

# From Induction to Graph Theory

## Motivation, Algorithms, Applications, and Correctness

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This is a handout for the lecture on graph theory for my fellows. It covers the basic concepts of graph theory, including the definition of graphs, trees, and the basic algorithms for graph traversal. The handout also includes the correctness proof of the algorithms. Before delve into the graph theory, we will first introduce the concept of structural induction, which is the foundation of the correctness proof of the graph algorithms, and other structural algorithms.

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## §1. From Induction to General Induction

### Remark 1.1.

This lecture note is compiled using typst, and has two versions, one for the lecturer and one for the student. The latter version will be used during the lecture as handouts for the students. After the lecture, the lecturer version will be shared with students for further study or reference, which contains hints for lecture and solution/proofs for examples and exercises.

### §1.1. Recap on Induction

#### Definition 1.1.1 (Induction).

Induction is a method of proof in which we prove that a statement is true for all natural numbers by proving that it is true for the smallest natural number and then proving that if it is true for some natural number, then it is true for the next natural number.

The most common use case of induction is to prove a statement defined on the natural numbers.

#### Example 1.1.1.

Prove that  $1 + 2 + 3 \dots + n = \frac{n(n+1)}{2}$  for all  $n \geq 1$ .

**Proof.** Not discussed as it is trivial. □

#### §1.1.1. Motivation & Assumption

The principle of induction is based on the completeness of the natural numbers, which is the foundation of the induction. The completeness of the natural numbers is the property that every non-empty subset of the natural numbers has a least element. This property is the foundation of the induction, which allows us to prove a statement for all natural numbers by proving it for the smallest natural number and then proving that if it is true for some natural number, then it is true for the next natural number.

#### Definition 1.1.1.1 (Naive Definition of Natural Numbers).

The natural numbers are the set of positive integers, possibly including zero.

Is  $0 \in \mathbb{N}$  is a question that has been debated for centuries until now. In different branches of mathematics, the definition of natural numbers varies. In this lecture, we will use  $\mathbb{N}_0$  for the set of natural numbers including zero, and  $\mathbb{N}$  for the set of natural numbers excluding zero.

#### §1.1.1.1. Peano Axioms

**Axiom 1.1.1.1.1 (Peano Axioms).**

The Peano axioms are a set of axioms for the natural numbers presented by the 19th-century Italian mathematician Giuseppe Peano. These axioms define the natural numbers as a set of objects, a number system, and a set of operations.

1.  $0 \in \mathbb{N}$
2.  $\forall n \in \mathbb{N}, n' \in \mathbb{N}$ , where  $n'$  is called the successor of  $n$
3.  $\forall n \in \mathbb{N}, n' \neq 0$
4.  $\forall n, m \in \mathbb{N}, n' = m' \Rightarrow n = m$
5.  $\forall K \subseteq \mathbb{N}, [0 \in K \wedge \forall n(n \in K \Rightarrow n' \in K) \Rightarrow K = \mathbb{N}]$

**Remark 1.1.1.1.1.**

It is quite normal in both computer science and mathematics that a extremely complex system can be built on a few simple rules, or we say axioms here. Some examples are systems of differential equations, recurrence relations, etc.

**Problem 1.1.1.1.1 (Some Counter Examples).**

- For a number system consists of only  $\{0\}$ , what axioms are violated?
- For a number system consists of only  $\{0, 1\}$ , what axioms are violated?
- For a number system consists of only  $\{0, 1, 2\}$ , what axioms are violated?
- How can we find a counter example to show that axiom 5 is necessary?

**§1.1.1.2. Define Arithmetic Operations on Natural Numbers**

We can define the arithmetic operations on natural numbers using the Peano axioms.

**Notation 1.1.1.2.1 (pred and succ).**

$\text{pred}()$  and  $\text{succ}()$  are the predecessor and successor functions on natural numbers, respectively. formally,  $\text{pred} : \mathbb{N} \rightarrow \mathbb{N}$  and  $\text{succ} : \mathbb{N} \rightarrow \mathbb{N}$ . We will use  $\text{pred}(n)$  and  $\text{succ}(n)$  to denote the predecessor and successor of  $n$  in the following.

**Definition 1.1.1.2.1 (Addition on Natural Numbers).**

The addition of two natural numbers  $m$  and  $n$  is defined recursively as follows:

1.  $m + 0 = m$
2.  $m + \text{succ}(n) = \text{succ}(m + n)$

**Definition 1.1.1.2.2 (Multiplication on Natural Numbers).**

The multiplication of two natural numbers  $m$  and  $n$  is defined recursively as follows:

1.  $m \times 0 = 0$
2.  $m \times \text{succ}(n) = m \times n + m$

**Problem 1.1.1.2.1.**

How can we define the **subtraction** and **integer division** on natural numbers using the Peano axioms?

**§1.1.2. Weak Induction****Definition 1.1.2.1 (Weak Induction).**

Weak induction is a method of proof in which we prove that a statement is true for all natural numbers by proving that it is true for the smallest natural number and then proving that if it is true for some natural number, then it is true for the next natural number. Formally, let  $P(n)$  be a statement for each  $n \in \mathbb{N}_0$ . If  $P(0)$  is true, and  $\forall k \in \mathbb{N}_0, P(k) \Rightarrow P(k+1)$ , then  $\forall n \in \mathbb{N}_0, P(n)$  is true.

**Example 1.1.2.1.**

Prove that  $\forall n \in \mathbb{N}_0, 3 \mid n^3 + 2n$ .

**Remark 1.1.2.1.**

The statement  $3 \mid n^3 + 2n$  means that  $n^3 + 2n$  is divisible by 3, which means that

$$\exists m \in \mathbb{Z} : n^3 + 2n = 3m.$$

Accordingly, if  $3 \nmid n^3 + 2n$ , then  $n^3 + 2n$  is not divisible by 3, which means that

$$\exists m \in \mathbb{Z} : n^3 + 2n = 3m + r, r \in \mathbb{Z}_{>0}^{\leq 3}$$

- Chain of logic
  - Base case:  $P(0)$  holds.
  - Inductive step: Assume  $P(k)$  is true, prove  $P(k+1)$  is true. Finally we have

$$\forall k \geq 0, P(k) \Rightarrow P(k+1)$$

- Conclusion: by the principle of induction, we have  $\forall k \geq 0, P(k)$  is true.

**§1.1.3. Strong Induction****Definition 1.1.3.1 (Strong Induction).**

Strong induction is a method of proof in which we prove that a statement is true for all natural numbers by proving that it is true for the smallest natural number and then proving that if it is true for all natural numbers less than or equal to some natural number, then it is true for the next natural number. Formally, let  $P(n)$  be a statement for each  $n \in \mathbb{N}_0$ . If  $P(0)$  is true, and  $\forall k \in \mathbb{N}_0, (\forall m \leq k, P(m)) \Rightarrow P(k+1)$ , then  $\forall n \in \mathbb{N}, P(n)$  is true.

**Example 1.1.3.1.**

Prove that every integer greater than 1 can be written as a product of prime numbers.

- Chain of logic:
  - Base case:  $P(0)$  holds.
  - Inductive step: Assume  $P(0), P(1), \dots, P(k)$  are true, prove  $P(k+1)$  is true. Finally we have

$$\begin{aligned} & \forall k \geq 0, (\forall m \leq k, P(m)) \Rightarrow P(k+1) \text{ or} \\ & \forall k \geq 0, (P(0) \wedge P(1) \wedge \dots \wedge P(k)) \Rightarrow P(k+1) \text{ or} \\ & \forall k \geq 0, \bigwedge_{m \leq k} P(m) \Rightarrow P(k+1) \end{aligned}$$

#### §1.1.4. Generalised Induction

##### Definition 1.1.4.1 (Generalised Induction).

Generalised induction is a method of proof in which we prove that a statement is true for all objects in a set by proving that it is true for the smallest object and then proving that if it is true for all objects smaller than or equal to some object, then it is true for the next object. Formally, we implicitly define a bijection between the set of objects and the natural numbers, and then prove the statement for all natural numbers, as what we do in normal induction.

- pattern:
  - The conclusion holds when the structure is minimized.
  - Assume the conclusion holds for all smaller sub-structures, prove the conclusion holds for the current structure.
  - The conclusion holds for all structures.
- Why Generalize Induction?
  - Natural numbers are insufficient for complex structures (e.g., proving properties of graphs or programs).
  - Unified framework: Well-foundedness captures the essence of induction, allowing it to apply broadly.

##### §1.1.4.1. Structural Induction

##### Definition 1.1.4.1.1 (Structural Induction).

Structural induction is a generalisation of mathematical induction to data structures. It is a method of proof in which we prove that a property holds for all elements of a data structure by proving that it holds for the smallest elements and then proving that if it holds for all sub-structures of some element, then it holds for the element itself.

##### Remark 1.1.4.1.1.

Using structural induction is always dependent on the recursive definition of the data structure we are working on.

In the context of computer science, we often use structural induction, which is a kind of generalised induction, to prove properties of data structures including strings, trees, and graphs.

**Example 1.1.4.1.1 (Well-formed Parentheses).**

A Well-formed string of parentheses is a string that consists of a series of opening and closing parentheses, such that each closing parenthesis matches the most recent unmatched opening parenthesis. For example, the strings “(())” and “((()))” are well-formed, while the strings “()”( and “(())” are not well-formed. Prove that every well-formed string of parentheses has an equal number of opening and closing parentheses.

