An Overview Graphs Theory and Its Application in Various Scientific Field

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Abstract: As part of mathematics, the use of graphic theory at the present time in various other scientific fields such as chemistry, physics, engineering and social science, is very widespread. This paper is trying to reveal some of the uses of graph theory in several fields of science. It is realized that at this time, graph theory has become one of the topics that attract attention because the models contained in graph theory can be applied to problems such as transportation, electrical circuit networks, computer science, and many other fields. Briefly stated that the graph is a representation of a picture of a system that uses two basic elements, namely points and edges. A point represents a circle and an edge is represented by a line connecting two points. This paper highlights various views on the application of graphs in the fields of chemistry and physics, research operations and some general descriptions are presented.

1 INTRODUCTION

As one of the branches of science that is quite old, graph theory has many applications in various fields of science. Graph is useful for representing objects and relationships contained in these objects. Visual representation of a graph is to declare an object as a point, circle or dot and the relationship that occurs between these points is described as a line. An easy example that can be found in everyday life is a map of the highway network in a city. As a graph, cities on the map are expressed by points while lines connecting the points are edges. In this paper, we review the notions of graph theory and its use in several fields by referring to some of the materials mentioned in the references.

2 GRAPH THEORY

Diagrams that consist of a set of points and lines connecting certain pairs of points are widely used in real-world situations. The focus here is about the two points connected by one line, the way the two points are connected is not important. It is this mathematical abstraction that gave rise to the concept of graphics.

Graph G is sequential triple [V(G), E(G), \emptyset_G] consisting of non-empty vertices V(G), set E(G), disjoint from V(G), edges, and \emptyset_G functions events related to each edge G of the unordered pair of vertices (not necessarily different) from G. If *e* is the edge and *u* and *v* are vertices such that PG(e) = uv, then *e* is said to join *u* and *v*; vertices *u* and *v* are called ends *e*. The following are two examples of graphs that serve to clarify the situation.

 $G = (V(G), E(G), \phi_G), \text{ where } V(G) = \{v_1, v_2, v_3, v_4, v_5\} \text{ and } E(G) = \{e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8\}, \text{ and } \phi_G \text{ defined by } \\ \phi_G(e_1) = v_1 v_2, \phi_G(e_2) = v_2 v_3, \phi_G(e_3) \\ = v_3 v_3, \phi_G(e_4) = v_3 v_4 \\ \phi_G(e_5) = v_2 v_4, \phi_G(e_6) = v_4 v_5, \phi_G(e_7) \\ = v_2 v_5, \phi_G(e_8) = v_2 v_5 \\ \text{Example 2, } \\ H = (V(H), E(H), \phi_H), \text{ where } V(H) = \{v_1 v_2, v_3, v_4, v_5, v_6, v_6\}$

 $\{u, v, w, x, y\}$, and $E(H) = \{a, b, c, d, e, f, g, h\}$, and \emptyset_G defined by $\emptyset_H(a) = uv, \ \emptyset_H(b) = uu, \ \emptyset_H(c) = vw, \ \emptyset_H(d)$

$$\phi_H(a) = uv, \ \phi_H(b) = uu, \ \phi_H(c) = vw, \ \phi_H(a)$$
$$= wx$$
$$\phi_H(e) = vx, \ \phi_H(f) = wx, \ \phi_H(g) = ux, \ \phi_H(h)$$
$$= xy$$

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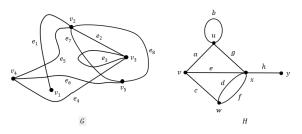


Figure 1: Diagrams of graphs G and H.

Graphs represented graphically help to understand the properties of the graphs. Each vertex is represented by a point, and each edge by a line connecting the points represent the edges. In Figure 1, diagrams G and H are shown in Figure 1. Another G diagram, is given in Figure 2. The graph diagram illustrates the relationship between the vertices and their edges. Note that the two sides in the diagram of the graph can intersect at points that are not vertices (for example e_1 and e_6 of graph G in figure 1).

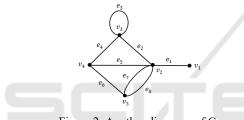


Figure 2: Another diagrams of G.

Graphs that have diagrams whose edges only intersect at the edges are called planar, because such graphs can be represented in simple fields. The graphic image (3.i) is planar, and the graphic image (3.i), on the other hand, is nonplanar. Most of the definitions and concepts in graph theory are given by graphical representations. The edges are called incident with edges, and vice versa. Two vertices that are adjacent to the same edge are adjacent, as are the two edges that intersect the common node. Edges with identical ends are called loops, and edges with different ends are links. For example, the e_3 edge of G (figure 2) is a loop; all other G edges are links.

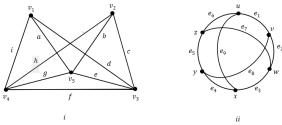


Figure 3: Planar and nonplanar graphs.

The graph is limited if the set of vertices and set of edges is also limited. A graph is called simple if it does not have a loop and no two links join the same node pair. Graphic figure 1 is not simple, while the graphic in figure 3 is simple.

