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Investigation into topological uses of graphic theory

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Abstract

Some physical and chemical qualities, that critical mass and durability of chemical substances, correlated with topological indices. It is common to link topological indices with QSPR and QSAR, which stand for quantitative structure activity relationships, when discussing their importance. The ability to traverse edges in just one direction characterizes directed graphs. An internal graph structure known as a rooted tree for any set G where the nodes are vertices, a normal tree is one in which the tree-order of the nodes' ends is similar. One of the most valuable nanomaterials in many fields, A human hair is one millionth of its thickness. the neighborhood zeroth order index (NZ(ſ)), and the fifth geometric-arithmetic index (GA5).

Keywords: Topological, Graphic Theory, chemical, (NZ(ſ)), and machine

Introduction

Graphs are defined as G is defined as the set of all edges (E) and all vertices (V), also known as nodes. If a vertex connects to an edge, we say that it is adjacent to that edge; otherwise, we say that it is not. A link edge has two end vertices, while a loop edge only has one. When the last vertex of a pair of edges is the same, we say that they are many or parallel. "Adjacent vertices" are two nodes that have a competitive advantage and are therefore linked. If there are no gaps in graph H, then the vertices and edges of graph G, then H is a subgraph of graph G. of G. A finite graph is one in which the sets of all possible ends, both vertex and edge, are finite. All graphs are nontrivial unless they have exactly one vertex.

A walk is a set of G-graph edges and vertices that alternate between v1 to vn with each iteration of n ranging from 1 to n+1. Along with v1, v2, v3..., vn+1, the 0 The origin is located at vertex v1 and the terminal is at vertex vn+1. The stroll is closed if and only if v1v= vn+1. The office is available. The walk's length is directly proportional to the walk's edge count. A zero-length stroll is a very short walk. An unbroken path is called a trail. A walk devoid of repeated vertices is referred to as a route. In a simple circuit, there is just one vertex and no edges; this is called a closed trail. A Eulerian path is one that makes full use of all of the data map's edges. Given the presence of a Eulerian circuit, we say that it is Eulerian.

A Hamilton route of G is a path that includes all of the vertices of "G" and "a" A Hamilton cycle of G is a cycle that contains all of the vertices in G. The graph's Hamiltonian presence cycle, we say that it is Hamilton. "Simple graphs" are those that lack many edges or loop edges. The Any cycle that includes A Hamilton cycle of G is defined as each vertex in G. If a graph has a Hamiltonian, it may be used to characterize the edge. A multigraph is a network in graph theory where every pair of vertices has several edges. The sum of all edges that traverse a vertex is denoted as deg (v) or (). its degree. each loop counts as two edges. The symbol () Δ () represents the lowest and highest degrees of G. respectively.

The ability to traverse edges in just one direction characterizes directed graphs. In a basic directed graph, an edge may be defined as a connection between two vertices denoted by an ordered pair (,). That is said to be near to. A vertex's in-degree the out-degree of a directed graph is, and the total number of edges across it is the same except for the direction in which those edges originate.

An internal graph structure known as a rooted tree for any

set G where the nodes are vertices, a normal tree is one in which the tree-order of the nodes' ends is similar. Each node in a rooted tree has its own unique parent, starting at the root and continuing all the way to every other node. An offspring of a node the set v includes all vertices with v as their parent. Rooted trees may only have one parent at each node. If a graph may be shown on a plane with just end-to-end overlap of its edges, we state that it is suitable for planar embedding. Planar embeddings of graphs G are drawings of this kind.

Literature Review

Santiago-Valentin, *et al*. (2018) [10]. The Santiago-Portilla Method (SPM), This work introduces a graph theory-based approach for representing planar processes. SPM generates an extended matrix including all topological and geometric information about a planar mechanism from the corresponding adjacency matrix. This matrix structure allows computational tools such as metaheuristic algorithms to do topological and dimensional synthesis simultaneously, which is useful for optimal mechanism design. To ensure that the proposed technique is successful, a case study modelled after the construction of a fixed-linear-trajectory tracker mechanism is employed. To implement it, we used the Differential Evolution technique to solve the design optimization issue, with SPM-generated matrices serving as population representations.

Stoilova, Svetla & Stoev, Veselin. (2015) [11]. With the use of graph theory, we may examine transport networks mathematically and learn more about their properties. Using graph theory, the paper investigates the metro system's architecture. Subways in twenty-two European capitals are part of the research. The study has identified new metrics such as routing degree, route connectedness, average link length (which accounts for route count), route intensity, and route density. In order to study and categories the metro networks, both new and old indicators have been used. The networks have been categorized using the statistical approach known as cluster analysis. In order to conduct the study, ten indicators were used.