**Remark 1.1.4.1.2.**

Let  $\Sigma = \{ (, ) \}$ . Let  $\Sigma^*$  be the set of all finite strings over  $\Sigma$ . Let  $\text{open} : \Sigma^* \rightarrow \mathbb{N}_0$  and  $\text{close} : \Sigma^* \rightarrow \mathbb{N}_0$  be functions counting the number of opening and closing parentheses in a string  $S$ , respectively. ( $\mathbb{N}_0$  denotes the set of non-negative integers). The set of **Well-Formed Parentheses** strings, denoted WFP, is a subset of  $\Sigma^*$  defined recursively as the smallest set satisfying:

[Base Case:] The empty string  $\lambda$  is in WFP.

[Recursive Step 1:] If  $S'$  is in WFP, then the string  $(S')$  is in WFP, where  $(S')$  is the concatenation of  $S'$  with an opening and closing parenthesis.

[Recursive Step 2:] If  $S'$  and  $T'$  are in WFP, then their concatenation  $S'T'$  is in WFP.

**Example 1.1.4.1.2.**

Let  $\Sigma$  be a finite alphabet. A string over  $\Sigma$  is a finite sequence of characters from  $\Sigma$  recursively defined by the alphabet. We use  $\Sigma^*$  to denote the set of all strings over  $\Sigma$ . For some string  $w \in \Sigma^*$ , let  $w^R$  denote the reversed string of  $w$ . Prove that for any two strings  $w_1, w_2 \in \Sigma^*$ ,

$$w_1^R w_2^R = (w_2 w_1)^R$$

Note: you may use  $\lambda$  to denote the empty string. Additionally,  $w^R$  is recursively defined as follows:

- If  $w = \lambda$ , then  $w^R = \lambda$ .
- If  $w = xw'$ , where  $x \in \Sigma$  and  $w' \in \Sigma^*$ , then  $w^R = w'^R x$ .

- Other generalised induction(not covered in this lecture):
  - Transfinite Induction
  - Noetherian Induction

## §2. Introduction to Graph Theory

**Definition 2.1 (Graph).**

A graph  $G$  is an ordered pair  $G = (V, E)$ , where  $V$  is a set of vertices and  $E$  is a set of edges. Each edge is a pair of vertices  $(u, v)$ , where  $u, v \in V$ . We use  $V(G)$  and  $E(G)$  to denote the set of vertices and edges of  $G$ , respectively.

- In a nutshell, a graph is an abstraction of some tangible or intangible objects and their relationships.
- The vertices represent the objects, and the edges represent the relationships between the objects.

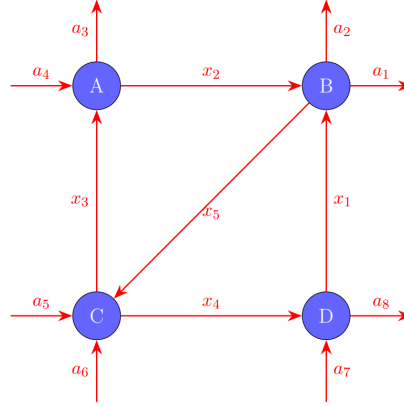


Figure 1: An example of a graph for road traffic

- The above is a Directed Graph, where the edges have directions.
- The graph is also weighted, meaning that the edges have weights, or attached with a value.
- Using the notation  $G = (V, E)$ , we can represent the graph as  $G = (\{A, B, C, D\}, \{(A, B), (B, C), (C, A), (C, D), (D, B)\})$ .

## §2.1. Some Basic Notions

### Definition 2.1.1 (Weight of Edges).

The weight of an edge in a graph is a value associated with the edge. The weight can represent the cost, distance, probability or any other value associated with the edge.

### Definition 2.1.2 (Direction of Edges).

The edges of a graph can be directed or undirected. In a **directed graph**, the edges have directions, meaning that the edge  $(u, v)$  is different from the edge  $(v, u)$ . In an **undirected graph**, the edges do not have directions, meaning that the edge  $(u, v)$  is the same as the edge  $(v, u)$ .

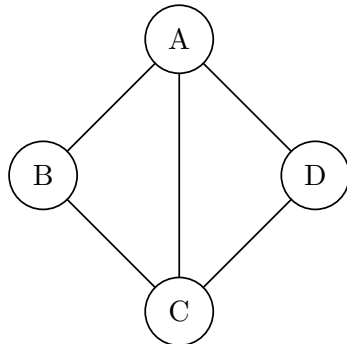


Figure 3: Undirected Graph

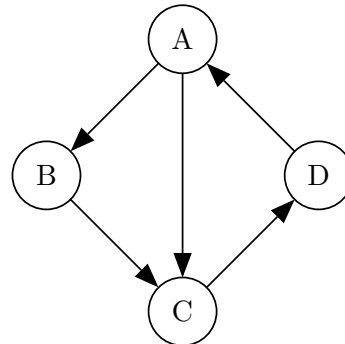


Figure 4: Directed Graph

**Definition 2.1.3 (Loop).**

A loop is an edge that connects a vertex to itself. In a graph, a loop is an edge of the form  $(v, v)$ , where  $v \in V$ .

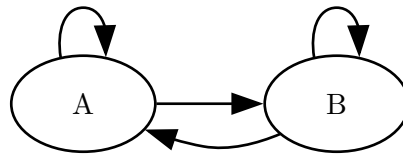


Figure 5: Graph with a loop

**Definition 2.1.4 (Simple Graph).**

A simple graph is a graph in which there is at most one edge between any two vertices and no edge from a vertex to itself.

| Type                  | Edges                   | Multiple Edges? | Loops Allowed? |
|-----------------------|-------------------------|-----------------|----------------|
| Simple graph          | Undirected              | No              | No             |
| Multigraph            | Undirected              | Yes             | No             |
| Pseudograph           | Undirected              | Yes             | Yes            |
| Simple directed graph | Directed                | No              | No             |
| Directed multigraph   | Directed                | Yes             | Yes            |
| Mixed graph           | Directed and undirected | Yes             | Yes            |

Table 1: Graph Typology

## §2.2. Applications of Graph

Graphs are widely used in computer science, mathematics, and other fields to model relationships between objects. Some common applications of graphs include:

- Social networks: representing relationships between people.
- Road networks: representing roads and intersections.
- Network traffic: representing data flow between devices.
- Computer networks: representing connections between computers.
- Scheduling: representing tasks and dependencies between tasks.
- Circuit design: representing components and connections between components.

**Example 2.2.1.**

An example of a graph for network traffic is the webpage ranking. Webpage ranking is an algorithm used by search engines to rank web pages in search results. The algorithm uses a graph to represent the web pages and the links between them. We cannot discuss the details of the algorithm here, but in this algorithm, we use a directed weighted graph to represent possibility of a user visiting a webpage from another webpage.



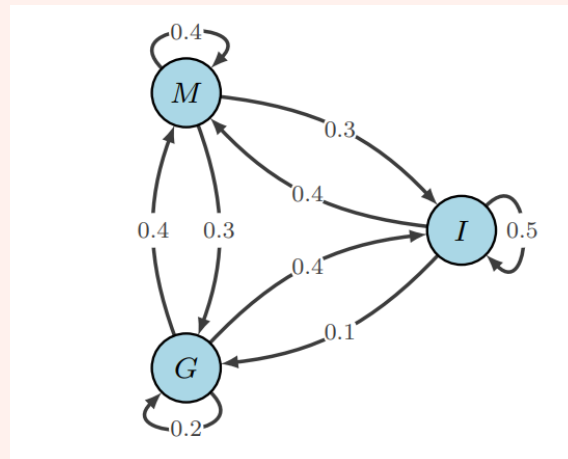


Figure 6: An example of a graph for network traffic

We will look into the details of this example in matrix representation of a graph.

## §2.3. More Terminologies

### Definition 2.3.1 (Degree of a Vertex).

The degree of a vertex  $v$  in a graph is the number of edges incident to  $v$ . In an undirected graph, the degree of a vertex is the number of edges connected to the vertex. In a directed graph, the degree of a vertex is the sum of the in-degree and out-degree of the vertex, where the in-degree is the number of edges pointing to the vertex, and the out-degree is the number of edges pointing from the vertex.

### §2.3.1. Path and Cycle

#### Definition 2.3.1.1 (Path).

A path in a graph is a sequence of vertices in which each vertex is connected to the next vertex by an edge. A path is simple if it does not contain any repeated vertices.

For example, in the graph below, the sequence  $A \rightarrow B \rightarrow C \rightarrow D$  is a path.

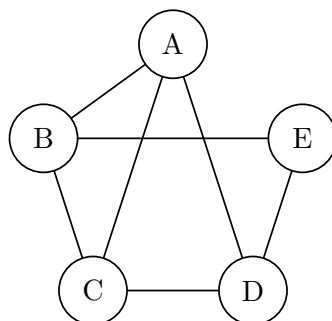


Figure 7: A graph with cycle

We also introduce some special subsets of paths.

**Definition 2.3.1.2 (Cycle).**

A cycle in a graph is a path that starts and ends at the same vertex. A cycle is simple if it does not contain any repeated vertices except the starting and ending vertex.

For example, in the previous graph, the sequence  $A \rightarrow B \rightarrow C \rightarrow D \rightarrow A$  is a cycle.

**§2.3.1.1. Euler Path and Circuit****Definition 2.3.1.1.1 (Euler Path).**

An Euler path in a graph is a path that visits every edge exactly once. An Euler path may start and end at different vertices.

**Definition 2.3.1.1.2 (Euler Circuit).**

An Euler circuit in a graph is a cycle that visits every edge exactly once. An Euler circuit starts and ends at the same vertex.

**Problem 2.3.1.1.1.**

Can you find an Euler path/cycle in Figure 7?

