ISSN: 1672 - 6553

JOURNAL OF DYNAMICS AND CONTROL

VOLUME 9 ISSUE 8: 29 - 41

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https://doi.org/10.71058/jodac.v9i8004

MOLECULAR DESCRIPTORS ASSOCIATED WITH GRAPHS DERIVED FROM VECTOR SPACE

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Abstract: *Molecular descriptor is a numerical value obtained from a molecular graph. In recent years' molecular descriptors are playing vital role in QSPR studies of certain physcio-chemical properties of molecules due to their high predicting power. In this paper we have considered three types of molecular descriptors namely, degree-based, distance –based and eigenvalue-based to compute explicit formulae for the graphs obtained from algebraic structures like vector space.*

Keywords: *Molecular descriptor, algebraic structure, vector space.*

MSC: *05C10; 05C92;*

1. Introduction

Algebraic graph theory is a branch of mathematics, in which graph theory problems are studied using algebraic structures. Cayley graphs were constructed using finite groups and used to study underlying network for routing problems in parallel computing. The interrelation between graph theory and algebraic structures was first studied by Beck [5] by defining graph using commutative rings, later Anderson and Livingston [6] renamed it as zero divisor graph. Angsuman Das [1,2,3,4] introduced nonzero component graph of a finite dimensional vector space and studied the domination and chromatic number, relation between graph and vector space isomorphism, also determined clique, girth etc. Further defined nonzero union and subspace component graph of finite dimensional vector space. Tamizh and Prabha [10] introduced Complement of the reduced non-zero component graph of free semimodules and studied various results on isomorphism, distance, girth, perfectness, genus etc. Until then a lot of work has done in connecting graph theory with algebraic structures. In this article, we define complement nonzero component graph of a finite dimensional vector space $\bar{\Gamma}(G_\alpha)$ over field $\mathbb{F}$ of $\dim(\mathbb{V}) = n$ with basis $\{\alpha_1, \alpha_2, \dots, \alpha_n\}$ and study various properties and results.

2. Definitions and Preliminaries

Let $G = (V, E)$ be a graph with order $|V| = n$ and size $|E| = m$, two vertices u and v in V are said to be adjacent if $(u, v) \in E$. If order is finite then the graph is finite or else it is infinite. The open neighbourhood of a vertex $v \in V$ is $N(v) = \{u/uv \in E\}$. The degree of a vertex v is $d_v = |N(v)|$. The maximum degree of G denoted by $\Delta(G)$, is the degree of the vertex with the greatest number of edges incident to it and minimum degree of G denoted by $\delta(G)$, is the degree of

 https://doi.org/10.71058/jodac.v9i8004

the vertex with the least number of edges incident to it. A vertex with degree zero is isolated vertex and graph with isolated vertices is a null graph. G is complete if every vertex is pairwise adjacent and is a clique if subgraph of G is complete. A graph G is said to be planar if it can be drawn on a plane without crossing the edges. Two graphs $G = (V, E)$ and $H = (V', E')$ are said to be isomorphic if ∃ a bijective function $\phi: V \to V'$ such that $(u, v) \in E$ iff $(\phi(u), \phi(v)) \in E'$. Girth of a graph is the length of the shortest cycle contained in the graph, if the graph is tree (forest) then the girth is infinite.

Across this article, $\mathbb{V}$ is a n dimension vector space (dim($\mathbb{V}$) = n) over the eld F of order (($O(F) = k$). Let $B = \{b_1, b_2, \dots, b_n\}$ as a basis of $\mathbb{V}$. Any vector $v \in \mathbb{V}$ is represented as $v = \alpha_1 b_1 + \alpha_2 b_2 +, \dots \dots + \alpha_n b_n$, where $\alpha_i \in F$ (simply denoted $v = (\alpha_1, \alpha_2, \dots \dots, \alpha_n)$). The skeleton of any vector in $\mathbb{V}^* = \mathbb{V} - \{0\}$ based on B' is described by $S_{B'}(u) = \{b_i : \alpha_i \neq 0, 1 \leq i \leq n\}$. Moreover, a vector v with skeleton j means $|S_{B'}(u)| = j$. The non- zero component union graph of $\mathbb{V}$ based on the basis B' is defined as a simple graph with $V = \mathbb{V}^*$ and different non zero vectors u and v in V are adjacent if and only if $S_{B'}(u) \cup S_{B'}(v) = B'$. This graph is denoted by $\mathcal{G}(\mathbb{V}_{B'})$.