Gowda, Dr. Dankan, *et al*. (2021) [13]. Mathematics is an important subject in many different industries. A major subfield of mathematics, graph theory that structural models draw upon. Recent advances and shifts in these fields are the result of the structural structure of various things or technology. It was in 1735, with the Konigsberg Bridge issue, that field graph theory was born. Information technology, electrical engineering, linguistics, computer network science, biotechnology, and graphical theoretical applications. are the primary foci of this article, which describes graphical theory implementations in a variety of diverse fields.

Al-khafaji, Saba *et al*. (2018) [14]. We have built a graph topology and a subgraph topology with examples in this work. Our proof states that connections in graphs may only be established when be linked with regard to its topology. A new topological notion, symmetric with examples, was also introduced; it is based on two topologies. We also demonstrated that isomorphism guarantees symmetric topologies for two graphs and provided an example demonstrating that this is not always the case.

Sarma, Salako. (2012) [15]. This article details the methods used by Bharat Sanchar Nigam Limited, a GSM (Group Special Mobile) operator, in their theoretical planning of the network's architecture. The approaches address determining the base station identification code (BSIC), hopping sequence number (HSN), and location. area code (LAC), in addition to a novel variation of the now-classic use of graph coloring to frequency assignment. Graph theory approaches are shown to be applicable to a variety of optimization and time table scheduling challenges encountered in GSM radio network design.

Computation of graphene network topological indices

Here, we want to calculate graphene yardsticks constructed from the sums of nearby degrees. One of the most important materials in most conductive and lightest substance known to man. One of the most valuable nanomaterials in many fields, A human hair is one millionth of its thickness. When compared to steel, it performs better. in terms of strength and has remarkable electrical and magnetic characteristics. Researchers have so been very interested in learning more about its characteristics. Here is the graph of graphene molecules.

Case 1. Consider p > 1; q > 1. Graphene framework incorporating p > 1; q > 1 is shown in Figure 1

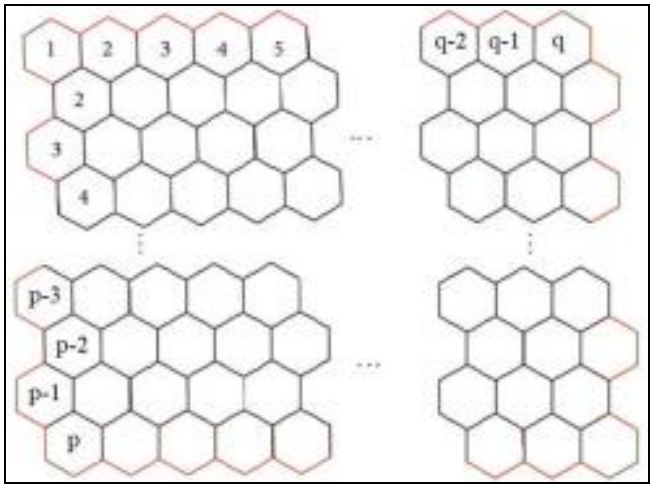

Fig 1: Graphene structure with p > 1 rows and q > 1 table cell.

Let $jV_ij = n_i$ and $jE_{(i;j)}j = m_{i;j}$, then

$$n_4 = 2,\ n_5 = 2p + 4,\ n_6 = 2q - 4,\ n_7 = 2q,\ n_8 = 2p - 4,$$

$$n_9 = (2q - 2)(p - 1).$$

and

$m_{4;5} = 4$; $m_{5;5} = p$; $m_{5;7} = 8$; $m_{5;8} = 2p\ 4$; $m_{6;7} = 4q\ 8$;
$m_{7;9} = 2q$; $m_{8;8} = p\ 2$; $m_{8;9} = 2p\ 4$; $m_{9;9} = 3qp\ 4q\ 4p + 5$:

Case 2. Think about the options The graphene structure with p= 1 and q > 1 is Figure 2 illustrates this.

Fig 2: Graphene structure with p = 1 rows and q > 1 columns.

Here,

$n_4 = 4$; $n_5 = 4$; $n_6 = 2q\ 4$; $n_7 = 2q\ 2$:

and
$m_{4;4} = 2$; $m_{4;5} = 4$; $m_{5;7} = 4$; $m_{6;7} = 4q\ 8$; $m_{7;7} = q\ 1$:

Chemical significance using machine learning algorithm based on multiple linear regression

In 2020, some chemical properties were predicted using three machine learning models. Similarly, other works related to finding topological indices using machine learning are seen in Motivated by this, a machine learning model has been developed in this section using multiple linear regression for three different cases.

