Directed and Undirected Graphical Models

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MLSALT4 Lecture
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With thanks to David Sontag (NYU) and Tony Jebara (Columbia)
for use of many slides and illustrations

For more information, see
http://mlg.eng.cam.ac.uk/adrian/

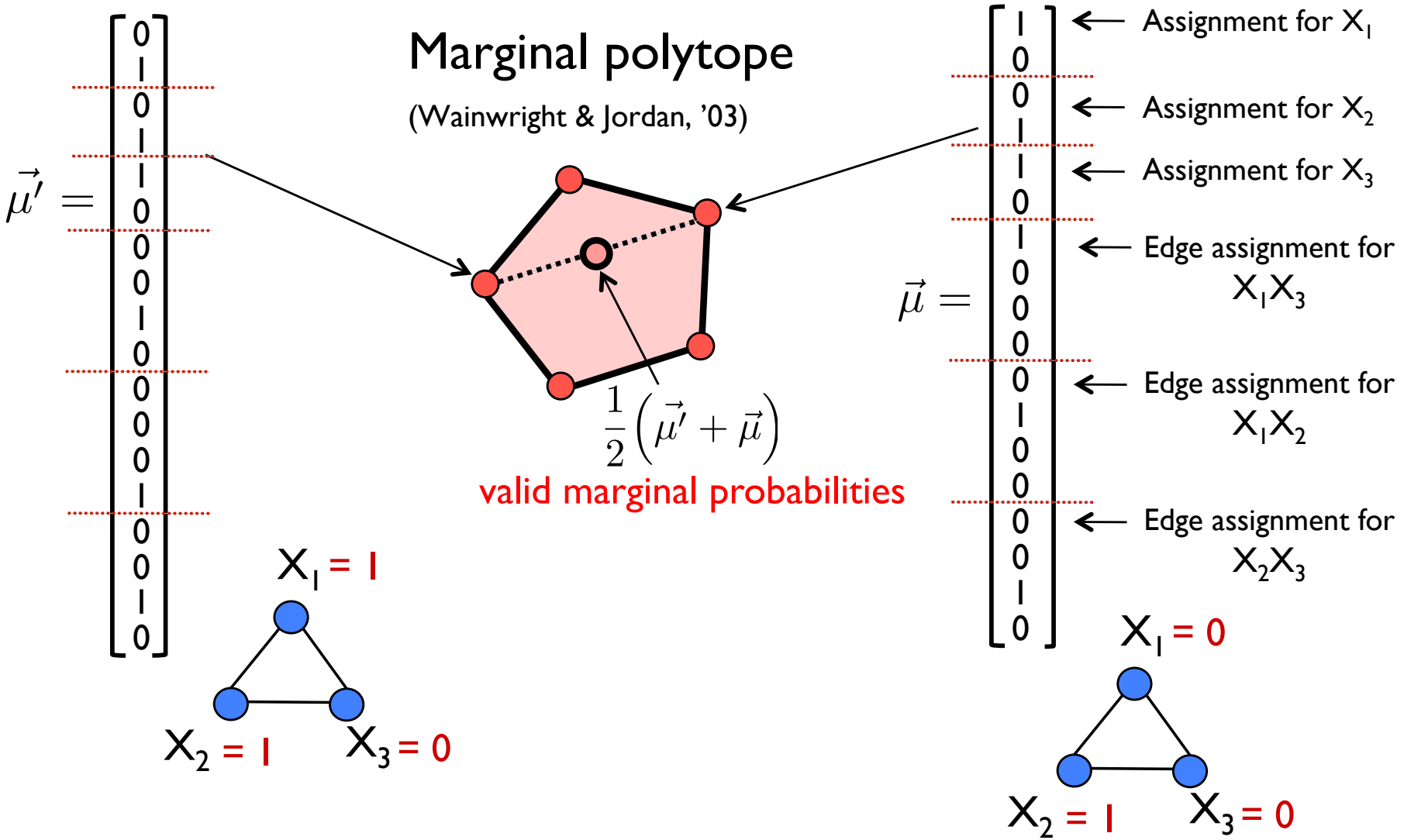
High level overview of our 3 lectures

- 1. LP relaxations for MAP inference (last week)
- 2. Directed and undirected graphical models (today)
- 3. Junction tree algorithm for exact inference, belief propagation, variational methods for approximate inference (Monday)

