Chapter 1

Introduction
1.1 Introduction

Graph theory has well-grooved itself as an significant mathematical tool in a wide miscellanea of subjects, ranging from operational research and chemistry to genetics and linguistics, and from electrical engineering and geography to sociology and architecture. At the same time it has also emerged as a worthwhile mathematical discipline in its own right. Graphs are very useful tools for depicting the relationships among objects, which are represented by vertices. Vertex typically means a point where lines meet. It is also called as node.

In order, relationships among vertices are represented by connections. In general, one simple way of representing the structure of any system is graph.

For a great diversification of problems such pictorial representations may lead to a solution. Examples of such applications include signal-flow graphs, map colorings, databases, physical networks, web graphs, organic molecules, tracing mazes as well as less tangible interactions occurring in social networks, ecosystems and in a flow of a computer program.

The field Graph theory may be said to have its beginning in 1736 when Leonhard Euler considered the (general case of the) Königsberg bridge problem: Does there exist a walk crossing each of the seven bridges of Königsberg exactly once?
Swiss Mathematician, Leonhard Euler proposed the solution which led to the birth of a branch of mathematics called graph theory. Euler proved that there is no solution to the problem based on the number of bridges connecting each land area. Euler also noticed that the number of bridges at every land area would add up to twice the number of bridges. This appear as the hand-shaking lemma in graph theory, which states that the sum of the vertex degrees in a graph is equal to twice the number of edges. This result implies to the formulation of a frequently used result in graph theory that states that the sum of vertex degrees in a graph is always even [16, 18, 39, 42, 133].

The results from the solution of the Königsberg bridge problem have been extended to various concepts in graph theory.

At present, graph theory is a dynamic field in both theory and applications. Graphs can be used as a modelling tool for many problems of practical importance. For instance, a network of cities, which are represented by vertices, and connections among them make a weighted graph. The well-known traveling salesman problem asks for the shortest possible tour, which visits all the cities exactly once. Graph theory can solve majority of computational problems in industry. Because every system is based on some relations, consequently every system is a graph topology. For example: traffic organization, social relations, artificial intelligence and so on and there are numerous applications like this.
Molecular graph is the skeleton of the molecule and is obtained according as, every carbon atom is represented by a vertex and every carbon-carbon bond by an edge. Hydrogen atoms are ignored.

In the context of new technologies for molecular discovery, such as combinatorial chemistry and high-throughput screening, topological indices play an important role for the analysis of molecular diversity and lead to optimization through well-established structure-property relationships [3, 25]. A graph can be represented by a matrix, a sequence, a polynomial and a numeric number (often called a topological index) which represents the whole graph and these representations are aimed to be uniquely defined for that graph.

The study of topological indices play a prominent role in Quantitative structure-activity relationships (QSAR) and Quantitative structure-
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property relationships (QSPR) study. Topological indices correlate the certain physico-chemical properties (boiling point, enthalpy of vaporization, stability, strain energy etc) of chemical compounds specially organic family. To study and computing topological indices of molecular graphs and networks is a respected problem in mathematical and computational chemistry. There are some special classes of topological indices such as distance based, degree based and counting related topological indices which have their own chemical significance.

1.2 Definitions and terminology

For definitions and terminologies of graphs and spectra of graphs we refer the books [6, 9, 20, 64, 78, 84, 131].

A graph $G$ consists of a finite nonempty set $V(G) = \{v_1, v_2, \ldots, v_n\}$ of $n$ vertices together with a prescribed set $E(G)$ of $m$ unordered pairs of distinct vertices of $V(G)$. Each pair of vertices in $E(G)$ is an edge of $G$. We consider only simple, undirected graphs without loops. Two vertices are said to be adjacent if there is an edge joining them. An edge and its end vertex are incident with each other. Two edges are adjacent, if they are incident with common vertex.

The degree of a vertex is the number of edges incident to it. A vertex of degree zero is called an isolated vertex. A vertex with degree one is called a pendant vertex. A loop is an edge that
connects a vertex to itself. **Order** is the number of vertices of a graph \( G \) and is written as \( |G| \).

If all the vertices have same degree equal to \( r \), then \( G \) is called a **regular graph** of degree \( r \) or \( r \)-regular graph.

Two graphs \( G \) and \( H \) are said to be **isomorphic** if there is one-to-one correspondence between their vertex sets which preserves the adjacency, and it is written as \( G \cong H \) or \( G = H \).

A **subgraph** of \( G \) is a graph having vertex set as a subset of vertex set of \( G \) and edge set as a subset of edge set of \( G \). A **spanning subgraph** is a subgraph containing all the vertices of \( G \). For any set \( S \) of vertices of \( G \), the **induced subgraph** \( < S > \) is the maximal subgraph of \( G \) with vertex set \( S \).

A **walk** of a graph \( G \) is an alternating sequence of vertices and edges, beginning and ending with vertices, in which each edge is incident with the two vertices immediately preceding and following it. It is **closed** if end vertices are same and is **open**, otherwise. A walk is a **trail** if all the edges are distinct and it is a **path** if all the vertices are distinct. A path with \( n \) vertices is denoted by \( P_n \). A closed walk is called the **cycle** provided all its \( n \) vertices are distinct and \( n \geq 3 \). A cycle with \( n \) vertices is denoted by \( C_n \).

