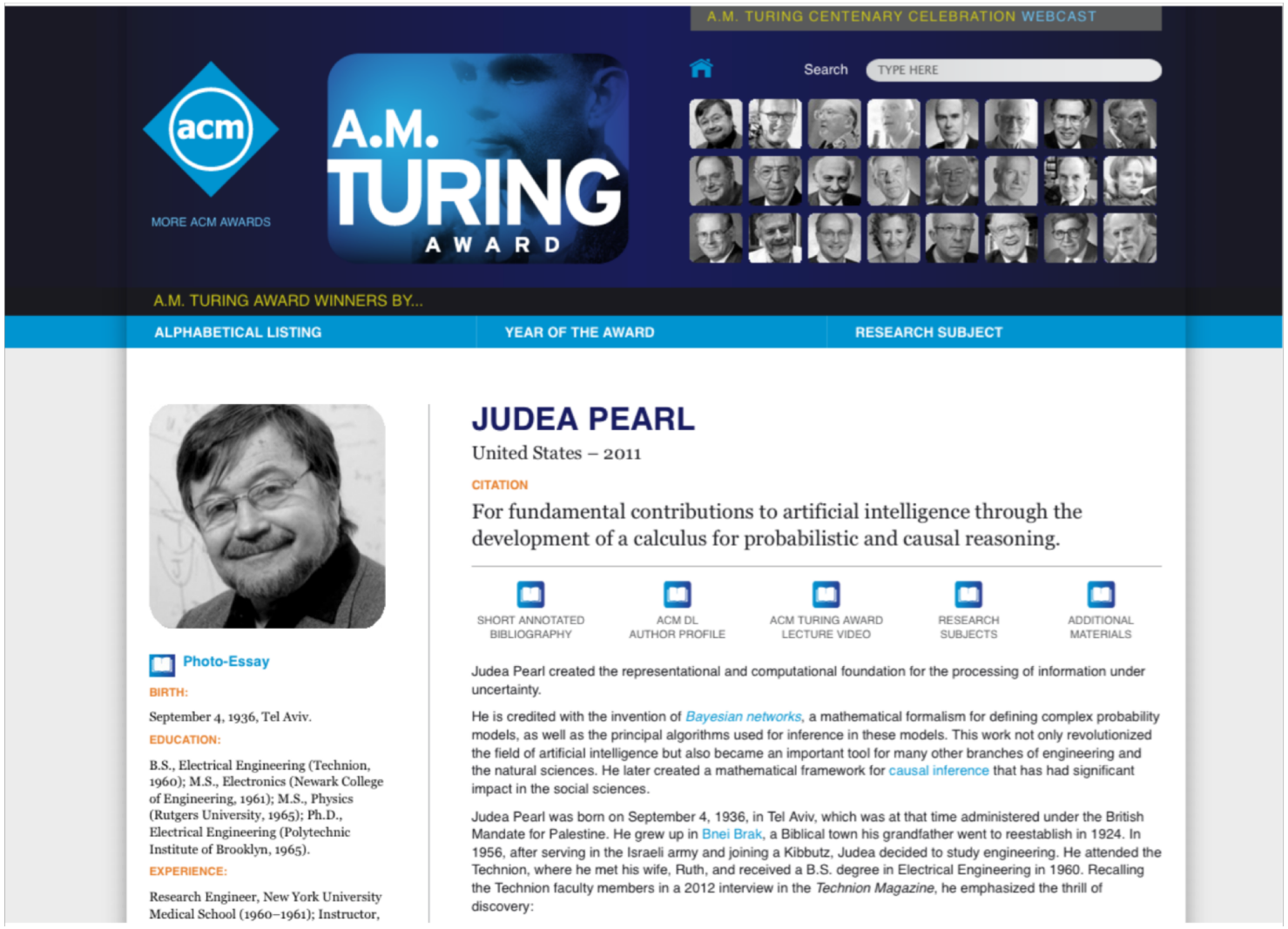
Advanced Prediction Models

Deep Learning, Graphical Models and Reinforcement Learning

Today's Outline

- Motivation
- Primer on Graphs
- Directed Graphical Models
- Undirected Graphical Models

Recent Turing Award (highest in the CS discipline)



[1]Reference: David Sontag, (2013)

Why Graphical Models

- We have seen deep learning techniques for unstructured data
  - Predominantly vision and text/audio
  - We will see control in the last part of the course
    - (Reinforcement Learning)

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- For structured data, graphical models are the most versatile framework
  - Successfully applications:
    - Kalman filtering in engineering
    - Decoding in cell phones (channel codes)
    - Hidden Markov models for time series
    - …

Graphical Models vs Deep Learning

Graphical Models	Deep Neural Networks
■ Probabilistic	■ Deterministic
■ Dependencies btw. RVs	■ Input/Output Mapping
■ Low capacity	■ High capacity
■ Domain knowledge: easy to encode	■ Domain knowledge: hard

[1]Reference: Andreas Geiger, Autonomous Vision Group, MPI (2017)

Graphical Models Landscape

- Three parts to the story:
  - Representation (this lecture)
    - Capture uncertainty (joint distribution)
    - Capture conditional independences (metadata)
    - Visualization of metadata for a distribution

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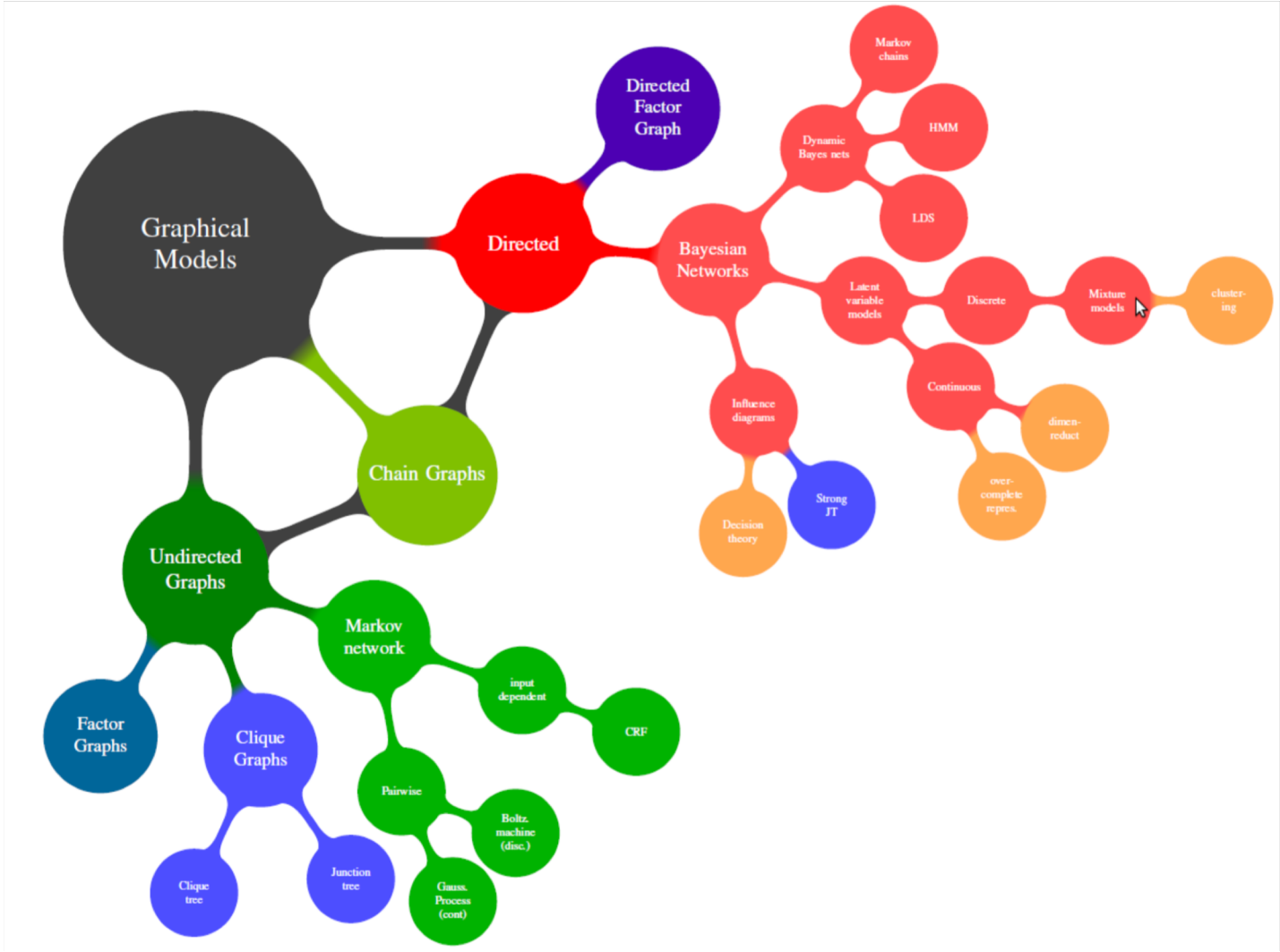
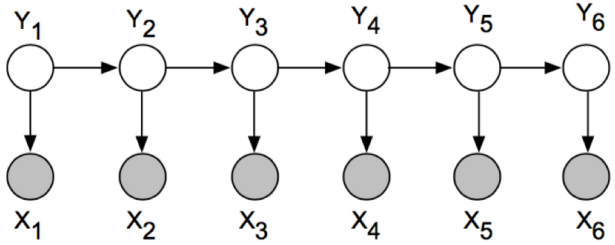
  - Inference
    - Create data structures for computing marginal or conditional distributions quickly
  - Learning
    - Learning the parameters of the distribution can be aided by graph techniques

Graphical Models Landscape



[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Application 1: Hidden Markov Model



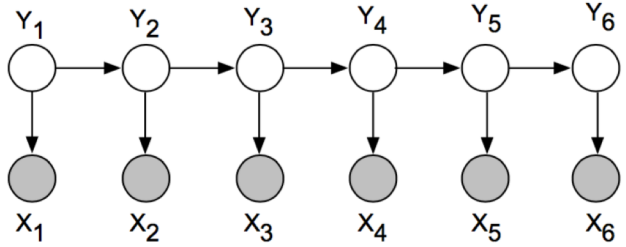
- Frequently used for speech recognition and part-of-speech tagging
- Joint distribution factors as:

$$p(\mathbf{y}, \mathbf{x}) = p(y_1)p(x_1 \mid y_1) \prod_{t=2}^{T} p(y_t \mid y_{t-1})p(x_t \mid y_t)$$

  - $p(y_1)$ is the distribution for the starting state
  - $p(y_t \mid y_{t-1})$ is the *transition* probability between any two states
  - $p(x_t \mid y_t)$ is the *emission* probability
- What are the conditional independencies here? For example, $Y_1 \perp \{Y_3, \ldots, Y_6\} \mid Y_2$

[1]Reference: David Sontag (2013)

Application 1: Hidden Markov Model



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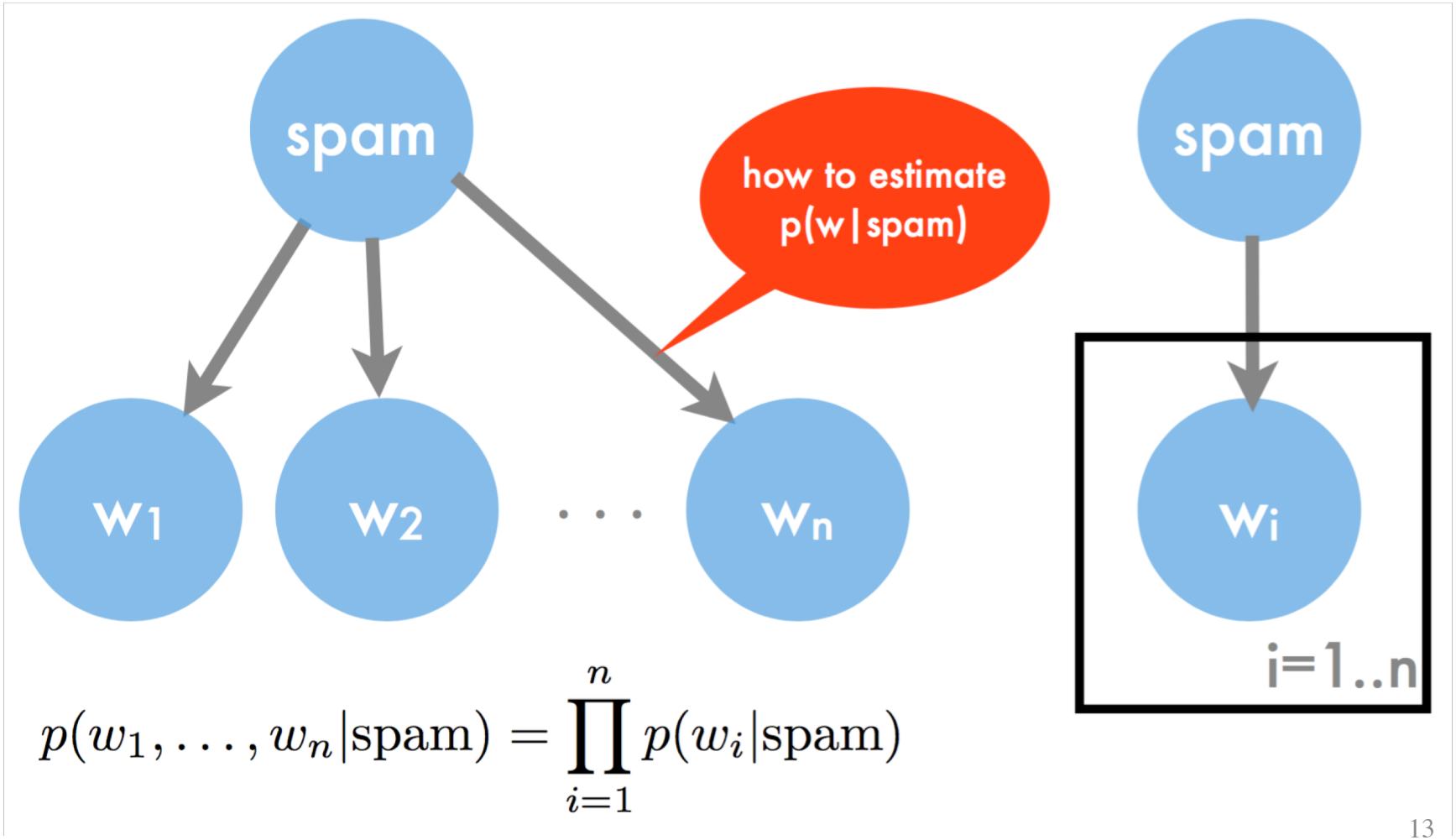
- A **homogeneous** HMM uses the same parameters (β and α below) for each transition and emission distribution (**parameter sharing**):

$$p(\mathbf{y}, \mathbf{x}) = p(y_1)\alpha_{x_1,y_1} \prod_{t=2}^{T} \beta_{y_t,y_{t-1}}\alpha_{x_t,y_t}$$

How many parameters need to be learned?

