Contents

1. Graph neural networks

1.1. Graph definition

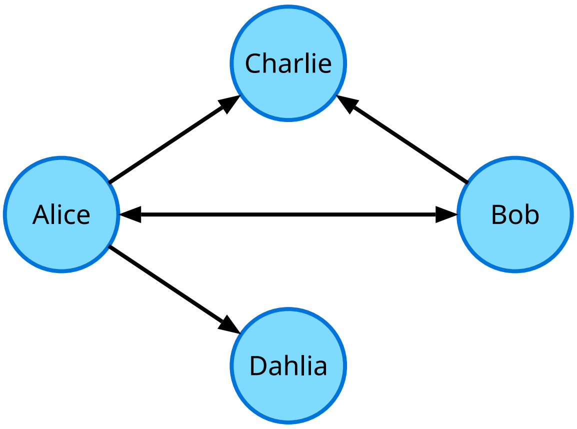
A **graph** G is defined as an ordered couple (V, E), where V is the set of **vertices** or **nodes** and E is the set of **edges**. Each edge represents the existence of a relationship betweeen two vertices. An edge $e \in E$ is therefore defined as an ordered couple $(u, v) \in V \times V$.

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:



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

$\square$

The **neighborhood** of a node is the set of all nodes that connected to that node. Given a graph $G = (V, E)$, for any node $v \in V$ the neighborhood $N(v) \subseteq V$ is defined as the set $\{u \mid (v, u) \in E\}$ or, equivalently with respect to its adjacency matrix A, $\{u \mid A[v, u] \neq 0\}$.

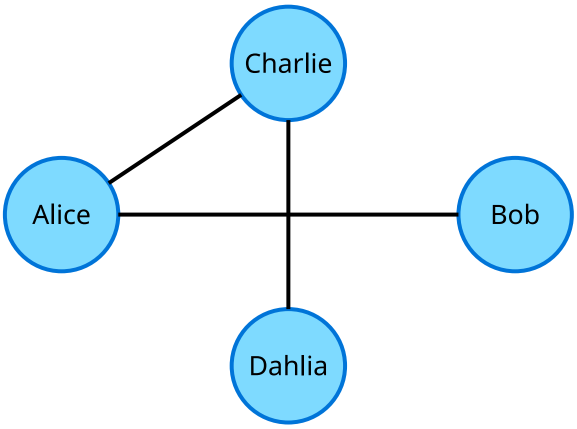
A graph is said to be **connected** if every node appears in at least one edge, except for **loops** (an edge connecting a node to itself). Formally, a graph $G = (V, E)$ is connected if, for any $v \in V$, exists $u \in V - \{v\}$ such that $(u, v) \in E$ or $(v, u) \in E$.

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.



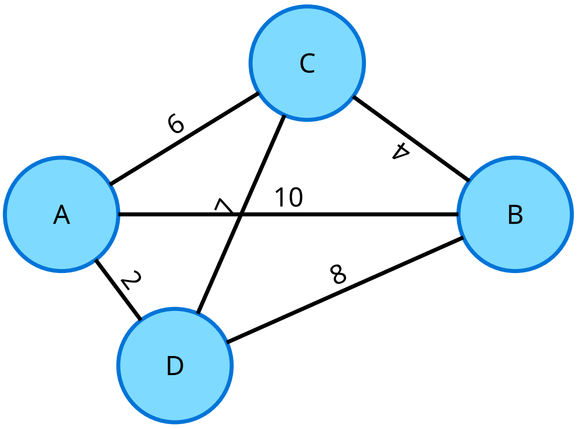
$$\begin{array}{c c} & \begin{array}{cccc} \text{Alice} & \text{Bob} & \text{Charlie} & \text{Dahlia} \end{array} \\ \begin{array}{c} \text{Alice} \\ \text{Bob} \\ \text{Charlie} \\ \text{Dahlia} \end{array} & \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}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

□

A graph $G = (V, E, W)$, that has a function $W : E \to \mathbb{R} - \{0\}$ that associates a real non-zero number to any edge of the graph is called **weighted graph**. The adjacency matrix of a weighted graph has $W(i, j)$ instead of 1 as the value of the (i, j)-th cell. The graphical representation of a weighted graph has the weight of each edge nenoted on the size of the corresponding arrow and, in general, the lenght of the arrow is scaled with respect to the weight.

Exercise 1.1.3: The town of A dists 10 from B, 6 from C and 2 from D, B dists 4 from C and 8 from D and D dists 7 from C. Represent the relationship with a graph.