2.1 Graphs in Chemistry and Physics

Graph Theory in Chemistry Graphs are used in chemistry to model chemical compounds and their structures. In computational biochemistry, the same sequence of cell samples must be issued to resolve conflicts between two sequences. This is modeled in a graphical form where vertices represent sequences in the sample. An edge will be drawn between two vertices if and only if there is a conflict between the corresponding order. The goal is to remove the possibility of a node to eliminate all conflicts.

In physics, graphs are used in condensed matter physics. Usually describes solid state and molecular systems as a strict binding model. Graph theory is also widely used in the field of statistical physics. Statistical physics in the branch of science that deals with methods of using probability and statistical theories, and especially mathematical tools for dealing with large populations and forecasts, in solving physical problems. The main areas of statistical physics that use graph theory are statistical mechanics, particle physics, and statistical analysis problems and thermodynamic results.

2.2 Graphs in Switching Theory

Ehrenfest (1910), presented a paper on switching theory where he stated that Boolean algebra could be applied to automatic telephone exchange. Next Shannon (1938) introduced a mathematical formulation of contact network behavior (a particular type of switching network). Since then, switching theory has developed very rapidly. Initially, this was intended for engineers of communication tools to analyze and synthesize large scale relay switching networks, such as telephone exchanges. And, in recent years, the rapid growth of switching theory was motivated because of its use in digital computer design. Unlike a signal in a classical network (say, in a radio receiver), a switching network signal has only two values defined as 0 and 1. A switching network is designed to process and store the binary signal.

Switching networks can be classified as combinational networks and / or sequential networks. Combinational switching networks are networks that output at a certain time only depend on the input at that time. Sequential switching networks, on the other hand, are those that output at a particular time are a function of the inputs at that time and during the entire past history. In other words, sequential networks have memory, whereas combinational networks do not. All digital systems, are built from these two basic types of circuits combinations and sequences.

Combinational switching networks can then be classified as (1) contact networks, or (2) gateway networks. Here we limit ourselves to the contact network only.

2.2.1 Contact Networks

Relay contacts (or contacts, for short) can be likened to ordinary household switches that are used to control light. This is a two-terminal device that has two statuses; in the open state where there is no conductive path between the terminals; and in a closed state where there is a path that will allow electric current to flow in both directions. So contact is a bilateral device. Usually, a contact is represented by one of the symbols shown in Figure 4 below.



Figure 4: Symbol used to represent a switch or contact.

Contact networks are interconnected networks where each contact network can be represented by a graph, where the ends are contacts and the node is the terminal. For the purpose of writing, a definition of contact network is given, namely: the contact network is a directed, connected graph (without its own loop) where each side has a binary variable x_i associated with it, which can be assumed to have only two values, 1 or 0 The binary variable x_i specified for a contact is 1 when the contact is closed and 0 when the contact is open.

The input-ouput behavior of the contact network is usually expressed in terms of functions,

$$f_i(x_1, x_2, \ldots, x_k),$$

from binary variables. The f_i function is called the switching function (or Boolean) and is assumed to have a value of 0 or 1, and where the Boolean algebra consists of a limited set of $x_1, x_2, ..., x_k$ and two binary + operations (called Boolean addition) and . (called Boolean duplication) that meets the following postulates:

1. Either $x_i = 1$ or $x_i = 0$

For each x_i there is another variable x_i', called the complementary x_i, so that if x_i = 0, x'₁ = 1, and if x_i = 1, x_i' = 0.

3. (a). Sum
$$x_i + x_j = \begin{cases} 0, & \text{if } x_i = x_j = 0, \\ 1, & \text{otherwise} \end{cases}$$

(b). Product $x_i x_j = \begin{cases} 1, & \text{if } x_i = x_j = 1, \\ 0, & \text{otherwise} \end{cases}$

with this postulate a number of results can be derived, which is useful in simplifying the expression of switching. For example, it can be easily shown that $x_i + x_i x_j = x_i$.

In the contact network, two types of problems will be found, namely the problem of analysis and synthesis. Here we will discuss only the problem of analysis only, where in the analysis given the G contact network and how to find conditions where there is an electrical conduction path between a pair of vertices (v_i, v_j) in G.

Consider two nodes in the G contact network, because G is connected, there is one or more paths between these two nodes. Each path can be identified by a Boolean product from variables related to edges in the path. For example, in figure 5, eight different paths between vertices a and b are (x_1x_5) , $(x_1x'_3x_1)$, $(x_2x_3x_1)$, $(x_2x_3x'_3x_5)$, $(x_2x'_1x_1)$, $(x_2x'_1x'_3x_5)$, $(x_3x_4x_1)$, $(x_3x_4x'_3x_5)$, (*)

each of these products is called the path product between nodes a and b in the contact network of G. Obviously, the value of the path product is 1 if and only if each variable in the path product has a value of 1; if not, it is 0. The value 1 of the product line implies the existence of an electric conduction path between a and b through the appropriate contacts in the network.

