Principles of Computer Science II Introduction to Graph Theory

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Lecture 16

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?



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Chess Diagrams

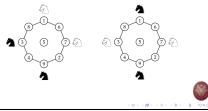
- A Chess Diagram is used to represent movements of chess pieces on the board.
- Example of a 3 × 3 chessboard.
- Two points are connected by a line if moving from one point to another is a valid knight move.





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



Hydrocarbons as Graphs and Structural Isomers









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)}



- ▶ 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.



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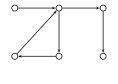
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Degree of the Vertex

- 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), ∑_{u∈V} d(u) = 2 · |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:

- indegree(u) the number of incoming edges,
- outdegree(u) the number of outgoing edges.
- ▶ For every directed graph G = G(V, E),

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

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.



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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 (v₀, v₁,..., v_k), where we have (v_i, v_{i+1}) ∈ E.
- ▶ If $v_i \neq v_j$ for all $0 \le i < j \le k$ we call the path simple.
- If v₀ = v_k for all 0 ≤ i < j ≤ k and v₀ = 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 $v_k = v$.



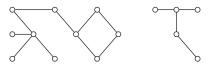
Graph Connectivity

- 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.





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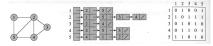
Forests & Trees

- 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

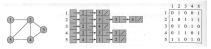
- Two standard ways to represent a graph G(V, E):
 - 1. A collection of adjacency lists.
 - Usually prefered for sparse graphs.
 - Sparse graph: |E| is much less than |V|².
 - 2. An adjacency matrix.
 - Usually prefered for dense graphs.
 - Dense graph: |E| is close to |V|².





Adjacency List

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



Adjacency Matrix

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

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







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