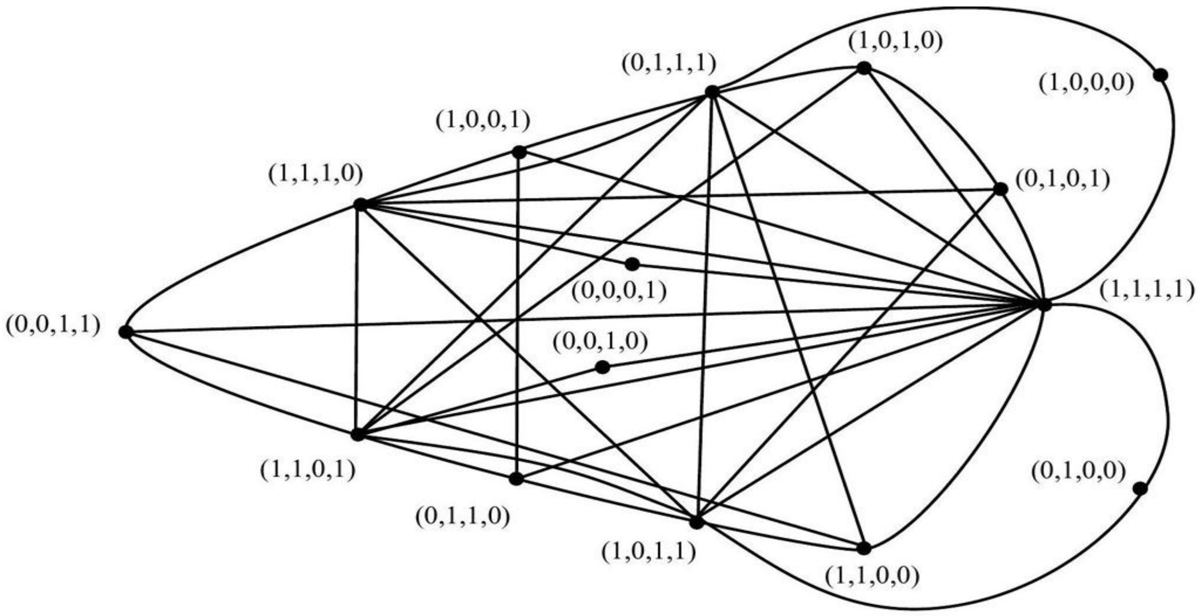

Figure 1: Nonzero component graph of a finite dimensional vector space $\mathcal{G}(\mathbb{V}_{B'})$ with $n = 4$ and $k = 2$.

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3. Preliminary Results

The following definitions and theorems were used to determine the topological indices for the graphs under discussion. We put up a few current findings that will be discussed in this section.

Theorem A ([13]). Let $\mathcal{G}(\mathbb{V}_{B'})$ be the nonzero component union graph of $\mathbb{V}$ based $B = \{b_1, b_2, \ldots, b_n\}$. Let $v = \beta_1 b_{i1} + \beta_2 b_{i2} + \ldots \ldots + \beta_j b_{ij}$ be a vertex in $\mathcal{G}(\mathbb{V}_{B'})$ with $\beta_i \neq 0$ where $1 \leq i \leq j$. Then $\deg(v) = \begin{cases} (k-1)^{n-j} k^j, & 1 \leq j \leq n \\ k^n - 2, & j = n \end{cases}$.

Theorem B ([13]). Let O(F) = k and dim($\mathbb{V}$) = n. Then, order and size of $\mathcal{G}(\mathbb{V}_{B'})$ is $k^n - 1$ and $\frac{(k-1)^n[(k+1)^n - 3]}{2}$, respectively.

We have considered the following molecular descriptors for our study. One can refer to [2, 9-12, 18].

Sl. No	Name	Formula
1	Wiener index	$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v).$
2	First Zagreb index	$M_1(G) = \sum_{u \in V(G)} (d(u))^2$
3	Second Zagreb index	$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$
4	Wiener polynomial	$W(G, x) = \sum_{u,v \in V(G)} x^{d(u,v)} = \sum_{J=1}^{diam(G)} d(G, J)x^J$ The amount of unordered vertex pairs in G that are accurately J distances apart is specified as $d(G, J)$.
5	Hyper-Wiener index	$WW(G) = \frac{1}{2} W(G) + \frac{1}{2} \sum_{u \in V(G)} (d(u, v))^2 + \frac{1}{2} \sum_{j=1}^{diam(G)} j(j+1) d(G, j)$
6	Eccentricity index	$\xi(G) = \sum_{v \in V(G)} d(u)\, ecc(u)$
7	New version (eccentricity based) of Zagreb index	$M_1^*(G) = \sum_{uv \in E(G)} (ecc(u) + ecc(v))$ $M_1^{**}(G) = \sum_{u \in V(G)} (ecc(u))^2$ $M_2^*(G) = \sum_{uv \in E(G)} ecc(u)\, ecc(v)$
8	Average eccentricity index	$\text{aveg(G)} = \frac{1}{n} \sum_{u \in V(G)} ecc(u)$

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9	Eccentric distance sum index	$\xi^{DS}(G) = \sum_{u \in V(G)} ecc(u)\, D(u\|G)$
10	The ABC index	$ABC(\mathcal{G}(\mathbb{v}_{B'})) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$

4. Main Results

Theorem 1: Let $G = \mathcal{G}(\mathbb{v}_{B'})$, then,

$$W(\mathcal{G}(\mathbb{v}_{B'})) = (k^n - 2)\left(k^n - \frac{(k-1)^n - 2}{2}\right) - (k-1)^n((k+1)^n - k^n - 1)$$

Proof: Clealry,

$$W(\mathcal{G}(\mathbb{v}_{B'})) = \frac{1}{2}[(\sum_{j=1}^{n-1} C_n^j (k-1)^j k^j (k-1)^{n-j}) + 2(\sum_{j=1}^{n-1} C_n^j (k-1)^j (k^n - 2 - (k-1)^{n-1} k^j)$$
$$+ (k-1)^n (k^n - 2)].$$

$$W(\mathcal{G}(\mathbb{v}_{B'})) = (k^n - 2)\left(k^n - \frac{(k-1)^n - 2}{2}\right) - (k-1)^n((k+1)^n - k^n - 1).$$

Now, consider the following Figure 2 to visualize $W(\mathcal{G}(\mathbb{v}_{B'}))$ with n dimension over the field of order k

