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Thesis Title

by

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A thesis submitted in partial fulfillment for the
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in the
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School of Physics

Supervising Professor: Dr. Panagiotis Argyrakis

Date

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Abstract

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Abbreviations

Acronym	**W**hat (it) **S**tands **F**or

Dedication (optional)

Chapter 1

Introduction

1.1 Graphs

In this subsection, the main aspects of graph theory are briefly presented.

1.1.1 Introduction

In the real world, many problems can be described by a diagram connecting a set of points with lines, joining pairs of these points, or even creating loops on a single point. A simple example of that would be a set of points representing people with lines connecting acquintances, or points representing atoms and lines representing chemical bonds, creating a representation of a molecule as a graph attribute. In the examples above, the only information contained is whether two points are associated, with the manner being disregarded. The concept of a graph consists of a mathematical abstraction of the above. [1]

Definition 1.1. Mathematically, in its simplest form, a **graph** is an ordered pair[1] $G = (V, E)$ of:

- **V**, a set of vertices (also known as nodes).
- $E \subseteq \{\{x, y\} | x, y \in V \; x \neq y\}$, which is the set of **edges** which consists of unordered pairs of vertices that connect two nodes.

This type of object is called an **undirected simple graph** to avoid confusion with other types.

[1] An ordered pair (a, b) is a pair of objects in which the order of appearance or insertion is significant; the ordered pair (a, b) is different than (b, a) unless $a = b$. An unordered pair is a set of the form a, b is a set having two elements with no relation between them and $a, b = b, a$.

Definition 1.2. A *graph* G is an ordered pair $(V(G), E(G))$ consisting of a set $V(G)$ of *vertices* (also called *nodes* or *points*) and a set $E(G)$, disjoint from $V(G)$ which consists of *edges* (also called *links* or *lines*) together with an incidence function ψ_G that associates with each edge of G an unordered pair of not necesserily distinct vertices of G. If e is an edge and u and v are vertices such that $\psi_G = u, v$ then e is said to *join* u and v, and the vertices u and v are called the *ends* of e. We denote the numbers of vertices and edges G by $u(G)$ and $e(G)$ which two parameters are called the *order* and *size* of G, respectively [1].

In short, we can define a **graph** as an ordered triple $G = (V, E, \phi_G)$ consisting of:

- V, a set of *vertices*
- E, a set of *edges*
- $\phi_G : E \to \{\{x, y\}|x, y \in V \; and \; x \neq y\}$ an *incidence function* mapping every edge to an unordered pair of vertices - an edge associated with two distinct vertices. The incidence function is a function of the edges.

This type of object is called an *undirected multigraph*, to avoid confusion. Note, that the above definition of the *incidence function* does not allow for *loops* (mappings of an edge on the same vertex).

A *loop* is a an edge that allows a connection of a vertex to itself and a graph can be defined to either allow or disallow the presence of loops. Some authors allow for loops to exist on *multigraphs* [2], while other consider these kind of graphs to exist in a different category, called *pseudographs* [3]. Allowing loops requires modifying the incidence function so they can be supported. The new incidence function can be written as:

$$\phi_G : E \to \{\{x, y\}|x, y \in V\} \tag{1.1}$$

The example presented below should better illustrate clarify the definition (of a pseudograph).

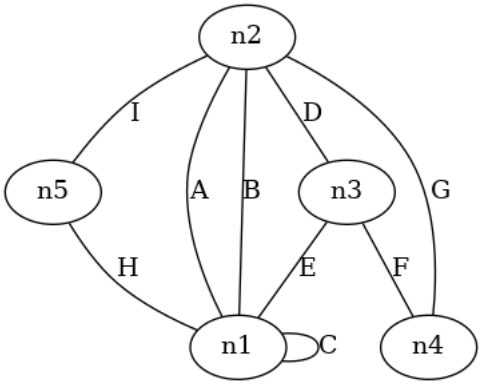


FIGURE 1.1: An undirected pseudograph with labeled nodes and edges.

Example 1.1.