[1]Reference: David Sontag (2013)

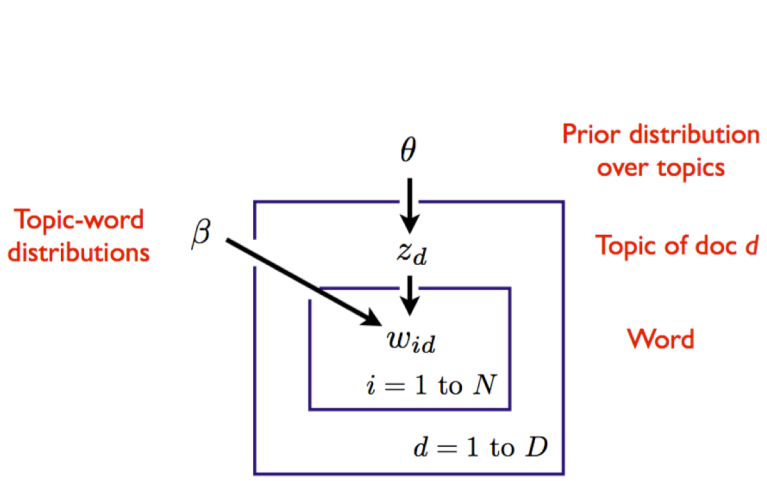
Application 2: Naïve Bayes Spam Filter

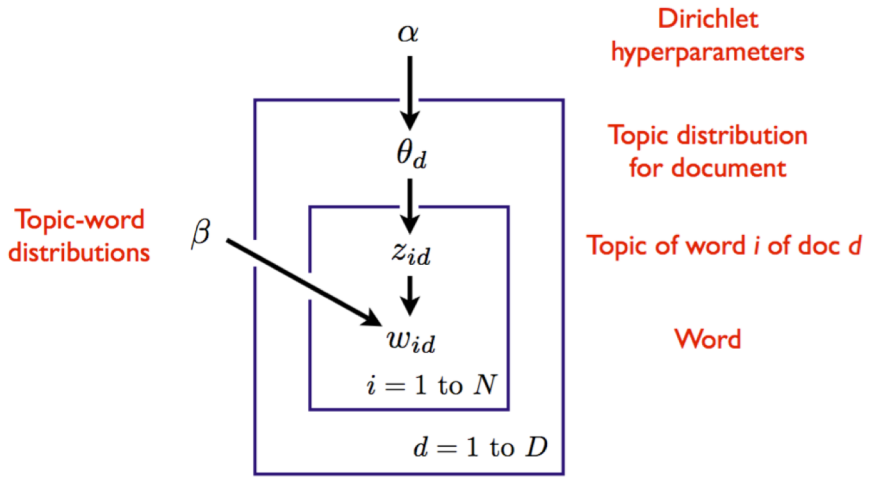


$$p(w_1, \ldots, w_n|\text{spam}) = \prod_{i=1}^{n} p(w_i|\text{spam})$$

[1]Reference: Alex Smola (2011)

Application 3: Latent Dirichlet Allocation





- Model on left is a **mixture model**
  - Called *multinomial* naive Bayes (a word can appear multiple times)
  - Document is generated from a single topic
- Model on right (LDA) is an **admixture model**
  - Document is generated from a distribution over topics

[1]Reference: David Sontag (2013)

Application 4: Conditional Random Field

- **Conditional random fields** are undirected graphical models of conditional distributions $p(\mathbf{Y} \mid \mathbf{X})$
  - $\mathbf{Y}$ is a set of **target variables**
  - $\mathbf{X}$ is a set of **observed variables**
- A CRF is a Markov network on variables $\mathbf{X} \cup \mathbf{Y}$, which specifies the conditional distribution

$$P(\mathbf{y} \mid \mathbf{x}) = \frac{1}{Z(\mathbf{x})} \prod_{c \in C} \phi_c(\mathbf{x}_c, \mathbf{y}_c)$$

with partition function

$$Z(\mathbf{x}) = \sum_{\hat{\mathbf{y}}} \prod_{c \in C} \phi_c(\mathbf{x}_c, \hat{\mathbf{y}}_c).$$

[1]Reference: David Sontag (2013)

Questions?

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- Directed Graphical Models
- Undirected Graphical Models

Primer on Graphs

Graph

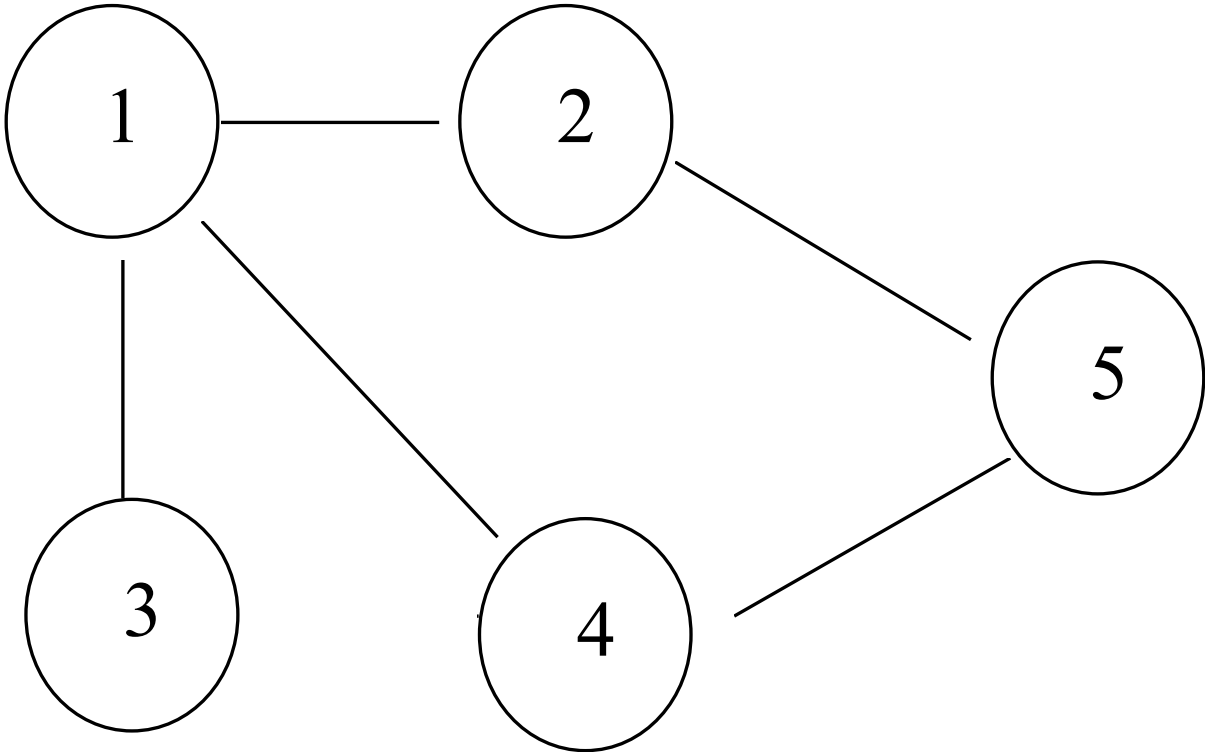
- A network with
  - Edges (links)
  - Vertices (nodes)

- Heavily used in Computer Science for algorithms and data structures

- Here, we will only need the terminology of graphs.
  - As we will see, their primary purpose will be visualization and encoding domain knowledge

Undirected Graph

- An undirected graph
  - Edges have no direction information

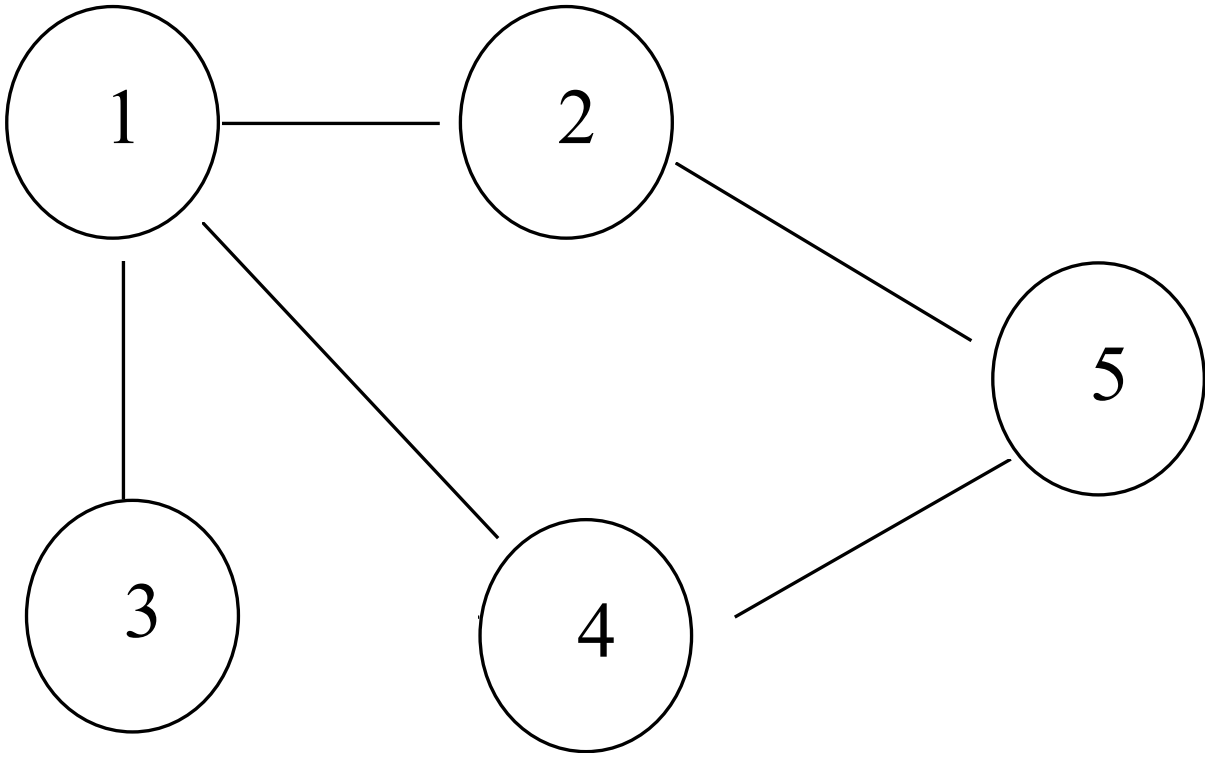


Notation for Undirected Graphs

- Set of vertices denoted $1, \ldots, N$
- Size of graph is N
- Edge is an (unordered) pair (i, j)
  - (i, j) is the same as (j, i)
  - indicates that i and j are directly connected
- Maximum number of edges: $N(N-1)/2$ (order N^2)
- i and j connected if there is a path of edges between them
- Subgraph of G:
  - restrict attention to certain vertices and edges between them

Path

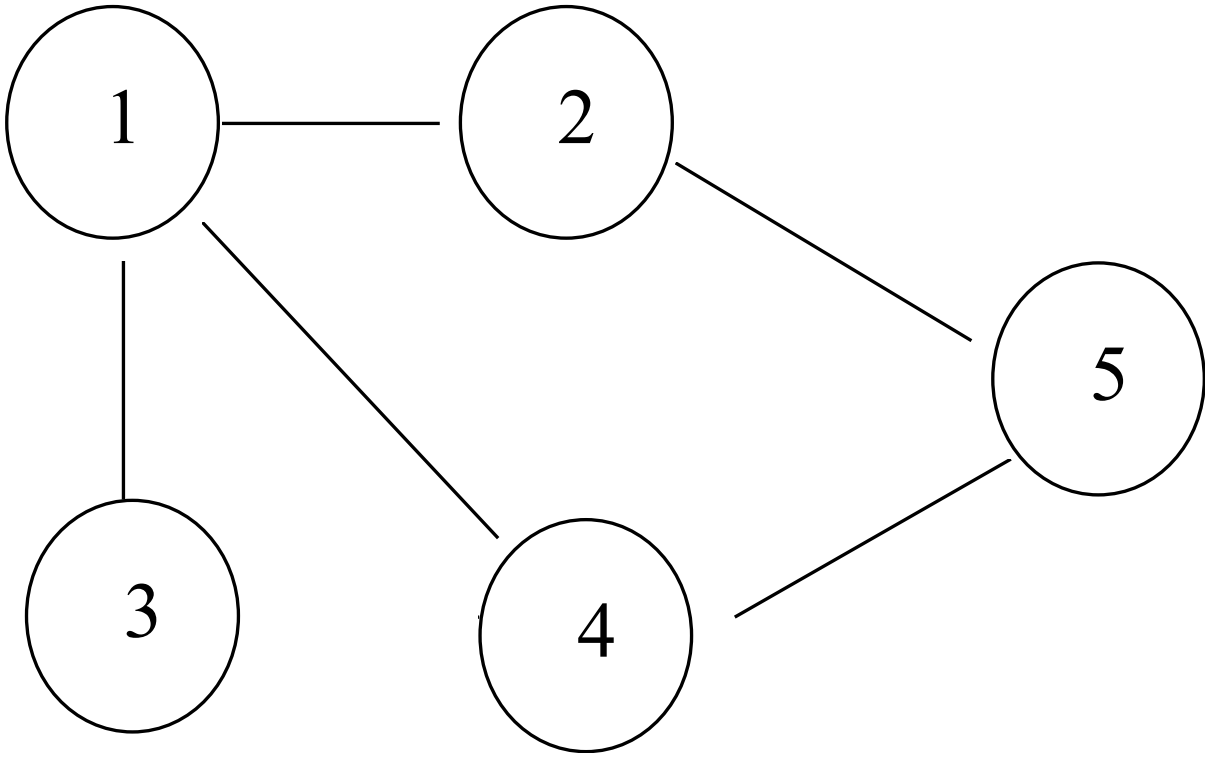
- A sequence of vertices where each successive pair are connected by an edge



- For example, (3,4,5) is not a path. (3,1,4,5) is a path

Neighbor

- All vertices that share an edge with the node are its neighbors. Denote as $nbhd(X)$



- For example, $(3,4,2)$ are neighbors of 1.
  - $nbhd(1) = (3,4,2)$

Cliques and Independent Sets

- A clique in a graph G is a set of vertices:
  - informal: that are all directly connected to each other
  - formal: whose induced subgraph is complete
  - an edge is a clique of just 2 vertices

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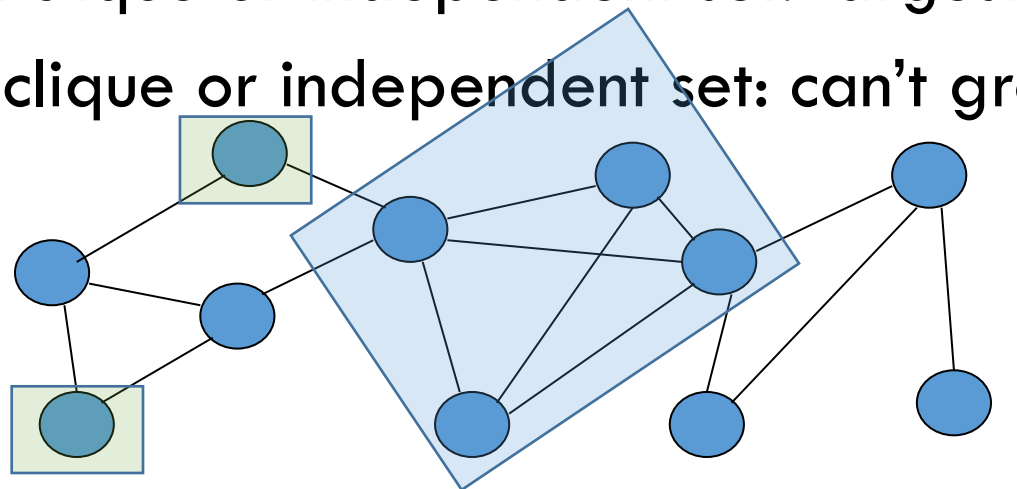
- A clique in a graph G is a set of vertices:
  - informal: that are all directly connected to each other
  - formal: whose induced subgraph is complete
  - an edge is a clique of just 2 vertices
- Independent set:
  - set of vertices whose induced subgraph is empty (no edges)
- Maximum clique or independent set: largest in the graph
- Maximal clique or independent set: can't grow any larger



