrt{16\times 16}}{16+16}(4mn-4n-4m+4).$$

$$GA_5\left(L(\mathrm{O}_n^m)\right) = \frac{2\sqrt{20}}{9}(8) + \frac{2\sqrt{45}}{14}(4n+4m-8) + \frac{2\sqrt{81}}{18}(2n+2m-4) + \frac{2\sqrt{126}}{23}(4n+4m-8) + \frac{2\sqrt{224}}{30}(8mn-8n-8m+8) + \frac{2\sqrt{256}}{32}(4mn-4n-4m+4).$$

$$GA_5\left(L(\mathrm{O}_n^m)\right) = \frac{32\sqrt{5}}{9} + \frac{12\sqrt{5}}{7}(n+m-2) + \frac{24\sqrt{14}}{23}(n+m-2) + \frac{32\sqrt{14}}{15}(mn-n-m+1 + (4mn-2n-2m).$$

7. By using Table 4, we can easily prove fifth arithmetic geometric index, i.e.,

$$AG_5 = \sum_{xy\in E(G)} \frac{S_x + S_y}{2\sqrt{S_x \times S_y}}$$

$$AG_5\left(L(\mathrm{O}_n^m)\right) = \frac{4+5}{2\sqrt{4\times 5}}(8) + \frac{5+9}{2\sqrt{5\times 9}}(4n+4m-8) + \frac{9+9}{2\sqrt{9\times 9}}(2n+2m-4) + \frac{9+14}{2\sqrt{9\times 14}}(4n+4m-8) + \frac{14+16}{2\sqrt{14\times 16}}(8mn-8n-8m+8) + \frac{16+16}{2\sqrt{16\times 16}}(4mn-4n-4m+4).$$

$$AG_5\big(L(\mathrm{O}_n^m)\big) = \frac{36}{\sqrt{20}} + \frac{7}{\sqrt{45}}(4n+4m-8) + \frac{9}{\sqrt{81}}(2n+2m-4) + \frac{23}{2\sqrt{126}}(4n+4m-8) + \frac{30}{2\sqrt{224}}(8mn-8n-8m+8) + \frac{16}{\sqrt{256}}(4mn-4n-4m+4).$$

$$AG_5\big(L(\mathrm{O}_n^m)\big) = \frac{18}{\sqrt{5}} + \frac{28}{\sqrt{45}}(n+m-2) + \frac{46}{\sqrt{126}}(n+m-2) + \frac{15\sqrt{14}}{7}(mn-n-m+) + 2(2mn-n-m).$$

8. By using Table 4, we can easily prove sanskruti index, i.e.,

$$\sum_{xy\in E(L(G))} \left(\frac{S_x \times S_y}{S_x + S_y - 2}\right)^3.$$

$$S\big(L(\mathrm{O}_n^m)\big) = \left(\frac{4\times 5}{4+5-2}\right)^3 (8) + \left(\frac{5\times 9}{5+9-2}\right)^3 (4n+4m-8) + \left(\frac{9\times 9}{9+9-2}\right)^3 (2n+2m-4) + \left(\frac{9\times 14}{9+14-2}\right)^3 (4n+4m-8) + \left(\frac{14\times 16}{14+16-2}\right)^3 (8mn-8n-8m+8) + \left(\frac{16\times 16}{16+16-2}\right)^3 (4mn-4n-4m+4).$$

$$S\big(L(\mathrm{O}_n^m)\big) = \left(\frac{20}{7}\right)^3 (8) + \left(\frac{15}{4}\right)^3 (4n+4m-8) + \left(\frac{81}{16}\right)^3 (2n+2m-4) + 216(4n+4m-8) + 512(8mn-8n-8m+8) + \left(\frac{128}{15}\right)^3 (4mn-4n-4m+4).$$

$$S\big(L(\mathrm{O}_n^m)\big) = 6581.5mn - 5247.1n - 5247.1m + 4099.2$$

3. Comparison

Here, we give graphically representation of the above computed topological indices which based on the degree of the vertices (see Figures 3-6) and neighbourhood degree of vertices (see Figures 7-10), for the line graph of octagonal network (O_n^m), where, *m* = 1, 2, 3, 4,..., 10 and *n* = 1, 2, 3, 4,..., 10.