For the graph presented in Figure 1.1 the following can be assumed:

$$G = (V(G), E(G))$$

and

$$V(G) = \{n_1, n_2, n_3, n_4, n_5\}$$
$$E(G) = \{A, B, C, D, E, F, G, H, I\}$$

and the incidence function is defined as:

$$\psi_G(A) = n_1n_2, \quad \psi_G(B) = n_1n_2, \quad \psi_G(C) = n_1n_1, \quad \psi_G(D) = n_2n_3,$$
$$\psi_G(E) = n_1n_3, \quad \psi_G(F) = n_3n_4, \quad \psi_G(G) = n_2n_4, \quad \psi_G(H) = n_1n_5,$$
$$\psi_G(I) = n_2n_5$$

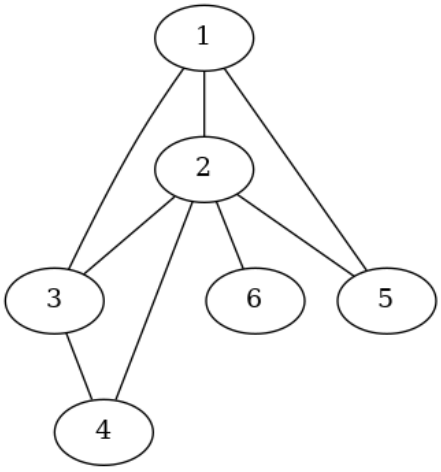
It should now be clear that with the newer definition of ϕ_G, self loops are now possible. Additionaly, even though this was not prohibited by the previous definition, it is worth noting that a node can be connected to another with multiple edges (or multiedges), or that it can have zero connections to other nodes. Generally, V is assumed to be a non-empty set, but E can be empty.

It is now possible to define some characteristic attributes of graphs:

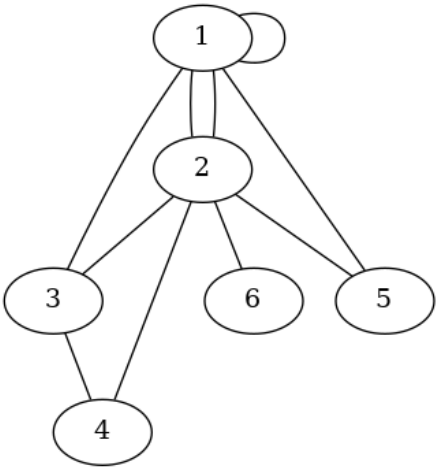
- $|V|$: the **order** of a graph is the number of its vertices.
- $|E|$: the **size** of a graph is the number of its edges.
- The **degree** (or **valency**) of a single node is the number of edges connected to it. The **degree** of a graph is the maximum number of edges connected to a single vertex that belongs to it.
- The edges of create a *homogenous relation*[2] $\sim$ on the vertices of the graph that is called **adjacency relation**; for each edge (x, y), its endpoints *x, y* are said to be **adjacent** to each other, denoted by $x \sim y$. This property will be particulary useful when the adjacency matrix is defined in the following section.

It can be inferred from the above definitions and attributes that for an undirected graph of order *n*, the maximum *degree* of a node is $n - 1$ and and maximum *size* of a graph is $n(n - 1)/2$.

[2] A **homogenous relation** (or **endorelation**) over a set *X* is a set of assignments (binary relations) over *X* and itself; i.e. it is a subset of the cartesian product $X \times X$



(A) Multigraph with no loops and multiple edges.



(B) Mutligraph with loops and multiple edges.

FIGURE 1.2: Two undirected multigraphs.

In this section only *undirected* graphs were considered, which are graphs with edges with no orientation. A whole other class of graph objects with edges which have orientation exists, called *directed graphs*. These kind of graphs objects are out of scope for this thesis and will not be presented.

1.1.2 Adjacency Matrix

Definition 1.3. The *adjacency matrix* is the fundamental mathematical representation of a graph. It is a square matrix, the elements of which represent which pair of nodes are *adjacent* or not. Thus, the adjacency matrix **A** of a graph of order n is the $n \times n$ matrix with elements A_{ij} such that:

$$A_{ij} = \begin{cases} 1 & \text{if there exists at least one edge connecting } i \text{ and } j \\ 0 & \text{if there no edges connecting those edges directly.} \end{cases} \tag{1.2}$$

Considering the simple undirected graph of Figure 1.3a we can construct the following adjacency matrix:

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

TABLE 1.1: Adjacency matrix for Figure 1.3a

For this simple network, which has no loops and only one edge connect two nodes, the diagonal matrix elements are always zero and the matrix is symmetric, as for each edge connecting i and j there is a representation for the j to i connection as well.

