



## APPLICATIONS OF GRAPH THEORY

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### Abstract

Graph appears in a many domains whenever it is useful to represent how things are either physically or logically linked to one another in a network structure. Graph theory has a very wide range of applications in engineering, in physical and biological sciences, in linguistics and in numerous other areas. A graph can be used to represent almost any physical situation involving discrete and a relationship among them [1]. Applications of graph theory in different fields is studied in this paper.

**Keywords:** Graph theory applications, tree, matrix, graph, molecular topology, degree.

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### INTRODUCTION

A graph is a collection of points and lines connecting a subset of them. If  $e$  is an edge of  $G$ , connecting the vertices  $u$  and  $v$  then we write  $e = uv$  and say  $u$  is adjacent to  $v$ . The vertex-set and edge-set of  $G$  is denoted by  $V(G)$  and  $E(G)$ . The degree of vertex  $u \in V(G)$  is the number of vertices joining to  $u$  and denoted by  $\delta(u)$ . Distance is an important concept in graph theory and it has applications to computer science, chemistry and variety of other fields [2,3]. Graph theory is birth in 1736 with the publication of the work of the Swiss mathematician Leonhard Euler on the problem of finding a round trip path that would cross all the seven bridges of the city of Königsberg exactly once [4].

Graph theory has found many applications in engineering and science, such as chemical, electrical and mechanical engineering, architecture, management and control, communication, operational research, sparse matrix technology, combinatorial optimization and computer research. As far as the application in the computer science is concern it has unlimited applications whether it is related to software or hardware [5]. Graph theory has also been used in economics ,logistics ,cybernetics, artificial intelligence ,pattern recognition ,genetics, reliability theory, fault diagnosis in computers studying the structure of computer memory. The terminology and notations in this paper are standard and mainly taken from [6-13].

Trees are simple graph structure, are the most common structure used. There are two special types of graphs, which play a central role in graph theory; they are the complete graphs and the complete bipartite graphs. There are  $n^{n-2}$  distinct labeled trees with n-vertices .Trees has been widely used in many situations and lots of results have been proven for trees. For simple graphs with n-nodes have  $\frac{n(n-1)}{2}$  different edges. In this paper various applications of graph theory has been investigated.

**RESULTS AND DISCUSSION:**

Euler generalized the Konigsberg bridge problem and developed a criterion for a given graph to be so traversable; namely it is connected and every number of lines incident with an even number of lines ( Fig.1) .Euler was the first to prove the impossibility of starting from any node in this graph, passing every edge exactly once and returning the starting point [14].Euler remains one of the most prolific writers in mathematics , aside from graph ,we owe him the notation  $f(x)$  for a function ,I for square root of -1 ,and for Pi .He worked hard throughout his entire life only to become blind; “ Now I will have fewer distractions ,” and proceeded to write hundreds of papers more[15].

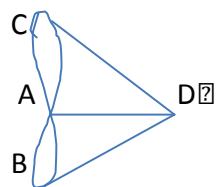


Fig.1:The graph of the Konigsberg Bridge Problem

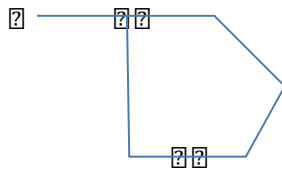


Fig.2: A drawing of graph

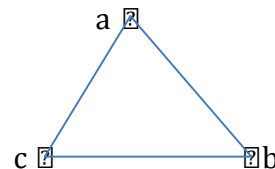


Fig.3: Simple graph

Representing a problem as a graph can make a problem much simpler (Fig.2). Graph theory gives a set of techniques for analyzing graph. Graph theory is an essential tool for

definition, systemization and enumeration of chemical compounds. In addition it helps for codification and nomenclature purposes [16]. A simple graph is an unweighted, undirected graph without loops or multiple edges (Fig.3). A tree is a connected acyclic graph. The edges of a tree called branches (Fig.4). For matrix representation of graph, Incidence matrix, Distance matrix, Circuit matrix, Path matrix, Laplacian matrix and Adjacency matrix are used. The adjacency matrix of a graph  $G$  with  $n$  vertices and no parallel edges is an  $n \times n$  symmetric matrix.