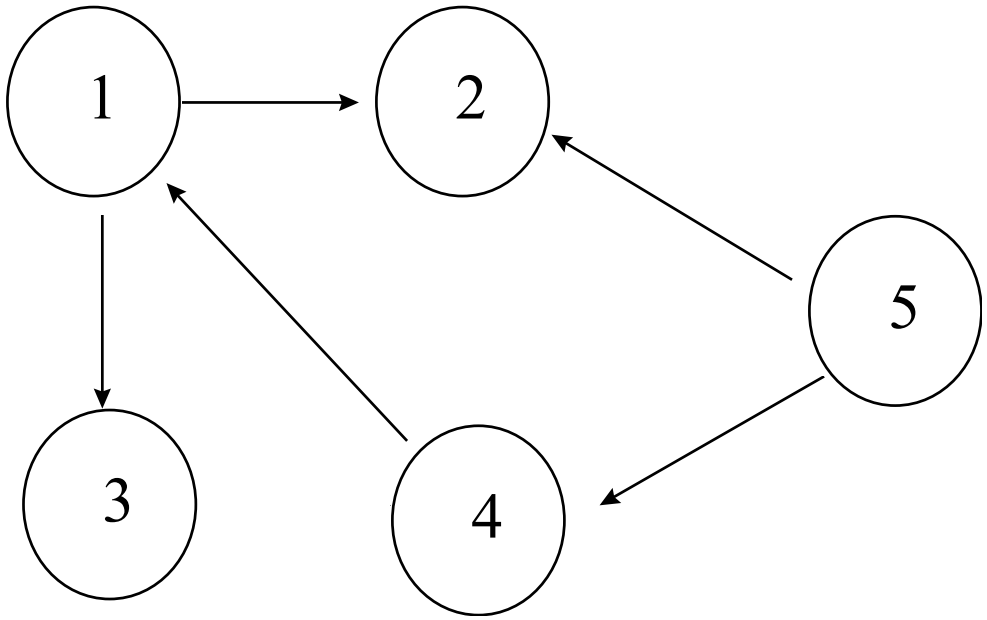
Directed Acyclic Graph

- A directed graph
  - Edges have directions or orientations
  - Edge (u,v) means u $\rightarrow$v
  - May also have edge (v,u)
  - Common for capturing asymmetric relations

- A directed acyclic graph (DAG)
  - No directed cycles
  - No way to follow the oriented edges and come back to the starting node

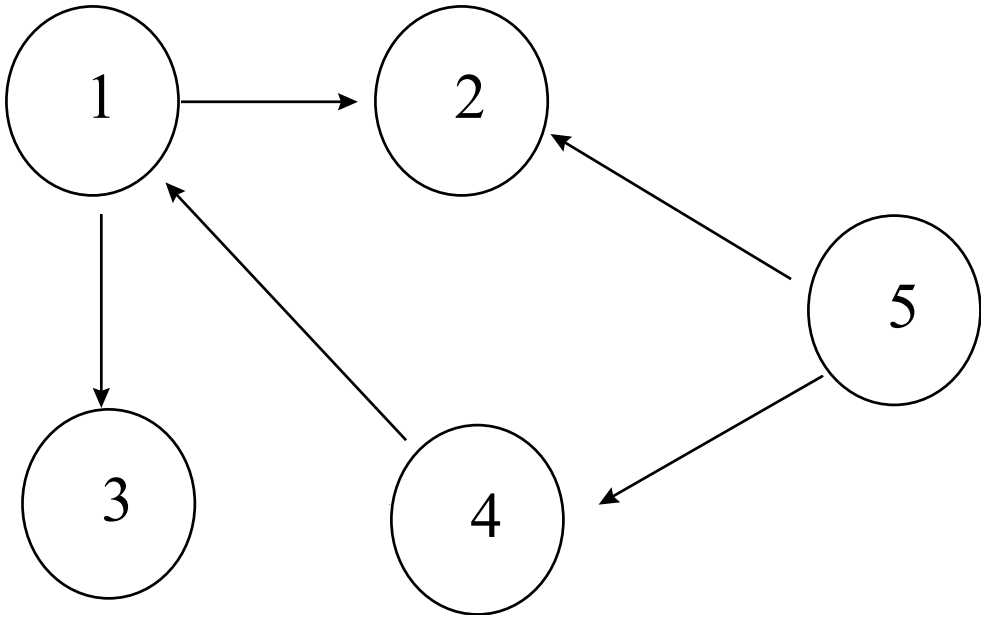
DAG

- A directed acyclic graph (DAG)



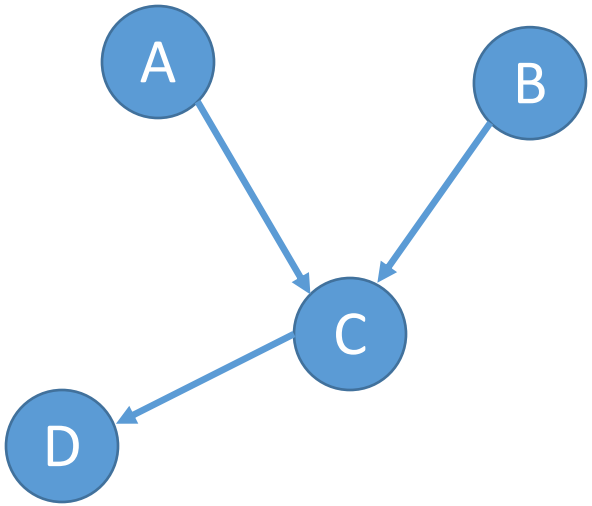
DAG Paths vs Directed Paths

- Path:
  - Same as undirected graph. Ignore directions
  - Example: (3,1,2) is a path
- Directed path
  - Take direction into account. E.g., (5,4,1,3) is a directed path



Parents of a Node

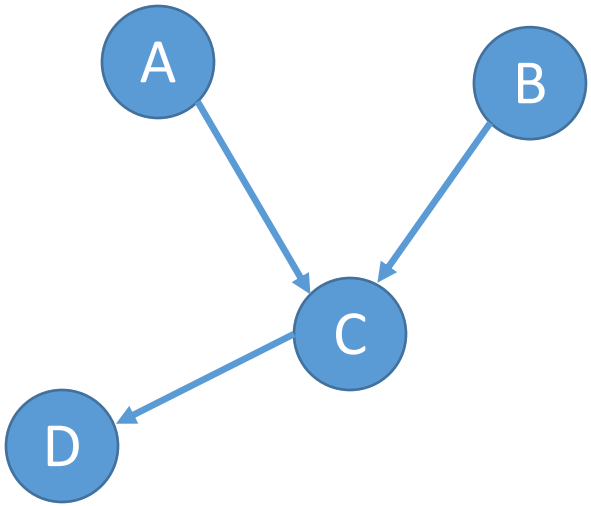
- Notation:
  - $pa(J)$ = Parents of node J

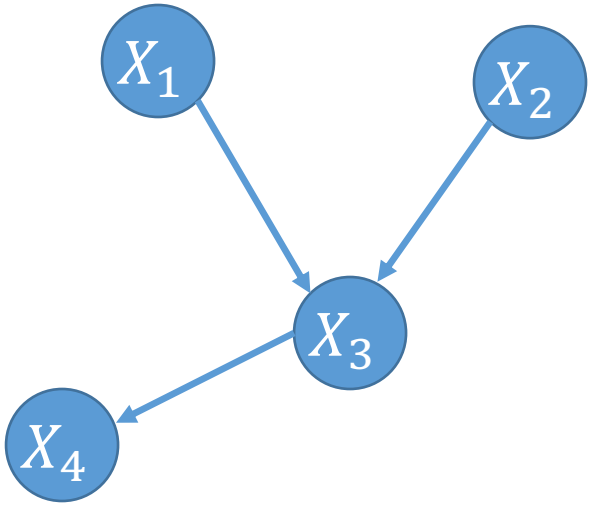


  - In this graph, parents of C are (A, B)
    - Neighbors of that vertex that point to that vertex

Parents of a Node

- In the below graph, parents of A is the empty set ϕ

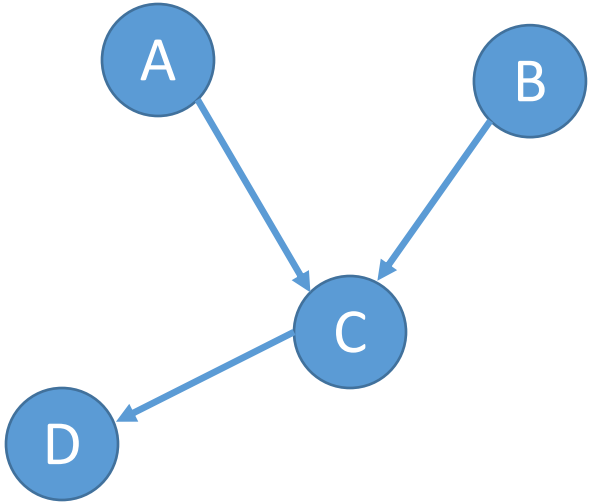


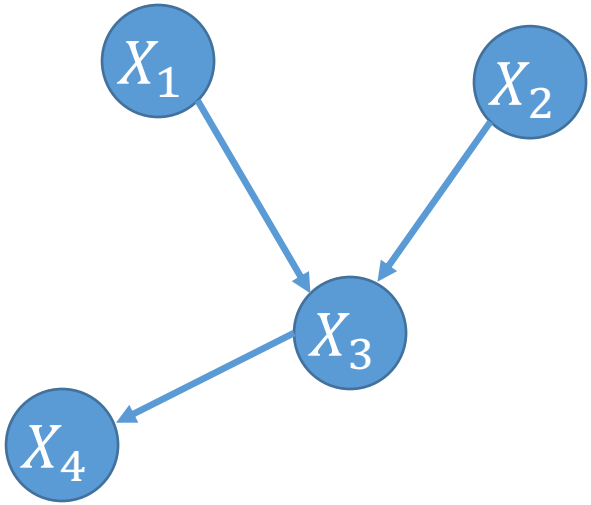


- In the graph on the right, $pa(X_4) = (X_3)$

Descendants of a Node

- All nodes that can be reached by following the arrow directions
- In the below graph, descendants of A are $\{C, D\}$

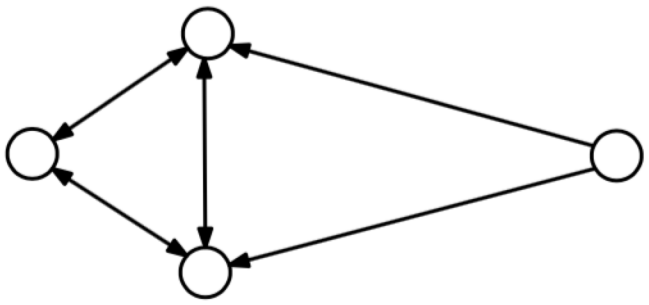




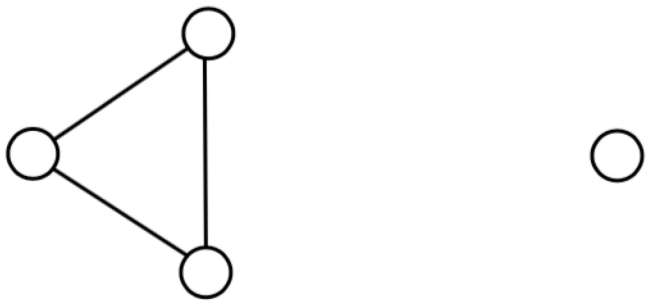
- In the graph on the right, $\text{Desc}(X_3) = (X_4)$

Connected Graphs

- G (directed or undirected) is connected if there is a path between any two vertices.
- Otherwise, we have connected components.
    - subgraphs determined by mutual connectivity
- Complete graph: edge between all pairs of vertices



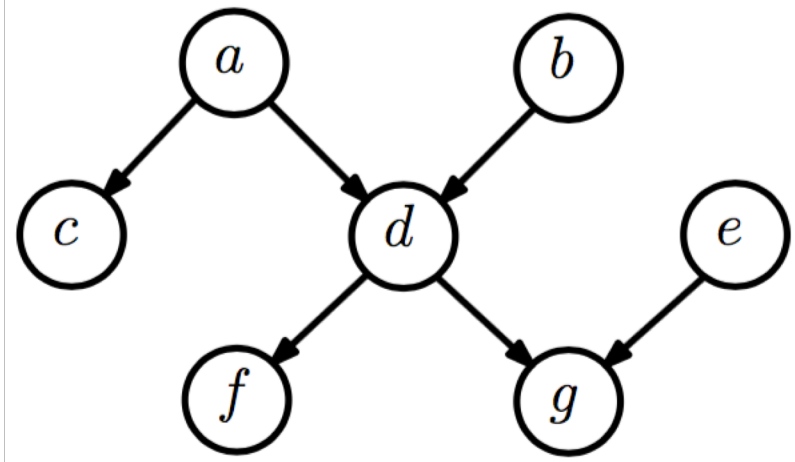
connected graph



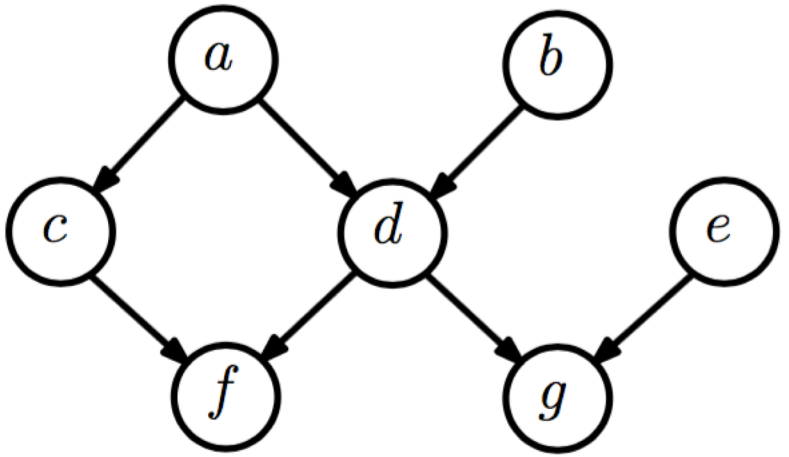
graph with two connected components

Tree Graph (Singly-Connected)

- If for any vertex pair, there is no more than one path between them. This is also called a tree.



singly-connected



multiply-connected

- Otherwise, it is multiply-connected. Also called loopy.
- Similar definition for undirected graphs as well.