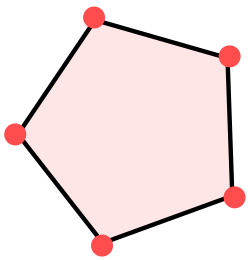
Further reading / viewing:

- Murphy, Machine Learning: a Probabilistic Perspective
- Barber, Bayesian Reasoning and Machine Learning
- Bishop, Pattern Recognition and Machine Learning
- Koller and Friedman, Probabilistic Graphical Models
  `https://www.coursera.org/course/pgm`
- Wainwright and Jordan, Graphical Models, Exponential Families, and Variational Inference

Background: *the marginal polytope* (all valid marginals)

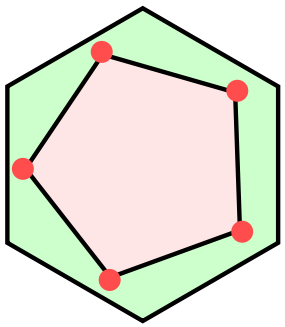


Stylized illustration of polytopes

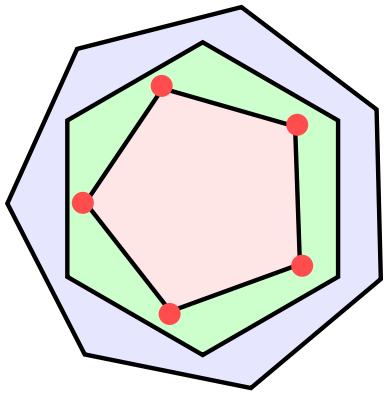


marginal polytope $\mathbb{M} = \mathbb{L}_n$
global consistency

...



triplet polytope $\mathbb{L}_3$
triplet consistency

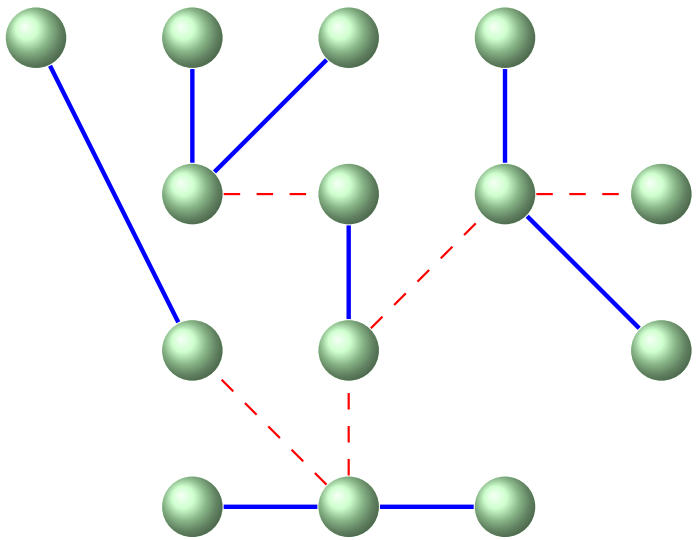


local polytope $\mathbb{L}_2$
pair consistency

More accurate $\leftrightarrow$ Less accurate

More computationally intensive $\leftrightarrow$ Less computationally intensive

When is MAP inference (relatively) easy?



Tree

Key ideas for graphical models

1. **Represent** the world as a collection of random variables $X_1, \ldots, X_n$ with joint distribution $p(X_1, \ldots, X_n)$
2. **Learn** the distribution from data
3. Perform **inference** (typically MAP or marginal)

Challenges

1. **Represent** the world as a collection of random variables $X_1, \ldots, X_n$ with joint distribution $p(X_1, \ldots, X_n)$
   - How can we compactly describe this joint distribution?
   - Directed graphical models (Bayesian networks)
   - Undirected graphical models (Markov random fields, factor graphs)
2. **Learn** the distribution from data
   - Maximum likelihood estimation, other methods?
   - How much data do we need?
   - How much computation does it take?
3. Perform **inference** (typically MAP or marginal)
   - Exact inference: Junction Tree Algorithm
   - Approximate inference (belief propagation, variational methods...)

How can we compactly describe the joint distribution?