**Theorem 2.3.1.1.1 (Euler's Theorem).**

Let  $G = (V, E)$  be a finite, connected, undirected graph, then  $G$ :

- Has an Euler path if and only if it has exactly two or zero vertices of odd degree.
- Has an Euler circuit if and only if all vertices have even degree.

**Lemma 2.3.1.1.1 (Maximum possible edges in a graph).**

Let  $G = (V, E)$  be a graph with  $n$  vertices.

If  $G$  is undirected, then the maximum number of edges in  $G$  is  $\frac{|V|(|V|-1)}{2} = \frac{n(n-1)}{2}$ .

If  $G$  is directed, then the maximum number of edges in  $G$  is  $|V|(|V|-1) = n(n-1)$ .

**Proof.** We use combinatorial proof techniques to prove this lemma.

- For an undirected graph, the number of edges is the number of ways to choose two vertices from  $V$ . This is given by the binomial coefficient  $\binom{n}{2} = \frac{n(n-1)}{2}$ .
- For a directed graph, the number of edges is the number of ways to choose an ordered pair of vertices from  $V$ . This is given by the product  $n(n-1)$ , by the rule of product from combinatorics.

□

**§2.3.2. Connected & Acyclic Graph**

**Definition 2.3.2.1 (Connected Graph).**

A graph is connected if there is a path between every pair of vertices in the graph.

**Definition 2.3.2.2 (Acyclic Graph).**

A graph is acyclic if it does not contain any cycles.

**Definition 2.3.2.3 (Complete Acyclic Graph).**

A complete acyclic graph is a graph in which every pair of vertices is connected by a **unique** path.

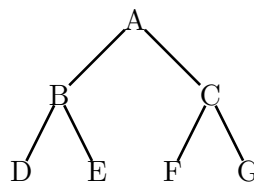


Figure 8: A tree with 7 vertices

**Remark 2.3.2.1.**

A more well-known name for a complete acyclic graph is a **tree**. Figure 8 is called a binary tree, as each vertex has at most two child nodes. It is also a complete or full binary tree, as all levels are fully filled except possibly for the last level, which is filled from left to right.

**Problem 2.3.2.1.**

Can you give a recursive definition of a tree? Thus, give a formal definition of a binary tree.

**§2.3.2.1. Binary Tree**

Binary tree is one of the most common tree structures in computer science.

We have already discussed the recursive definition of a binary tree. Here is another definition of a binary tree:

**Definition 2.3.2.1.1 (Binary Tree).**

A binary tree is a tree in which each node has at most two children, which are referred to as the left child and the right child.

The top vertex of the tree is called the **root** of the tree. The vertices that have no children are called **leaves** (node).

- A binary tree is called a **full binary tree** if each node has either zero or two children.
- A binary tree is called a **complete binary tree** if all levels are fully filled except possibly for the last level, which is filled from left to right.
- A binary tree is called a **perfect binary tree** if all internal nodes have two children and all leaves are at the same level.

**Example 2.3.2.1.1.**

The tree Figure 8 is a binary tree. It is also a complete binary tree, as all levels are fully filled except possibly for the last level, which is filled from left to right. Node A

**Problem 2.3.2.1.1.**

Prove that a tree with  $n$  vertices has  $n - 1$  edges.

**Problem 2.3.2.1.2.**

The level of a node in a tree is the number of edges on the path from the root to the leaf node. The root is at level 0.

For a binary tree of  $n$  nodes, the maximum height of the tree is  $n - 1$ . Prove this proposition.

**Problem 2.3.2.1.3.**

Prove that at the  $i$ -th level of a binary tree, the maximum number of nodes is  $2^i$  (counting from 0).

**Problem 2.3.2.1.4.**

If a binary tree of height  $h$  has  $l$  leaves, then  $h \geq \lceil \log_2 l \rceil$ , if the binary tree is full and balanced, then  $h = \lceil \log_2 l \rceil$ .

Prove this proposition.

**§2.3.3. Subgraph****Definition 2.3.3.1 (Subgraph).**

A subgraph of a graph  $G = (V, E)$  is a graph  $G' = (V', E')$  such that  $V' \subseteq V$  and  $E' \subseteq E$ . That is, a subgraph is a graph that contains a subset of the vertices and edges of the original graph.

In a straightforward way, a subgraph is a graph that can be obtained by removing some vertices and edges from the original graph.

**§2.3.4. Complete Graph****Definition 2.3.4.1 (Complete Graph).**

A complete graph is a graph in which every pair of vertices is connected by an edge. The number of edges in a complete graph with  $n$  vertices is

$$\binom{n}{2} = \frac{n(n-1)}{2}.$$

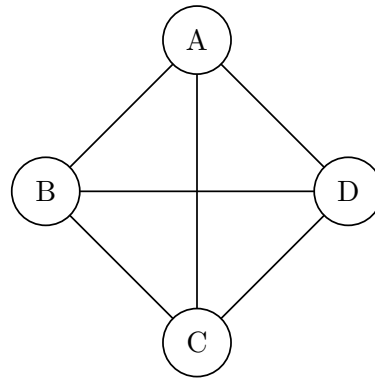


Figure 9: A complete graph with 4 vertices

**Remark 2.3.4.1.**

A complete graph with  $n$  vertices is denoted by  $K_n$ .

**§2.3.5. Bipartite Graph****Definition 2.3.5.1 (Bipartite Graph).**

A bipartite graph is a graph whose vertices can be divided into two disjoint sets  $V_1$  and  $V_2$  such that every edge connects a vertex in  $V_1$  to a vertex in  $V_2$ .

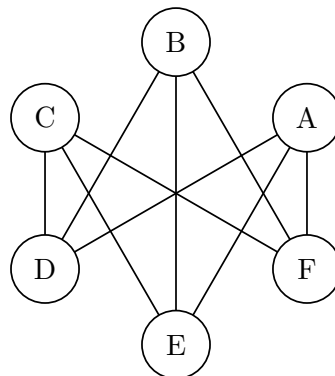


Figure 10: A bipartite graph with 3 vertices in each set

**Notation 2.3.5.1.**

A complete bipartite graph, by convention, is denoted by  $K_{\{m,n\}}$ , where  $m$  and  $n$  are the number of vertices in the two sets  $V_1$  and  $V_2$ , respectively.

For example, the graph above is denoted by  $K_{\{3,3\}}$ .

**§2.3.6. Finite and Infinite Graph****Definition 2.3.6.1 (Finite Graph).**

A graph is finite if it has a finite number of vertices and edges.

**Definition 2.3.6.2 (Infinite Graph).**

A graph is infinite if it has an infinite number of vertices or edges.

**Remark 2.3.6.1.**

The concept of infinite graphs is essential in mathematics and computer science, especially in the study of infinite structures and algorithms on infinite structures.

**Problem 2.3.6.1.**

Anything discussed earlier in the lecture can be abstract by a infinite graph?

## §2.4. Useful Results on Graph

### §2.4.1. Handshaking Theorem

**Theorem 2.4.1.1 (Handshaking Theorem).**

The handshaking theorem states that for any graph, the sum of the degrees of all vertices is equal to twice the number of edges. A loop at a vertex  $v$  is typically counted as contributing 2 to  $\deg(v)$ .

Formally, let  $G = (V, E)$  be an undirected graph with  $m = |E|$  edges. Then

$$\sum_{v \in V} \deg(v) = 2m.$$

How can we prove it? Eventhough it is trivial, we can prove it by structural induction on the definition of a undirected graph.

**Problem 2.4.1.1.**

There are 605 people in a party. Each person shakes hands with some other people. Suppose that each of them shakes hands with at least one person. Prove that there must be someone who shakes hands with at least two persons.

**Theorem 2.4.1.2 (Number of Vertices with Odd Degree).**

In any simple graph  $G$ , the number of vertices with odd degree is always even.

**Problem 2.4.1.2.**

Prove that among a group of people ( $n > 2$ ), there are at least 2 persons where the number of people they know is the same.

## §2.5. Representation of Graph

Graph can be represented in different ways, including adjacency matrix, adjacency list, and incidence matrix. Each representation has its own advantages and disadvantages, and the choice of representation depends on the specific problem being solved. We introduce two of the most common representations: adjacency matrix and adjacency list.

### §2.5.1. Adjacency Matrix

#### Definition 2.5.1.1 (Adjacency Matrix).

An adjacency matrix is a square matrix used to represent a graph. The rows and columns of the matrix correspond to the vertices of the graph, and the entries of the matrix indicate whether there is an edge between the corresponding vertices. If there is an edge between vertices  $u$  and  $v$ , the entry  $a_{uv}$  is 1; otherwise, it is 0.

If the graph is weighted, the entries of the adjacency matrix can be the weights of the edges instead of 0 or 1.

Formally, for a un weighted graph, the adjacency matrix  $A$  of a graph  $G = (V, E)$  with  $n$  vertices is an  $n \times n$  matrix defined as

$$A = (a_{ij}) = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix},$$

where  $a_{ij} = 1$  if  $(v_i, v_j) \in E$  and  $a_{ij} = 0$  otherwise.

For a weighted graph, the adjacency matrix  $A$  of a graph  $G = (V, E)$  with  $n$  vertices is an  $n \times n$  matrix defined as

$$A = (a_{ij}) = \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{n1} & w_{n2} & \cdots & w_{nn} \end{pmatrix},$$

where  $w_{ij}$  is the weight of the edge  $(v_i, v_j)$  if  $(v_i, v_j) \in E$  and  $w_{ij} = 0$  otherwise.