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Directed (Probabilistic) Graphical Models

Based on notes by MathematicalMonk[1]

[1]Reference: https://www.youtube.com/playlist?list=PLD0F06AA0D2E8FFBA

DPGM

- DPGM: Directed Probabilistic Graphical Model
- Also called a Bayesian Network or Belief Net
  - Nothing Bayesian here
- Directed graphs tell us about conditional independence properties of a probability distribution

Why Conditional Independence?

- Why do we care about conditional independence?

- Because we can perform tractable or efficient inference (we will address this next lecture!)

Joint Distribution

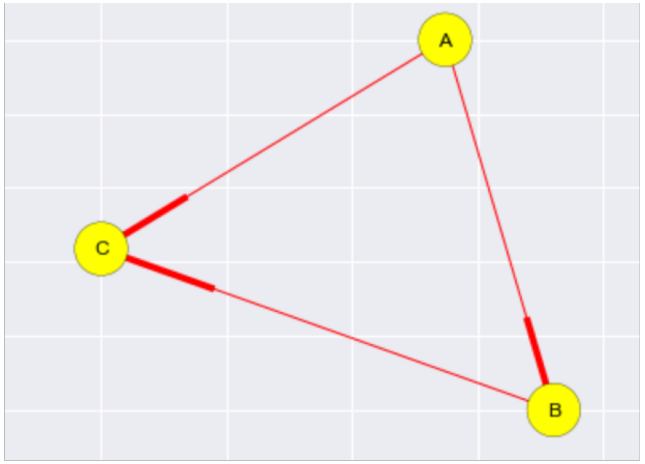
- Let A, B, C be RVs

- Joint distribution
  - $P(A = a, B = b, C = c)$
    - $= P(c|a, b)P(a, b)$
    - $= P(c|a, b)P(b|a)P(a)$

  - This is a factorization
    - We can always do this

Factorizations are not Unique

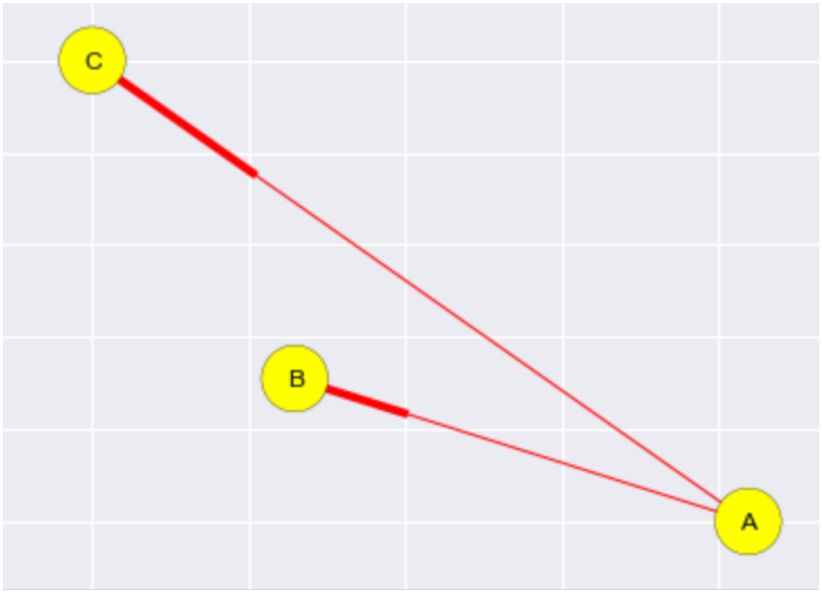
- $P(c|a,b)P(b|a)P(a)$
- Create a node for each factor
- Graph has directed edges
- No cycles
  - Can't return to a node



- Nothing special about this factorization
  - We could have factored in a completely different way

Conditional Independence Changes the Graph

- If C is conditionally independent of B given A
- Use notation $C \perp B \mid A$
- Then $P(c|a,b) = P(c|a)$
- So we got a different graph



- Not every distribution could have lead to this graph.

Non-unique Graphs

- Given $X = (X_1, \ldots, X_n) \sim P$, and a DAG G
- We say X respects G (or P respects G) if
  - $P(x_1, \ldots, x_n) = \prod P(x_i | pa(x_i)) \ \forall i = 1, \ldots, n$

Non-unique Graphs

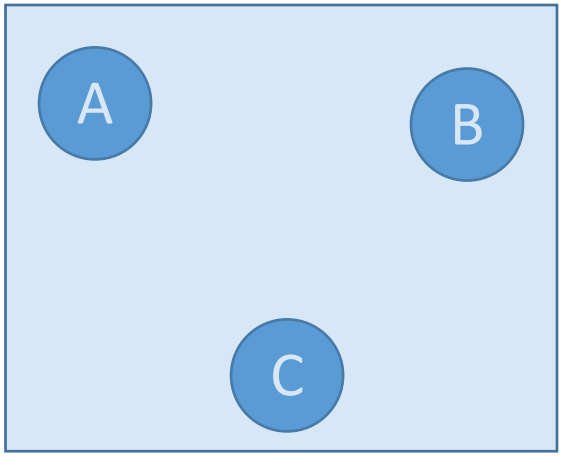
- Given $X = (X_1, \ldots, X_n) \sim P$, and a DAG G
- We say X respects G (or P respects G) if
  - $P(x_1, \ldots, x_n) = \prod P(x_i | pa\,(x_i)) \;\; \forall i = 1, \ldots, n$

- The graph G does not imply that any RVs are conditionally dependent.
  - At most, it will imply is conditional independence

- The graph G does not uniquely determine the probability distribution P

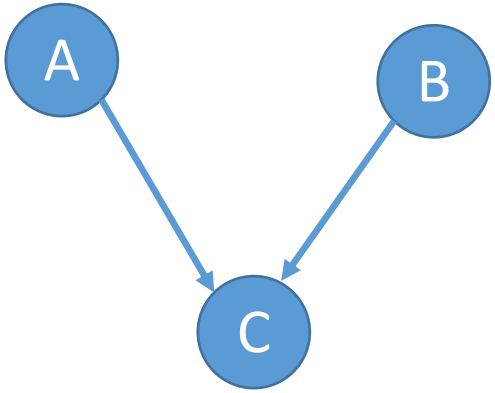
Non-unique Graphs: Example

- Say A,B,C are independent
  - $P(a, b, c) = P(a)P(b)P(c)$



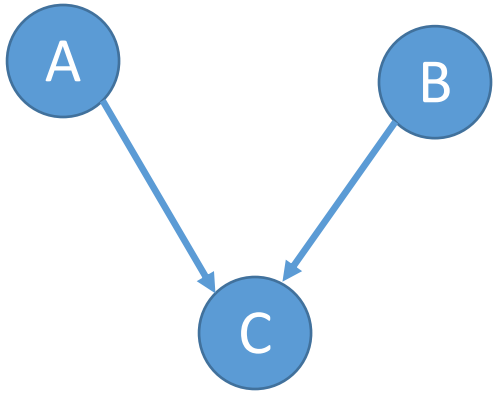
- Let X = (A,B,C)
- Then X respects the graph G

- X also respects G'

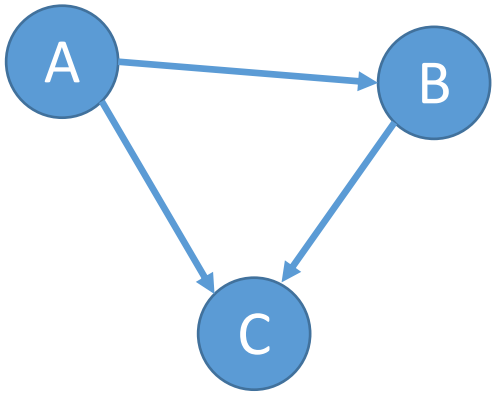


Non-unique Graphs: Example

- Graph G' is not saying C depends on A and B



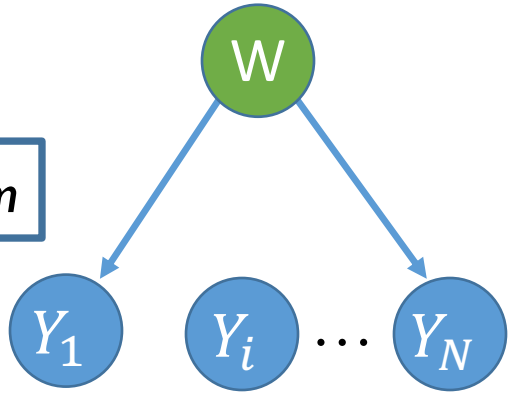
- It only says that the distribution of X = (A,B,C) factors in a way that can be represented by G'
- X also respects G''



Example: Linear Regression

- Graphical model for (Bayesian) linear regression
  - Data: $\{x_i, y_i\}_{i=1}^N$ where x_i is d dimensional
  - Model: $f_W(x) = W^T \phi(x)$
    - Linear in W (not a matrix, a random vector)
- Let $W \sim N(0, \sigma_0^2 I)$
- Let $Y_i \sim N(W^T \phi(x_i), \sigma^2)$
  - Let Y_i be conditionally independent of Y_j given W

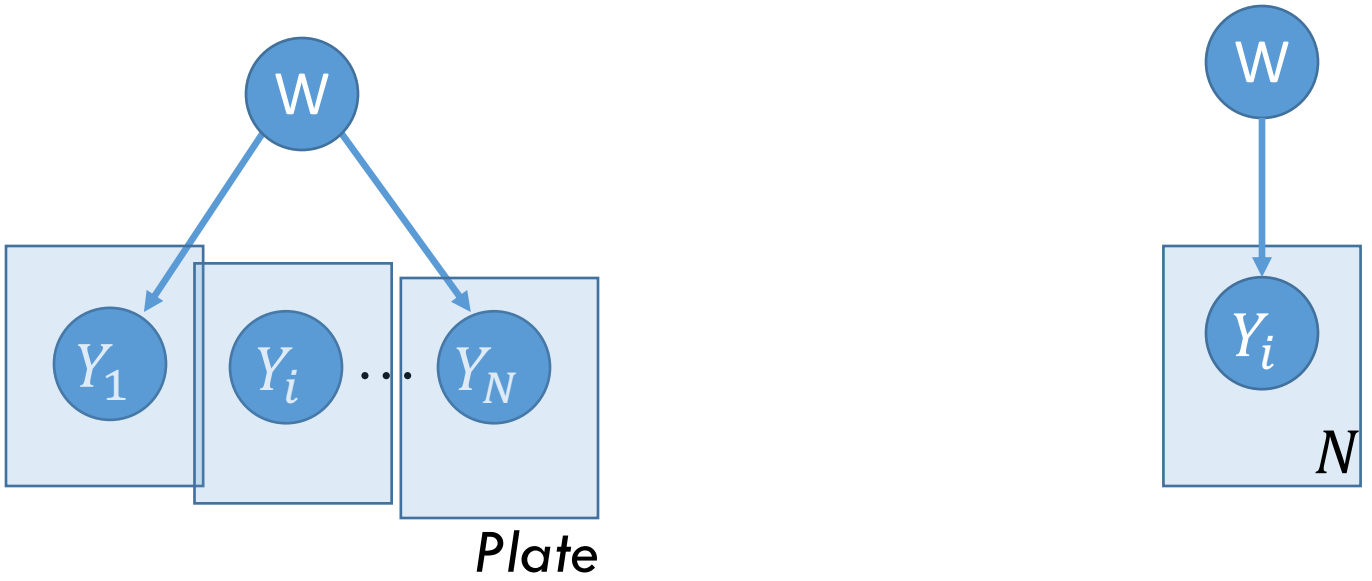
σ_0, σ and x_i are not random



Example: Linear Regression

- $P(w, y_1, \ldots, y_N) = P(w) \prod P(y_i|w)$

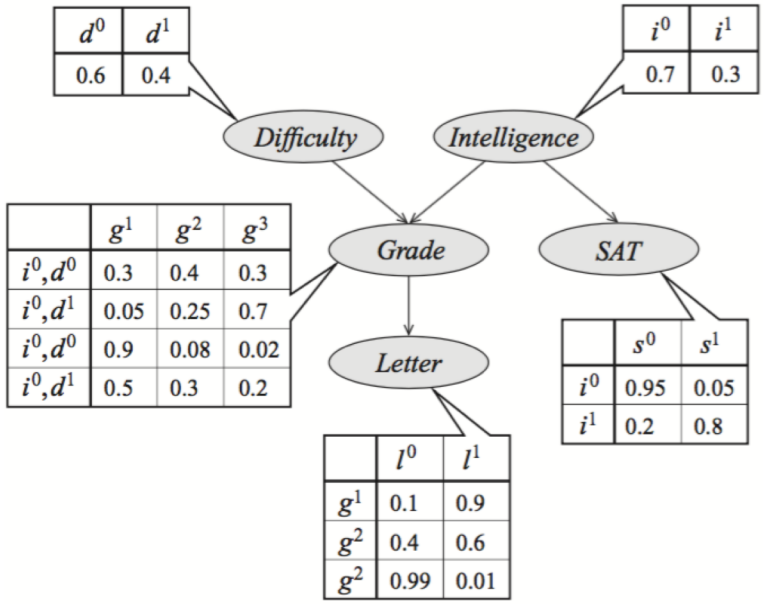
- Can also use a plate notation
  - Stack the plates on top of each other



- Variable W is called a latent or hidden variable
- Variables Y_i are called observed variables

Example: Student Network

- Consider the following Bayesian network:



d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3

	g^1	g^2	g^3
i^0, d^0	0.3	0.4	0.3
i^0, d^1	0.05	0.25	0.7
i^0, d^0	0.9	0.08	0.02
i^0, d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^2	0.99	0.01

- What is its joint distribution?

$$p(x_1, \ldots x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{\mathrm{Pa}(i)})$$

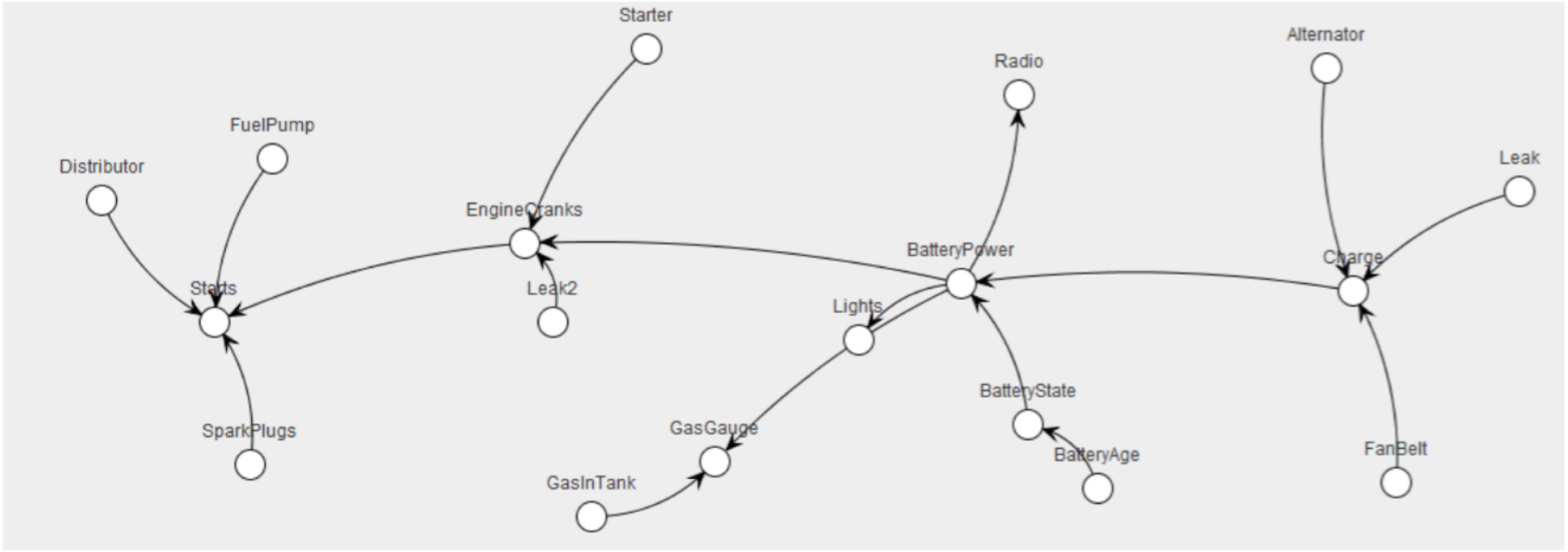
$$p(d, i, g, s, l) = p(d)p(i)p(g \mid i, d)p(s \mid i)p(l \mid g)$$

[1]Reference: David Sontag (2013)

Example: Car Network

$$p(x_1, \ldots x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{\mathrm{Pa}(i)})$$

Will my car start this morning?