$X = [X_{ij}]$  defined as

$$X = 1, \text{ if there is an edge between } i^{\text{th}} \text{ and } j^{\text{th}} \text{ vertices, and} \\ = 0, \text{ if there is no edge between them.}$$

Adjacency matrix is useful for computer representation, entrée to linear to linear algebra, especially Eigen values and Eigen vectors. Matrix is the basis to compute topological indices and other parameters. Topological index can be used to evaluate structural similarity and diversity. Its main role is to work as a numeral molecular descriptor in QSAR/QSPR model [17]. Let  $G = (V, E)$  be a graph. There are two degree values that are of interest in graph theory: the largest and smallest vertex degrees usually denoted  $\Delta(G)$  and  $\delta(G)$ : that is

$$\Delta(G) = \max_{v \in V} \text{deg}(v)$$

$$\delta(G) = \min_{v \in V} \text{deg}(v)$$

Some binary operations between two simple graphs  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  are:

- 1) The union is  $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$  simple graph
- 2) The intersection is  $G_1 \cap G_2 = (V_1 \cap V_2, E_1 \cap E_2)$  simple graph
- 3) The ring sum  $G_1 \oplus G_2$  is the sub graph of  $G_1 \cup G_2$  induced by the edge set  $(E_1 \oplus E_2)$  simple graph, The set operation  $\oplus$  is the symmetric difference i.e.  $E_1 \oplus E_2 = (E_1 - E_2) \cup (E_2 - E_1)$ .
- 4) Product of graphs for  $G_1 * G_2$ , two points  $u = (u_1, u_2)$ ,  $v = (v_1, v_2)$  in  $v = v_1 * v_2$ . Then  $u$  and  $v$  are adjacent in  $G_1 * G_2$  whenever  $[u_1 = v_1 \text{ and } u_2 \text{ adj. } v_2]$  or  $[u_2 = v_2 \text{ and } u_1 \text{ adj. } v_1]$ .

## APPLICATIONS

### CHEMISTRY

In chemistry graph theory makes natural model for a molecule, where vertices represent atoms and edges bonds. This approach is especially used in a computer processing of molecular structures, ranging from chemical editors to database searching. In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural

formula of a chemical compound in terms of graph theory [18]. Molecular topology is an application of graph theory in fields like chemistry, biology and pharmacology, in which molecular structure matters [19]. An inherent problem in the development of a QSAR model is the quantification of chemical structure this problem of QSAR can be solved by utilizing the area of molecular connectivity wherein chemical structures are treated as graphs [20]. QSAR /QSPR are mathematical models relating the biological activity measurements of a set of chemical structures [21].

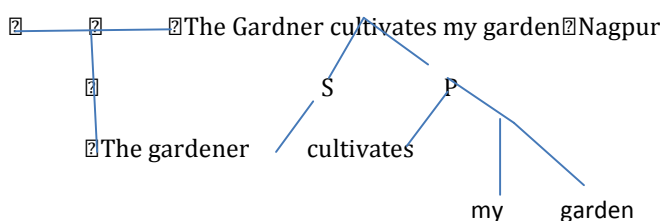
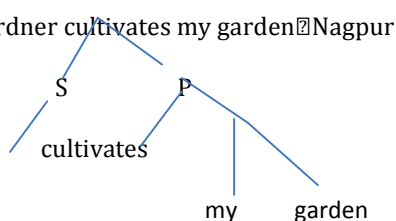


Fig.(4):Tree with five vertices



Fig(5):Tree in linguistics

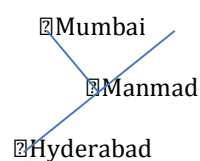


Fig.(6):Simple graph between cities

## PHYSICS

In condensed matter physics, the three dimensional structure of complicated simulated atomic structures can be quantitatively described by gathering statistics on graph theoretic problems related to the topology of atoms .Suppose that we are given the electrical network and we wish to find the current in each branch as is done in electrical network analysis. By applying Kirchoff's laws, current, voltage and resistance can be computed with drawing of graphs. In statistical physics graphs can represent connections between particular parts of a physical process or such systems.

## COMPUTER SCIENCE

In computer science graphs are used to represent networks of communications, the flow of computation, data organization, computational devices etc. Trees as graphs have much applications especially in data storage, searching and communication [8]. Graph spectra appear in internet technologies, pattern recognition, computer vision and many other areas .Rooted trees are used in many other applications of computer science to store data in a computer's memory. Trees are also used extensively to organize data in computer systems. For example: Consider the following quadratic equation  $ax^2+bx+c, x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ . Computers used to process such expressions to which end they first need to be stored. This can be done conveniently in the form of the rooted tree [10].The matrices are commonly used to represent graphs for computation of Eigen values

and Eigen vectors usually accomplished by computer and several algorithms have been developed. Trees used in data base designing, software engineering and network.