In a more complex case, such as the one presented in Figure 1.2b where loops and multiedges are present an adjacency matrix can still be constructed. In this case, a multiedge is represented by setting the value of the corresponding A_{ij} value equal to the multiplicity of the edge. In this case, $A_{12} = A_{21} = 2$.

For loops, the most common representation in the case of undirected graphs is to still set the value of the A_{ii} element equal to 2 (i.e. $A_{11} = 2$ in the example presented). Essentially, an edge of a loop has two ends that connect to the same node, thus the result [4, p. 68]. Additionaly, defining the matrix in such manner, allows for better computations and is consistent with the definition of the representation of an edge connecting two nodes of an undirected graph [5, p. 108].

Thus, the adjacency matrix for the graph of Figure 1.2b is

$$A = \begin{pmatrix} 2 & 2 & 1 & 0 & 1 & 0 \\ 2 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

TABLE 1.2: Adjacency matrix for Figure 1.2b

Remark 1.4. Note that the degree of a node can be easily found by summing the values of the column or row of the adjacency matrix that correspond to said node.

1.1.2.1 Adjacency List

An alternative to the adjacency matrix is the *adjacency list.* An adjacency list is a collection of lists, one for each node i. Each list contains the labels of the nodes that i is connected to, and its the most common method for storing networks on computers as it requires less space. It is also possible to represent edge attributes in an adjacency list by appending an extra column which holds these values. An example for the graph presented in Figure 1.2b with multiedges and loops:

Node	Neighbors
1	1,2,2,5,3
2	1,1,3,5,6,4
3	1,2,4
4	3,2
5	1,2
6	2

TABLE 1.3: Adjacency list for Figure 1.2b

Each edge of the network appears twice, thus for a network with m edges the size of the adjacency list would be $2m$, much smaller compared to the $n \times n$ matrix required to build an adjacency matrix. This is particularly useful in networks which are relatively *sparse*[3], but have a high order.

1.1.3 Graph Laplacian

The graph lacplacian is another representation matrix representation of a graph. In its simplest form, for a simple, undirected and unweigheted network of order n, is a $n \times n$ matrix **L** with elements:

$$L_{ij} = \begin{cases} k_i, & \text{if } i = j \\ -1, & \text{if i} \neq \text{j and there exists an edge connecting } i \text{ and } j \\ 0, & \text{everywhere else} \end{cases}$$

where k_i is the degree of the node. Another way to write the graph Lacplacian is as

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

where **D** is a diagonal matrix containing the degrees of the nodes.

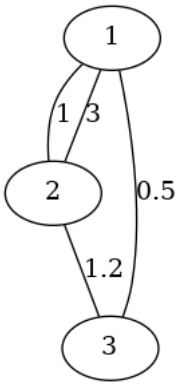
[3] *Sparse* networks are networks with a much lower number of edges than those possible.

In a similar manner the Laplacian matrix can be constructed for weighted networks, by replacing the the degree k_i of a node with the relevant matrix elements.

The Laplacian matrix has many applications in the study of dynamical systems, random walks and graph visualization. It has also found applications in graph neural networks, as its spectral decomposition allows the construction of low dimensional embeddings with applications in graph neural networks, such as ChebNet [6] which will be discussed in depth later.

1.1.4 Edge weights

So far, while presenting edges, we have considered graphs where connections between nodes represented binary relations between them; they either existed or they did not. In many situations when studying graphs, it is useful to represent edges as connections which carry some kind of attribute or value, commonly called *weight*. This weight could be any real number that fits a particular example, such as the distance between two airfields on an airline network, the kinship of connections on a social network (negative values can represent animosity and vice versa) or any type of relational attribute that can be quantified and characterizes the connection between nodes that belong in the same network[5, p. 109]. A simple example is presented in the figure below.



(A) Multigraph with no loops and multiple edges.

$$A = \begin{pmatrix} 0 & 4 & 0.5 \\ 4 & 0 & 1.2 \\ 0.5 & 1.2 & 0 \end{pmatrix}$$

(B) Corresponding adjacency matrix.