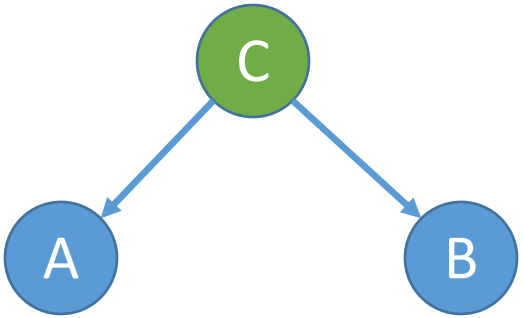


Heckerman *et al.*, Decision-Theoretic Troubleshooting, 1995

[1]Reference: David Sontag (2013)

Conditional Independence (I)

- Given a graphical model, we can determine if two sets of RVs are conditionally independent or not

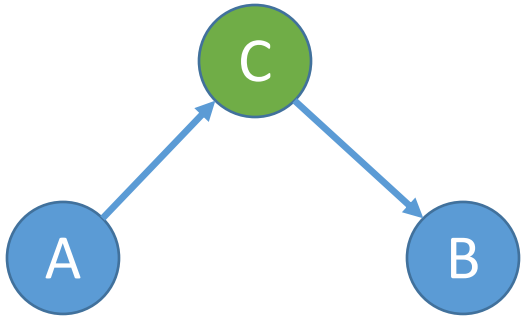


Tail-to-tail

- $P(a, b, c) = P(a|c)P(b|c)P(c)$ is a joint distribution that respects this graph
- What happens when we condition on C?
  - $P(a, b|c) = \frac{P(a,b,c)}{P(c)} = P(a|c)P(b|c)$
  - Thus, A and B are conditionally independent given C
  - Use notation $A \perp B \mid C$

Conditional Independence (II)

- Given a graphical model, we can determine if two sets of RVs are conditionally independent or not

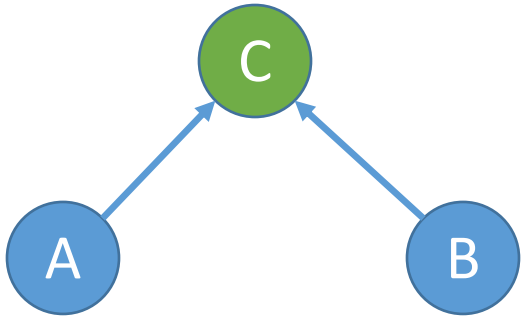


Head-to-tail

- $P(a,b,c) = P(a)P(c|a)P(b|c) = [P(a|c)P(c)]P(b|c)$ is the joint distribution that respects this graph
- What happens when we condition on C?
  - $P(a,b|c) = \frac{P(a,b,c)}{P(c)} = P(a|c)P(b|c)$
  - Thus, A and B are conditionally independent given C
  - Use notation $A \perp B \mid C$

Conditional Independence (III)

- Given a graphical model, we can determine if two sets of RVs are conditionally independent or not

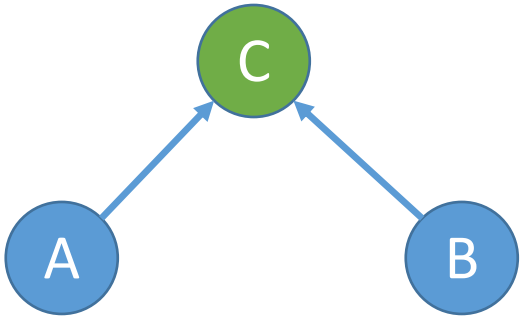


Head-to-head

- $P(a, b, c) = P(a)P(b)P(c|a, b)$ is the joint distribution that respects this graph
- What happens when we condition on C?
  - $P(a, b|c) = \frac{P(a,b,c)}{P(c)} \neq P(a|c)P(b|c)$
  - Cannot say A & B are conditionally independent given C

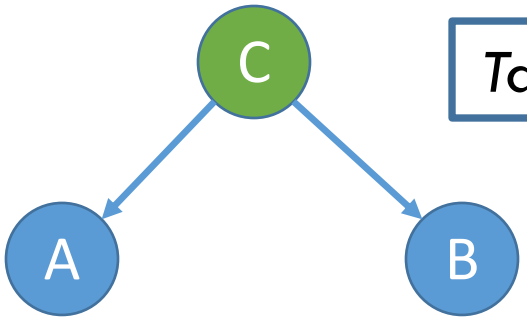
Head-to-Head Example

- Say $A \sim Bern\left(\frac{1}{2}\right), B \sim Bern(\frac{1}{2})$
- Say $C = 1$ if $A = B$ and 0 otherwise
- Conditioned on C
  - If we know A, we know B.
    - They are dependent!
  - Similarly, if we know B, we know A.
- Hence, $A \not\perp B \mid C$ (i.e., not true for every distribution that respects the graph)
- But unconditionally, $A \perp B$
  - $P(a,b) = \sum_c P(a,b,c) = \sum_c P(a)P(b)P(c|a,b)$
  - $= P(a)P(b)\sum_c P(c|a,b) = P(a)P(b)$

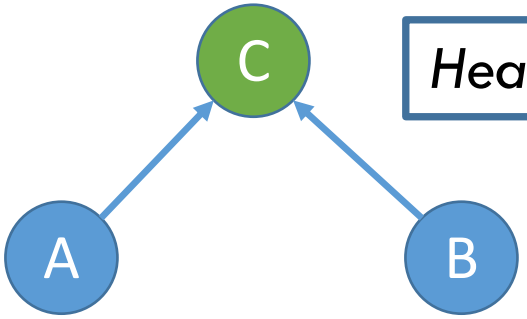


Conditional Independence: Summary for 3 Node Graphical models

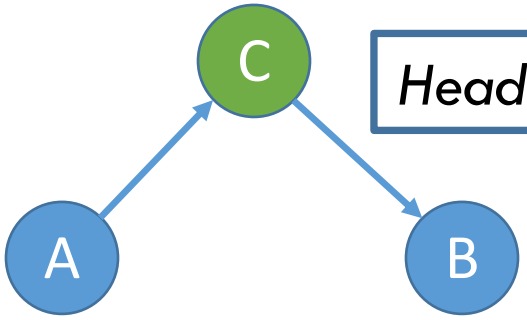
- Given a graphical model, we can determine if two sets of RVs are conditionally independent or not



Tail-to-tail: $\mathrm{A} \perp B \mid C$



Head-to-head: $\mathrm{A} \not\perp B \mid C$



Head-to-tail: $\mathrm{A} \perp B \mid C$

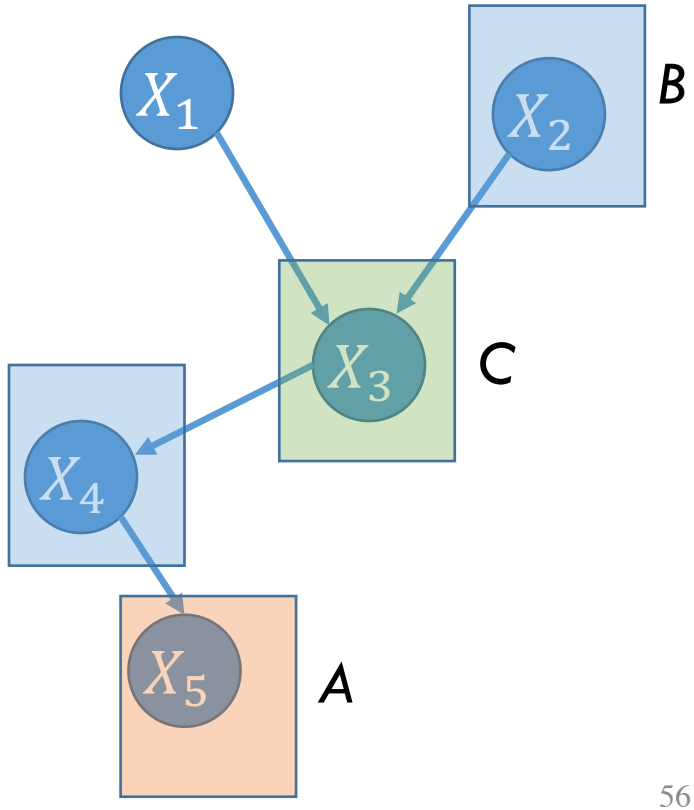
D-Separation Criterion: N Node Setting

- We saw how conditional independence properties unfold due to graph structure
  - This was only for three node graphs
- We will now move to larger DAGs
- We will look at the general idea of d-separation

D-Separation (I)

- Helps you read off the conditional independence properties

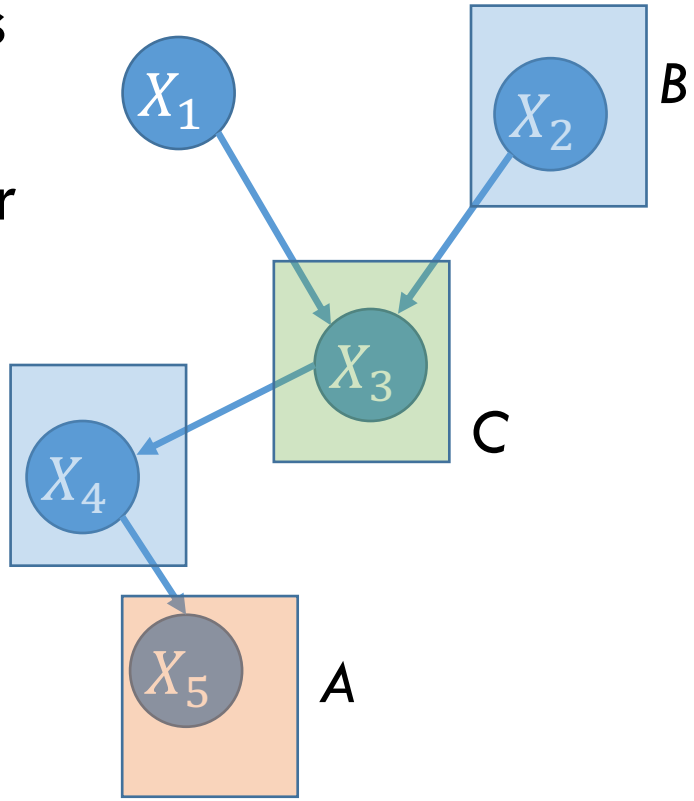
- Notation
  - Sets of RVs A,B and C
  - Disjoint
  - Not necessarily covering all



D-Separation (II)

- A path between two vertices is blocked with respect to C if it passes through a node v such that
  - v $\in$ C, arrows are head-to-tail or tail-to-tail
  - OR, $v \notin C$, arrows are head-to-head, and Descendants(v) $\notin C$

- Example
  - X_4, X_3 and X_2 are in head-tail
  - So path is blocked



D-Separation (III)

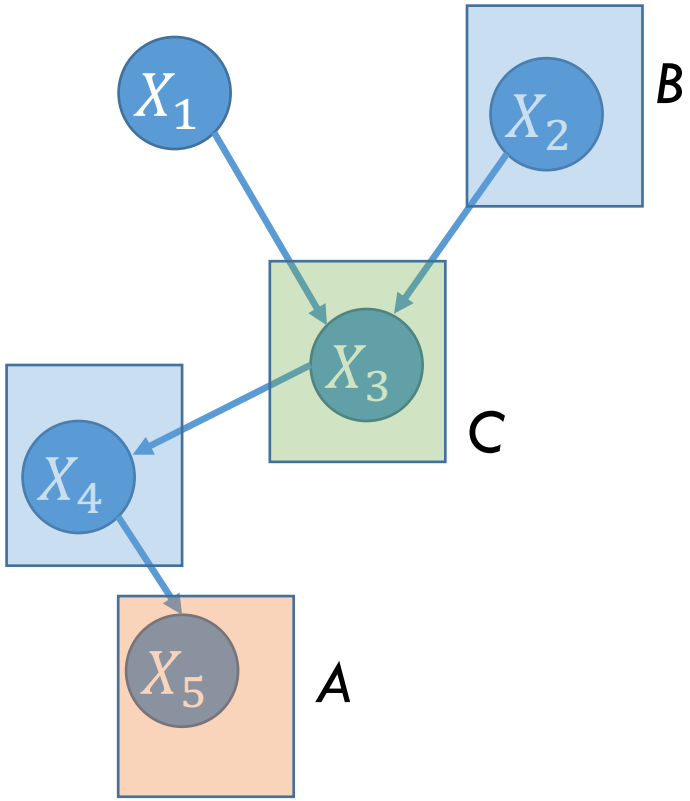
- Definition of D-Separation
  - A and B are d-separated by C if all paths from vertices in A to vertices in B are blocked with respect to C

- Key result
  - If A and B are d-separated by C, then $A \perp B \mid C$

  - Note: the above result is only 'necessary' not 'sufficient'

D-Separation Example I

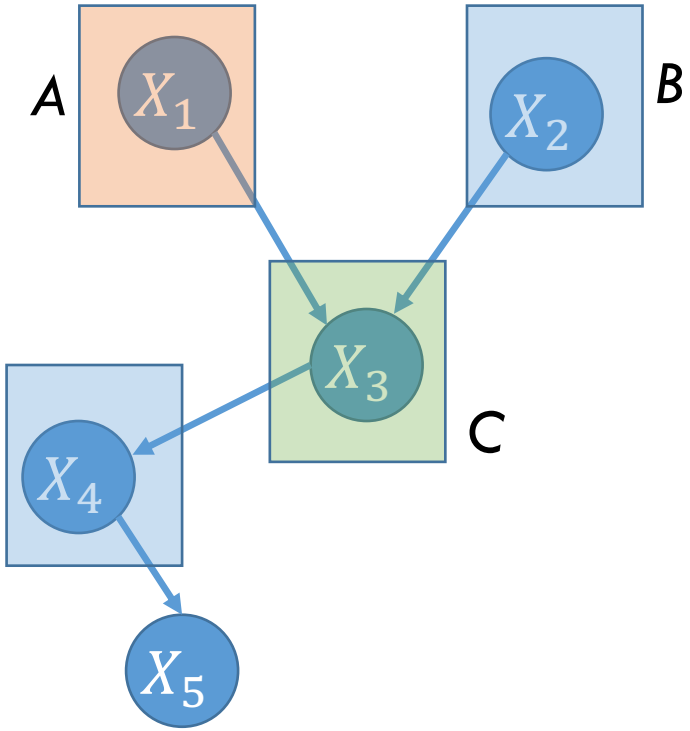
- Let C $= \{X_3\}$
- Is A $\perp B \mid C$?
- We can check that by checking d-separation for all pairs of vertices $X_i \perp X_j \mid C$?
  - $i = \{5\}$
  - $j = \{2,4\}$



- Easy to see that
  - X_2, X_5 are blocked by C
  - X_4, X_5 are not blocked by C
- Hence, not d-separated
- Hence cannot say A $\perp B \mid C$

D-Separation Example II

- Let C = $\{X_3\}$
- Is $A \perp B \mid C$?
- We can check that by checking d-separation for all pairs of vertices $X_i \perp X_j \mid C$?
  - $i = \{1\}$
  - $j = \{2,4\}$



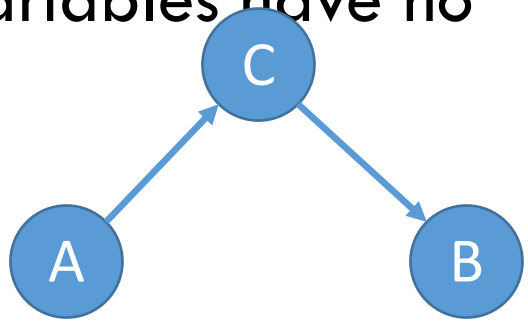
- We can see that
  - X_1, X_2 are not blocked by C
  - X_1, X_4 are blocked by C
- Hence, not d-separated
- Hence cannot say $A \perp B \mid C$

DAG and Probability (I)

- We have showed that the structure of the DAG corresponds to a set of conditional independence assumptions
  - We can read conditional independence easily!