#### Example 2.5.1.1.

Consider the graph  $G = (V, E)$  with

$$V = \{A, B, C, D\}$$

and

$$E = \{(A, B), (B, C), (C, A), (C, D), (D, B)\}.$$

The adjacency matrix of  $G$  is

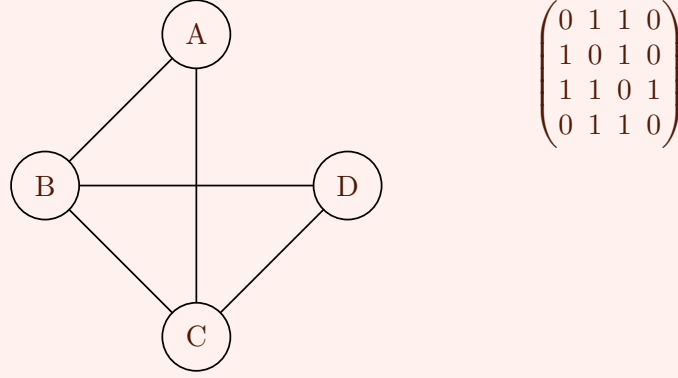


Figure 11: A graph and its adjacency matrix

### §2.5.1.1. Adjacency Matrix Power

#### Definition 2.5.1.1.1 (Matrix Power).

The power of a matrix  $A$  is defined as the matrix obtained by multiplying  $A$  by itself  $n$  times. The power of a matrix  $A$  to the  $n$ th power is denoted as  $A^n$ . For example, for a  $n$  dimensional square matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix},$$

The matrix  $A^2$  is obtained by multiplying  $A$  by itself:

$$A^2 = A \cdot A = \begin{pmatrix} \sum_{k=1}^n a_{1k}a_{k1} & \sum_{k=1}^n a_{1k}a_{k2} & \cdots & \sum_{k=1}^n a_{1k}a_{kn} \\ \sum_{k=1}^n a_{2k}a_{k1} & \sum_{k=1}^n a_{2k}a_{k2} & \cdots & \sum_{k=1}^n a_{2k}a_{kn} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{k=1}^n a_{nk}a_{k1} & \sum_{k=1}^n a_{nk}a_{k2} & \cdots & \sum_{k=1}^n a_{nk}a_{kn} \end{pmatrix}$$

#### Example 2.5.1.1.1 (Matrix Power).

A simple example of 3 by 3 matrix  $A$  is

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

The matrix  $A^2$  is

$$A^2 = A \cdot A = \begin{pmatrix} 30 & 36 & 42 \\ 66 & 81 & 96 \\ 102 & 126 & 150 \end{pmatrix}.$$

Let's decompose the calculation of each entry:

- The entry  $a_{11} = a_{11}a_{11} + a_{12}a_{21} + a_{13}a_{31} = 1 \times 1 + 2 \times 4 + 3 \times 7 = 30$ .



- The entry  $a_{12} = a_{11}a_{12} + a_{12}a_{22} + a_{13}a_{32} = 1 \times 2 + 2 \times 5 + 3 \times 8 = 36$ .
- The entry  $a_{13} = a_{11}a_{13} + a_{12}a_{23} + a_{13}a_{33} = 1 \times 3 + 2 \times 6 + 3 \times 9 = 42$ .
- The entry  $a_{21} = a_{21}a_{11} + a_{22}a_{21} + a_{23}a_{31} = 4 \times 1 + 5 \times 4 + 6 \times 7 = 66$ .
- The entry  $a_{22} = a_{21}a_{12} + a_{22}a_{22} + a_{23}a_{32} = 4 \times 2 + 5 \times 5 + 6 \times 8 = 81$ .
- The entry  $a_{23} = a_{21}a_{13} + a_{22}a_{23} + a_{23}a_{33} = 4 \times 3 + 5 \times 6 + 6 \times 9 = 96$ .
- The entry  $a_{31} = a_{31}a_{11} + a_{32}a_{21} + a_{33}a_{31} = 7 \times 1 + 8 \times 4 + 9 \times 7 = 102$ .
- The entry  $a_{32} = a_{31}a_{12} + a_{32}a_{22} + a_{33}a_{32} = 7 \times 2 + 8 \times 5 + 9 \times 8 = 126$ .
- The entry  $a_{33} = a_{31}a_{13} + a_{32}a_{23} + a_{33}a_{33} = 7 \times 3 + 8 \times 6 + 9 \times 9 = 150$ .

**Problem 2.5.1.1.1.**

Consider the previous matrix, what is the trend of the matrix power  $A^n$  as  $n$  increases? That is to say, how do we evaluate

$$\lim_{n \rightarrow \infty} A^n.$$

Also think about:

- what is the adjacency matrix of graph in Example 2.2.1?
- What is the adjacency matrix of the graph in Figure 7? Work on it and try to find is there any interesting property of the matrix and its power.

**Proposition 2.5.1.1.1 (Significance of Matrix Power).**

For a simple undirected graph  $G$ , the matrix power  $M^n$  will have some interesting properties:

- the  $(i, j)$  entry of  $M^n$  is the number of paths of length  $n$  from vertex  $i$  to vertex  $j$ .
- the  $(i, i)$  entry of  $M^n$  is the number of circuits of length  $n$  starting and ending at vertex  $i$ .

**Proof.** We will prove the proposition by induction on  $n$ .

**Base case:** For  $n = 1$ , the matrix  $M^1$  is the adjacency matrix of the graph  $G$ , and the  $(i, j)$  entry of  $M^1$  is 1 if there is an edge between vertex  $i$  and vertex  $j$  and 0 otherwise. Therefore, the base case holds.

**Inductive step:** Assume the proposition holds for some  $n = k$ . We need to prove that the proposition holds for  $n = k + 1$ .

Let  $M^k$  be the matrix obtained by raising the adjacency matrix  $M$  to the  $k$ th power. The  $(i, j)$  entry of  $M^k$  is the number of paths of length  $k$  from vertex  $i$  to vertex  $j$ . The  $(i, i)$  entry of  $M^k$  is the number of circuits of length  $k$  starting and ending at vertex  $i$ .

The  $(i, j)$  entry of  $M^{k+1}$  is the sum of the products of the  $(i, k)$  entry of  $M^k$  and the  $(k, j)$  entry of  $M$ . Therefore, the  $(i, j)$  entry of  $M^{k+1}$  is the number of paths of length  $k + 1$  from vertex  $i$  to vertex  $j$ . The  $(i, i)$  entry of  $M^{k+1}$  is the sum of the products of the  $(i, k)$  entry of  $M^k$  and the  $(k, i)$  entry of  $M$ . Therefore, the  $(i, i)$  entry of  $M^{k+1}$  is the number of circuits of length  $k + 1$  starting and ending at vertex  $i$ . Therefore, the proposition holds for  $n = k + 1$ .

By the principle of mathematical induction, the proposition holds for all  $n \in \mathbb{N}$ .  $\square$

## §2.5.1.2. Implementation

```

1  from typing import TypeVar, Generic, List, Optional, Tuple, Dict,
   Set, Any
2
3  V = TypeVar('V') # Type for vertex identifiers
4  E = TypeVar('E') # Type for edge weights (can be float, int, etc.)
5
6  class MatrixGraph(Generic[V, E]):
7      """
8      A graph implementation using an adjacency matrix.
9
10     Handles directed/undirected and weighted/unweighted graphs.
11     For unweighted graphs, the edge value '1' is used in the matrix.
12     For weighted graphs, the edge weight is stored.
13     'None' indicates the absence of an edge.
14
15     Note: Adding/removing vertices is  $O(V^2)$  due to matrix resizing.
16           Edge lookups/updates are  $O(1)$  after vertex index lookup.
17           Space complexity is  $O(V^2)$ .
18           This representation is generally better for dense graphs.
19     """
20
21     def __init__(self, directed: bool = False, weighted: bool = False):
22         """
23         Initializes an empty graph.
24
25         Args:
26             directed: True if the graph is directed, False otherwise.
27             weighted: True if the graph edges have weights, False otherwise.
28
29         Complexity:  $O(1)$ 
30         """
31         self._is_directed: bool = directed
32         self._is_weighted: bool = weighted
33         self._adj_matrix: List[List[Optional[E]]] = []
34         self._vertex_to_index: Dict[V, int] = {}
35         self._index_to_vertex: List[V] = []
36         self._num_vertices: int = 0
37         self._num_edges: int = 0
38
39     def num_vertices(self) -> int:
40         """
41         Returns the number of vertices in the graph.
42         Complexity:  $O(1)$ 
43         """
44         return self._num_vertices

```

```

45
46     def num_edges(self) -> int:
47         """
48         Returns the number of edges in the graph.
49         Complexity: O(1)
50         """
51         return self._num_edges
52
53     def is_directed(self) -> bool:
54         """
55         Returns True if the graph is directed, False otherwise.
56         Complexity: O(1)
57         """
58         return self._is_directed
59
60     def is_weighted(self) -> bool:
61         """
62         Returns True if the graph is weighted, False otherwise.
63         Complexity: O(1)
64         """
65         return self._is_weighted
66
67     def get_vertices(self) -> List[V]:
68         """
69         Returns a list of all vertices in the graph.
70         Complexity: O(V) - due to copying the list of vertices.
71         """
72         # Return a copy to prevent external modification of internal list
73         return list(self._index_to_vertex)
74
75     def has_vertex(self, vertex: V) -> bool:
76         """
77         Checks if a vertex exists in the graph.
78         Complexity: O(1) average - dictionary lookup. O(V) worst case (highly
79         unlikely with standard hash functions).
80         """
81         return vertex in self._vertex_to_index
82
83     def _get_vertex_index(self, vertex: V) -> int:
84         """
85         Helper to get the index of a vertex, raising ValueError if not found.
86         Complexity: O(1) average - dictionary lookup. O(V) worst case.
87         """
88         index = self._vertex_to_index.get(vertex)
89         if index is None:
90             raise ValueError(f"Vertex '{vertex}' not found in the graph.")