Example: Medical diagnosis

- Binary variable for each **symptom** (e.g. "fever", "cough", "fast breathing", "shaking", "nausea", "vomiting")
- Binary variable for each **disease** (e.g. "pneumonia", "flu", "common cold", "bronchitis", "tuberculosis")
- Diagnosis is performed by **inference** in the model:

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

- One famous model, Quick Medical Reference (QMR-DT), has 600 diseases and 4000 symptoms

Representing the distribution

- Naively, we could represent the distribution with a big table of probabilities for every possible outcome
- How many outcomes are there in QMR-DT? 2^{4600}
- **Learning** of the distribution would require a huge amount of data
- **Inference** of conditional probabilities, e.g.

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

  would require summing over exponentially many values
- Moreover, gives no way to make predictions with previously unseen observations
- We need structure

Structure through independence

- If $X_1, \ldots, X_n$ are independent, then

$$p(x_1, \ldots, x_n) = p(x_1)p(x_2) \cdots p(x_n)$$

- For binary variables, probabilities for 2^n outcomes can be described by how many parameters?

Structure through independence

- If $X_1, \ldots, X_n$ are independent, then

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- For binary variables, probabilities for 2^n outcomes can be described by how many parameters? n
- However, this is not a very *useful* model – observing a variable X_i cannot influence our predictions of X_j

- Instead: if $X_1, \ldots, X_n$ are **conditionally independent** given Y, denoted as $X_i \perp \mathbf{X}_{-i} \mid Y$, then

$$p(y, x_1, \ldots, x_n) = p(y) \prod_{i=1}^{n} p(x_i \mid y)$$

- This is a simple yet powerful model

Example: naive Bayes for classification

- Classify e-mails as spam ($Y = 1$) or not spam ($Y = 0$)
  - Let $i \in \{1, \ldots, n\}$ index the words in our vocabulary
  - $X_i = 1$ if word i appears in an e-mail, and 0 otherwise
  - E-mails are drawn according to some distribution $p(Y, X_1, \ldots, X_n)$
- Suppose that the words are conditionally independent given Y
  Then,

$$p(y, x_1, \ldots x_n) = p(y) \prod_{i=1}^{n} p(x_i \mid y)$$

  Easy to **learn** the model with maximum likelihood. **Predict** with:

$$p(Y = 1 \mid x_1, \ldots x_n) = \frac{p(Y = 1) \prod_{i=1}^{n} p(x_i \mid Y = 1)}{\sum_{y=\{0,1\}} p(Y = y) \prod_{i=1}^{n} p(x_i \mid Y = y)}$$

- Is conditional independence a reasonable assumption?

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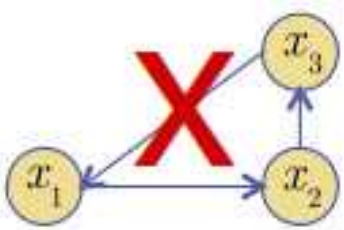
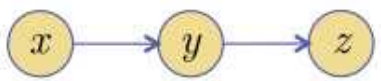
- Is conditional independence a reasonable assumption?
- A model may be "wrong" but still useful

Directed graphical models = Bayesian networks

- A **Bayesian network** is specified by a directed *acyclic* graph DAG$= (V, \vec{E})$ with:
  1. One node $i \in V$ for each random variable X_i
  2. One conditional probability distribution (CPD) per node, $p(x_i \mid \mathbf{x}_{\mathrm{Pa}(i)})$, specifying the variable's probability conditioned on its parents' values
- The DAG corresponds 1-1 with a particular factorization of the joint distribution:

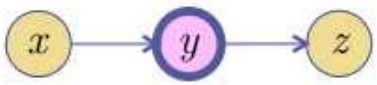
$$p(x_1, \ldots x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{\mathrm{Pa}(i)})$$