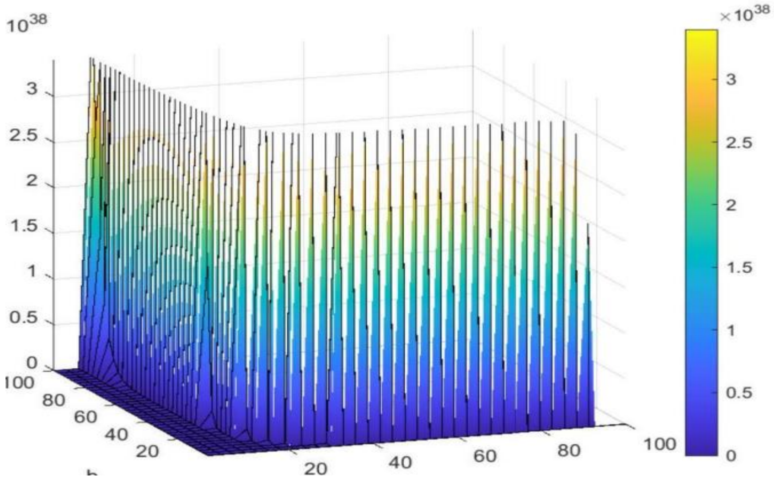

Figure 2: Wiener index of $\mathcal{G}(\mathbb{v}_{B'})$

Theorem 2. Let $G = \mathcal{G}(\mathbb{v}_{B'})$, then the first Zagreb index

$$M_1(\mathcal{G}(\mathbb{v}_{B'})) = (k-1)^n((k^2 + k - 1)^n - (k-1)^n - 4(k^n - 1))$$

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Proof: Let $v = \beta_1 b_{i1} + \beta_2 b_{i2} +, \ldots \ldots + \beta_j b_{ij}$ be a vertex in $\mathcal{G}(\mathbb{v}_{B'})$ with $\beta_i \neq 0$ where $1 \leq i \leq j$.

Then, by Theorem A, the degree of the vertex u is $\deg(u) = \begin{cases} (k-1)^{n-j}k^j, & 1 \leq j \leq n \\ k^n - 2, & j = n \end{cases}$; Therefore, the first Zareb index $M_1(\mathcal{G}(\mathbb{v}_{B'})) = \sum_{j=1}^{n-1} C_n^j (k-1)^j \left((k-1)^{n-j}k^j\right)^2 + (k-1)^n (k^n-2)^2$

$$= (k-1)^{2n} \sum_{j=1}^{n-1} C_n^j \left(\frac{k^2}{k-1}\right)^j + (k-1)^n (k^n-2)^2$$

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

$$M_1(\mathcal{G}(\mathbb{v}_{B'})) = (k-1)^n((k^2+k-1)^n - (k-1)^n - 4(k^n-1)).$$

This completes the proof.

Now, consider the following Figure 3 to visualize $M_1(\mathcal{G}(\mathbb{v}_{B'}))$ with n dimension over the field of order k

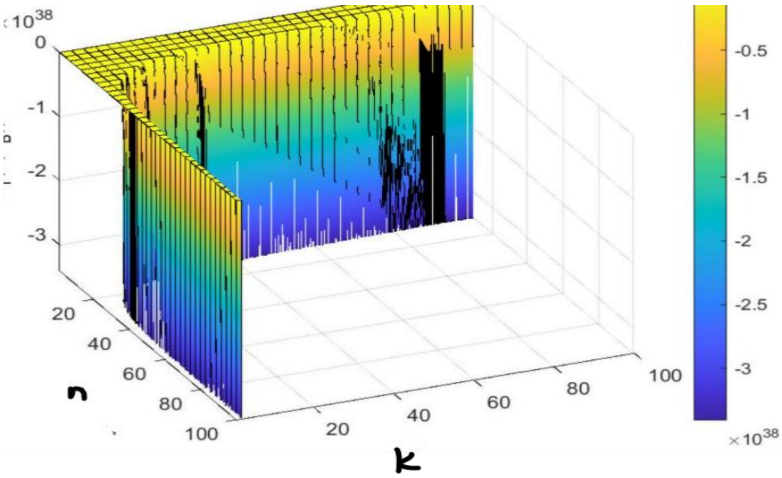

Figure 3: First Zagreb index of $\mathcal{G}(\mathbb{v}_{B'})$

Theorem 3. Let $G = \mathcal{G}(\mathbb{v}_{B'})$, then the second Zagreb index

$$M_2(\mathcal{G}(\mathbb{v}_{B'})) = \frac{1}{2}\Big[\sum_{j=1}^{n-1} C_n^j (k-1)^j \left(\sum_{t=n-1}^{n-1} C_n^{|t+j-n|} (k-1)^n k^t + (k-1)^n (k^n-2)\right) + (k-1)^n (k^n-2) \left(\sum_{j=1}^{n-1} C_n^j (k-1)^n k^j + ((k-1)^n - 1)(k^n-2)\right)\Big]$$

Theorem 4. Let $G = \mathcal{G}(\mathbb{v}_{B'})$, then the Wiener polynomial

$$W(\mathcal{G}(\mathbb{v}_{B'}); x) = \frac{1}{2}(k-1)^n((k+1)^n - 3)x + \frac{1}{2}((k^n-2)k^n - (k-1)^n(k+1)^n)x^2$$

Proof: We know the result: $W(\mathcal{G}(\mathbb{v}_{B'}); x) = \sum_{j=1}^{diam(\mathcal{G}(\mathbb{v}_{B'}))} d(\mathcal{G}(\mathbb{v}_{B'}), j)\, x^j$

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$$= d(\mathcal{G}(\mathbb{v}_{B'}),1)x + d(\mathcal{G}(\mathbb{v}_{B'}),2)x^2$$

$$= \frac{x}{2}\left[\left(\sum_{j=1}^{n-1} C_n^j (k-1)^j (k-1)^{n-j} k^j\right) + (k-1)^n (k^n - 2)\right]$$

$$+ \frac{x^2}{2}\left(\sum_{j=1}^{n-1} C_n^j (k-1)^j (k^n - 2 - (k-1)^{n-j} k^j\right)$$

$$W(\mathcal{G}(\mathbb{v}_{B'});x) = \frac{1}{2}(k-1)^n((k+1)^n - 3)x + \frac{1}{2}((k^n-2)k^n - (k-1)^n(k+1)^n)x^2$$

