Graph Theory Intro Practice

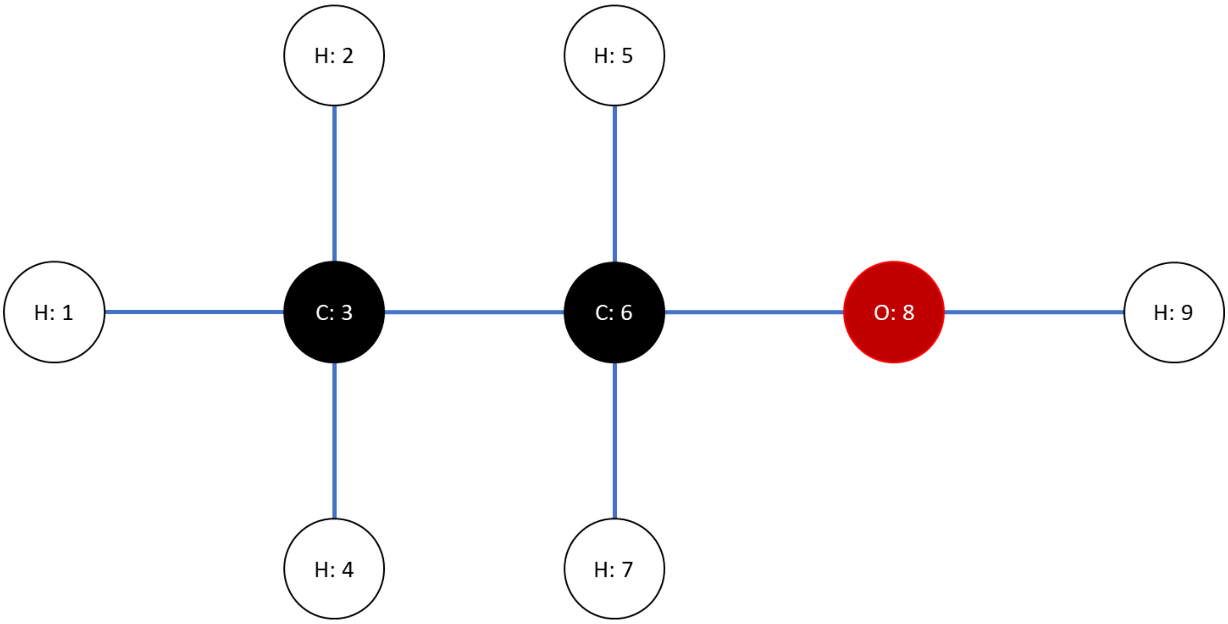
Extras

Exercises

Below are a few exercises for autonomous practice of the graph theory concepts we introduced earlier.

1. Defining a graph

Let us consider the following molecule, below, the beloved ethanol.



This molecule could be represented as a graph. But to do so, it requires to answer a few questions first, listed below.

A. We denote N, the number of vertices in this graph.
How many vertices does this graph contain?

B. Is this graph directed or undirected?

C. Assuming we refer to nodes as x_i, with $i \in \{1, 2, \dots, N\}$, what could the node features h_i consist of? Discuss.

D. What is the adjacency matrix A of this graph?

E. What is the degree matrix D of this graph?

F. Consider the sentence below.

"A Carbon atom can form four covalent bonds, an Oxygen atom can form two and an Hydrogen atom can form one."

How does this concept of covalent bonds relate to graph theory?

2. Laplacian matrix of a complete graph

Consider the definition below.

"A complete graph is a graph in which each pair of graph nodes is connected by an edge."

Let us now consider a complete undirected graph with N nodes, $N > 3$.

A. What is the degree of each node in the graph?
B. What is the adjacency matrix A for this complete graph looking like?
C. What is the Laplacian matrix L for this complete graph looking like?
D. (Optional challenge) What are the eigenvalues of the Laplacian matrix for this graph?

3. Degree of a graph

Let us consider a group of 8 friends, who decide to shake hands with each other.
How many handshakes took place in the end?
How does this question relate to graph theory?

4. Diameter of a graph

Consider the definition below.

"The diameter D_G of a graph G the maximum hop-distance $d(x_i \rightarrow x_j)$ between any two pair of distinct vertices x_i and x_j in the graph G, or in other words

$$D_G = \max_{\substack{i,j \\ i \neq j}}(d(x_i \rightarrow x_j))$$

A. What is the diameter of the ethanol graph from Q1?

B. What is the diameter of a complete graph with N nodes?

Solutions

Below are the solutions for each exercise.

1. Defining a graph

A. We have $N = 9$ vertices in the graph, corresponding to the 9 atoms in the molecule.

B. This graph is undirected. The undirected property holds here: atom x_i is connected to atom x_j if and only if atom x_j is connected to atom x_i.

C. The node features h_i could simply consist of the atom name (C, O or H), for each atom x_i.

D. The adjacency matrix A is

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

E. The degree matrix D is

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

F. The number of covalent bonds for atom h_i corresponds to the degree d_{ii} of each node x_i of the graph. This holds true for any index $i \in \{1, 2, \dots, N\}$.

2. Degree of a graph

A. Each node has a degree value equal to $N - 1$.
B. The adjacency matrix A of a complete graph is a $N \times N$ matrix with zeroes on the diagonal and ones everywhere else.

C. The Laplacian matrix of a complete graph a $N \times N$ matrix with value $N - 1$ on its diagonal elements and -1 everywhere else.

D. Only two eigenvalues for the Laplacian matrix of a complete graph with N nodes. The first eigenvalue is 0, which appears only once. We then have the eigenvalue N, which appears $N - 1$ times.

   The proof for this requires a bit of linear algebra, but is a good practice for the eigenvalues, eigenvectors and null space concepts: https://saadquader.wordpress.com/2013/04/25/eigenvalues-of-the-laplacian-matrix-of-the-complete-graph/

3. Degree of a graph

We could define a graph, where each of the 8 friends are nodes, and the edges represent the handshakes. This graph appears to be a complete graph with $N = 8$ nodes, and each node would have a degree $d = 7$.

The degree of the undirected graph would then be

$$D = \frac{Nd}{2} = \frac{8 \times 7}{2} = 28.$$

This is the total number of handshakes, which could have also been calculated as

$$\sum_{i=1}^{7} i = 1 + 2 + 3 + 4 + 5 + 6 + 7 = 28.$$

Reason for second equation: First friend shakes hands with 7 friends, second friend has only 6 friends left to shake hands with, etc.

4. Diameter of a graph

A. $R_G = 4$. The maximal hop-distance appears, for instance, between nodes 1 and 9.

B. All the nodes are immediately connected to each other in a complete graph. More specifically, we could prove quite easily that the hop-*distance* $d(x_i \to x_j)$ between any two pair of distinct vertices x_i and x_j of a complete graph is 1. Its radius $\mathrm{R_G}$ is therefore 1 as well.