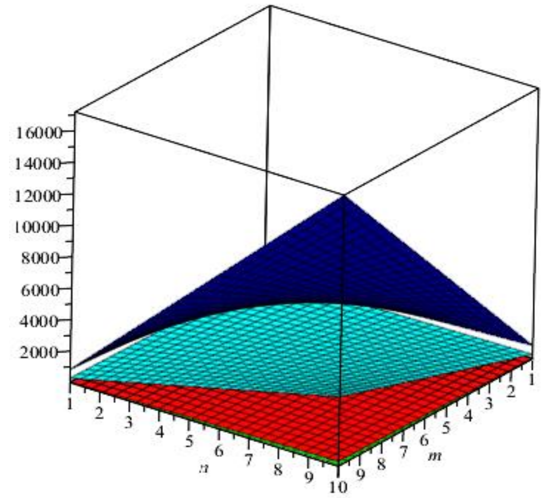

Figure 3: Graphically representation of general randic index

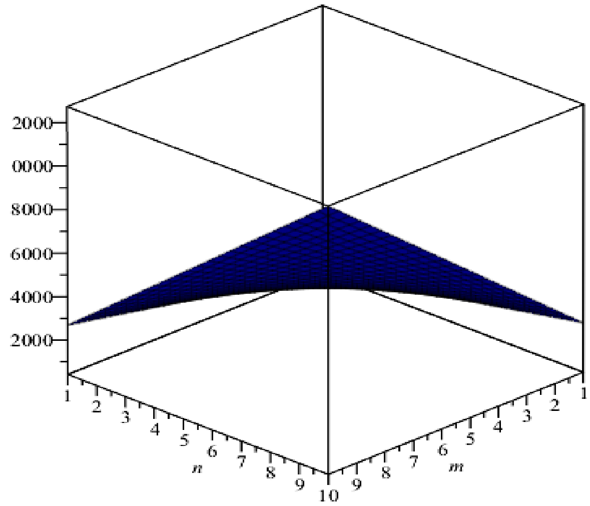

Figure 4: Graphically representation of first zegreb index

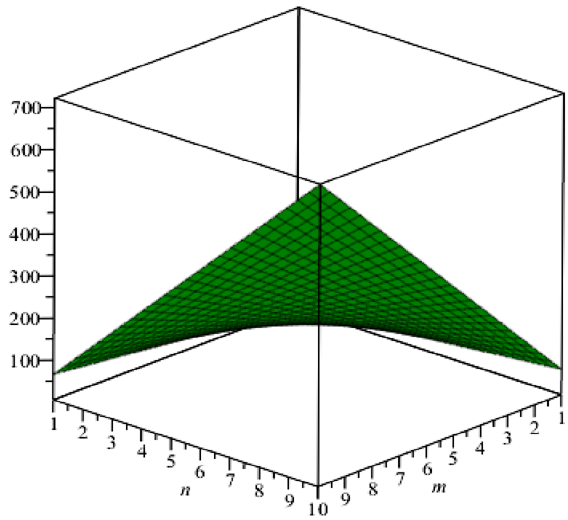

Figure 5: Graphically representation of atom bond connectivity index

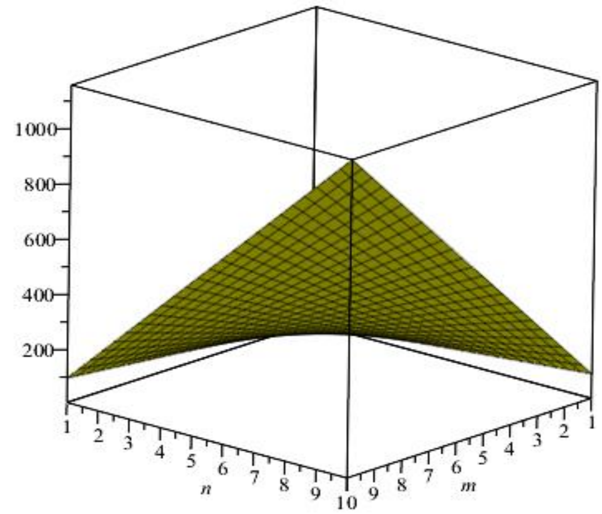

Figure 6: Graphically representation of geometric arithmetic index

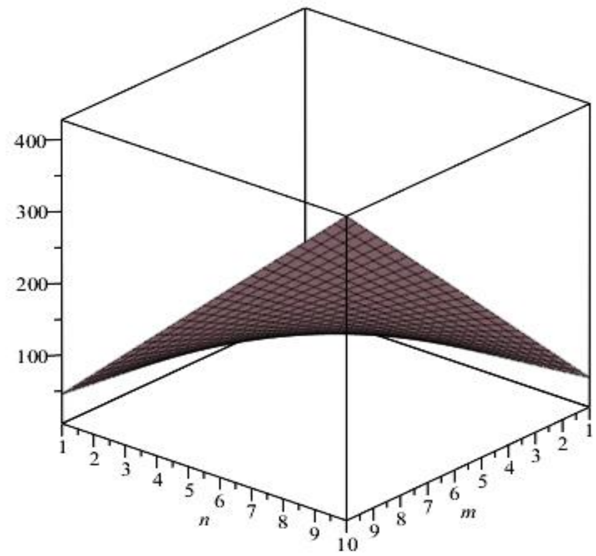

Figure 7: Graphically representation of fourth atom bond connectivity index

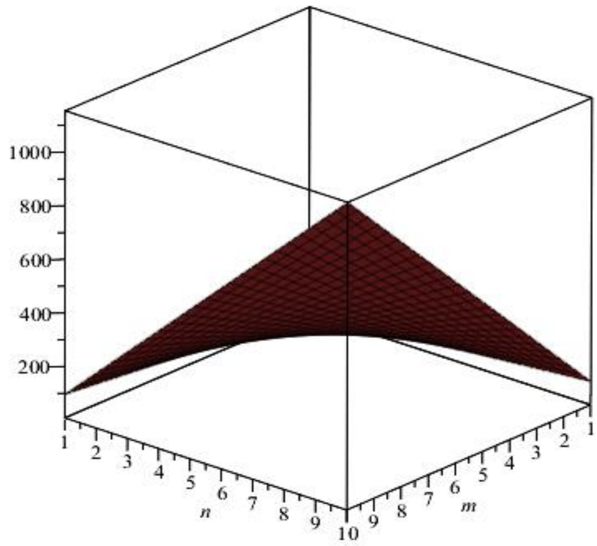

Figure 8: Graphically representation of fifth geometric arithmetic index

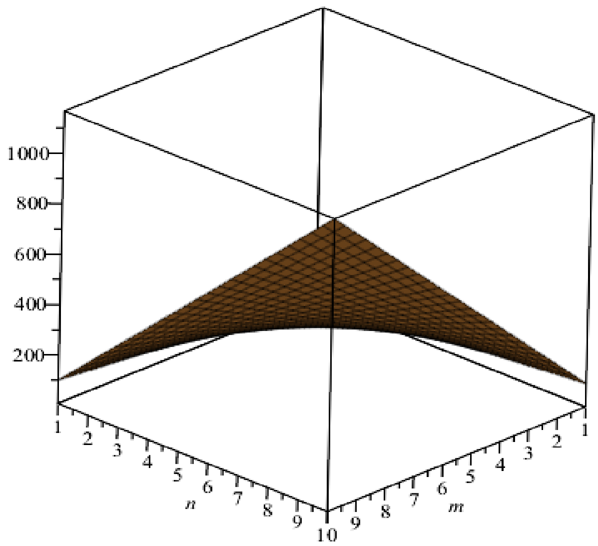

Figure 9: Graphically representation of arithmetic geometric index

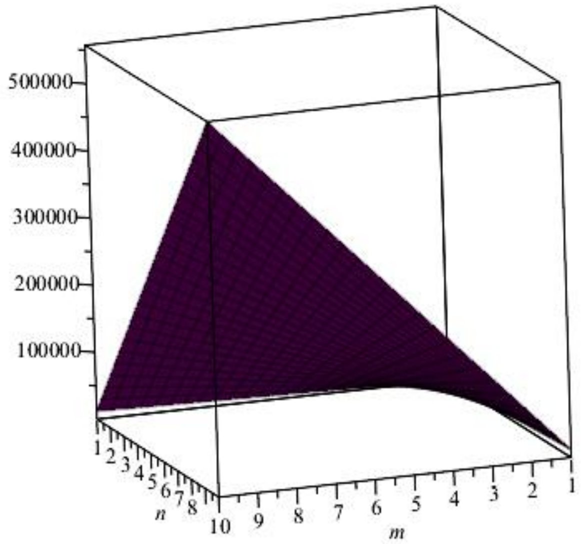

Figure 10: Graphically representation of sanskruti index

Conclusion

We have constructed the line graph of octagonal network and computed the closed formulae of degree-based topological indices like as general Randic index (R_α), first-Zagreb index (M_1), atom bond connectivity index (ABC), geometric arithmetic index (GA) and neighbourhood degree-based topological indices like as fourth atom bond connectivity index (ABC_4), fifth geometric arithmetic index (GA_5), fifth arithmetic geometric index (AG_5) and sanskruti index (S) of line graph of octagonal network (O_n^m). The geometric structures of attained results are presented graphically.

Statements and Declarations

We confirm that the manuscript has been read and approved by all named authors and that there are no other persons who satisfied the criteria for authorship but are not listed. We further confirm that the order of authors listed in the manuscript has been approved by all of us.

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