Markov chain: 

$$p(x, y, z) = p(x)\,p(y \mid x)\,p(z \mid y)$$

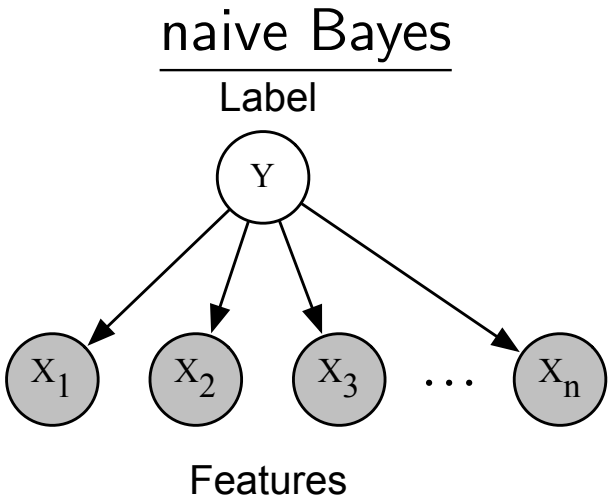
Example binary events:
x = president says war
y = general orders attack
z = soldier shoots gun



$$x \perp\!\!\!\perp z \mid y$$

$$p(x \mid y, z) = \frac{p(x, y, z)}{p(y, z)} = p(x \mid y)$$

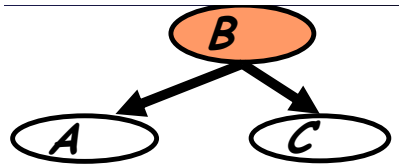
Bayesian networks are *generative models*



- Evidence is denoted by shading in a node
- Can interpret Bayesian network as a **generative process**. For example, to *generate* an e-mail, we
  1. Decide whether it is spam or not spam, by samping $y \sim p(Y)$
  2. For each word $i = 1$ to n, sample $x_i \sim p(X_i \mid Y = y)$

Bayesian network structure ⇒ conditional independencies

- Generalizing earlier example, can show that a variable is independent from its non-descendants given its parents

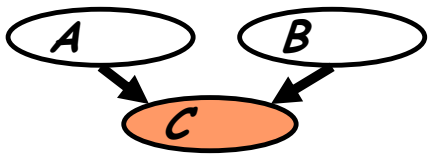


- **Common parent** – fixing B decouples A and C

tail to tail

- **Cascade** – knowing B decouples A and C

head to tail



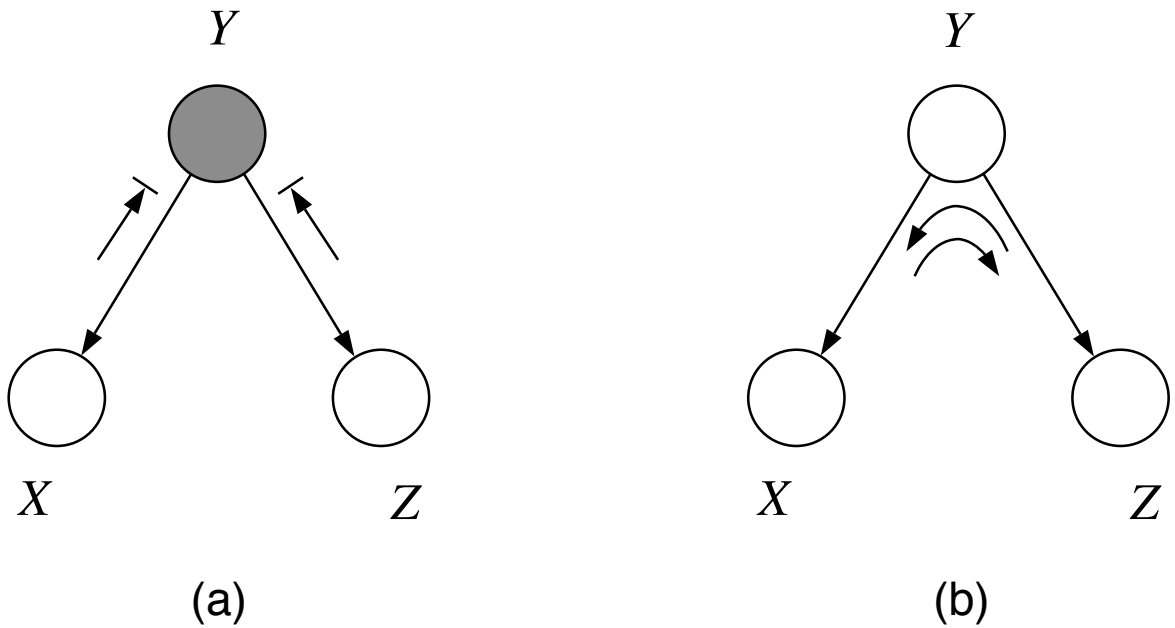
- **V-structure** – Knowing C couples A and B
  - This important phenomona is called **explaining away**