```

```

90         return index
91
92     def add_vertex(self, vertex: V) -> None:
93         """
94         Adds a vertex to the graph.
95
96         If the vertex already exists, this method does nothing.
97         Complexity:  $O(V^2)$  - dominated by matrix resizing (adding a row and
98         column).
99
100         0(1) average if vertex already exists.
101
102         Args:
103         vertex: The vertex identifier to add.
104         """
105         if self.has_vertex(vertex): # 0(1) avg
106             return
107
108         new_index = self._num_vertices
109         self._vertex_to_index[vertex] = new_index # 0(1) avg
110         self._index_to_vertex.append(vertex)      # 0(1) avg (amortized)
111
112         # Resize matrix: Add a new column to existing rows - 0(V)
113         for row in self._adj_matrix:
114             row.append(None) # 0(1) for each row
115
116         # Add a new row for the new vertex - 0(V) creation + 0(V) append = 0(V)
117         new_row = [None] * (self._num_vertices + 1)
118         self._adj_matrix.append(new_row) # 0(1) avg (amortized for list append)
119
120         # Overall: 0(1) + 0(V) + 0(V) = 0(V), BUT standard analysis often
121         # assumes
122         # matrix allocation/copying dominates, leading to  $O(V^2)$  practical view
123         # if
124         # underlying memory needs reallocation or if we consider creating the
125         # new row/col elements.
126         # Let's stick to  $O(V^2)$  as the most common analysis for matrix
127         # resizing.
128         # If implemented without full reallocation (e.g., pre-allocating larger
129         # blocks),
130         # it could be closer to 0(V), but the standard matrix model implies  $V^2$ 
131         # for resizing.
132
133         self._num_vertices += 1 # 0(1)
134
135     def remove_vertex(self, vertex: V) -> None:
136         """
137         Removes a vertex and all incident edges from the graph.

```

```

130
131     Complexity:  $O(V^2)$  - dominated by creating the new smaller matrix and
132                recalculating edges. Index remapping is  $O(V)$ .
133
134     Args:
135         vertex: The vertex identifier to remove.
136
137     Raises:
138         ValueError: If the vertex does not exist.
139     """
140     if not self.has_vertex(vertex): #  $O(1)$  avg
141         raise ValueError(f"Vertex '{vertex}' not found for removal.")
142
143     idx_to_remove = self._vertex_to_index[vertex] #  $O(1)$  avg
144
145     # 1. Adjust edge count ( preliminary check, full recalc below) -  $O(V)$ 
146     # edges_removed = 0 ... (omitted for brevity, recalc is dominant)
147
148     # 2. Remove vertex from mappings -  $O(1)$  avg dict del,  $O(V)$  list pop
149     del self._vertex_to_index[vertex]
150     self._index_to_vertex.pop(idx_to_remove)
151
152     # 3. Remap indices -  $O(V)$ 
153     for v, i in self._vertex_to_index.items():
154         if i > idx_to_remove:
155             self._vertex_to_index[v] = i - 1
156
157     # 4. Create a new smaller matrix -  $O(V^2)$ 
158     new_size = self._num_vertices - 1
159     new_matrix = [[None for _ in range(new_size)] for _ in range(new_size)]
160     current_new_row = 0
161     for old_row_idx in range(self._num_vertices):
162         if old_row_idx == idx_to_remove: continue
163         current_new_col = 0
164         for old_col_idx in range(self._num_vertices):
165             if old_col_idx == idx_to_remove: continue
166             new_matrix[current_new_row][current_new_col] =
167                 self._adj_matrix[old_row_idx][old_col_idx]
168             current_new_col += 1
169         current_new_row += 1
170
171     self._adj_matrix = new_matrix #  $O(1)$  reference assignment
172     self._num_vertices -= 1 #  $O(1)$ 
173
174     # 5. Recalculate edge count -  $O(V^2)$ 
175     self._recalculate_num_edges()

```

```

175
176
177     def _recalculate_num_edges(self):
178         """
179         Helper to recalculate the edge count by iterating the matrix.
180         Complexity:  $O(V^2)$  - iterates through the entire matrix.
181         """
182         count = 0
183         for r in range(self._num_vertices):
184             for c in range(self._num_vertices):
185                 if self._adj_matrix[r][c] is not None:
186                     if self._is_directed:
187                         count += 1
188                     else:
189                         if r <= c: # Count undirected edges once
190                             count += 1
191         self._num_edges = count
192
193
194     def add_edge(self, source: V, destination: V, weight: Optional[E] = 1) ->
None:
195         """
196         Adds an edge between source and destination vertices.
197
198         If the graph is unweighted, the weight parameter is ignored, and 1 is
199         stored.
200         If the graph is weighted, a weight must be provided (defaults to 1 if
201         None).
202         If the edge already exists, its weight is updated (if weighted).
203
204         Complexity:  $O(1)$  average - after vertex index lookups (which are  $O(1)$ 
205         avg).
206
207         Args:
208             source: The source vertex identifier.
209             destination: The destination vertex identifier.
210             weight: The weight of the edge (used only if graph is weighted).
211             Defaults to 1.
212
213         Raises:
214             ValueError: If source or destination vertices do not exist.
215             ValueError: If the graph is weighted and weight is None.
216         """
217         u_idx = self._get_vertex_index(source) #  $O(1)$  avg
218         v_idx = self._get_vertex_index(destination) #  $O(1)$  avg
219
220         edge_value: Optional[E]

```

```

217         if self._is_weighted:
218             if weight is None:
219                 edge_value = 1 # Defaulting to 1
220             else:
221                 edge_value = weight
222         else:
223             edge_value = 1 # Use 1 for unweighted graphs
224
225         # Check if edge is newly added - O(1)
226         is_new_edge = self._adj_matrix[u_idx][v_idx] is None
227
228         # Matrix update - O(1)
229         self._adj_matrix[u_idx][v_idx] = edge_value
230         if not self._is_directed:
231             # Additional matrix update - O(1)
232             is_new_reverse = self._adj_matrix[v_idx][u_idx] is None if u_idx !=
                v_idx else False
233             self._adj_matrix[v_idx][u_idx] = edge_value
234             # Edge count update - O(1)
235             if is_new_edge or is_new_reverse:
236                 self._num_edges += 1
237             elif is_new_edge: # Directed
238                 # Edge count update - O(1)
239                 self._num_edges += 1
240
241     def remove_edge(self, source: V, destination: V) -> None:
242         """
243         Removes the edge between source and destination.
244
245         If the graph is undirected, removes the edge in both directions.
246         Does nothing if the edge doesn't exist.
247
248         Complexity: O(1) average - after vertex index lookups (which are O(1)
                avg).
249
250         Args:
251             source: The source vertex identifier.
252             destination: The destination vertex identifier.
253
254         Raises:
255             ValueError: If source or destination vertices do not exist.
256         """
257         u_idx = self._get_vertex_index(source) # O(1) avg
258         v_idx = self._get_vertex_index(destination) # O(1) avg
259
260         # Check existence - O(1)

```

```

261         edge_existed = self._adj_matrix[u_idx][v_idx] is not None
262
263         if edge_existed:
264             # Matrix update(s) - O(1)
265             self._adj_matrix[u_idx][v_idx] = None
266             if not self._is_directed:
267                 if u_idx != v_idx:
268                     self._adj_matrix[v_idx][u_idx] = None
269             # Edge count update - O(1)
270             self._num_edges -= 1
271         else: # Directed
272             # Edge count update - O(1)
273             self._num_edges += 1
274
275
276     def has_edge(self, source: V, destination: V) -> bool:
277         """
278         Checks if an edge exists between source and destination.
279
280         Complexity: O(1) average - after vertex index lookups (which are O(1)
281         avg).
282
283         Args:
284             source: The source vertex identifier.
285             destination: The destination vertex identifier.
286
287         Returns:
288             True if the edge exists, False otherwise.
289
290         Raises:
291             ValueError: If source or destination vertices do not exist.
292         """
293         u_idx = self._get_vertex_index(source) # O(1) avg
294         v_idx = self._get_vertex_index(destination) # O(1) avg
295         # Matrix access - O(1)
296         return self._adj_matrix[u_idx][v_idx] is not None
297
298     def get_edge_data(self, source: V, destination: V) -> Optional[E]:
299         """
300         Gets the weight or data associated with the edge.
301
302         Returns None if the edge does not exist.
303         For unweighted graphs, returns 1 if the edge exists.
304
305         Complexity: O(1) average - after vertex index lookups (which are O(1)
306         avg).