A graph is **connected** if every pair of vertices is joined by a path. The **length of a path** is the number of edges in it. The **distance**
$d(u, v)$ between two vertices $u$ and $v$ of $G$ is the length of shortest path joining $u$ and $v$ if any, otherwise $d(u, v) = \infty$. A shortest $u-v$ path is often called a geodesic. The diameter of a connected graph $G$ denoted by $D = \text{diam}(G)$, is the length of any longest geodesic.

The complement $\overline{G}$ of a graph $G$ is a graph with vertex set $V(G)$ and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in $G$. A self complementary graph is isomorphic with its complement.

The complete graph $K_n$ is a graph with $n$ vertices in which every pair of vertices is adjacent. Thus $K_n$ has $\frac{n(n-1)}{2}$ edges and it is regular graph of degree $n - 1$.

A bipartite graph is a graph whose vertex set can be partitioned into two subsets $V_1$ and $V_2$ such that no two vertices in either sets are adjacent. If every vertex of $V_1$ is adjacent to each vertex of $V_2$ then $G$ is a complete bipartite graph and is denoted by $K_{p,q}$, where $|V_1| = p$ and $|V_2| = q$. A star on $n$ vertices is a complete bipartite graph $K_{1,n-1}$.

A tree is a connected graph without cycles. A graph without cycles is a forest (or acyclic graph).

The line graph of $G$, denoted by $L(G)$ is the graph whose vertices has one-to-one correspondance with the edges of $G$ and two vertices of $L(G)$ are adjacent whenever the corresponding edges of $G$ are adjacent. If $G$ is an $r$-regular graph then $L(G)$ is $(2r-2)$-regular graph.
The subdivision graph $S(G)$ is the graph obtained from $G$ by replacing each of its edge by a path of length 2, or equivalently, by inserting an additional vertex into each edge of $G$.

The adjacency matrix of $G$ is the square matrix $A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if $v_i$ is adjacent to $v_j$ and $a_{ij} = 0$ otherwise. The eigenvalues of $A(G)$ will be referred to as the adjacency eigenvalues of $G$ and labeled as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. These form the adjacency spectrum of $G$ [20]. Two graphs are said to be cospectral if they have same spectra.

The ordinary graph energy $E_\pi(G)$ of a graph $G$ is defined as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$ [54]. Two graphs $G_1$ and $G_2$ are said to be equienergetic if $E_\pi(G_1) = E_\pi(G_2)$. Trivially cospectral graphs are equienergetic. The theory of ordinary graph energy is extensively elaborated in the book [84].

1.3 Outline of the present work

In this thesis we have obtained the results on topological indices such as Zagreb index, Forgotten index, Randić index, Harmonic index, Geometric-Arithmetic index, Sum-Connectivity index, Atom-Bond Connectivity index, Augmented Zagreb index. Also worked on Harary
energy, Harary equienergetic graphs, Seidel Laplacian spectra. The thesis consists of eight chapters followed by the list of references.

Chapter 1. This chapter mainly deals with introduction, basic terminologies and definitions that are used in the thesis.

Chapter 2. This chapter is associated with generalized transformation graphs and degree based topological indices. We obtain the expressions for the Randić index, harmonic index, Geometric-Arithmetic index, Sum-connectivity index, Atom-bond connectivity index and Augmented Zagreb index of generalized transformation graphs $G_{xy}$ and of their complements $\overline{G_{xy}}$ in terms of the parameters of underlying graph $G$.

Chapter 3. This chapter mainly deals with some chemical structure graphs, we correct the result regarding triangular benzenoid. Also a simple expression for the forgotten topological index of graphene sheet is derived and with this carried out the further studies of the previous work done by W. Gao et al. and obtained forgotten index of subdivision graph and line graph of some drug structures.

Chapter 4. In this Chapter, we study the association between harmonic index and Randić index. We attempt to quantify the association between harmonic index and Randić index by considering benzenoid hydrocarbons. Also obtained explicit formulas for Randić index and harmonic index of certain class of trees. Further an algorithm with
the help of adjacency matrix is given to compute the Randić index of graph.

**Chapter 5.** This Chapter mainly deals with Harary Matrix, we show that the Harary matrix of complement of the line graph of certain regular graphs has exactly one positive eigenvalue. Further we obtain the Harary energy of line graphs and of complement of line graphs of certain regular graphs and thus constructs pairs of Harary equienergetic graphs of same order and having different Harary eigenvalues.

**Chapter 6.** This Chapter associated with Seidel matrix. We introduce Seidel Laplacian Matrix and its energy, obtain the bounds for the energy.

**Chapter 7.** In this chapter, our aim is to present an algorithm for differential equations using linearly independent Hosoya polynomials obtained from trees. Proposed algorithm expands the desired solution in terms of a set of continuous polynomials over a interval. However, accuracy and efficiency are dependent on the size of the set of Hosoya polynomials and the procedure is much simpler compared to other existing methods for solving differential equations. The current procedure has implemented to solve linear and nonlinear equations and excellent agreement is found between the exact and approximate solutions.

**Chapter 8.** In this chapter we developed a method called Hosoya
polynomial method (HPM) using Hosoya polynomial of paths and is applied for the numerical solution of Fredholm integral equations and compared with the simple Haar Wavelet Method (HWM)). The present methods reduces an integral equation into a set of algebraic equations. HPM gives higher accuracy with exact ones and existing method (HWM). The numerical result shows that, the accuracy improves with increasing $n$ the number of verticies of polynomial for better accuracy. Error analysis justifies the comparative study of a new developed method is effective, validity and applicability of the new technique with existing method (HWM).