Theorem 5. Let $G = \mathcal{G}(\mathbb{v}_{B'})$, then the Hyper-Wiener index

$$WW(\mathcal{G}(\mathbb{v}_{B'})) = 3(k^n - 2)\left(k^n - \frac{2(k-1)^n}{3} - 1\right) - 2(k-1)^n((k+1)^n - k^n - 1)$$

Proof: We have the following result:

$$WW(\mathcal{G}(\mathbb{v}_{B'})) = \frac{1}{2}\sum_{j=1}^{diam(\mathcal{G}(\mathbb{v}_{B'}))} j(j+1) d(\mathcal{G}(\mathbb{v}_{B'}),j)$$

$$= \frac{1}{2}(2d(\mathcal{G}(\mathbb{v}_{B'}),1) + 6d(\mathcal{G}(\mathbb{v}_{B'}),2))$$

$$= \frac{1}{2}\left[2\left(\sum_{j=1}^{n-1} C_n^j (k-1)^j (k-1)^{n-j} k^j\right) + 2(k-1)^n (k^n - 2)\right]$$

$$+6\left(\sum_{j=1}^{n-1} C_n^j (k-1)^j ((k^n - 2) - (k-1)^{n-j} k^j\right)$$

$$= 3(k^n - 2)(k^n - (k-1)^n - 1) - 2(k-1)^n((k+1)^n - 1 - k^n)$$

$$+(k-1)^n(k^n - 2)$$

$$WW(\mathcal{G}(\mathbb{v}_{B'})) = 3(k^n - 2)\left(k^n - \frac{2(k-1)^n}{3} - 1\right) - 2(k-1)^n((k+1)^n - k^n - 1)$$

Now, consider the following Figure 4 to visualize $WW(\mathcal{G}(\mathbb{v}_{B'}))$ with n dimension over the field of order k

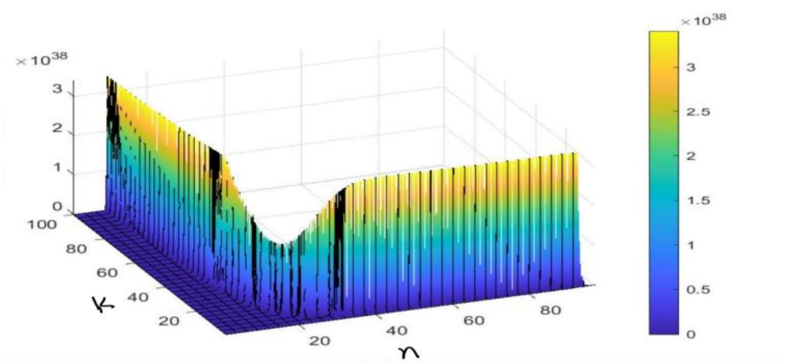

Figure 4: Hyper-Wiener index of $\mathcal{G}(\mathbb{v}_{B'})$

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Theorem 6. Let $G = \mathcal{G}(\mathbb{V}_{B'})$, then the eccentricity index

$$\xi\big(\mathcal{G}(\mathbb{V}_{B'})\big) = (k-1)^n[2(k+1)^n - k^n - 4]$$

Proof. We obtain the following relation:

$$\xi\left(\mathcal{G}(\mathbb{V}_{B'})\right) = \sum_{u\in V(\mathcal{G}(\mathbb{V}_{B'}))} d(u)\mathrm{ecc}(u)$$

$$= 2\sum_{j=1}^{n-1}(k-1)^{n-1}C_n^j k^j(k-1)^j + (k-1)^n(k^n-2)$$

$$= 2(k-1)^n\sum_{j=1}^{n-1}C_n^j k^j + (k-1)^n(k^n-2)$$

$$\xi\big(\mathcal{G}(\mathbb{V}_{B'})\big) = (k-1)^n[2(k+1)^n - k^n - 4].$$

Theorem 7. Let $G = \mathcal{G}(\mathbb{V}_{B'})$, then the total eccentricity index

$$\zeta\big(\mathcal{G}(\mathbb{V}_{B'})\big) = 2(k^n-1) - (k-1)^n$$

Proof. We obtain the following relation:

$$\zeta\left(\mathcal{G}(\mathbb{V}_{B'})\right) = \sum_{u\in V(\mathcal{G}(\mathbb{V}_{B'}))} \mathrm{ecc}(u)$$

$$= 2[(k^n-1) - (k-1)^n] + (k-1)^n$$

$$\zeta\big(\mathcal{G}(\mathbb{V}_{B'})\big) = 2(k^n-1) - (k-1)^n.$$

Theorem 8. If dim $(\mathbb{V}) = n$ and O(F) = k, then

$$M_1^*\big(\mathcal{G}(\mathbb{V}_{B'})\big) = (k-1)^n(2(k+1)^n - (k-1)^n - k^n - 2)$$

Prof: We have

$$M_1^*\big(\mathcal{G}(\mathbb{V}_{B'})\big) = (k-1)^n((k-1)^n - 1) + 3((k^n-2) - (k-1)^n + 1)(k-1)^n)$$

$$+4\left((k-1)^n\left(\frac{(k+1)^n+(k-1)^n-2}{2} - k^n + 1\right)\right)$$

$$M_1^*\big(\mathcal{G}(\mathbb{V}_{B'})\big) = (k-1)^n(2(k+1)^n - (k-1)^n - k^n - 2)$$