- We just need to specify $P(X_i|pa(X_i))$

- This does not mean that non-parent variables have no influence
  - Thus, the DAG does not imply
    - $P(c|a,b) = P(c|a)$



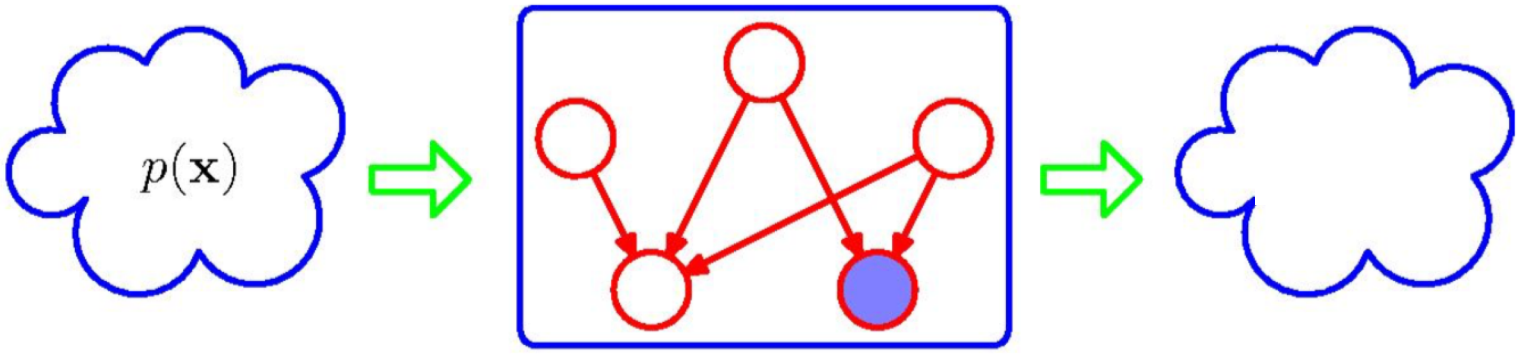
DAG and Probability (II)

- DPGMs are good for representing independence, not for representing dependence

- We have seen this
  - Multiple graphs for the same distribution

  - D-separation only says conditional independence if true. If not true, then no conclusion is drawn.

Filter view of DPGM



- Only distributions that satisfy conditional independences are allowed to pass
- One graph can describe many probability distributions
- Edge cases:
  - When DAG is fully connected, all distributions pass
  - When DAG is fully disconnected, only the product distribution ($\prod_i P(X_i)$) passes

[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Continuous Distributions

- We never had to state whether $P(X|Y)$ was continuous or discrete
- The graph is agonistic to the support of the random variables!

Questions?

Today's Outline

- Motivation
- Primer on Graphs
- Directed Graphical Models
- Undirected Graphical Models

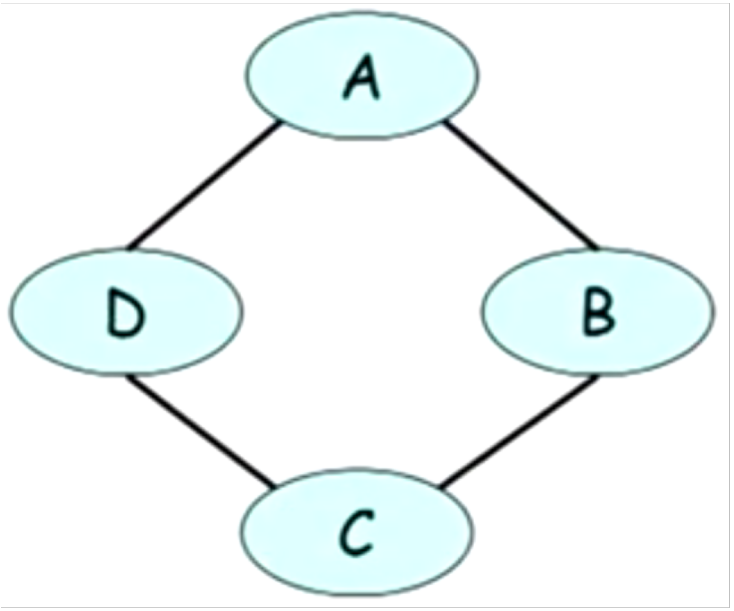
Undirected (Probabilistic) Graphical Models

Based on notes from Bjoern Andres and Bernt Schiele (2016)

[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

UPGM

- Also called Markov Networks or Markov Random Fields
- No edge directions
- Again, diagrams of probability distributions that capture conditional independences



[1]Reference: Daphne Koller (2011)

UPGM vs DPGM

- DPGMs have been used in data analytics, ML, statistics
- UPGMs have been used in computer vision and physics, and have applications in data analytics as well

- DPGM
  - Factor of the distribution was a (cond.) distribution

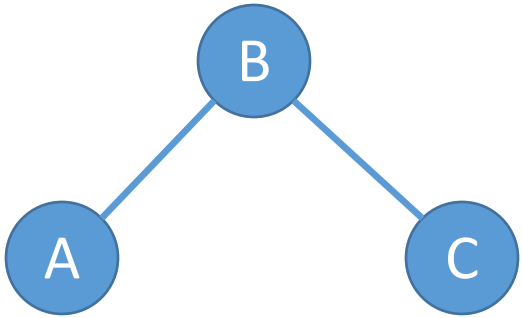
- UPGM
  - Factor (also called potential) need not be a distribution
  - Let $P(a,b,c) = \frac{1}{Z}\phi_1(a,b)\phi_2(b,c)$
  - Here Z is the normalization constant or partition function. $Z = \sum_{a,b,c}\phi_1(a,b)\phi_2(b,c)$

[1]Reference: Daphne Koller (2011)

Notion of a Potential

- Potential $\phi(x)$ is a non-negative function of variable x. Joint potential $\phi(x_1, \ldots, x_D)$ is a non-negative function of a set of variables.

- Let $P(a, b, c) = \frac{1}{Z}\phi_1(a, b)\phi_2(b, c)$



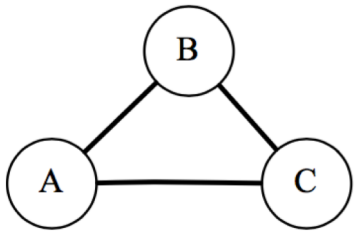
Potentials Over Cliques

- For RVs $X_1, \ldots, X_D$, an UPGM is defined as a product of potentials over the cliques of graph G

- $P(X_1, \ldots, X_D) = \frac{1}{Z} \prod_c \phi_c(\mathcal{X}_c)$
  - Here $Z = \sum_{x_1,\ldots,x_D} \prod_c \phi_c(\{x_i : X_i \in \mathcal{X}_c\})$

- Special cases:
  - When cliques are of size 2: the UPGM is called a pairwise UPGM
  - When all potentials are strictly positive: the distribution is called a Gibbs distribution

Example Potentials



$\phi_{A,B}(a,b) =$

A \ B	0	1
0	10	1
1	1	10

$\phi_{B,C}(b,c) =$

B \ C	0	1
0	10	1
1	1	10

$\phi_{A,C}(a,c) =$

A \ C	0	1
0	10	1
1	1	10

$$p(a,b,c) = \frac{1}{Z}\phi_{A,B}(a,b) \cdot \phi_{B,C}(b,c) \cdot \phi_{A,C}(a,c),$$

where

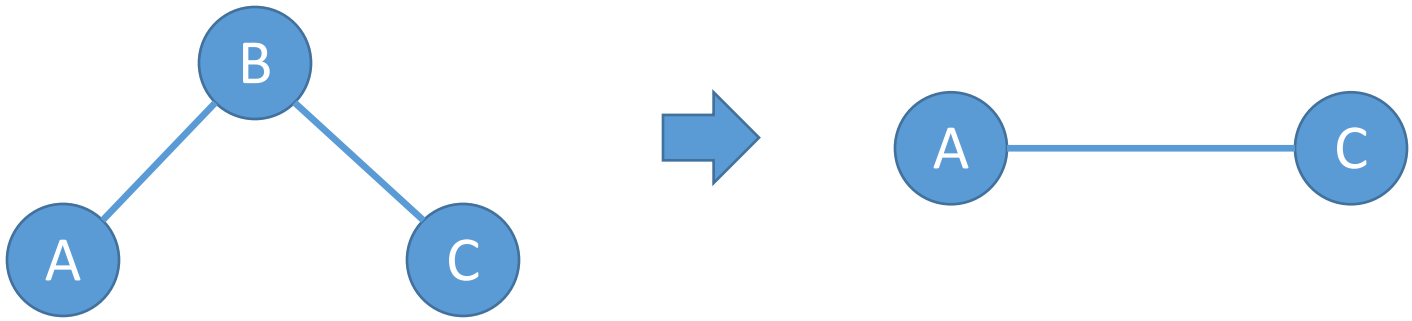
$$Z = \sum_{\hat{a},\hat{b},\hat{c} \in \{0,1\}^3} \phi_{A,B}(\hat{a},\hat{b}) \cdot \phi_{B,C}(\hat{b},\hat{c}) \cdot \phi_{A,C}(\hat{a},\hat{c}) = 2 \cdot 1000 + 6 \cdot 10 = 2060.$$

[1]Reference: David Sontag (2013)

Marginalization

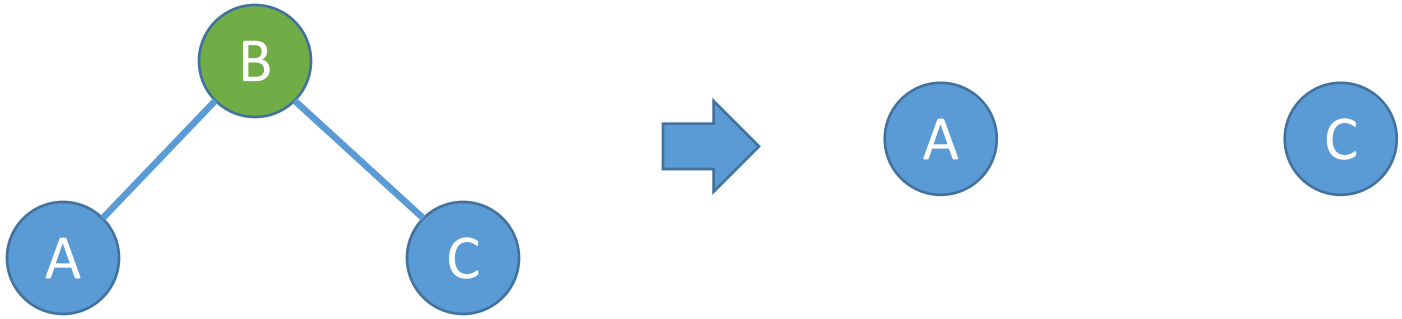
- Marginalizing over B makes A and C graphically dependent

- $P(a,c) = \sum_b P(a,b,c) = \frac{1}{Z}\phi_3(a,c)$



Conditional Independence (I)

- Conditioning on B makes A and C independent
- $P(a, c|b) = P(a|b)P(c|b)$



- Key: This is different from the head-to-head directed graph example, where conditioning introduced dependency!

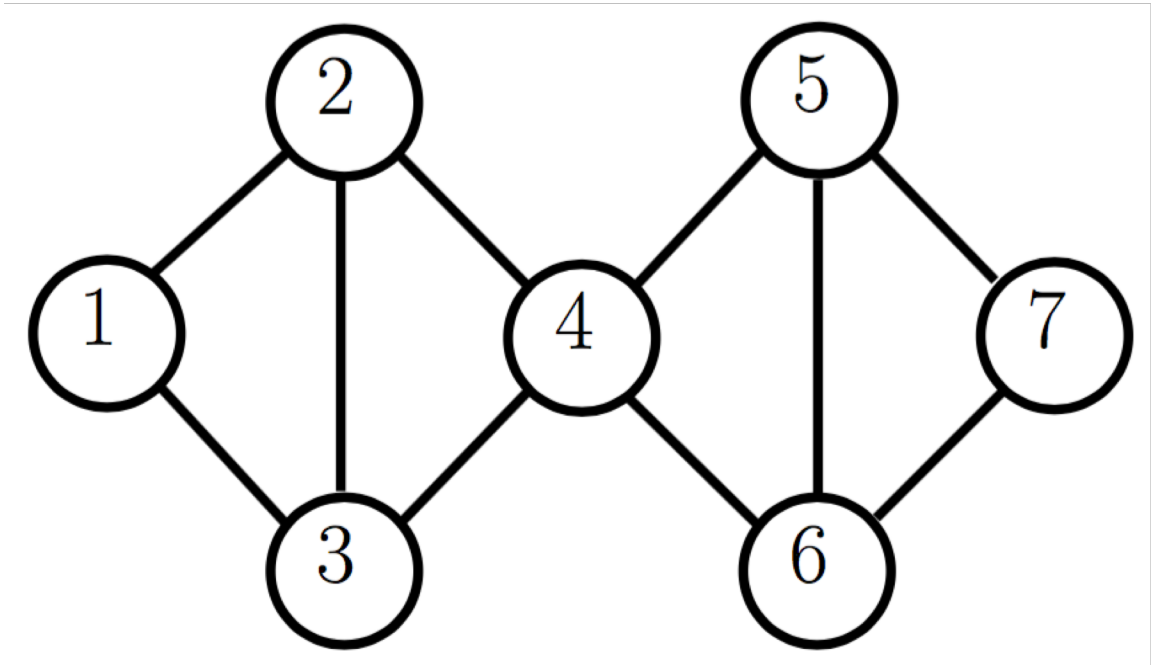
Conditional Independence (II)