Solution:



$$\begin{array}{c c} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \end{array} & \begin{bmatrix} 0 & 10 & 6 & 2 \\ 10 & 0 & 4 & 8 \\ 6 & 4 & 0 & 7 \\ 2 & 8 & 7 & 0 \end{bmatrix} \end{array}$$

□

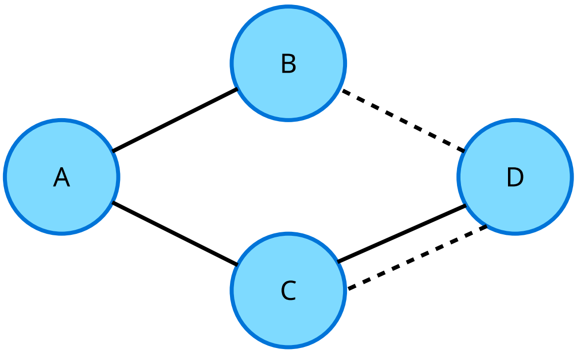
A graph can represent more than one relationship with the same entities at once; a graph with this characteristic is called a **multirelational graph**. Formally, a graph $G = (V, E, T)$ is a multirelational graph if each edge e is defined as a tuple $e = (u, v, \tau)$, where $u, v \in V$ and $\tau \in T$ is the type of the relationship. A multirelational graph is encoded as $|T|$ adjacency matrices, each representing one type of relation. Said matrices can be combined into a single tensor, an **adjacency tensor** $A \in \mathbb{R}^{|V| \times |V| \times |T|}$.

Exercise 1.1.4: Drugs can interact with each other, inducing certain side effects when taken together. Suppose that:

- Drug A induces headache when taken with drug B or with drug C, and vice versa;
- Drug B induces tachychardia when taken with drug D, and vice versa;
- Drug C induces both tachychardia and headache when taken with drug D and vice versa.

Represent this relationship in a multirelational graph.

Solution:



$$\begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \end{array} & \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

$$\begin{array}{cc} & \begin{array}{cccc} A & B & C & D \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \end{array} & \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

□

An **eterogeneous graph** is a multirelational graph where nodes have a type, partitioning the set of nodes. Formally, a (multirelational) graph $G = (V, E, T)$ is an eterogeneous graph where the set V is constructed as the union of n sets V_i, with $i \in \{1, ..., n\}$, such that:

$$V = \bigcup_i V_i \qquad\qquad V_i \cap V_j = \emptyset, \forall i, j \text{ when } i \neq j$$

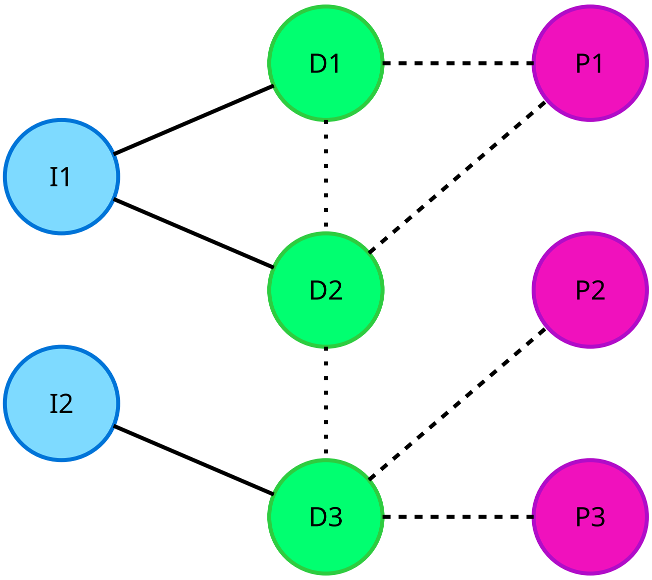
An eterogeneous graph whose edges can only connect nodes of different types is called a **multipartite graph**. Formally, an eterogeneous graph $G = (V, E, T)$ is a multipartite graph if, for any edge $e = (u, v, \tau) \in E$, it follows that $u \in V_i, v \in V_j, i \neq j$.

Exercise 1.1.5: Certain illnesses are treated using certain drugs. Drugs can be incompatible with each other and influence the behaviour of certain proteins. Suppose that:

- Illness I_1 is treated using either drug D_1 or drug D_2;
- Illness I_2 is treated using drug D_3;
- Drug D_1 is incompatible with drug D_2 (and vice versa);
- Drug D_2 is incompatible with drug D_3 (and vice versa);
- Protein P_1 is influenced by drug D_1 and drug D_2;
- Protein P_2 is influenced by drug D_2;
- Protein P_3 is influenced by drug D_3.

Represent this relationship in a multirelational graph. Is it a multipartite graph?

Solution: No, because the relationship "being incompatible with" relates entities of the same type (drugs).



$$\begin{array}{cc} & \begin{matrix} \mathrm{I1} & \mathrm{I2} & \mathrm{D1} & \mathrm{D2} & \mathrm{D3} \end{matrix} \\ \begin{matrix} \mathrm{I1} \\ \mathrm{I2} \\ \mathrm{D1} \\ \mathrm{D2} \\ \mathrm{D3} \end{matrix} & \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$\begin{array}{cc} & \begin{matrix} \mathrm{D1} & \mathrm{D2} & \mathrm{D3} \end{matrix} \\ \begin{matrix} \mathrm{D1} \\ \mathrm{D2} \\ \mathrm{D3} \end{matrix} & \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \end{array}$$

$$\begin{array}{cc} & \begin{matrix} \mathrm{D1} & \mathrm{D2} & \mathrm{D3} & \mathrm{P1} & \mathrm{P2} & \mathrm{P3} \end{matrix} \\ \begin{matrix} \mathrm{D1} \\ \mathrm{D2} \\ \mathrm{D3} \\ \mathrm{P1} \\ \mathrm{P2} \\ \mathrm{P3} \end{matrix} & \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

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