ECE 175B: Probabilistic Reasoning and Graphical Models
Lecture 3: Basic Graph Theory

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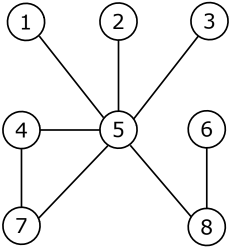
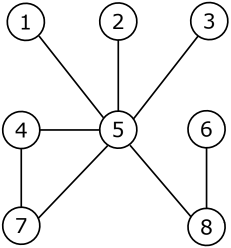
Nodes and Edges

Definition: A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ consists of nodes (vertices) and undirected or directed links (edges) between nodes. The vertex set and the edge set are denoted as $\mathcal{V}$ and $\mathcal{E}$, respectively

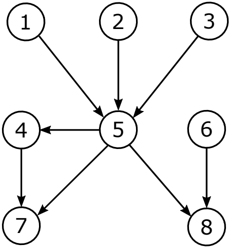


Example: The vertex set $\mathcal{V} \triangleq \{j\}_{j=1}^{N}$, consists of $N = |\mathcal{V}| = 8$ nodes with indexes j. The edge set $\mathcal{E} = \big\{\{1,5\}, \{2,5\}, \{3,5\}, \dots\big\} = \{(i_k, j_k)\}_{k=1}^{M}$ consists of $M = |\mathcal{E}| = 8$ node pairs.

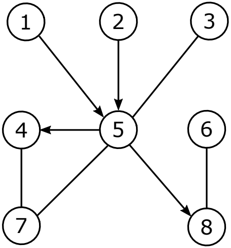
Directed and Undirected Graphs



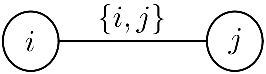
(a) undirected, e.g., $\{1, 5\} \in \mathcal{E}$



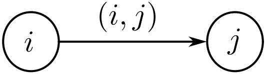
(b) directed, e.g., $(1, 5) \in \mathcal{E}$, $(5, 1) \notin \mathcal{E}$



(c) mixed



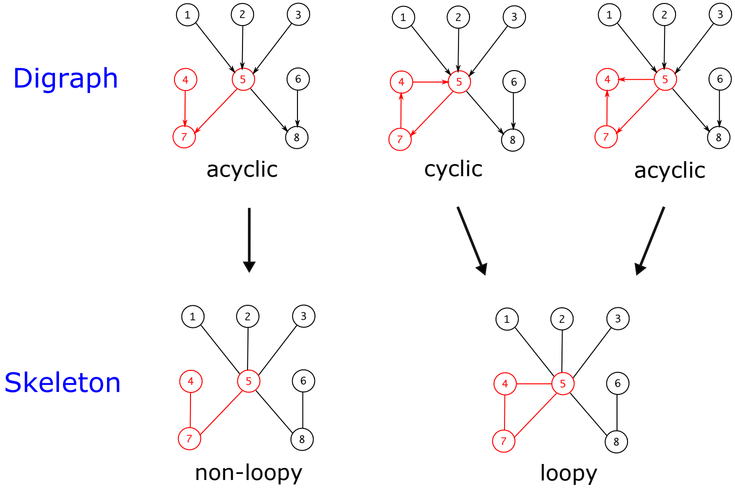
undirected edge: $\{i, j\} \in \mathcal{E}$



directed edge: $(i, j) \in \mathcal{E}$, $(j, i) \notin \mathcal{E}$

The Skeleton of a Directed Graph

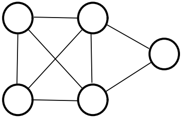
- Directed graphs (digraphs) and their skeletons



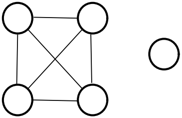
Terminology

- The skeleton of a directed graph is a undirected graph with all arrow heads dropped. An undirected graph is its own skeleton
- A path is a sequence of connected nodes on the skeleton
- A directed path on a directed graph must "follow the arrows"
- A loop is a closed path on the skeleton
- A cycle is a closed directed path on a directed graph
- A directed acyclic graph (DAG) can be either loopy or non-loopy

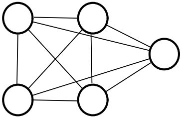
Connectivity



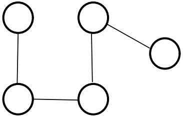
connected



not-connected



fully-connected

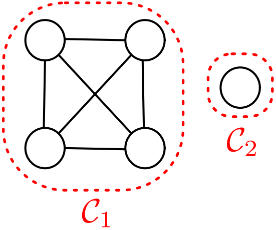


singly-connected

- In an connected graph there is a path between any two nodes
- In a fully-connected (complete) graph there is an edge between any two nodes
- In a singly-connected graph (tree) there is only one path from any node to any other node

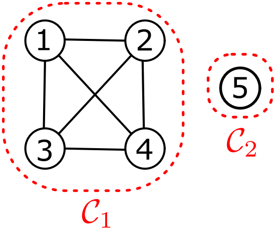
Connected Components

- Connected components are connected subgraphs in a non-connected graph
- In the non-connected graph $\mathcal{G}$ below, both $\mathcal{C}_1$ and $\mathcal{C}_2$ are connected components and $\mathcal{G} = \mathcal{C}_1 \cup \mathcal{C}_2$