```



```

305
306     Args:
307         source: The source vertex identifier.
308         destination: The destination vertex identifier.
309
310     Returns:
311         The edge weight/data, or None if the edge doesn't exist.
312
313     Raises:
314         ValueError: If source or destination vertices do not exist.
315     """
316     u_idx = self._get_vertex_index(source) # O(1) avg
317     v_idx = self._get_vertex_index(destination) # O(1) avg
318     # Matrix access - O(1)
319     return self._adj_matrix[u_idx][v_idx]
320
321     def get_neighbors(self, vertex: V) -> List[Tuple[V, Optional[E]]]:
322         """
323         Gets a list of neighbors for a given vertex, along with edge data.
324
325         Complexity: O(V) - Must iterate through a full row of the matrix.
326
327     Args:
328         vertex: The vertex identifier.
329
330     Returns:
331         A list of tuples, where each tuple is (neighbor_vertex,
332         edge_weight).
333         Returns an empty list if the vertex has no neighbors.
334
335     Raises:
336         ValueError: If the vertex does not exist.
337     """
338     u_idx = self._get_vertex_index(vertex) # O(1) avg
339     neighbors = []
340     # Iterate through row - O(V)
341     for v_idx in range(self._num_vertices):
342         edge_data = self._adj_matrix[u_idx][v_idx] # O(1) access
343         if edge_data is not None:
344             neighbor_vertex = self._index_to_vertex[v_idx] # O(1) access
345             neighbors.append((neighbor_vertex, edge_data)) # O(1) avg
346             append
347     return neighbors
348
349     def get_edges(self) -> List[Tuple[V, V, Optional[E]]]:
350         """

```

```

349         Gets a list of all edges in the graph.
350
351         For undirected graphs, each edge is listed only once (e.g., (u, v, w)
           but not (v, u, w)).
352
353         Complexity:  $O(V^2)$  - Must iterate through the relevant portion of the
           matrix
354                     (whole matrix for directed, roughly half for undirected).
355
356         Returns:
357             A list of tuples, where each tuple is (source_vertex,
           destination_vertex, edge_weight).
358         """
359         edges = []
360         # Nested loops iterate  $O(V^2)$  times (or  $O(V^2/2)$  for undirected)
361         for u_idx in range(self._num_vertices):
362             start_j = u_idx if not self._is_directed else 0
363             for v_idx in range(start_j, self._num_vertices):
364                 edge_data = self._adj_matrix[u_idx][v_idx] #  $O(1)$  access
365                 if edge_data is not None:
366                     source = self._index_to_vertex[u_idx] #  $O(1)$  access
367                     destination = self._index_to_vertex[v_idx] #  $O(1)$  access
368                     edges.append((source, destination, edge_data)) #  $O(1)$  avg
           append
369         return edges
370
371     def __len__(self) -> int:
372         """
373         Returns the number of vertices in the graph.
374         Complexity:  $O(1)$ 
375         """
376         return self._num_vertices()

```

## §2.5.2. Adjacency List

### Definition 2.5.2.1 (Adjacency List).

An adjacency list is a collection of lists used to represent a graph. Each list in the collection corresponds to a vertex of the graph, and the elements of the list are the vertices adjacent to the corresponding vertex. In an undirected graph, the adjacency list of a vertex  $v$  contains all the vertices adjacent to  $v$ . In a directed graph, the adjacency list of a vertex  $v$  contains all the vertices that have an edge pointing to  $v$ .

### Example 2.5.2.1.

Consider the graph  $G = (V, E)$  with

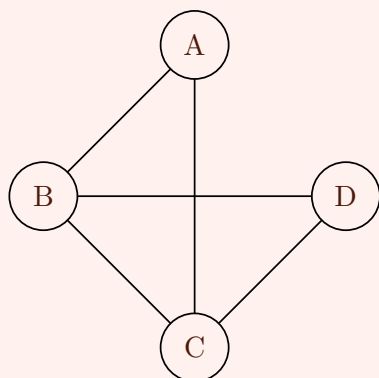
$$V = \{A, B, C, D\}$$

and

$$E = \{(A, B), (B, C), (C, A), (C, D), (D, B)\}.$$

The adjacency list of  $G$  is

$$A : \{B, C\}, B : \{A, C, D\}, C : \{A, B, D\}, D : \{B\}.$$



| Node | Adjacency List |
|------|----------------|
| A    | {B, C}         |
| B    | {A, C, D}      |
| C    | {A, B, D}      |
| D    | {B}            |

Table 2: A graph and its adjacency list

### §2.5.2.1. Implementation

#### Remark 2.5.2.1.1.


Do note that, the adjacency list attached to each vertex can be implemented as a list, set, or any other data structure that supports efficient insertion and deletion of elements. The choice of data structure depends on the specific problem being solved. In our occasion, we use dictionaries to represent the adjacency list:

```
[Vertex, Dict[Neighbor, EdgeWeight]]
```

```

1  from typing import TypeVar, Generic, List, Optional, Tuple, Dict,
   Set, Any, Iterable, Hashable
2
3  V = TypeVar('V', bound=Hashable) # Type for vertex identifiers (must be
   hashable)
4  E = TypeVar('E')                  # Type for edge weights (can be float, int,
   etc.)
5
6  class ListGraph(Generic[V, E]):
7      """
8      A graph implementation using adjacency lists represented by dictionaries.
9      The structure is: {vertex: {neighbor: weight/data, ...}, ...}
10
11     Handles directed/undirected and weighted/unweighted graphs.
12     For unweighted graphs, the edge value '1' (or True) is often used, here we
   use 1.
13     'None' edge data is possible if explicitly added but generally avoided.
14

```

 Python

```

15     Note: Vertex addition/lookup is  $O(1)$  avg. Edge addition/lookup is  $O(1)$  avg.
16         Getting neighbors is  $O(\text{degree}(V))$ . Vertex removal is  $O(V + E)$  in the
17         worst case
18         (must check all other vertices for incoming edges). Space complexity
19         is  $O(V + E)$ .
20
21         This representation is generally better for sparse graphs.
22     """
23
24     def __init__(self, directed: bool = False, weighted: bool = False):
25         """
26         Initializes an empty graph.
27
28         Args:
29             directed: True if the graph is directed, False otherwise.
30             weighted: True if the graph edges have weights, False otherwise.
31
32         Complexity:  $O(1)$ 
33         """
34         self._is_directed: bool = directed
35         self._is_weighted: bool = weighted
36
37         # The core adjacency list structure: Dict[Vertex, Dict[Neighbor,
38         # EdgeData]]
39         self._adj_list: Dict[V, Dict[V, Optional[E]]] = {}
40
41         self._num_vertices: int = 0
42         self._num_edges: int = 0
43
44     def num_vertices(self) -> int:
45         """
46         Returns the number of vertices in the graph.
47         Complexity:  $O(1)$ 
48         """
49         # Alternatively, could use len(self._adj_list), but keeping a counter
50         # is safer
51         return self._num_vertices
52
53     def num_edges(self) -> int:
54         """
55         Returns the number of edges in the graph.
56         Complexity:  $O(1)$ 
57         """
58         return self._num_edges
59
60     def is_directed(self) -> bool:
61         """

```

```

57         Returns True if the graph is directed, False otherwise.
58         Complexity:  $O(1)$ 
59         """
60         return self._is_directed
61
62     def is_weighted(self) -> bool:
63         """
64         Returns True if the graph is weighted, False otherwise.
65         Complexity:  $O(1)$ 
66         """
67         return self._is_weighted
68
69     def get_vertices(self) -> List[V]:
70         """
71         Returns a list of all vertices in the graph.
72         Complexity:  $O(V)$  - Collects keys from the dictionary.
73         """
74         return list(self._adj_list.keys())
75
76     def has_vertex(self, vertex: V) -> bool:
77         """
78         Checks if a vertex exists in the graph.
79         Complexity:  $O(1)$  average - dictionary key lookup.
80         """
81         return vertex in self._adj_list
82
83     def add_vertex(self, vertex: V) -> None:
84         """
85         Adds a vertex to the graph.
86
87         If the vertex already exists, this method does nothing.
88         Complexity:  $O(1)$  average - dictionary insertion/check.
89
90         Args:
91             vertex: The vertex identifier to add. Must be hashable.
92         """
93         if vertex not in self._adj_list: #  $O(1)$  avg check
94             self._adj_list[vertex] = {} # Add vertex with an empty neighbor
95                                     dict -  $O(1)$  avg insert
96             self._num_vertices += 1 #  $O(1)$ 
97
98     def remove_vertex(self, vertex: V) -> None:
99         """
100         Removes a vertex and all incident edges from the graph.

```

```

101      Complexity:  $O(V + E)$  worst case.  $O(V + \text{degree}(\text{vertex}))$  average if graph
      is sparse.
102      Need to iterate through all vertices potentially ( $O(V)$ ) to
      remove
103      incoming edges. Each incoming edge removal is  $O(1)$  avg.
104      Removing outgoing edges is  $O(\text{degree}(\text{vertex}))$ .
105
106      Args:
107          vertex: The vertex identifier to remove.
108
109      Raises:
110          ValueError: If the vertex does not exist.
111      """
112      if not self.has_vertex(vertex): #  $O(1)$  avg check
113          raise ValueError(f"Vertex '{vertex}' not found for removal.")
114
115      # 1. Count and remove outgoing edges from the vertex being removed
116      # Complexity:  $O(\text{degree}(\text{vertex}))$  to count, affects edge counter later
117      outgoing_edges_data = self._adj_list[vertex]
118      outgoing_edge_count = len(outgoing_edges_data) #  $O(1)$  for dict len
      usually, but conceptually  $O(\text{degree})$  related work
119
120      # 2. Remove the vertex itself and its outgoing edges list from the main
      dictionary
121      # Complexity:  $O(1)$  average deletion
122      del self._adj_list[vertex]
123      self._num_vertices -= 1 #  $O(1)$ 
124
125      # 3. Remove all incoming edges pointing to the removed vertex
126      # Complexity:  $O(V + E_{\text{in}})$  worst case where  $E_{\text{in}}$  is incoming edges,  $O(V)$ 
      average for sparse graphs
127      # Need to check every *other* vertex's neighbor list
128      incoming_removed_count = 0
129      vertices_to_check = list(self._adj_list.keys()) #  $O(V)$  to create list
130      for u in vertices_to_check: #  $O(V)$  iteration
131          if vertex in self._adj_list[u]: #  $O(1)$  avg check
132              del self._adj_list[u][vertex] #  $O(1)$  avg deletion
133              incoming_removed_count += 1 #  $O(1)$ 
134
135      # 4. Adjust edge count carefully based on directedness
136      #  $O(1)$  operations
137      if self._is_directed:
138          # Total edges removed = outgoing + incoming
139          self._num_edges -= (outgoing_edge_count + incoming_removed_count)
140      else: # Undirected
141          # Each edge (u, v) was represented as u->v and v->u.

