Principles of Computer Science II

Introduction to Graph Theory

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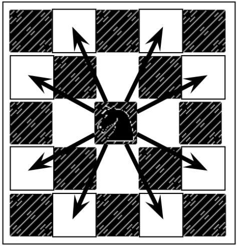
Lecture 6

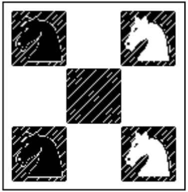
A little bit of Chess

- Knights move using a particular pattern.
- Knights can move two steps in any of four directions (left, right, up, and down) followed by one step in a perpendicular direction,
- Two points are connected by a line if moving from one point to another is a valid knight move.



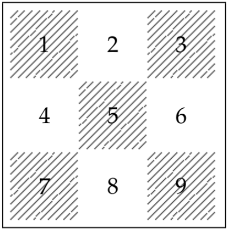
A Chess Puzzle

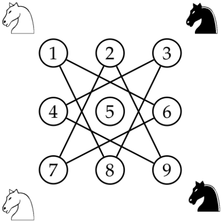
- Two white and two black knights on a 3×3 chessboard.
- Two Knights cannot occupy the same square.
- Starting from the top configuration,
- Can they move, using the usual chess knight's moves, to occupy the bottom configuration?

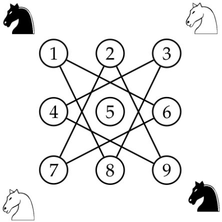


Chess Diagrams

- A Chess Diagram is used to represent movements of chess pieces on the board.
- Example of a 3×3 chessboard.
- Two points are connected by a line if moving from one point to another is a valid knight move.

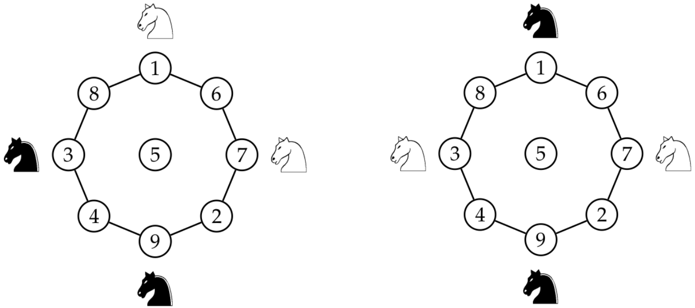






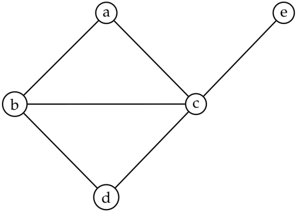
Chess Diagrams – Equivalent Representations

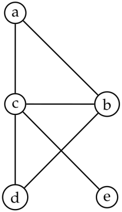
- An equivalent representation of the resulting diagram.
- Now it is easy to see that knights move around a “cycle”.
- Every knight’s move corresponds to moving to a neighboring point in the diagram – clockwise or counterclockwise
- white-white-black-black cannot be transformed into white-black-white-black



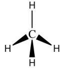
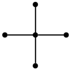
Chess Diagrams & Graphs

- Chess Diagrams are examples of *graphs*.
- The points are called vertices and lines are called edges.
- A simple graph of five vertices and six edges.
- We denote a graph by $G = G(V, E)$, where
  - V represents the set of vertices
    $V = \{a, b, c, d, e\}$
  - E represents the set of edges
    $E = \{(a, b), (a, c), (b, c), (b, d), (c, d), (c, e)\}$

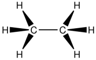
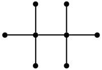




Hydrocarbons as Graphs and Structural Isomers

Methane

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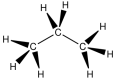
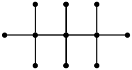
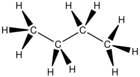
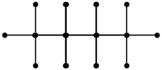
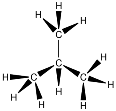
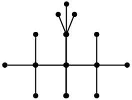