## **BIOLOGY**

Graph models are used extensively in many areas of the biological sciences, e.g. niche overlap graph for a forest ecosystem. In conservation efforts, the overall movement and sustenance of the species is studied. Graphs can be used in drug target identification, determining a protein's or gene's function, designing effective strategies for treating various diseases or providing early diagnosis of disorders as well as for describing a different biological networks ,biochemical networks, transcriptional regulation networks etc.[22].In systems biology, in the context of genetic circuits or gene networks, a node represents an active biological species such as gene ,enzyme or signal molecule , and an edge depicts the connection and the nature of connection for between them as self-edge and directed edge ,e.g. current opinion in cell biology [23 ].Graphs as secondary RNA structures, Graphs as amino acids, graphs as proteins, are the recent applications. The study of RNA of molecules is at the forefront of the field of systems biology [24].Application of graph theory in QSAR covers variety of topics from the study of various physico-chemical data to biological activity and toxicity including graph theoretical descriptors and pattern recognition [25].Three classes of bimolecular networks has attracted the most attention: metabolic networks, protein interaction network and the transcriptional regulatory networks. In biology these networks comprise nodes that are biological quantities i.e. proteins, metabolites and edges that are interactions: protein-protein interactions, metabolic reactions.

## **MEDICAL SCIENCE**

Graph theory provides models for complex networks in the brain and allows one to better understand the relations between network structure and processes taking place on those networks.

## **LINGUISTICS**

In modern linguistics, immediate constituent analysis, the structuralists combines the categorical labeling and functional labeling in a system which is known as (Fig.5) Immediate Constituent Analysis, IC Analysis in short. A structure prediction contains two constituents: a subject (s) and a predicate (P).The constituent can be shown by a tree diagram or a topless box diagram, for example: The gardener cultivates my garden [26].The tree represents parsing of an English sentence [27].

## **OPERATIONAL RESEARCH**

Graphs are used as models for assignment problems, (assigning people to jobs, arranging programs, finding proper schools for children, finding professional colleges and finding proper business schools). Graphically how can we represent a track system of railways connecting tourist spots? A graph with edge indicating a direct train connection between two cities is used (Fig.6). Graph theory is applied to the problems in engineering, economics and war science to find optimal way to perform certain tasks in competitive environments. Frequency assignment: Assignment of channels is modeled by graph coloring.

## **ARGO-ECOSYSTEM**

An agro-ecosystem is directed by the interactions among the populations living in it and depending on many abiotic factors. Using well known graph theory theorems and having the help of computers is especially powerful for controlling huge systems that are difficult to survey by existing methods [28]. The recent advances in network science, a multidisciplinary motivated intention to understand the universal architectural principles of different kinds on real networks encouraged ecologists to study the number of networks of species in food webs and distribution.

## **SOCIAL SCIENCES**

Social network analysis has been important for the further development of graph theory, e.g. in relative importance, influence, proximity, structural balance etc. Social network is graph between working relationship between different faculty members in an institute. A sociologist ponders a diagram illustrating the power of a large corporation. Sociologists use graphs in order to model social networks, to represent the interaction between people in a specific graph. Graph models are between, friendship graphs on social media, collaboration graphs—where two or more people are connected for preparatory work for cracking competitive examination /CAT-examination.

## **MATHEMATICS**

Graph theory is one of the most important areas in mathematics which is used to study different structural models or configurations. These structural arrangements of various objects of technologies lead to new inventions and modifications in the existing environment for enhancement in those fields [29]. The exciting and rapidly growing area of graph is rich in theoretical results as well as applications to real-world problems. The coloring theory brings one immediate application to mind. For example: If you want to make a time table for choice based credit system classes for undergraduate classes, one common condition that you cannot

have two subjects attended by students at a time, if one or more of the students has to attend both subjects. If you recast the problem correctly it turns out to be a simple coloring matter. The idea of using the minimum number of colors then translates to, “What is the minimum number of different periods you need to put in the timetable “? Graph theory has been used to model and address in the problem of flows in networks. A network could be the movements of vehicles from the city to another on the roads or an electrical distribution grid and so on.

### CONCLUSIONS:

Graph theory is a branch of mathematics that has a wealth of applications from science to engineering, natural science to social sciences. There is hardly any field in which graph theory is inapplicable. Graph theory is used in economics, logistics, and cybernetics, artificial intelligence pattern recognition, genetics, reliability theory, and fault diagnosis in computer memory. Graph theory has developed into a subject itself with a variety of applications. Applying graph theory gives a set of techniques for analyzing graphs. Applying graph theory to a system means using a graph-theoretic representation.

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