Cliques

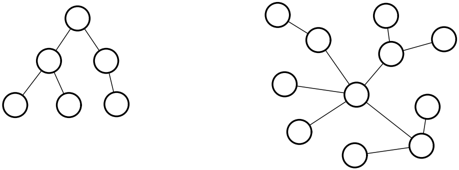
- A clique is a fully-connected subset of nodes
  - In the graph below, the nodes $\{1,2,3,4\}$, $\{1,2,3\}$, $\{1,2\}$, $\{1,3\}$, $\{1,4\}$, $\{2,3\}$, $\{2,4\}$, $\{3,4\}$, $\{1\}$, $\{2\}$, $\{3\}$, $\{4\}$, $\{5\}$ form cliques
- A maximal clique is a clique that is not a subset of a larger clique
  - In the graph below, the nodes $\{1,2,3,4\}, \{5\}$ form maximal cliques, and, e.g., the nodes $\{1,2,3\}, \{1,2\}$ form non-maximal cliques



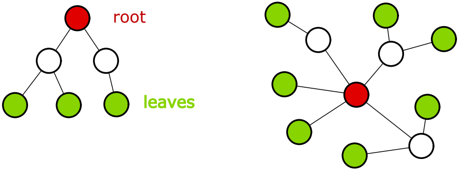
- A complete graph is itself a single, “giant” maximal clique; any subsets of nodes also forms a clique

Trees

- A tree is an undirected connected graph with no loops
  - Since a tree is a singly connected graph, there is only one path between any two nodes in a tree

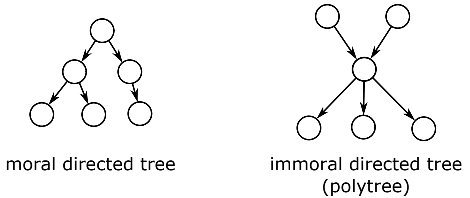


- Leaves are defined as nodes that only yield a single edge
- In a rooted tree, after the root node has been selected, the leaves are the nodes that only have a single edge and are not the root node

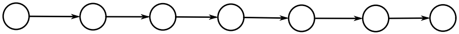


Directed Trees

- A directed tree is a directed graph whose skeleton is a tree
  - In any directed tree "parent", "child", "ancestor", and "descendent" nodes are naturally defined
  - In a moral tree every node has at most one parent
  - In a immoral tree or polytree some nodes have more than one parent

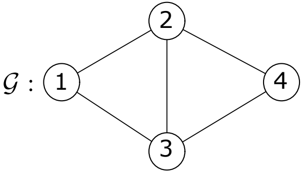


- A serial chain is a special case of a tree where there is a single child node for every parent node



The Adjacency Matrix of a Graph

- The adjacency matrix $A \triangleq A(\mathcal{G})$ of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a Boolean $N \times N$ matrix $N = |\mathcal{V}|$
  - if $\mathcal{G}$ is an undirected graph, the elements a_{ij} and a_{ji} of A are equal to 1 if there is an undirected edge between nodes i and j, i.e., $\{i, j\} \in \mathcal{E}$ and 0 otherwise
  - if $\mathcal{G}$ is an directed graph, the element a_{ij} of A is equal to 1 if there is a directed edge from node i to node j, i.e., $(i, j) \in \mathcal{E}$ and 0 otherwise
- Example: Consider the adjacenty matrix of the following undirected graph

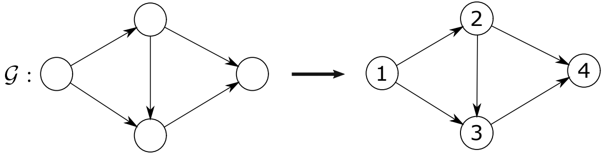


$$A = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

- Note that, for an undirected graph, we have $A = A^{\mathsf{T}}$

The Adjacency Matrix of a Graph

- In a directed graph, topological sorting is an enumeration of nodes such that they are in ancestral ordering, i.e., parents always have lower index numbers than children
- Example: Consider the adjacenty matrix of the following topological sorted directed graph



$$A = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

- In a directed graph, $(A^k)_{ij}$ is the number of paths from i to j that require k-edge hops
- Let $\tilde{A} = A + I$. In a directed graph, if $(\tilde{A}^{N-1})_{ij} \neq 0$ then there exists a path from i to j

Graphs and Probability Distributions

- Let $\mathcal{X} = \{x_1, \dots, x_N\}$ be a collection of N random variables with joint distribution $P(\mathcal{X}) = P(x_1, \dots, x_N)$
- We want to create a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ that
  - consists of one node $j \in \mathcal{V}$, $|\mathcal{V}| = N$ for each random variable x_j, $j = 1, \dots, N$
  - encodes dependency relationships between the random variables (as given by conditional probability statements) in the edges $\mathcal{E}$

graph	***probability distribution***
$\mathcal{G} = (\mathcal{V}, \mathcal{E})$	$P(\mathcal{X})$
$\mathcal{V} = \{1, \dots, N\}$	$\mathcal{X} = \{x_1, \dots, x_N\}$
separativity connectivity	independency dependency