FIGURE 1.3: Simple example of an unordered graph with weighted edges

Generally, edges and nodes can hold any type of variable as values, such as vectors, the usefulness of which will become apparent when computer algorithms for graph representations and graph neural networks are discussed in later sections and chapters.

1.1.5 Distance between nodes and shortest paths

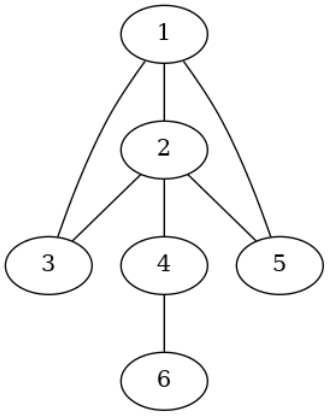
On a graph, any route that traverses nodes along the edges connecting them creates a sequence which is called a *walk*. Walks are not prohibited from traversing previously visited nodes and edges, but walks that do not intersect themselves are called *paths*.

Remark 1.5. *Adjacency Matrix Powers* Before continuing, it is worth mentioning that the powers of the adjacency matrix A^c directly provide the number of walks of length c among two nodes. If there is a connection between two nodes i and j, then $A_{ij} = 1$ else it is 0. Moving to the second power and taking for example an intermediate node k which might lie between i and j, the product $A_{ik}kj$ would be 1 if there is a node and 0 if there is not [5, p. 131]. Generalizing to walks of length c which traverse nodes i to j, their total number is:

$$N_{ij}^{(c)} = [A^c]_{ij}$$

The *shortest path* between two nodes is the shortest walk between those two nodes, the walk which traverses the least amount of nodes. In terms of edges, the least number that must be traversed is called *shortest distance* or often just "distance". Mathematically, the shortest distance between two nodes i and j is the walk with the smallest value c where $[A^c]_{ij} > 0$

Example 1.2. *For instance consider the following graph:*



$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

FIGURE 1.4: A graph with a maximum path of 3 (nodes 1 to 6).

In this example, it can be visiually determined that the minimum walk between nodes 1 and 6 is of length 3. Indeed, raising the adjacency matrix to a power of three yields for these nodes:

$$\dots$$

$$N_{1,6}^{(2)} = \sum^{n} A_{1k}A_{k6} = [A^2]_{1,6} = 0$$

$$N_{1,6}^{(3)} = \sum^{n} A_{1k}A_{kl}A_{l6} = [A^3]_{1,6} = 1$$

1.1.6 Node and edge properties

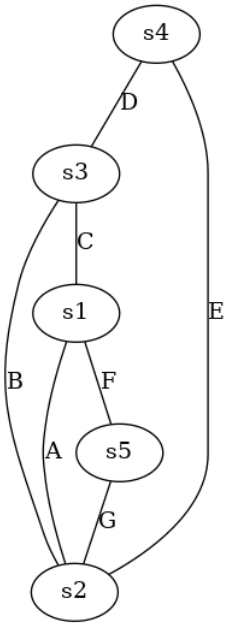
As mentioned in Section 1.1.4, edges can hold more information than just the binary relations between nodes. In fact, this concept can be generalized to nodes and even whole graphs. When studying graphs and networks, especially when using computational methods for applications like complex dynamics, it is the most natural way to phrase data on a graph. The data can be any real number or even categorical data, such as colors.

The matrices which hold the information mentioned before are

- **V: vertex (or node) attributes** (i.e. a label or number of neighbors)
- **E: edge (or link) attributes** (i.e. a label or edge weight)
- **U: global (or master node) attributes** (i.e. number of nodes or number of paths of length 2)

Global attributes usually get their values as an aggregation of the attributes of the nodes and edges, and methods applied on them. For instance, a molecule might have chemical elements as node attributes, types of bonds as edge attributes and the toxicity of the molecule as graph attributes. An example of a classroom should better illustrate the concept.