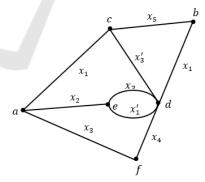


Figure 5: Contact network with six vertices and nine contacts.

For electrical conduction between two vertices, it is necessary and sufficient that at least one of the path products be 1. In other words, the Boolean number of path products between certain node pairs (v_i, v_j) is 1 if and only if terminals v_i and v_j are electrically connected in the contact network. Therefore, the number of Boolean line products is referred to as the contact network transmission between two nodes that are determined. For example, the transmission between vertices a and bin Figure 5 is

$$F_{ab} = x_1 x_5 + x_1 x'_3 x_1 + x_2 x_3 x_1 + x_2 x'_3 x'_3 x_5 + x_2 x'_1 x_1 + x_2 x'_1 x'_3 x_5 + x_3 x_4 x_1 + x_3 x_4 x'_3 x_5$$

Finding the transmission between the nodes specified in the given contact network consists of counting all the paths between the two nodes, and finding the Boolean number of product lines. Furthermore, the possibility of simplification based on Boolean algebraic postulates was also carried out. For example, in the product lines listed in (*), the following identities are clear:

$$\begin{aligned} x_1 x_3' x_1 &= x_1 x_3' \\ x_2 x_3' x_3' x_5 &= 0 \\ x_2 x_1' x_1 &= 0, \end{aligned}$$

and

$$x_3 x_4 x_3' x_5 = 0.$$

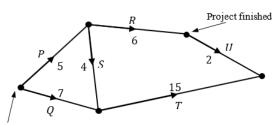
Therefore, the switching function between vertices a and b in Figure 5 is

 $F_{ab} = x_1x_5 + x_1x'_3 + x_1x_2x_3 + x'_1x_2x'_3x_5 + x_1x_3x_4$ Obviously, F_{ab} provides all different conditions where there is a conductive path between *a* and *b*.

2.3 Graphs in Operation Research - Activity Networks in Project Planning

One of the most popular network applications in operations research is the planning and scheduling of complex projects. A project is divided into many jobs called activities. Due to technical limitations, work must be completed before the others start, each activity also requires the duration or time of the activity. Several lists of activities in a project, including a list of direct prerequisites, and duration, a weighted digraph can be made to describe the project, as follows: each edge represents the activity, and the weight represents the duration of the activity, while the node represents the beginning and end of the activity. Activity (i, j) cannot start before all activities *i* have finished. Every event in the project is a well-defined event in time. Like a weight, connected graphs describe activities in a project called the activity network.

Suppose a project consists of six activities P, Q, R, S, T, and U, with the limitation that P must precede R and S; Q and S must precede T; and R must precede U. The duration for activities P, Q, R, S, T, and U are 5, 7, 6, 4, 15, and 2 days respectively. This network of project activities is shown in Figure 6.



Project begins

Figure 6: Activity network.

Note that network activity must be acyclic; if not, then there will be an impossible situation where no activity on the directed circuit can be started. Also note that the point indicating where the project starts must have a zero degree, because there are no activities that precede this point. Likewise, the point indicating where the project ends must have zero degrees, because there are no activities after this.

Dummy Activity; in the network activity example in Figure 6, suppose there is an additional limitation that activity U cannot begin before Q and S are completed. This main relationship can be described as an edge by connecting point x to y(Fig. 7). This is what is called a dummy activity.

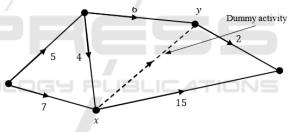


Figure 7: Dummy activity in a network.

Dummy activities are important when there are not enough activities to describe all the relationships that are prioritized accurately. All puppet activity has zero duration and is usually displayed in a dotted line. Two parallel edges (e.g., activities that have the same direct predecessor and the same direct successor) can be replaced by one edge, combining the two activities into one [Fig. 8 (a)]. However, if activities must be tracked separately, then dummy activities and dummy events must be created [Fig. 8 (b)]. And, because there is no self-loop in the activity network, we only have a simple digraph for the activity network.

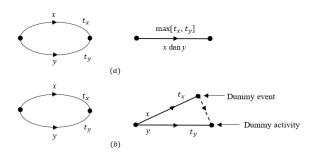


Figure 8: Replacement of parallel edges.

A network of activities can be assumed to have exactly one node with zero in degrees and exactly one node with zero outside degrees. If there is more than one node having zero degrees, someone arbitrarily chooses one of these for the initial event and draws the puppet activity from this to the other node. Vertices with zero degrees are handled equally.

In short, the activity network is a representation of two aspects of the project: (1) the priority relationship between activities, and (2) the time period. These are connected, weighted, simple, acyclic digraphs with exactly one zero point in degrees and exactly one zero point outside the degree.

3 CONCLUSION

In this paper the author has provided a basic understanding of graph theory. Understanding is quite easy to understand and provides a description of several types of graphs. This paper also explains where different graphs of graph theory can be used in various fields of science. In other words, an idea is given about the use of graphic theory terminology in its use in various fields of science. Furthermore, one can understand about this terminology and get other ideas related to their use in the real world.

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