Title :  **“A Study on Graph Structures and their underlying Geometry through Topological Indices”**

Introduction

* Graphs are any mathematical object involving points and connections among them.
* Applications of Graphs are databases, physical networks, organic molecules, map colorings, signal-flow graphs, web graphs, tracing mazes as well as less tangible interactions occurring in social networks, ecosystems and in a flow of a computer program.
* A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are also called topological indices.
* There are three types of topological indices have been studied so far.
* 1. Degree Based Topological Indices
* 2. Distance Based Topological Indices
* 3. Matrix and Eigen values based Topological Indices.
* Based on the applications of Topological Indices in QSPR analysis they are categorized into useful and non useful.
* In this proposed work we are concentrating on the useful degree based topological indices.

Problem Statement

Predicting the physical properties of chemical compounds without doing any experiment for example boiling point, tempetature, melting point of compound .

Proposed system

* Determining the physical properties of chemical Compound using Mathematics,i.e. Graph theory.
* Using molecular graph or Chemical graph theory i.e. usually chemical compound consist of carbon and hydrogen, by removing hydrogen replacing with carbon.consider the carbon atom as vertex and the link between two carbon atoms as edge and also using topological indices .

**Objectives**

* Comparison of earlier bounds with newly obtained bounds and characterize graphs which holds equality of the bounds.
* Comparison of degree based topological indices with the distance based topological indices.
* Obtain new distance and degree based topological indices and compare with the earlier indices.
* Obtain the mathematical properties of newly introduced topological indices and study their chemical applications.
* Study the mathematical properties of certain nanostructures through topological indices.
* Characterization of graphs through topological index values.

Molecular graph or Chemical Graph

* Chemical graph theory is a branch of mathematics which combines graph theory and chemistry.
* Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds.
* Some physical properties, such as the boiling point, are related to the geometric structure of the compound.
* This is especially true in the case of chemical compounds known as alkanes.
* Alkanes are organic compounds exclusively composed of carbon and hydrogen atoms.
* The structure of an alkane determines its physical properties.
* Physical properties of alkanes can be modeled using topological indices.
* There are three types of topological indices are present in the literature.
* According to the IUPAC definition, a topological index (or molecular structure descriptor) is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

**The Use of Degree Based Topological Indices in QSPR Studies**

There are 10 degree based topological indices,

* First Zagreb index
* Second Zagreb index
* Forgotten index
* Randi index
* Atom-bond connectivity index
* Augumented Zagreb index
* Geometric-arithmetic index
* Harmonic index
* Sum-connectivity index
* Reciprocal Randi index

**Work carried out so far**

* Study carried out so far is aimed at understanding the basic principles of manifolds applied in the analysis of space curves, surfaces in 3-dimensional Euclidean space.
* Literature survey has been conducted to study the basic ideology of manifolds associated with the study of Graph theory. Graphs of various forms applicable to Real life situations are considered in the present study.

Degree Based Topological Indices

* Consider the degree of each vertex and using first zagreb index make the summation of square of all the vertex values.
* perform the regression analysis i.e. find the corelation between the experimental values with the new values we got from first zagreb index.

Distance Based Topological Indices

* Consider the link between two vertices as edge and using second zagreb index make the summation of square of the values associated with the link.
* Perform the regression analysis i.e. find the corelation between the new values with the experimental values.

Matrix and Eigen values based Topological Indices.

* Here graph can be represented as matrix.Elements of matrix are 0 and 1.if any two vertices are adjacent then the value will be 1,if they are non adjacent its value will be 0 i.e.square symmetric matrix.
* Find the characteristic equation and eigen values,determine the sum of absolute eigen values.
* Perform the regression analysis i.e. find the corelation between the new values with the experimental values.

**Further work to be carried out**

The study of the research work aims at applying the principles and formulations in the field of Graph theory. And also aims at defining the new type of topological indices and comparing with the existing topological indices.

**Conclusion**

Our proposed work helps in finding the physical properties of chemical compounds without conducting any of the experiment. Using graph theory, branch of mathematics we are able to get those physical properties using topological indices. We are going to make comparison between existing topological indices values with the new topological index values using correlation and QSPR studies.

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