Theorem 9. If dim $(\mathbb{V}) = n$ and O(F) = k, then

$$M_1^{**}\big(\mathcal{G}(\mathbb{V}_{B'})\big) = 4k^n - 3(k-1)^n - 4$$

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Prof: We obtain the number of vertices having eccentricity 1 is $(\mathrm{k}-1)^{n}$ and the number of vertices having eccentricity 2 is $k^{n}-(\mathrm{k}-1)^{n}-1$.

$$M_1^{**}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=4(k^n-(k-1)^n-1)+(\mathrm{k}-1)^{n}$$

$$M_1^{**}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=4k^n-3(k-1)^n-4.$$

Theorem 10. Let $G=\mathcal{G}(\mathbb{v}_{B'})$, then $M_2^{*}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=(k-1)^n(2(k+1)^n-2k^n-1)$

Prof: We obtain

$$M_2^{*}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=(k-1)^n((k-1)^n-1)+2((k^n-2)-(k-1)^n+1)(k-1)^n)$$

$$+4\left((k-1)^n\left(\frac{(k+1)^n+(k-1)^n-2}{2}-k^n+1\right)\right)$$

$$M_2^{*}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=(k-1)^n(2(k+1)^n-2k^n-1)$$

Theorem 11. Let $G=\mathcal{G}(\mathbb{v}_{B'})$, then average eccentricity index, $\operatorname{aveg}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=2-\frac{(k-1)^n}{k^n-1}$.

Proof: We obtain the number of vertices having eccentricity 1 is $(\mathrm{k}-1)^{n}$ and the number of vertices having eccentricity 2 is $k^{n}-(\mathrm{k}-1)^{n}-1$.

$$\operatorname{aveg}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=\frac{1}{k^n-1}\sum_{u\in V(\mathcal{G}(\mathbb{v}_{B'}))}\operatorname{ecc}(u)$$

$$=\frac{2[(k^n-1)-(k-1)^n]+(k-1)^n}{k^n-1}$$

$$=\frac{2(k^n-1)-(k-1)^n}{k^n-1}$$

$$\operatorname{aveg}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=2-\frac{(k-1)^n}{k^n-1}$$

Theorem 12. Let $G=\mathcal{G}(\mathbb{v}_{B'})$, then the eccentricity distance sum index

$$\xi^{DS}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=4(k^n-2)\left(k^n-\frac{3}{4}-(k-1)^n\right)-2(k-1)^n[2(k+1)^n-1-k^n]$$

Proof: $\xi^{DS}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=\sum_{u\in V\left(\mathcal{G}(\mathbb{v}_{B'})\right)}\operatorname{ecc}(u)\,D\left(u|V\left(\mathcal{G}(\mathbb{v}_{B'})\right)\right)$

$$=\sum_{j=1}^{n-1}2C_n^j(2(k^n-2)-(k-1)^{n-j}k^j)+k^n-2$$

$$=4(k^n-2)\left(\sum_{j=1}^{n-1}2C_n^j\,(k-1)^j\right)-\left(2\sum_{j=1}^{n-1}2C_n^j\,(k-1)^nk^j\right)+(k^n-2)$$

$$\xi^{DS}\left(\mathcal{G}(\mathbb{v}_{B'})\right)=4(k^n-2)\left(k^n-\frac{3}{4}-(k-1)^n\right)-2(k-1)^n[2(k+1)^n-1-k^n]$$

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Theorem 13. Let $G = \mathcal{G}(\mathbb{V}_{B'})$, then ABC index

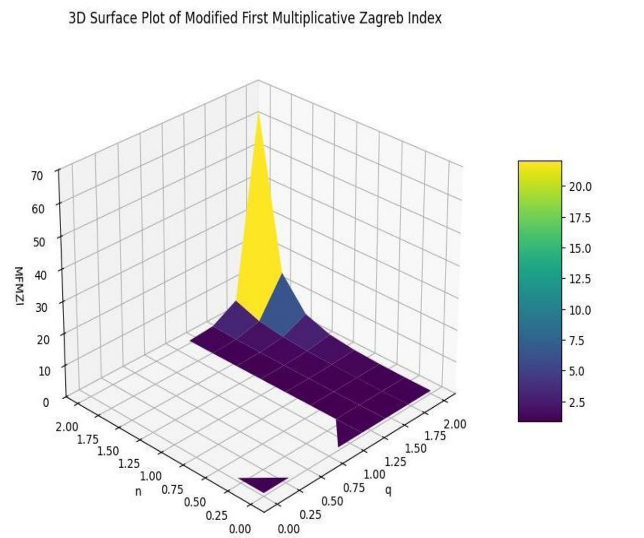
$$ABC\big(\mathcal{G}(\mathbb{V}_{B'})\big) = \frac{1}{2}\Bigg\{\Bigg[\sum_{j=1}^{n-1}\Bigg(\sum_{t=n-1}^{n-1} C_j^{|t+j-n|}(k-1)^t\sqrt{\frac{(k-1)^{n-j}k_1+(k-1)^{n-j}k^j-2}{(k-1)^{n-1}k_1+(k-1)^{n-t}k^t}}$$