Propane

Butane

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Basic Definitions

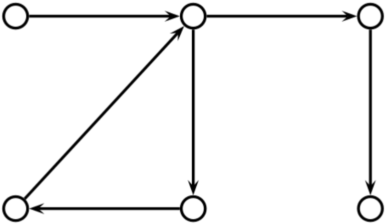
- We denote $|V| = n$ – the number of vertices.
- We denote $|E| = m$ – the number of edges.
- Two vertices u, v are called adjacent or neighboring vertices if there exists an edge $e = (u, v)$.
- We say that edge e is incident to vertices u and v.
- We say that vertices u and v are incident to edge e.
- A loop is an edge from a node to itself: (u, u).
- Two or more edges that have the same endpoints (u, v) are called multiple edges.
- The graph is called simple if it does not have any loops or multiple edges.

Degree of the Vertex

- The number of edges incident to a given vertex v is called the degree of the vertex and is denoted $d(v)$.
- For every graph $G = G(V, E)$, $\sum_{u \in V} d(u) = 2 \cdot |m|$.
- Notice that an edge connecting vertices v and w is counted in the sum twice: first in the term $d(v)$ and again in the term $d(w)$.

Directed & Undirected Graphs

- Many Bioinformatics problems make use of directed graphs.
- An edge can be undirected or directed.
- An undirected edge e is considered an unordered pair, in other words we assume that (u, v) and (v, u) are the same edge.
- A directed edge $e = (u, v)$ and $e' = (v, u)$ are different edges.
- If the edges have a direction, the graph is directed (digraph).
- If a graph has no direction, it is referred as undirected.



Directed Graphs

- In directed graphs, each vertex u has:
  - $\mathit{indegree}(u)$ – the number of incoming edges,
  - $\mathit{outdegree}(u)$ – the number of outgoing edges.
- For every directed graph $G = G(V, E)$,

$$\sum_{u \in V} \mathit{indegree}(u) = \sum_{u \in V} \mathit{outdegree}(u)$$

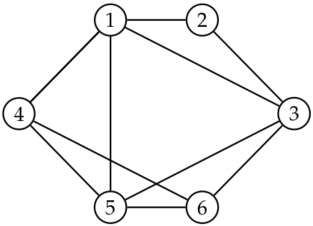
.

Subgraphs & Complete Graphs

- A subgraph G' of G consists of a subset of V and E. That is, $G' = (V', E')$ where $V' \subset V$ and $E' \subset E$.
- A spanning subgraph contains all the nodes of the original graph.
- If all the nodes in a graph are pairwise adjacent, the graph is called complete.

Triangles, Walks, Trails, Paths & Cycles

- A triangle in an undirected graph is a triplet (u, v, w), where $u, v, w \in V$ such that $(u, v), (v, w), (w, u) \in E$.
- A walk is a sequence of vertices and edges of a graph – Vertex can be repeated. Edges can be repeated.
- Trail is a walk in which no edge is repeated.
- Path is a trail in which no vertex is repeated.
- Paths that start and end at the same vertex are referred to as cycles.

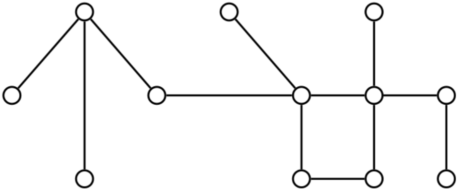


Paths

- A path of length k is a sequence of nodes $(v_0, v_1, \ldots, v_k)$, where we have $(v_i, v_{i+1}) \in E$.
- If $v_i \neq v_j$ for all $0 \leq i < j \leq k$ we call the path simple.
- If $v_0 = v_k$ for all $0 \leq i < j \leq k$ and $v_0 = v_k$ the path is a cycle.
- A path from node u to node v is a path $(v_0, v_1, \ldots, v_k)$ such that $v_0 = u$ and $v_k = v$.