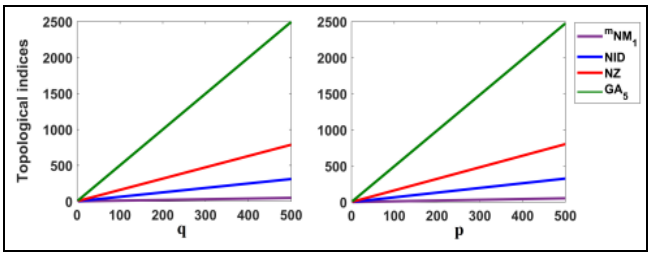

Fig 3: Plotting of topological indices for and p > 1; q = 1, and p = 1; q > 1. from left to right.

Chemical significance using machine learning

The purpose Using chemical graph theory, this section investigates the function of NID, NZ, mNM1, and GA5 as molecular descriptors. octane isomers and benzenoid hydrocarbons are the two categories of data sets. Several benzenoid hydrocarbons and octane isomers have their molecular graphs Figures 4 and 5 indicate this, respectively.

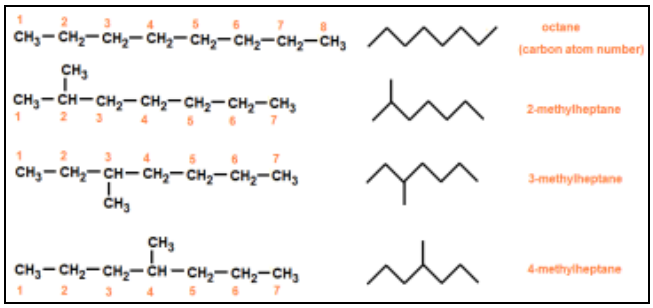

Fig 4: Molecular graphs of some octane isomers

An area of artificial intelligence known as machine learning (ML) allows computer systems to recognize trends and patterns, learn by training and perform required tasks without precise guidance.

Figure 6 shows the methodology adopted for the prediction process.

For both octanes include benzenoid hydrocarbons and indices serve as the input and the physical property as their output.

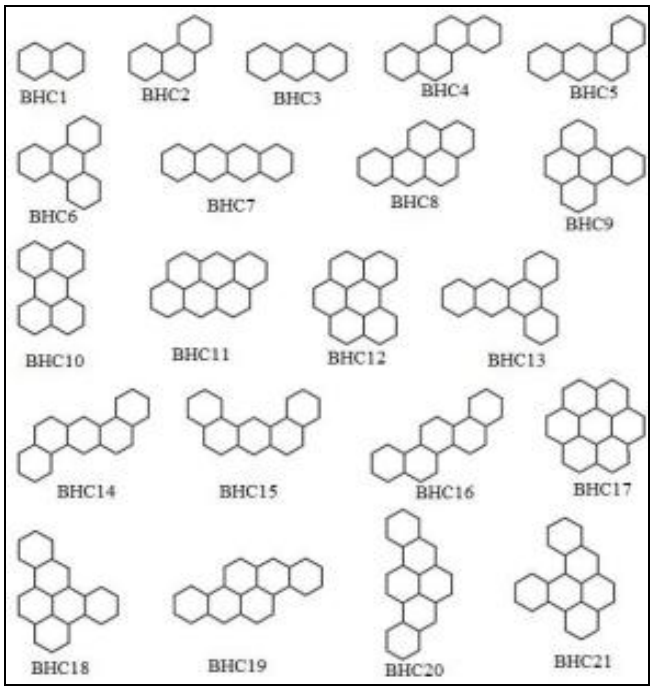

Fig 5: Molecular graphs of benzenoid hydrocarbons.

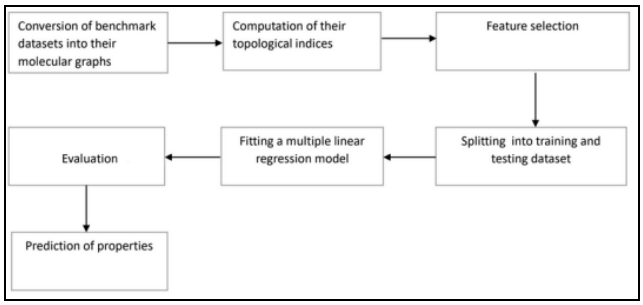

Fig 6: Proposed methodology for prediction of Physico-chemical properties.

First, the dataset consisting of the octane isomers, their corresponding NID, NZ, $^mNM_1$ and GA_5 values and the experimental values of the aforesaid properties (i.e., both inputs and outputs) are taken. Then it is split into two sets namely the datasets for training and testing purposes.