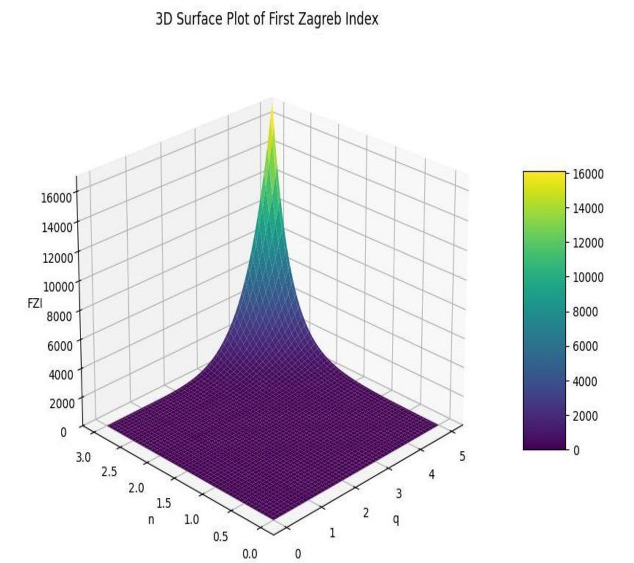
$$+(k-1)^n\sqrt{\frac{(k-1)^{n-j}k_1+(k^n-2)-2}{(k-1)^{n-1}k_1\,(k^n-2)}}\Bigg)\Bigg]$$

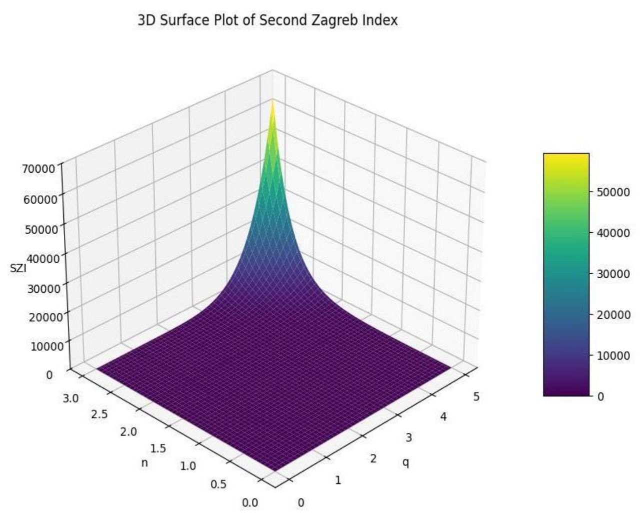
$$+\left(\sum_{j=1}^{n-1}(k-1)^j\sqrt{\frac{(k-1)^{n-1}k_1+(k^n-2)-2}{(k-1)^{n-1}k_1\,(k^n-2)}}\right)$$

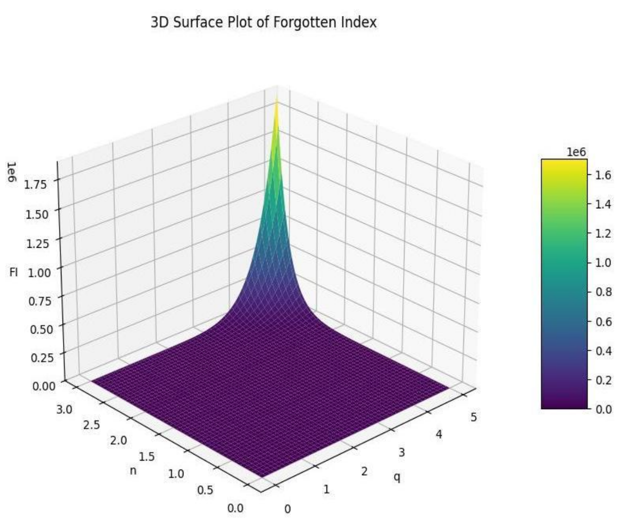
$$+(k-1)^n((k-1)^n-1)\sqrt{\frac{2(k^n-2)-2}{(k^n-2)^2}}\Bigg\}.$$

Following Figures are visualizations of different topological indices with n dimension over the field of order k.









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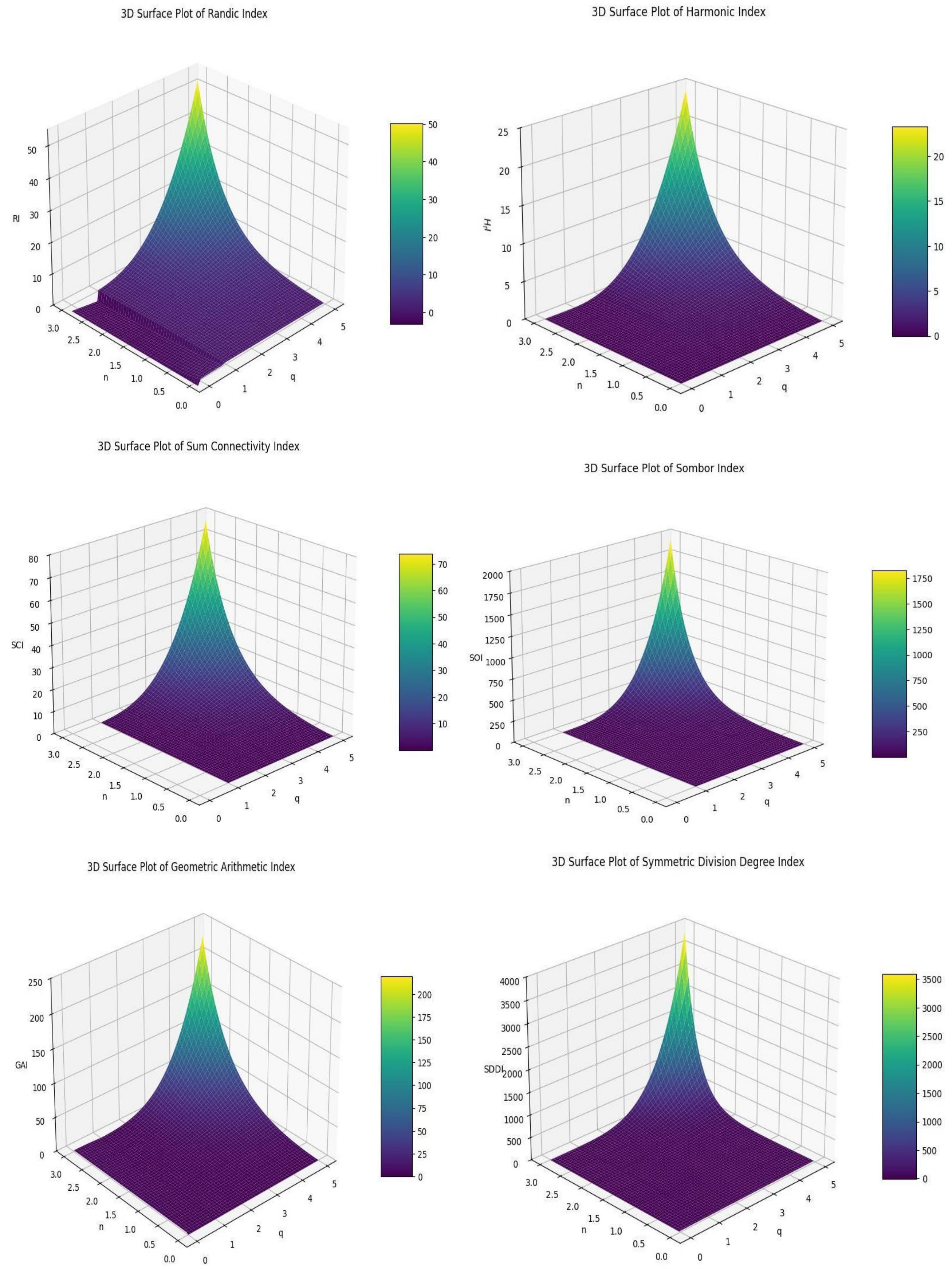