Graph Separation and Statistical Independence

- Let U, V, and W be disjoint subsets of nodes in $\mathcal{V}$, i.e., $\mathsf{U}, \mathsf{V}, \mathsf{W} \subset \mathcal{V}$ given as $\mathsf{U} = \{i_1, \ldots, i_u\}, \mathsf{V} = \{j_1, \ldots, j_v\}$, and $\mathsf{W} = \{k_1, \ldots, k_w\}$
- Similarly, we introduce the subsets $\mathcal{X}_\mathsf{U} = \{\mathsf{x}_{i_1}, \ldots, \mathsf{x}_{i_u}\}$, $\mathcal{X}_\mathsf{V} = \{\mathsf{x}_{j_1}, \ldots, \mathsf{x}_{j_v}\}$, and $\mathcal{X}_\mathsf{W} = \{\mathsf{x}_{k_1}, \ldots, \mathsf{x}_{k_w}\}$ of $\mathcal{X}$, i.e., $\mathcal{X}_\mathsf{U}, \mathcal{X}_\mathsf{V}, \mathcal{X}_\mathsf{W} \subset \mathcal{X}$
- For convenience, denote $\mathbf{X} = \mathcal{X}_\mathsf{U}, \mathbf{Y} = \mathcal{X}_\mathsf{V}$, and $\mathbf{Z} = \mathcal{X}_\mathsf{W}$
- We now have the correspondences $\mathsf{U} \leftrightarrow \mathbf{X}, \mathsf{V} \leftrightarrow \mathbf{Y}$, and $\mathsf{W} \leftrightarrow \mathbf{Z}$

Graph Separation and Statistical Independence

- The connectivity between nodes in the graph should give underlying information about the relationship between the corresponding random variables

- **Goal:** We want the graph separation statements to correspond to conditional independence statements among the random variables, i.e., we want to "step from node-to-node" along the edges in $\mathcal{E}$ to enable efficient computation of the conditional probabilities of random variables $\mathbf{X} = \mathcal{X}_{\mathsf{U}}, \mathbf{Y} = \mathcal{X}_{\mathsf{V}}$, and $\mathbf{Z} = \mathcal{X}_{\mathsf{W}}$

Graph Separation and Statistical Independence

- We recall that $\mathbf{X}$ is independent of $\mathbf{Y}$ conditioned on $\mathbf{Z}$, i.e., $\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z} = \mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}$, implies

$$
\begin{aligned}
& P(\mathbf{X}, \mathbf{Y} | \mathbf{Z}) = P(\mathbf{X}|\mathbf{Z}) P(\mathbf{Y}|\mathbf{Z}) \\
\iff \quad & P(\mathbf{X}|\mathbf{Y}, \mathbf{Z}) = P(\mathbf{X}|\mathbf{Z}) \\
\iff \quad & P(\mathbf{Y}|\mathbf{X}, \mathbf{Z}) = P(\mathbf{Y}|\mathbf{Z})
\end{aligned}
$$

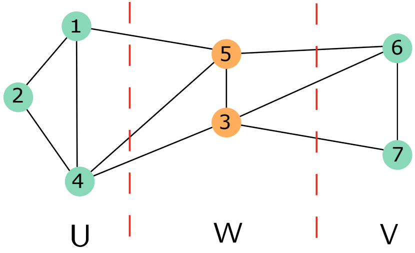
- Our goal is to find a purely graph-structural separation statement, denoted by $< \mathrm{U} \mid \mathrm{W} \mid \mathrm{V} >_{\mathrm{d}}$ such that

$$
< \mathrm{U} \mid \mathrm{W} \mid \mathrm{V} >_{\mathrm{d}} \quad \Longrightarrow \quad \mathcal{X}_u \perp\!\!\!\perp \mathcal{X}_v \mid \mathcal{X}_w = \mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}
$$

- Note that $< \cdot \mid \cdot \mid \cdot >_d$ stands for dependency(d)-separation

Graph Separation and Statistical Independence

- **Example:** Consider an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with node set $\mathcal{V} = \{1, 2, 3, 4, 5, 6, 7\}$ and edge set $\mathcal{E}$ as shown below



With $\mathsf{U} = \{1, 2, 4\}$, $\mathsf{W} = \{3, 5\}$, and $\mathsf{V} = \{6, 7\}$ from the graph we can see that W separates U and V. i.e., $< \mathsf{U} \mid \mathsf{W} \mid \mathsf{V} >_{\mathsf{d}}$

- Let $\mathcal{X} = \{\mathsf{x}_1, \ldots, \mathsf{x}_7\}$ be random variables whose joint distribution $P(\mathcal{X}) = P(\mathsf{x}_1, \ldots, \mathsf{x}_7)$ is represented by the graph shown above

- From $< \mathsf{U} \mid \mathsf{W} \mid \mathsf{V} >_{\mathsf{d}}$ it follows that $\mathcal{X}_u \perp\!\!\!\perp \mathcal{X}_v \mid \mathcal{X}_w$