Experimental analysis for octane isomers

Table 1: Correlation matrix of NID, NZ, $^mNM_1$ and GA_5 with some degree-based molecular descriptors for octane isomers.

	NID	NZ	$^mNM_1$	GA_5
NID	1			
NZ	0.96	1		
$^mNM_1$	0.98	0.99	1	
GA_5	-0.11	0.13	0.037	1

Case 1: When all the four indices are considered together, using the above model, the following regression equations are obtained:

$$S = \beta_0 + \beta_1(NZ) + \beta_2(NID) + \beta_3(GA_5) + \beta_4({}^mNM_1),$$

Table 2: The values of values of β0, β1, β2, β3, and β4 along the regression models and their statistical parameters.

	NZ	NID	GA5	mNM1	β0	R2	Adj.R2	F-statistic	Prob(F-stats)
S	-721.841	-490.813	38.030	989.210	985.414	0.958	0.939	51.12	$3{:}44 \times 10^{6}$
AF	0.718	0.213	0.128	-0.663	-2.213	0.993	0.989	306.6	$1{:}31 \times 10^{9}$
DHVAP	37.620	20.731	-1.394	-46.004	-50.002	0.913	0.875	23.73	$8{:}47 \times 10^{5}$

$$AF = \beta_0 + \beta_1(NZ) + \beta_2(NID) + \beta_3(GA_5) + \beta_4({}^mNM_1),$$

$$DHVAP = \beta_0 + \beta_1(NZ) + \beta_2(NID) + \beta_3(GA_5) + \beta_4({}^mNM_1).$$

The fitted values for the models are listed It was observed that for the above models, R^2 values were significant. Scatter plots of the above models are shown in Figure 7. However, the p -values for NZ and GA_5 were less than 0:05 at 5% significance level indicating that only these two indices are sufficient for the prediction of properties. We will analyse this in Case 3.

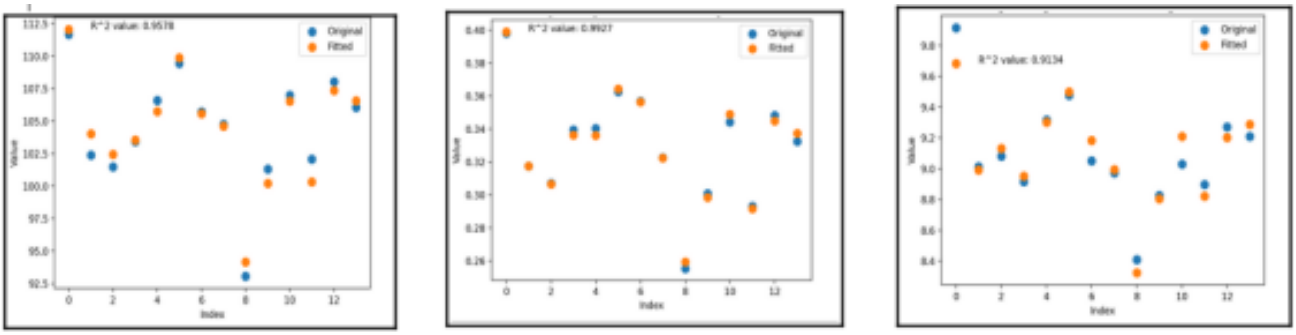

Fig 7: The original target values vs the predicted target values for S, AF and DHV AP of octane isomers for case 1.

Experimental analysis for benzenoid hydrocarbons

Here, we examine the performance of the aforesaid indices in modeling the BP and E of benzenoid hydrocarbons. Individually, GA_5 and NZ showed a significant correlation with BP and E of benzenoid hydrocarbons, which can be seen from the Table 2 and Table 3, respectively. From the values of statistical parameters, it is clear that GA_5 and NZ have significant correlation with BP and E, respectively.

Table 3: The values of β_0 and β_1 when only NZ is taken and some statistical parameters.

NZ	β_0	R^2	$Adj.R^2$	F-statistic	Prob(F-stats)
E4.175	-8.981	0.908	0.902	138.4	$1{:}21 \times 10^{8}$

However, other cases are also considered as given below for comparative analysis. First, we see the correlation matrix of these four indices for benzenoid hydrocarbons.

Table 4: Correlation matrix of NID, NZ, ${}^mNM_1$ and GA_5 with some degree-based molecular descriptors for benzenoid hydrocarbons.