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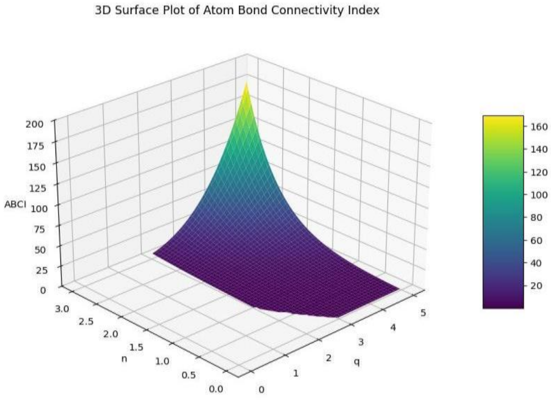
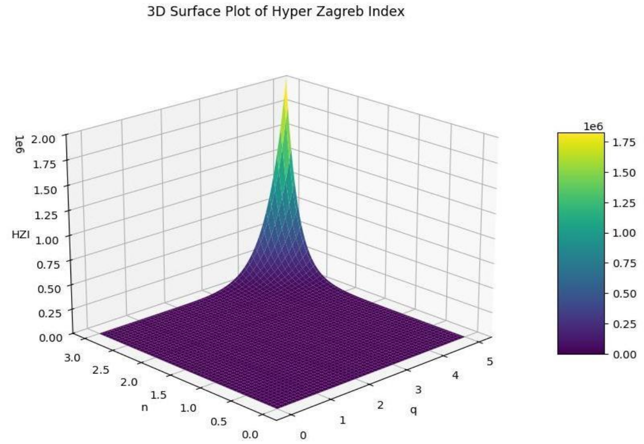
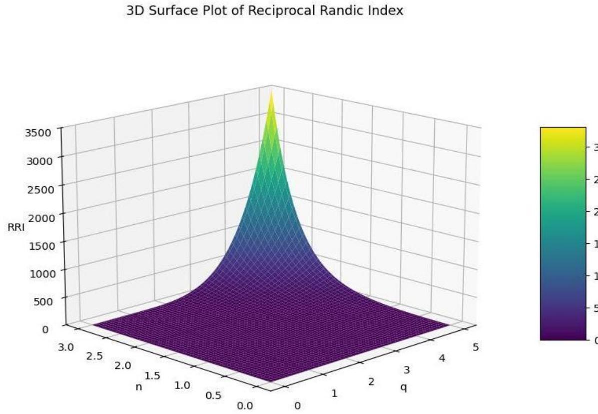
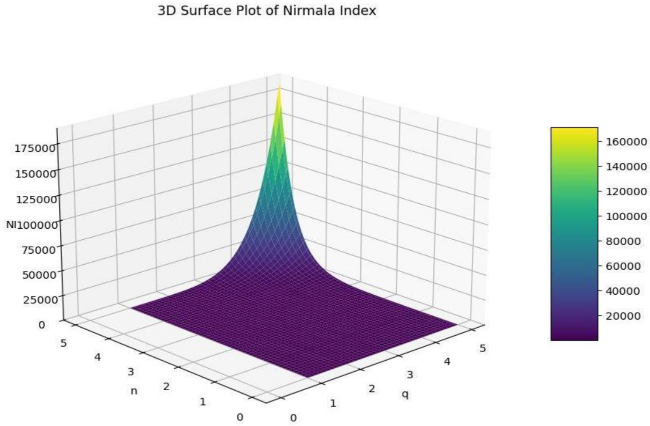
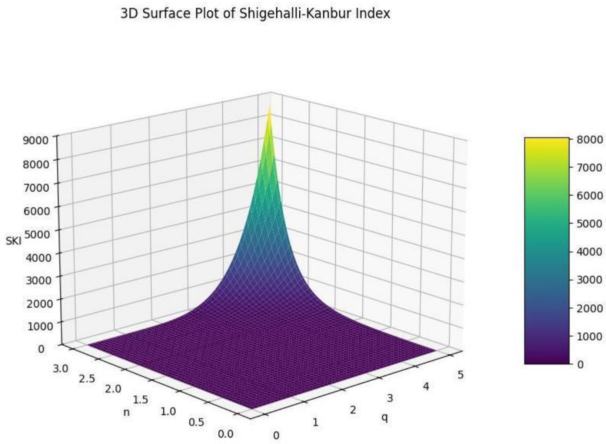
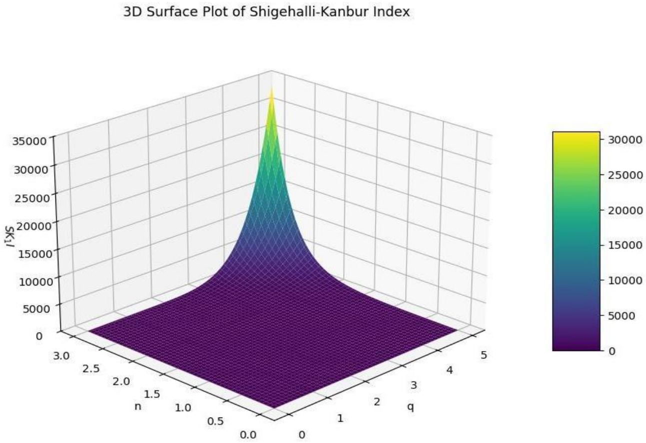