```

```

142         # Removing vertex 'v' deleted its entry (v -> neighbors),
           accounting for outgoing_edge_count edges.
143         # Iterating through others deleted incoming edges (u -> v).
144         # Since each edge is counted once, the total number of edges
           removed is simply outgoing_edge_count.
145         # (The incoming_removed_count should equal outgoing_edge_count if
           implemented correctly).
146         self._num_edges -= outgoing_edge_count
147
148
149     def add_edge(self, source: V, destination: V, weight: Optional[E] = 1) ->
       None:
150         """
151         Adds an edge between source and destination vertices.
152
153         If the graph is unweighted, the weight parameter is ignored and 1 is
           stored.
154         If the graph is weighted, the provided weight is stored (defaults to 1
           if None).
155         If the edge already exists, its weight is updated.
156
157         Complexity: O(1) average - Dictionary lookups and insertions.
158
159         Args:
160             source: The source vertex identifier.
161             destination: The destination vertex identifier.
162             weight: The weight of the edge (used only if graph is weighted).
                   Defaults to 1.
163
164         Raises:
165             ValueError: If source or destination vertices do not exist.
166         """
167         # Ensure vertices exist first - O(1) avg each
168         if source not in self._adj_list:
169             raise ValueError(f"Source vertex '{source}' not found.")
170         if destination not in self._adj_list:
171             raise ValueError(f"Destination vertex '{destination}' not found.")
172
173         edge_value: Optional[E]
174         if self._is_weighted:
175             edge_value = weight if weight is not None else 1 # Default weight 1
                           if None - O(1)
176         else:
177             edge_value = 1 # Use 1 for unweighted graphs - O(1)
178
179         # Check if edge is new before adding/updating - O(1) avg
180         is_new_edge = destination not in self._adj_list[source]

```

```

181
182     # Add/update the edge - O(1) avg
183     self._adj_list[source][destination] = edge_value
184
185     # Handle edge count and undirected case
186     if self._is_directed:
187         if is_new_edge:
188             self._num_edges += 1 # O(1)
189         else: # Undirected
190             # Also add/update the reverse edge, but only if not a self-loop
191             if source != destination:
192                 # Check if reverse is new *before* adding/adding it - O(1)
193                 # avg
194                 is_new_reverse = source not in self._adj_list[destination]
195                 # Add/update reverse edge - O(1) avg
196                 self._adj_list[destination][source] = edge_value
197             else:
198                 is_new_reverse = False # Self-loop already handled by
199                 is_new_edge
200
201     # Increment count only once if the edge was truly new (not just an
202     # update)
203     # For undirected, this means it didn't exist in *either* direction
204     # before.
205     # In our implementation, is_new_edge covers the source->dest check.
206     # If it's a self-loop, is_new_reverse is False.
207     # If not a self-loop, is_new_reverse checks dest->source.
208     # An edge is conceptually new if it wasn't present in the canonical
209     # direction (e.g., source->dest).
210     if is_new_edge:
211         self._num_edges += 1 # O(1)
212
213 def remove_edge(self, source: V, destination: V) -> None:
214     """
215     Removes the edge between source and destination.
216
217     If the graph is undirected, removes the edge in both directions.
218     Does nothing if the edge doesn't exist.
219
220     Complexity: O(1) average - Dictionary lookups and deletions.
221
222     Args:
223         source: The source vertex identifier.
224         destination: The destination vertex identifier.
225
226     Raises:
227         ValueError: If source or destination vertices do not exist.

```



```

223         """
224         # Check vertex existence -  $O(1)$  avg each
225         if source not in self._adj_list:
226             raise ValueError(f"Source vertex '{source}' not found.")
227         if destination not in self._adj_list:
228             raise ValueError(f"Destination vertex '{destination}' not found.")
229
230         # Check if edge exists before trying to delete -  $O(1)$  avg
231         if destination in self._adj_list[source]:
232             del self._adj_list[source][destination] #  $O(1)$  avg deletion
233             edge_was_removed = True
234         else:
235             edge_was_removed = False
236
237         # If edge existed and was removed, decrement count and handle
238         # undirected
239         if edge_was_removed:
240             self._num_edges -= 1 #  $O(1)$ 
241
242         # If undirected, remove the reverse edge as well (if not a self-
243         # loop)
244         if not self._is_directed and source != destination:
245             # Check existence before deleting reverse for robustness -  $O(1)$ 
246             # avg
247             if source in self._adj_list[destination]:
248                 del self._adj_list[destination][source] #  $O(1)$  avg deletion
249             # Do NOT decrement edge count again for undirected
250
251     def has_edge(self, source: V, destination: V) -> bool:
252         """
253         Checks if an edge exists between source and destination.
254
255         Complexity:  $O(1)$  average - Dictionary lookups.
256
257         Args:
258             source: The source vertex identifier.
259             destination: The destination vertex identifier.
260
261         Returns:
262             True if the edge exists, False otherwise. Returns False if vertices
263             don't exist.
264         """
265         if source not in self._adj_list: #  $O(1)$  avg check
266             return False
267         # Check if destination is a key in the source's neighbor dictionary -
268         #  $O(1)$  avg

```

```

265         return destination in self._adj_list[source]
266
267     def get_edge_data(self, source: V, destination: V) -> Optional[E]:
268         """
269         Gets the weight or data associated with the edge.
270
271         Returns None if the edge or vertices do not exist.
272         For unweighted graphs, returns 1 if the edge exists.
273
274         Complexity: O(1) average - Dictionary lookups.
275
276         Args:
277             source: The source vertex identifier.
278             destination: The destination vertex identifier.
279
280         Returns:
281             The edge weight/data, or None if the edge/vertex doesn't exist.
282         """
283         if source not in self._adj_list: # O(1) avg check
284             return None
285         # dict.get() returns None if key (destination) not found - O(1) avg
286         return self._adj_list[source].get(destination)
287
288     def get_neighbors(self, vertex: V) -> Iterable[Tuple[V, Optional[E]]]:
289         """
290         Gets an iterable of neighbors for a given vertex, along with edge data.
291
292         Complexity: O(degree(vertex)) - Iterates through the vertex's neighbor
293         dictionary items.
294
295         Getting the items view itself is O(1).
296
297         Args:
298             vertex: The vertex identifier.
299
300         Returns:
301             An iterable view (dict_items) of tuples (neighbor_vertex,
302             edge_weight).
303             Use list() around the result if a list copy is needed.
304
305         Raises:
306             ValueError: If the vertex does not exist.
307         """
308         if vertex not in self._adj_list: # O(1) avg check
309             raise ValueError(f"Vertex '{vertex}' not found.")

```

```

308      # .items() provides an efficient view for iteration -  $O(1)$  to create
      view
309      # Iteration over the view takes  $O(\text{degree}(\text{vertex}))$ 
310      return self._adj_list[vertex].items()
311
312  def get_edges(self) -> List[Tuple[V, V, Optional[E]]]:
313      """
314      Gets a list of all edges in the graph.
315
316      For undirected graphs, each edge is listed only once (conventionally).
317      Uses a set to track visited pairs for undirected graphs to avoid
      duplicates.
318
319      Complexity:  $O(V + E)$  - Iterates through all vertices ( $O(V)$ ) and then
      through
320          all neighbors for each vertex (totaling  $O(E)$  across all
          vertices).
321          Set operations are  $O(1)$  average.
322
323      Returns:
324          A list of tuples, where each tuple is (source_vertex,
          destination_vertex, edge_weight).
325      """
326      edges = []
327      # Used only for undirected graphs to avoid adding (u,v) and (v,u)
328      visited_undirected_pairs = set() #  $O(1)$  space overhead initially
329
330      #  $O(V)$  outer loop
331      for source, neighbors in self._adj_list.items():
332          #  $O(\text{degree}(\text{source}))$  inner loop -> totals  $O(E)$  over the outer loop
333          for destination, weight in neighbors.items():
334              if self._is_directed:
335                  edges.append((source, destination, weight)) #  $O(1)$  avg
                  append
336              else:
337                  # Ensure undirected edges are added only once
338                  # Create a canonical representation (frozenset for
                  hashability regardless of order)
339                  edge_pair = frozenset((source, destination)) #  $O(1)$ 
                  creation (assuming hashable V)
340                  if edge_pair not in visited_undirected_pairs: #  $O(1)$  avg
                  set lookup
341                      edges.append((source, destination, weight)) #  $O(1)$  avg
                      append
342                      visited_undirected_pairs.add(edge_pair) #  $O(1)$  avg set
                      add
343      return edges #  $O(E)$  size list returned
344

```

```

345     def __len__(self) -> int:
346         """
347         Returns the number of vertices in the graph.
348         Allows `len(graph)` syntax.
349         Complexity: O(1)
350         """
351         return self.num_vertices()

```

### §2.5.3. Trade-offs between Adjacency Matrix and Adjacency List

#### Definition 2.5.3.1 (Sparse and Dense Graph).

A graph is considered sparse if the number of edges is much less than the number of vertices squared, i.e.,  $|E| \ll |V|^2$ . Sparse graphs have relatively few edges compared to the number of possible edges.