	NID	NZ	${}^mNM_1$	GA_5
NID	1			
NZ	0.94	1		
${}^mNM_1$	0.97	0.99	1	
GA_5	0.86	0.98	0.96	1

Case 1: When all the four indices are considered together, using the above model, The following regression equations were obtained.:

$$BP = \beta_0 + \beta_1(NZ) + \beta_2(NID) + \beta_3(GA_5) + \beta_4({}^mNM_1),$$

$$E_\pi = \beta_0 + \beta_1(NZ) + \beta_2(NID) + \beta_3(GA_5) + \beta_4({}^mNM_1).$$

good fit. Also, for BP the p-values for all these indices were less than 0:05 at 5% significance level.

Table 5: The values of values of β0, β1, β2, β3, and β4 along the regression models and their statistical parameters.

	NZ	NID	GA5	mNM1	0	R2	Adj.R2	F-statistic	Prob(F-stats)
BP	4016.213	1.215×10^4	-222.950	-1.012×10^4	34.004	0.998	0.997	1438	7.19×10^{15}
E	75.016	88.134	-6.642	-138.508	-9.695	0.933	0.909	38.48	$2{:}09 \times 10^{6}$

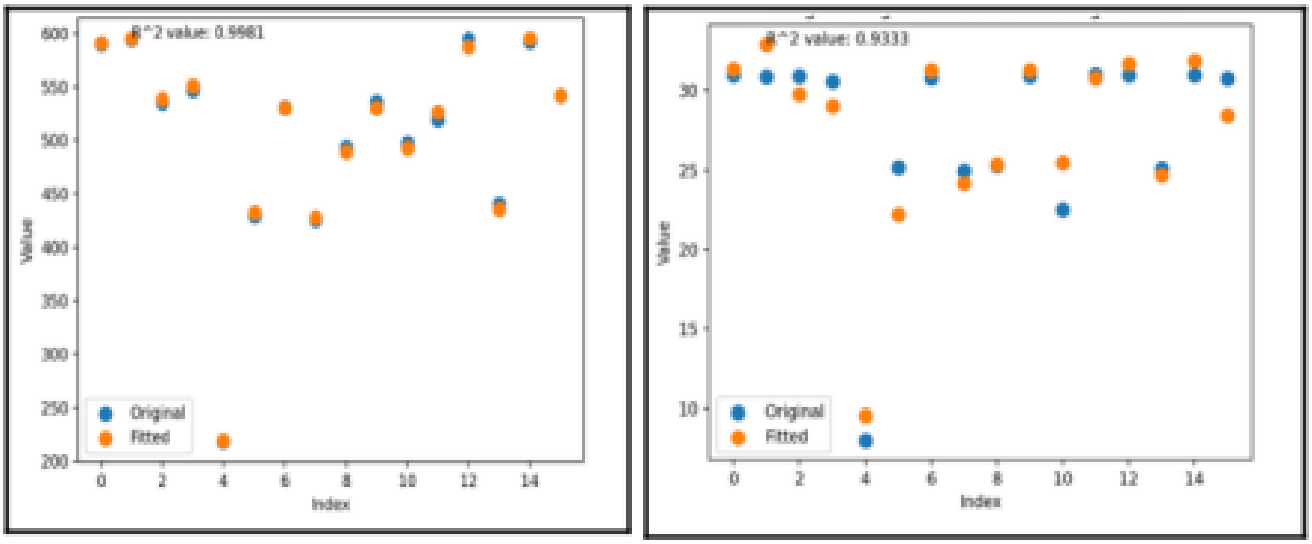

Fig 8: The original target values vs the predicted target values for BP and E of benzenoid hydrocarbons for case 1.

Table 6: The values of three values of β from the regression models and their statistical parameters.

	NID	GA5	β_0	R2	Adj.R2	F-statistic	Prob(F-stats)
BP	92.207	18.848	-24.788	0.995	0.995	1394	$6{:}80 \times 10^{16}$
E	17.835	0.909	-7.687	0.894	0.877	54.65	$4{:}7 \times 10^{7}$

However, for E, their p-values were greater than 0:05, indicating a discrepancy, which may have arisen due to a smaller number of data points. Therefore, we consider only two of the indices which is seen in case 3.

Conclusion

Molecular formulas provide a conceptual basis for the computation of topological indices, which are only numerical values. structure. In last 30 years the Topological indices play a significant role in chemical graph theory. because its tremendous applications. Chemical graph applications are the primary subject of this thesis. theory's topological indices. Four neighborhood-Degree-based indices, especially the neighborhood modified first Zagreb index (mNM1(Γ)), neighborhood Linear regression analysis was used to assess the chemical significance of the inverse degree index (NID (oe)), the neighborhood zeroth order index (NZ(ſ)), and the fifth geometric-arithmetic index (GA5).

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