- Global Markov property
  - Two sets of nodes (say A and B) are conditionally independent given a third set C if
    - All nodes in A and B are connected through nodes in C

- Local Markov property
  - Conditioning on the neighbors of X makes X independent of the rest of the graph.
  - $P(X_i|X_1, \ldots X_{i-1}, X_{i+1}, X_D) = P(X_i|nbhd(X_i))$

Global Markov Property

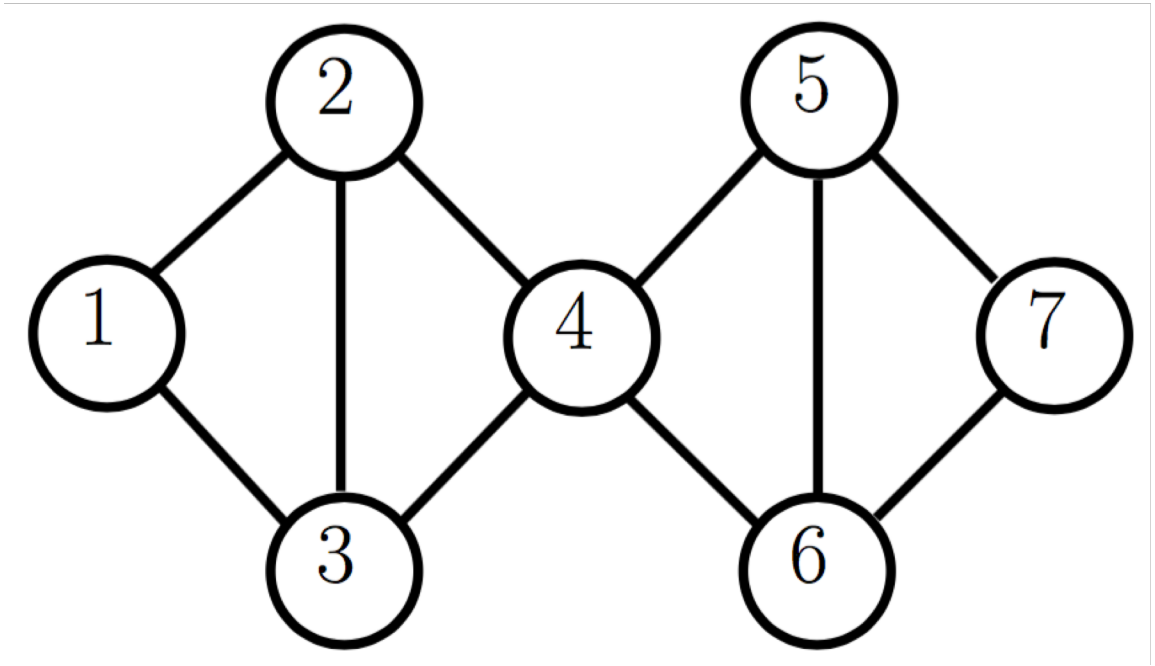
- In the following graph G, as a consequence of global Markov property:
  - $\{X_1, X_2, X_3\} \perp \{X_5, X_6, X_7\} | X_4$



[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Local Markov Property

- In the following graph G, as a consequence of local Markov property:
  - $X_4 \perp \{X_1, X_7\} | \{X_2, X_3, X_5, X_6\}$
  - $X_1 \perp \{X_4, X_5, X_6, X_7\}$



[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Graph to Distribution

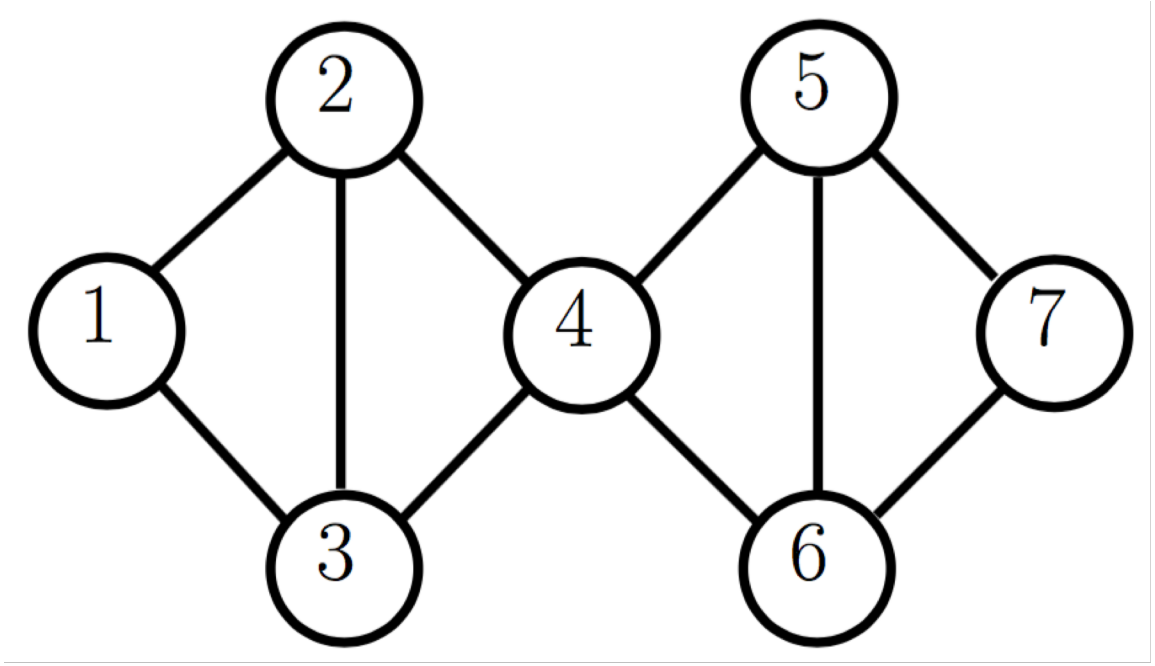
- So, the undirected graph specifies a set of conditional independence statements

- We can write down a joint distribution using the graph

- For example, we may consider a factorization involving maximal cliques.

Graph to Distribution

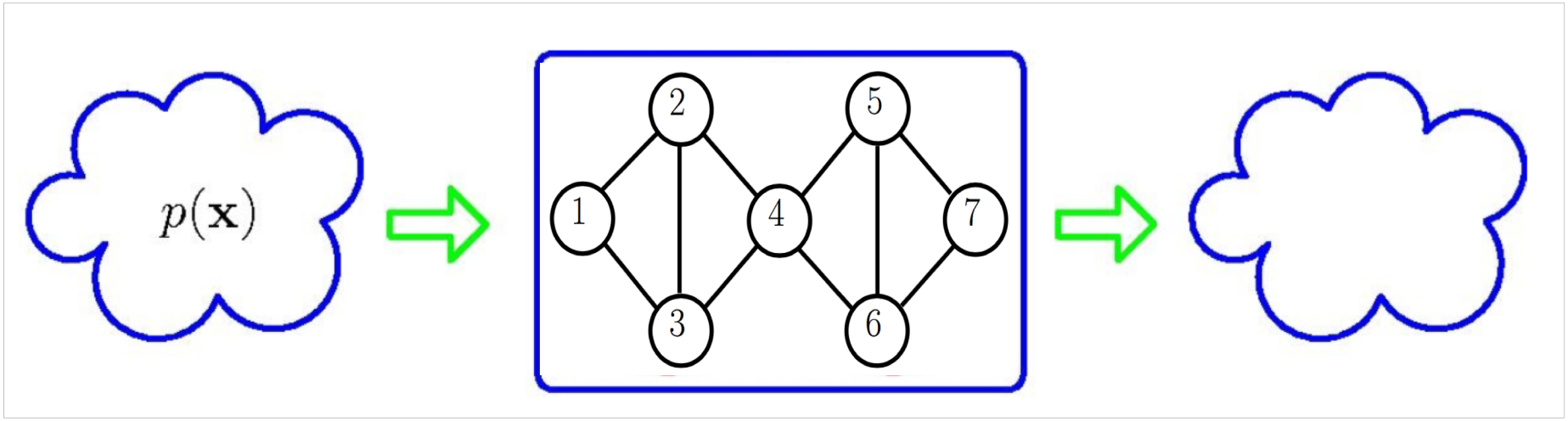
- $P(x_1, \dots, x_7) = \frac{1}{Z}\phi_1(x_1, x_2, x_3)\phi_2(x_2, x_3, x_4)\phi_3(x_4, x_5, x_6)\phi_4(x_5, x_6, x_7)$



- But, we could have also considered some other factorization

[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Filter view of UPGM



- Only distributions that satisfy conditional independences are allowed to pass

[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

Limitations of DPGM and UPGM

- Cannot always represent all conditional independences of a given joint distribution

- Example: we cannot draw a DPGM for the following distribution
  - $P(A, B, C, D)$ with $A \perp C | \{B, D\}$ and $B \perp D | \{A, C\}$

- Another example: we cannot represent the following using a UPGM
  - $P(A, B, C)$ with $A \not\perp C | \{B\}$ and $A \perp C$

- Homework: verify the above two statements!

[1]Reference: Bjoern Andres and Bernt Schiele, MPI (2016)

DPGM vs UPGM

Property	UPGMs	DPGMs
Form	Prod. potentials	Prod. potentials
Potentials	Arbitrary	Cond. probabilities
Cycles	Allowed	Forbidden
Partition func.	$Z = ?$	$Z = 1$
Indep. check	Graph separation	D-separation
Indep. props.	Some	Some
Inference	MCMC, BP, etc.	Convert to UPGM

[1]Reference: Pedro Domingos, CSE 515 (2017)

Questions?

Summary

- What are graphical models good at?
  - Capture complexity and uncertainty
  - Capture conditional independences
  - We can visualize what's happening with a distribution
- They unify many probabilistic techniques: mixture models, factor analysis, hidden Markov models, Kalman filters etc.

- Today we saw: visualization, conditional independence properties
- Next: computations (inference and learning)

Sample Exam Questions

- What is the need for graphical models?
- What is the significance of 'hidden' and 'Markov' in a HMM?
- What is the use of a Latent Dirichlet Allocation model?
- What is a clique?
- Which distributions respect a graph?
- What is the difference between a head-to-head and a tail-to-tail configuration in DPGMs?
- How is the factorization in a UPGM different from the factorization in a DPGM?
- How would you find conditional independence relationships in a UPGM?

Appendix

Additional Resources

- Book 1: *Graphical models, exponential families, and variational inference* by Martin J. Wainwright and Michael I. Jordan
  - See https://people.eecs.berkeley.edu/~wainwrig/Papers/WaiJor08_FTML.pdf
- Book 2: *Bayesian Reasoning and Machine Learning* by David Barber
  - See http://web4.cs.ucl.ac.uk/staff/D.Barber/pmwiki/pmwiki.php?n=Brml.Online

Review: Probability

Based on Sam Roweis's slides (2002)

Probability

- We use probabilities $p(x)$ to represent our beliefs $B(x)$ about the states x of the world.
- There is a formal calculus for manipulating uncertainties represented by probabilities.

[1]Reference: Sam Roweis (2002); Also see https://en.wikipedia.org/wiki/Cox%27s_theorem

Probability

- We use probabilities $p(x)$ to represent our beliefs $B(x)$ about the states x of the world.
- There is a formal calculus for manipulating uncertainties represented by probabilities.
- Any consistent set of beliefs obeying the *Cox Axioms* can be mapped into probabilities.
  1. Rationally ordered degrees of belief:
     if $B(x) > B(y)$ and $B(y) > B(z)$ then $B(x) > B(z)$
  2. Belief in x and its negation $\bar{x}$ are related: $B(x) = f[B(\bar{x})]$
  3. Belief in conjunction depends only on conditionals:
     $B(x \; and \; y) = g[B(x), B(y|x)] = g[B(y), B(x|y)]$

[1]Reference: Sam Roweis (2002); Also see https://en.wikipedia.org/wiki/Cox%27s_theorem

Probability

- An **outcome space** specifies the possible outcomes that we would like to reason about, e.g.

Ω = {  ,  } Coin toss

Ω = {  } Die toss

- We specify a **probability** $p(\omega)$ for each outcome ω such that

$$p(\omega) \geq 0, \quad \sum_{\omega \in \Omega} p(\omega) = 1$$

E.g., p() = .6

p() = .4

[1]Reference: David Sontag (2013)

Probability

- An **event** is a subset of the outcome space, e.g.

E = {  } Even die tosses

O = {  } Odd die tosses

- The **probability** of an event is given by the sum of the probabilities of the outcomes it contains,

$$p(E) = \sum_{\omega \in E} p(\omega)$$

E.g., p(E) = p() + p() + p()

= 1/2, if fair die

[1]Reference: David Sontag (2013)

Random Variables

- Random variables X represents outcomes or states of world.
  Instantiations of variables usually in lower case: x
  We will write $p(x)$ to mean probability$(X = x)$.
- Sample Space: the space of all possible outcomes/states.
  (May be discrete or continuous or mixed.)

[1]Reference: Sam Roweis (2002)

Random Variables

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- Sample Space: the space of all possible outcomes/states.
  (May be discrete or continuous or mixed.)
- Probability mass (density) function $p(x) \geq 0$
  Assigns a non-negative number to each point in sample space.
  Sums (integrates) to unity: $\sum_x p(x) = 1$ or $\int_x p(x)dx = 1$.
  Intuitively: how often does x occur, how much do we believe in x.
- Ensemble: random variable + sample space+ probability function

[1]Reference: Sam Roweis (2002)

Expectation

- Expectation of a function $a(x)$ is written $E[a]$ or $\langle a \rangle$

$$E[a] = \langle a \rangle = \sum_x p(x)a(x)$$

e.g. mean $= \sum_x xp(x)$, variance $= \sum_x (x - E[x])^2 p(x)$

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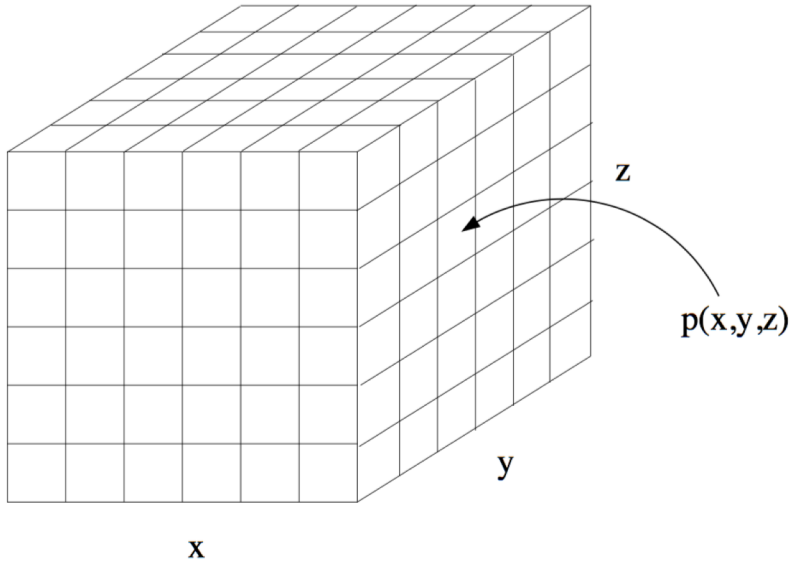
- Moments are expectations of higher order powers. (Mean is first moment. Autocorrelation is second moment.)
- Centralized moments have lower moments subtracted away (e.g. variance, skew, curtosis).
- Deep fact: Knowledge of all orders of moments completely defines the entire distribution.