Example 1.3. *In this example, a classroom of 5 classmates is presented. Each student has a number of* ***node*** *attributes, their age, heigh and average grade (from F to A).* ***Edge*** *attributes between students hold information about their physical proximity when seated for class, and their kinship (as a real number between* $0 - 1$*). Finally,* ***global*** *attributes consist of information about the classroom, such as total number of students and class's failure rate.*



$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

FIGURE 1.5: Example graph of a small classroom with labeled edges and nodes

Node	Age	Height	Grade
s1	11.5	135	C
s2	12	140	B
s3	12	142	A
s4	11.5	132	A
s5	12	143	B

(A)

Edge	Distance	Kinship
A	1.5	0.5
B	1.2	0.5
C	0.5	0.8
D	2	0.35
E	2	0.3
F	0.5	0.9

(B)

TABLE 1.4: A) Node properties B) Edge properties

	No. Nodes	Failure %
G	5	0

TABLE 1.5: Graph Properties

1.2 Network Dynamics

Frequently, it is useful to consider cases where the status of the networks studied changes over time. This could mean that the topology of the network changes (i.e. nodes and edges are added or removed), the internal state of the network changes (the properties discussed in the previous section) or both.

The main concern of this thesis is with networks with a fixed topology , but with elements (nodes and edges) whose properties constitute dynamical quantities which can change over time. Following some dynamical rule, nodes can interact with their neighbors or change their own properties, with edges dictating which interactions are possible. In fact, the study of network dynamics combines graph theory with non-linear dynamics [7].

For many real world situations, a proper model of their processes consists of dynamical systems acting on networks. This can range from opinion spreading, epidemics, flow of electricity on grids, spread of packages on internet networks and many more systems whose dynamics are evolving on a network. In fact, many network processes can be understood

Chapter 2

Graph Neural Networks

2.1 Background - Artificial Neural Networks

2.1.1 Introduction

2.1.1.1 Historical Background

Artificial Neural Networks (ANN), or sometimes simply called **neural networks** is a class of computational models that mimic the way biological neural networks work, such as the human brain. Interest on the subject sparked after the seminal paper *"A Logical Calculus of the Ideas Immanent in Nervous Activity"* [8] by Warren McCulloch and Walter Pitts, where they proposed a computationally functional model of neural networks. Their suggestions showed that in principle, any function a digital computer compute, a neural net should too. The models they described had weights and thresholds, but they lacked a training method.

The suggestions of McCulloch and Pitts lead Frank Rosenblatt to create the *Perceptron* in 1958 [9], a binary classifier algorithm based on supervised learning[1]. Although initially promising, single layer perceptrons were not able to train on multiple classes of patterns and were eventually proven incapable of learning a XOR function [2] in the book *Perceptrons* [**?**], as the way they worked was by "separating" data linearly. This lead to a stagnation in machine learning research dubbed "AI winter", until the proposal of **backpropagation**[3] by Paul John Werbos in 1975 [**?**].

[1] Supervised learning is a machine learning training technique that optimizes a model based on examples input-output pairs.

[2] XOR (Exclusive or, $x \oplus y$) is a logical operation that is true only if its arguments differ.

[3] Backpropagation is a method of fine tuning a neural network based on the error rate obtained from previous runs of the program. It will be discussed in detail later in this thesis.

A renewed interest in the field lead to the development of the Cresceptron [**?**] in 1992, a method of training large networks with pooling layers (**max-pooling**) and down-sampling. GPU[4] usage made

2.1.1.2 Summary

One can think of ANNs as a directed graph, with a collection of nodes which are densely connected (called **artificial neurons**), transimiting signals to each other. These nodes are usually organized in sets of layers, with signals moving in one direction (i.e. *feed forward networks*) through weighted connections. Signals received on a single neuron are real numbers, and the output of a single neuron is the output of an aggregation of a non-linear function of the sum of its inputs. Thus, each neuron can be thought as a simple processing unit. The weighted connections between nodes might have an excitatory or inhibitory effect, based on these weights which can be positive, negative or very close to zero, having no effect. [10, Chap. 1].

[4]GPU - Graphics Processing Units is a specialized electronic circuit, a central part of modern computers which excels in efficient computation of algorithms which process large blocks of data parallelly, thus exceling in machine learning applications.

2.1.2 Convolutional Neural Networks

Chapter 3

Notation & Fundamentals

Chapter 4

Basic Principles and Implementation Framework for an [Problem to be Solved]

Chapter 5

Implementation and Core Components of [Platform Title]

Chapter 6

Experimentation & Validation

Chapter 7

Conclusions & Future Work

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