Contents

1. Graph neural networks

1.1. Graph definition

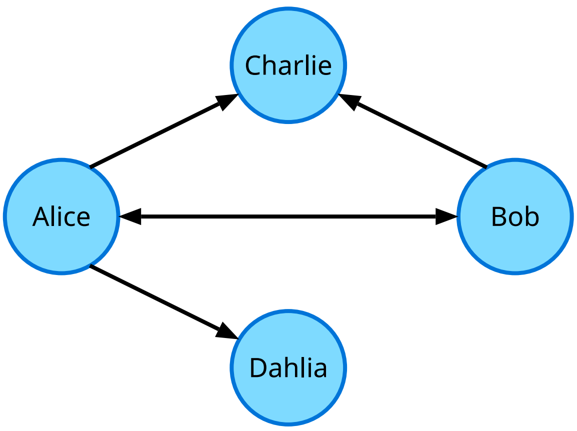
A **graph** G is defined as an ordered couple (V, E), where V is the set of **vertices** or **nodes** and E is the set of **edges**. Each edge represents the existence of a relationship betweeen two vertices. An edge $e \in E$ is therefore defined as an ordered couple $(u, v) \in V \times V$.

A graph is graphically represented using circles as nodes and using arrows as edges, whose tip is oriented in the direction of the edge. If the relationship holds both ways for a certain pair of nodes, the arrow is double-tipped.

A graph is matematically encoded in an **adjacency matrix**, a matrix that contains information concerning the existence of its edges. Formally, for a graph $G = (V, E)$ it is possible to construct an adjacency matrix $A \in \mathbb{R}^{|V| \times |V|}$ such that each entry (i, j) has the value 1 if $(i, j) \in E$ and 0 otherwise. Of course, the adjacency matrix of a graph can be constructed only if its edges can be enumerated.

Exercise 1.1.1: Alice knows Bob, Charlie and Dahlia, whereas Bob knows Alice and Charlie. Represent the relationship with a graph.

Solution:



$$\begin{array}{cc} & \begin{matrix}\text{Alice} & \text{Bob} & \text{Charlie} & \text{Dahlia}\end{matrix} \\ \begin{matrix}\text{Alice} \\ \text{Bob} \\ \text{Charlie} \\ \text{Dahlia}\end{matrix} & \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$\square$

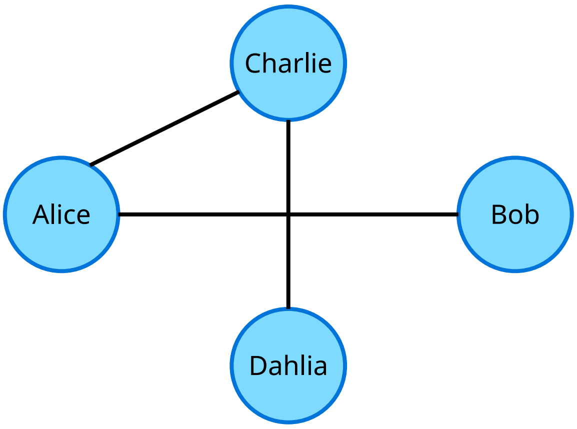
A graph is said to be **connected** if every node appears in at least one edge, except for **loops** (an edge connecting a node to itself). Formally, a graph $G = (V, E)$ is connected if, for any $v \in V$, exists $u \in V - \{v\}$ such that $(u, v) \in E$ or $(v, u) \in E$.

A graph is said to be **undirected** if the relationship between the nodes is symmetric, and holds both ways for every node. Formally, a graph $G = (V, E)$ is undirected if, for any $(u, v) \in E$, it is also true that $(v, u) \in E$. For clarity, the edges of an undirected graph are often drawn tipless. The adjacency matrix of an undirected graph will clearly be symmetric. If a graph is not undirected, it is said to be **directed**.

If a graph is connected, undirected and has no loops, it is called **simple**. It is easy to see that the adjacency matrix of a simple graph has 0 as each element of the diagonal.

Exercise 1.1.2: Alice is a friend of Bob and Charlie, whereas Dahlia is a friend of Charlie. Represent the relationship with a graph; is the graph simple?

Solution: Yes, the graph would be simple. This is because the "is a friend of" relationship is (assumed to be) symmetric, non reflexive and every person appears at least once as friend of someone else.



$$\begin{array}{c|cccc} & \text{Alice} & \text{Bob} & \text{Charlie} & \text{Dahlia} \\ \text{Alice} & 0 & 1 & 1 & 0 \\ \text{Bob} & 1 & 0 & 0 & 0 \\ \text{Charlie} & 1 & 0 & 0 & 1 \\ \text{Dahlia} & 0 & 0 & 1 & 0 \end{array}$$

$\square$