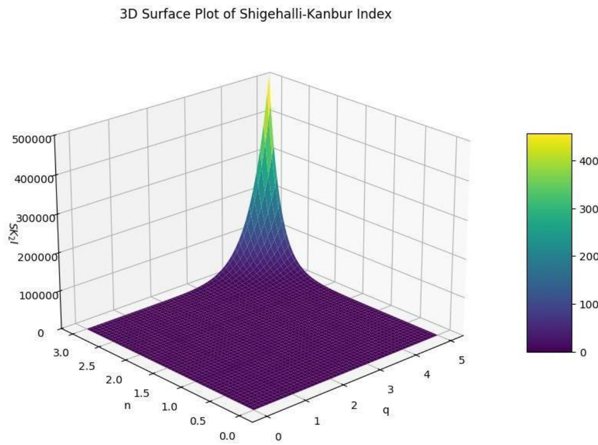


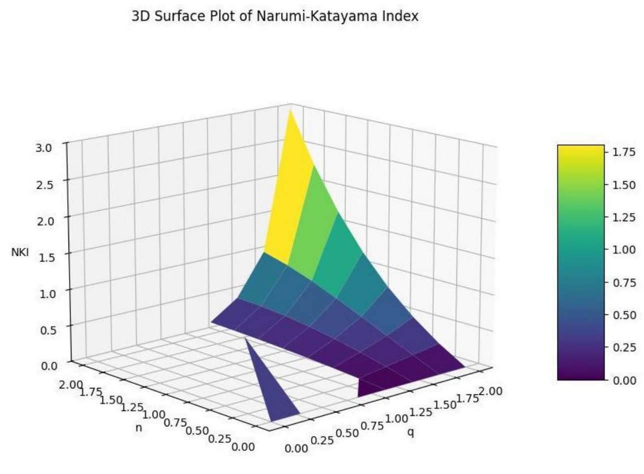




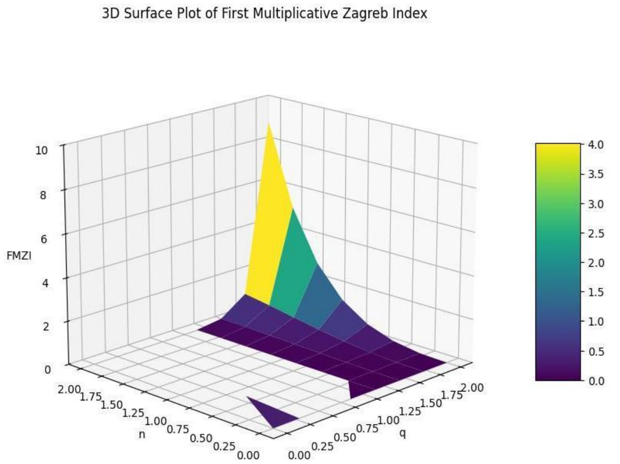


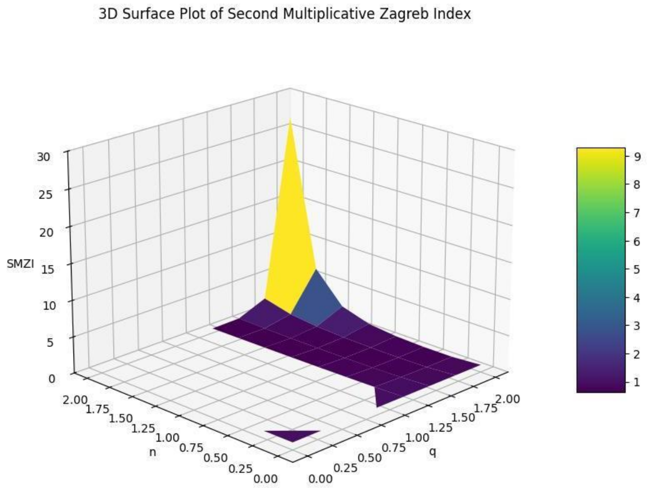






https://doi.org/10.71058/jodac.v9i8004





4. Conclusions

In this paper, we found the topological indices of nonzero component union graphs from vector spaces $\mathbb{V}$ with order n over the field F with order k, and we give the general formula and a comparison table for finding a different topological index to the number of graphs constructed from the vector space. Depending on the respective quantitative data, these resulting indices are graphically contrasted. Future scholars can build on our research of the indices for these structures to find and investigate other algebraic structures and their features.

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