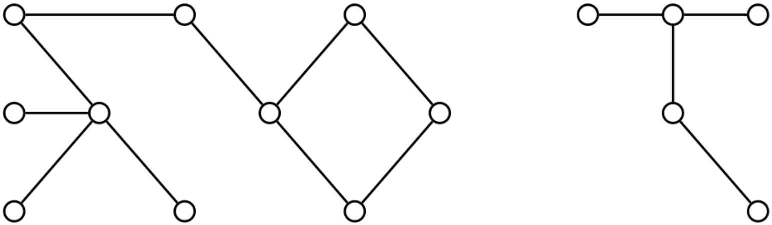
Graph Connectivity

- Two nodes u and v are connected if there is a path from u to v.
- A graph is called connected if all pairs of vertices can be connected by a path, otherwise we say that the graph is disconnected.
- A graph is called complete if there is an edge between every two vertices.



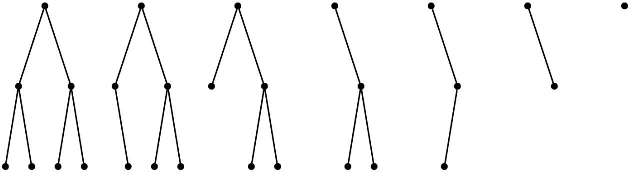
Graph Connectivity

- Disconnected graphs can be decomposed into a set of one or more connected components.



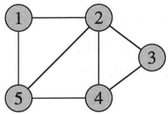
Forests & Trees

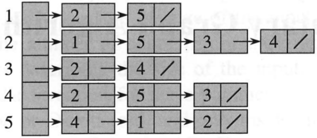
- A simple graph that does not contain any cycles is called a forest.
- A forest that is connected is called a tree.
- A tree has $n-1$ edges.
- Any two of the following three statements imply that a graph is a tree (and thus they also imply the third one):
  1. The graph has $n-1$ edges.
  2. The graph does not contain any cycles.
  3. The graph is connected.



Representation of Graphs

- Two standard ways to represent a graph $G(V, E)$:
  1. A collection of adjacency lists.
     - Usually prefered for sparse graphs.
     - Sparse graph: $|E|$ is much less than $|V|^2$.
  2. An adjacency matrix.
     - Usually prefered for dense graphs.
     - Dense graph: $|E|$ is close to $|V|^2$.

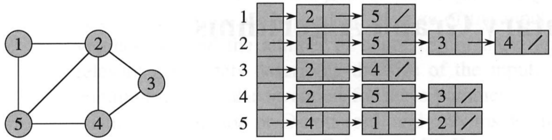




	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

Adjacency List

- Adjacency List Representation
- Consists of an array *Adj* of $|V|$ lists, one for each vertex in V.
- For each $u \in V$, the adjacency list $Adj[u]$ contains all the vertices adjacent to u in G.
- The vertices are stored in arbitrary order.

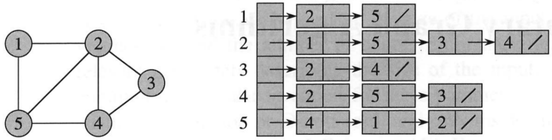


	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

Adjacency Matrix

- Adjacency Matrix Representation of $G(V, E)$
- We assume that vertices are numbered $1, 2, \ldots |V|$.
- The matrix $|V| \times |V|$ matrix.
- $A = (a_{i,j})$, where

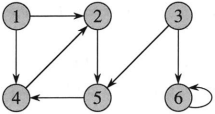
$$a_{i,j} = \begin{cases} 1, & \text{if } (i,j) \in E. \\ 0, & \text{otherwise.} \end{cases}$$

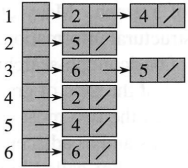


	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

Adjacency List and Adjacency Matrix Examples

- Adjacency Matrix Representation





	1	2	3	4	5	6
1	0	1	0	1	0	0
2	0	0	0	0	1	0
3	0	0	0	0	1	1
4	0	1	0	0	0	0
5	0	0	0	1	0	0
6	0	0	0	0	0	1

Graphs in Python

Open this Jupyter Notebook and let us see how to create and configure graphs: `https://drive.google.com/file/d/1cRjLIOGOA4ntOZVwzGhZBJT2yWhXVn9` `view?usp=sharing`