Accordingly, a graph is considered dense if the number of edges is close to the number of vertices squared, i.e.,  $|E| \sim |V|^2$ . Dense graphs have many edges compared to the number of possible edges.

| Feature / Operation     | Adjacency Matrix (MatrixGraph)  | Adjacency List (ListGraph) | Winner / Notes                       |
|-------------------------|---------------------------------|----------------------------|--------------------------------------|
| Space Complexity        | $O(V^2)$                        | $O(V + E)$                 | List (especially for sparse graphs)  |
| Add Edge                | $O(1)$ avg                      | $O(1)$ avg                 | Tie (both fast on average)           |
| Remove Edge             | $O(1)$ avg                      | $O(1)$ avg                 | Tie (both fast on average)           |
| Check Edge / Get Weight | $O(1)$ avg                      | $O(1)$ avg                 | Tie (both fast on average)           |
| Get Neighbors(u)        | $O(V)$                          | $O(\deg(u))$               | List (much faster for sparse graphs) |
| Get All Edges           | $O(V^2)$                        | $O(V + E)$                 | List (much faster for sparse graphs) |
| Add Vertex              | $O(V)$ or $O(V^2)$ if re-sizing | $O(1)$ avg                 | List (much faster & simpler)         |
| Remove Vertex           | $O(V^2)$                        | $O(V + E)$ or $O(V)$ avg   | List (generally better)              |

Table 3: Comparison of Adjacency Matrix and Adjacency List Graph Implementations

## §2.6. Basic Graph Algorithms

We discuss two fundamental graph traversal algorithms: Breadth-First Search (BFS) and Depth-First Search (DFS). These algorithms are used to explore and search a graph, and they can be applied to both directed and undirected graphs.

### §2.6.1. Breadth-First Search

## §2.6.1.1. Definition

**Definition 2.6.1.1.1** (Breadth-First Search (BFS)).

Breadth-First Search (BFS) is a graph traversal algorithm that explores the graph level by level. Starting from a source vertex, BFS visits all its neighbors first, then the neighbors' neighbors, and so on. The algorithm uses a **queue** to keep track of the vertices to visit next.

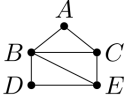
**Algorithm 1:** Breadth-First Search

```

1 function BFS(graph, initial_vertex):
2   visited = set()
3   queue = [initial_vertex]
4   visited.add(initial_vertex)
5   while queue is not empty:
6     current_vertex = queue.dequeue()
7     for neighbor in graph.get_neighbors(current_vertex):
8       if neighbor not in visited:
9         visited.add(neighbor)
10        queue.enqueue(neighbor)
11  return visited

```

**Example.**

If  $G =$  , with root vertex A.

Then  $Q$  and  $T$  grow as follows:


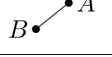

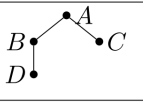
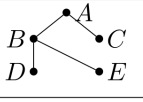
| Step | $Q$    | $T$   |
|------|--------|---|
| 1    | $A$    |  |
| 2    | $AB$   |  |
| 3    | $ABC$  |  |
| 4    | $BC$   |   |
| 5    | $BCD$  |  |
| 6    | $BCDE$ |  |
| 7    | $CDE$  |   |
| 8    | $DE$   |   |
| 9    | $E$    |   |

Figure 13: Breadth-First Search (BFS) traversal of a graph starting from vertex A.

## §2.6.1.2. Complexity Analysis

### §2.6.1.2.1. Space Complexity

For a graph with  $V$  vertices and  $E$  edges:

- If implemented by adjacency matrix, the space complexity of Breadth-First Search (BFS) is  $O(V)$ . This is because:
  - we maintain a queue of vertices to visit, which can contain all vertices in the worst case, contributing  $O(V)$  auxiliary space.
  - we maintain a set of visited vertices, which can contain all vertices in the worst case, contributing  $O(V)$  auxiliary space.
- If implemented by adjacency list, the space complexity of Breadth-First Search (BFS) is also  $O(V)$ . The reason is similar to the adjacency matrix case, but the space usage is more efficient for sparse graphs.

### §2.6.1.2.2. Time Complexity

#### Definition 2.6.1.2.2.1 (Big-O Notation).

By assuming the input of an algorithm is of variable size  $n$ , we use big-O notation to analyse the asymptotic upper bound of the time complexity when  $n \rightarrow \infty$ . We state that, in the worst case, the time complexity  $T(n)$  of an algorithm with input size  $n$  has  $T(n) = O(g(n))$ , if

$$\exists(c > 0 \wedge r \in \mathbb{N}^+) \text{ such that } \forall n > r, 0 \leq f(n) \leq c \cdot g(n),$$

where  $f(n)$  is the exact time complexity of the algorithm, and  $g(n)$  is the upper bound of the time complexity.

For a graph with  $V$  vertices and  $E$  edges:

- If implemented by adjacency matrix, the time complexity of Breadth-First Search (BFS) is  $O(V^2)$ . This is because:
  - The queue operations (enqueue and dequeue) will be executed for each vertex, contributing  $O(V)$  time.
  - The loop to visit neighbors of each vertex will be executed for each vertex. For adjacency matrix, we will run a outer loop of  $|V|$  and inner loop of  $|V|$  in the worst case, contributing  $O(V^2)$  time.
- If implemented by adjacency list, the time complexity of Breadth-First Search (BFS) is  $O(V + E)$ . This is because:
  - The queue operations (enqueue and dequeue) are will be executed for each vertex, contributing  $O(V)$  time.
  - The loop to visit neighbors of each vertex will be executed for each vertex. For adjacency list, we will run a outer loop of  $|V|$  and inner loop of  $\deg(V)$  in the worst case, and  $\max(\deg(V)) = E$  in the worst case, contributing  $O(V + E)$  time.

## §2.6.2. Depth-First Search

### §2.6.2.1. Definition

#### Definition 2.6.2.1.1 (Depth-First Search (DFS)).

Depth-First Search (DFS) is a graph traversal algorithm that explores the graph by going as deep as possible along each branch before backtracking. Starting from a source vertex,

DFS visits the first neighbor, then the neighbor's neighbor, and so on until it reaches a dead-end. The algorithm uses a **stack** to keep track of the vertices to visit next.

---

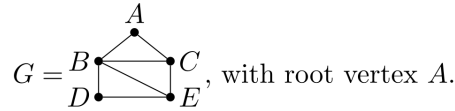
**Algorithm 2:** Depth-First Search
 

---

```

1 function DFS(graph, initial_vertex):
2   visited = set()
3   stack = [initial_vertex]
4   while stack is not empty:
5     current_vertex = stack.pop()
6     if current_vertex not in visited:
7       visited.add(current_vertex)
8       for neighbor in graph.get_neighbors(current_vertex):
9         if neighbor not in visited:
10          | stack.push(neighbor)
11   return visited
  
```

---

**Example.**

We use the same  $G$ , and take the top of  $S$  to its right hand end.

| Step | $S$     | $T$   |
|------|---------|---|
| 1    | $A$     | $\bullet A$   |
| 2    | $AB$    | $B \bullet \nearrow A$  |
| 3    | $ABC$   | $B \bullet \nearrow A$<br>$C \bullet$                             |
| 4    | $ABCE$  | $B \bullet \nearrow A$<br>$C \bullet \downarrow E$                |
| 4    | $ABCED$ | $B \bullet \nearrow A$<br>$C \bullet \downarrow E$<br>$D \bullet$ |
| 6    | $ABCE$  |   |
| 7    | $ABC$   |   |
| 8    | $AB$    |   |
| 9    | $A$     |   |

Figure 14: Depth-First Search (DFS) traversal of a graph starting from vertex  $A$ .

### §2.6.2.2. Complexity Analysis

#### §2.6.2.2.1. Space Complexity

For a graph with  $V$  vertices and  $E$  edges:

- If implemented by adjacency matrix, the space complexity of Depth-First Search (DFS) is  $O(V)$ . This is because:
  - we maintain a stack of vertices to visit, which can contain all vertices in the worst case, contributing  $O(V)$  auxiliary space.
  - we maintain a set of visited vertices, which can contain all vertices in the worst case, contributing  $O(V)$  auxiliary space.
- If implemented by adjacency list, the space complexity of Depth-First Search (DFS) is also  $O(V)$ . The reason is similar to the adjacency matrix case, but the space usage is more efficient for sparse graphs.

#### §2.6.2.2.2. Time Complexity

For a graph with  $V$  vertices and  $E$  edges:

- If implemented by adjacency matrix, the time complexity of Depth-First Search (DFS) is  $O(V^2)$ . This is because:
  - The stack operations (push and pop) are will be excecuted for each vertex, contributing  $O(V)$  time in the worst case.
  - The loop to visit neighbors of each vertex will be executed for each vertex. For adjacency matrix, we will run a outer loop of  $|V|$  and inner loop of  $|V|$  in the worst case, contributing  $O(V^2)$  time.
- If implemented by adjacency list, the time complexity of Depth-First Search (DFS) is  $O(V + E)$ . This is because:
  - The stack operations (push and pop) are will be excecuted for each vertex, contributing  $O(V)$  time.
  - The loop to visit neighbors of each vertex will be executed for each vertex. For adjacency list, we iterate through all vertices by accessing  $V$  times of  $O(1)$  operetion in the hash table, and iterate through all edges by accessing  $E$  times of  $O(1)$  operation in the inner hash table, contributing  $O(V + E)$  time.