[1]Reference: Sam Roweis (2002)

Joint Probability

- Key concept: two or more random variables may interact. Thus, the probability of one taking on a certain value depends on which value(s) the others are taking.
- We call this a joint ensemble and write

$$p(x, y) = \text{prob}(X = x \text{ and } Y = y)$$

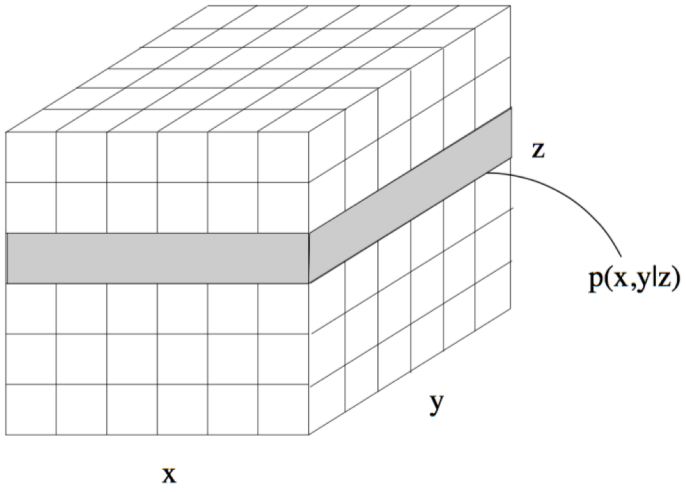


[1]Reference: Sam Roweis (2002)

Conditional Probability

- If we know that some event has occurred, it changes our belief about the probability of other events.
- This is like taking a "slice" through the joint table.

$$p(x|y) = p(x,y)/p(y)$$



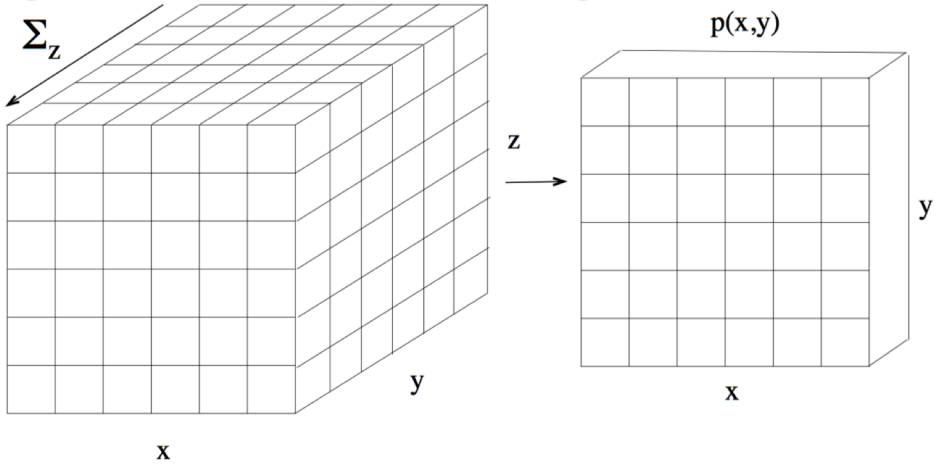
[1]Reference: Sam Roweis (2002)

Marginal Probability

- We can "sum out" part of a joint distribution to get the *marginal distribution* of a subset of variables:

$$p(x) = \sum_y p(x, y)$$

- This is like adding slices of the table together.



- Another equivalent definition: $p(x) = \sum_y p(x|y)p(y)$.

[1]Reference: Sam Roweis (2002)

Bayes Rule

- Manipulating the basic definition of conditional probability gives one of the most important formulas in probability theory:

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\sum_{x'} p(y|x')p(x')}$$

- This gives us a way of "reversing" conditional probabilities.
- Thus, all joint probabilities can be factored by selecting an ordering for the random variables and using the "chain rule":

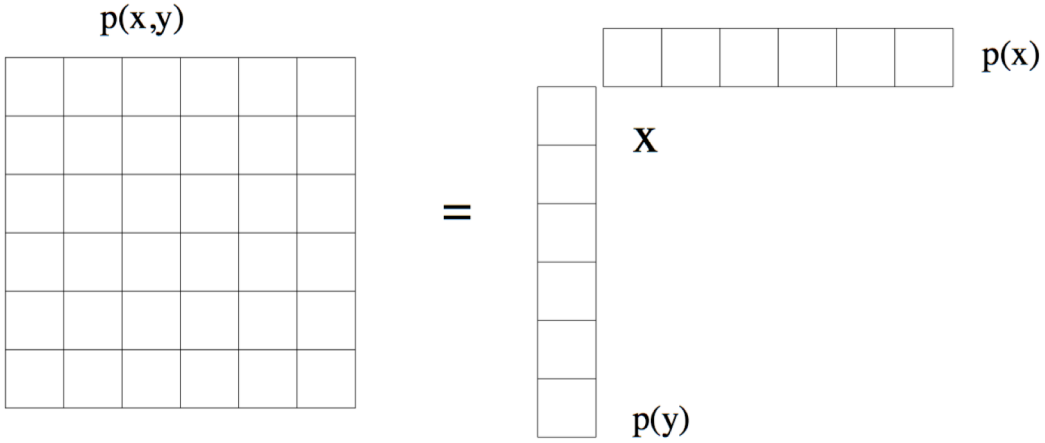
$$p(x, y, z, \ldots) = p(x)p(y|x)p(z|x, y)p(\ldots|x, y, z)$$

[1]Reference: Sam Roweis (2002)

Conditional Independence

- Two variables are independent iff their joint factors:

$$p(x, y) = p(x)p(y)$$



- Two variables are conditionally independent given a third one if for all values of the conditioning variable, the resulting slice factors:

$$p(x, y|z) = p(x|z)p(y|z) \qquad \forall z$$

[1]Reference: Sam Roweis (2002)

Independent Event Examples

- Independent event example
  - Hardware failures events in different data centers

- Dependent event examples
  - Queries to a search engine and news
  - Tweets and news
  - IM and email communications

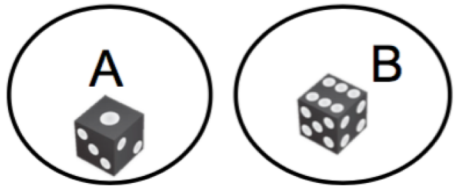
[1]Reference: Alex Smola (2011)

Independent Event Examples

- Two events A and B are **independent** if

$$p(A \cap B) = p(A)p(B)$$

- Are these two events independent?



No! $p(A \cap B) = 0, \quad p(A)p(B) = \left(\frac{1}{6}\right)^2$

- Now suppose our outcome space had two different die:

$\Omega = \{$  $\}$ 2 die tosses

$6^2 = 36$ outcomes

and the probability distribution is such that each die is independent,

p() = p() p()

p() = p() p()

[1]Reference: David Sontag(2013)

Independent Event Examples

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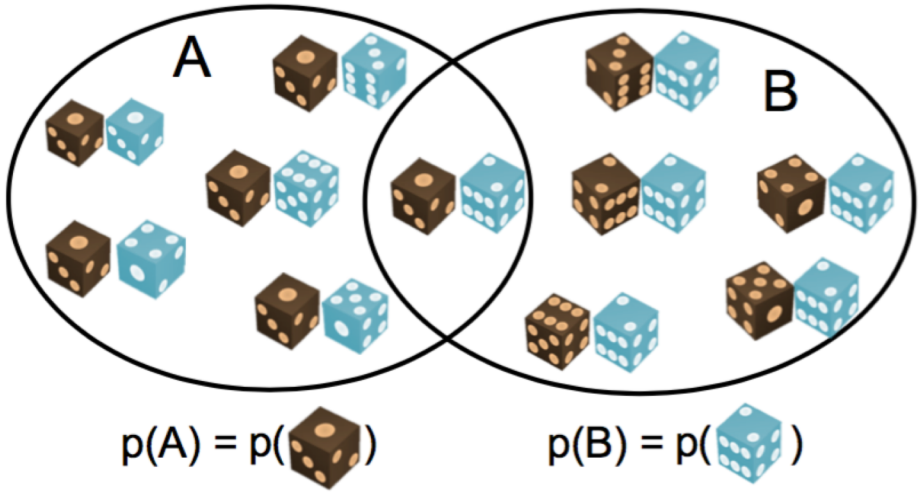

Yes!

$$p(A \cap B) = \text{p}($$  $$)$$

$$p(A)p(B) = \text{p}($$  $$)\ \text{p}($$  $$)$$

[1]Reference: David Sontag(2013)

Relation to Statistics

- Probability: inferring probabilistic quantities for data given fixed models (e.g. prob. of events, marginals, conditionals, etc).

[1]Reference: Sam Roweis (2002)

Relation to Statistics

- Probability: inferring probabilistic quantities for data given fixed models (e.g. prob. of events, marginals, conditionals, etc).
- Statistics: inferring a model given fixed data observations (e.g. clustering, classification, regression).
- Many approaches to statistics: *frequentist*, *Bayesian*, *decision theory*, ...

[1]Reference: Sam Roweis (2002)

Conditional Probability Table

- For discrete (categorical) quantities, the most basic parametrization is the probability table which lists $p(x_i = k^{th} \text{ value})$.
- Since PTs must be nonnegative and sum to 1, for k-ary variables there are $k - 1$ free parameters.

[1]Reference: Sam Roweis (2002)

Conditional Probability Table

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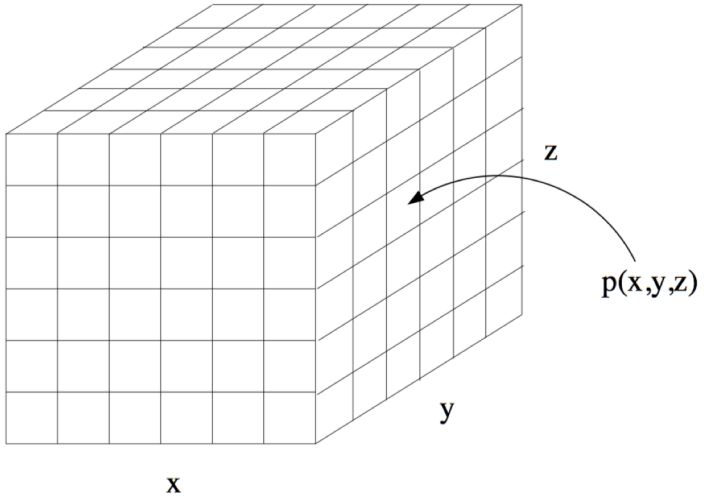
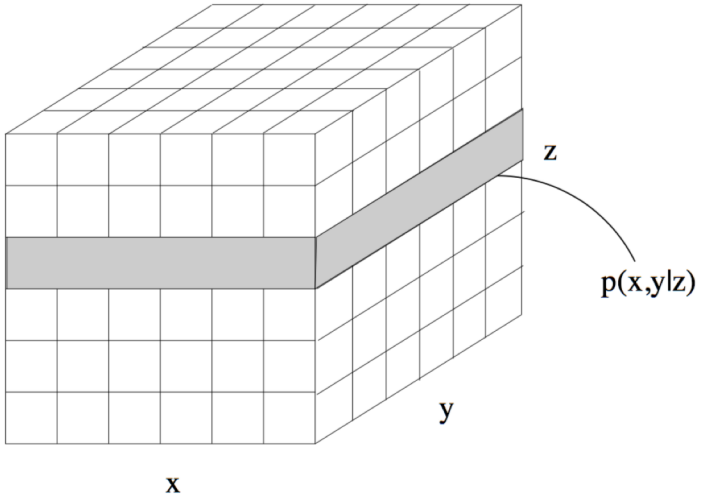
- Since PTs must be nonnegative and sum to 1, for k-ary variables there are $k - 1$ free parameters.
- If a discrete variable is conditioned on the values of some other discrete variables we make one table for each possible setting of the parents: these are called *conditional probability tables* or CPTs.





[1]Reference: Sam Roweis (2002)

Likelihood Function

- So far we have focused on the (log) probability function $p(\mathbf{x}|\theta)$ which assigns a probability (density) to any joint configuration of variables $\mathbf{x}$ given fixed parameters θ.
- But in learning we turn this on its head: we have some fixed data and we want to find parameters.
- Think of $p(\mathbf{x}|\theta)$ as a function of θ for fixed $\mathbf{x}$:

$$L(\theta; \mathbf{x}) = p(\mathbf{x}|\theta)$$
$$\ell(\theta; \mathbf{x}) = \log p(\mathbf{x}|\theta)$$

  This function is called the (log) "likelihood".

- Chose θ to maximize some cost function $c(\theta)$ which includes $\ell(\theta)$:

$c(\theta) = \ell(\theta; \mathcal{D})$ maximum likelihood (ML)

$c(\theta) = \ell(\theta; \mathcal{D}) + r(\theta)$ maximum a posteriori (MAP)/penalizedML

(also cross-validation, Bayesian estimators, BIC, AIC, ...)

[1]Reference: Sam Roweis (2002)

Complete Data, IID Sampling

- A single observation of the data $\mathbf{X}$ is rarely useful on its own.
- Generally we have data including many observations, which creates a *set of random variables*: $\mathcal{D} = \{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^M\}$
- Two very common assumptions:
  1. Observations are independently and identically distributed according to joint distribution of graphical model: IID samples.
  2. We observe all random variables in the domain on each observation: complete data.

[1]Reference: Sam Roweis (2002)

Maximum Likelihood

- For IID data:

$$p(\mathcal{D}|\theta) = \prod_m p(\mathbf{x}^m|\theta)$$

$$\ell(\theta; \mathcal{D}) = \sum_m \log p(\mathbf{x}^m|\theta)$$

- Idea of maximum likelihod estimation (MLE): pick the setting of parameters most likely to have generated the data we saw:

$$\theta^*_{\mathrm{ML}} = \mathrm{argmax}_\theta \ \ell(\theta; \mathcal{D})$$

- Very commonly used in statistics.
  Often leads to "intuitive", "appealing", or "natural" estimators.

[1]Reference: Sam Roweis (2002)

What to do with a Distribution

- *Generate data*: draw samples from the distribution. This often involves generating a uniformly distributed variable in the range [0,1] and transforming it. For more complex distributions it may involve an iterative procedure that takes a long time to produce a single sample (e.g. Gibbs sampling, MCMC).
- *Compute log probabilities.*
  When all variables are either observed or marginalized the result is a single number which is the log prob of the configuration.

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- *Compute log probabilities.*
  When all variables are either observed or marginalized the result is a single number which is the log prob of the configuration.
- *Inference*: Compute expectations of some variables given others which are observed or marginalized.
- *Learning.*
  Set the parameters of the density functions given some (partially) observed data to maximize likelihood or penalized likelihood.

[1]Reference: Sam Roweis (2002)

Aside: Observed vs Hidden Variables

- Observed variables:
  - For example, inputs in regression or classification

- Unobserved variables:
  - Also called hidden or latent
  - Can be marginalized out
  - Can make the modeling of observed variables easier (e.g., Gaussian mixture models)

[1]Reference: Sam Roweis (2002)