$p(A, B, C) = p(A)p(B)p(C \mid A, B)$

head to head

D-separation ("directed separation") in Bayesian networks

- Bayes Ball Algorithm to determine whether $X \perp Z \mid \mathbf{Y}$ by looking at graph d-separation
- Look to see if there is **active path** between X and Z when variables $\mathbf{Y}$ are observed:



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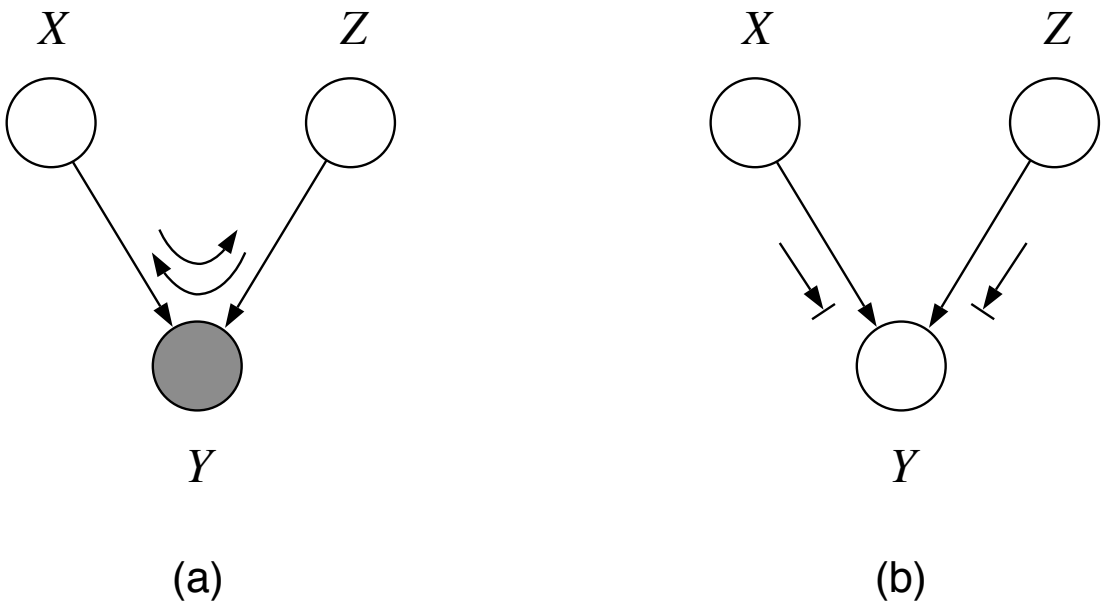

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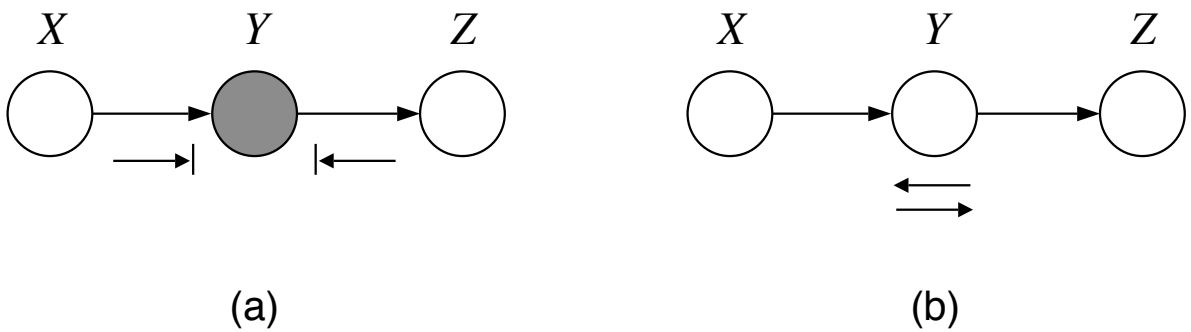
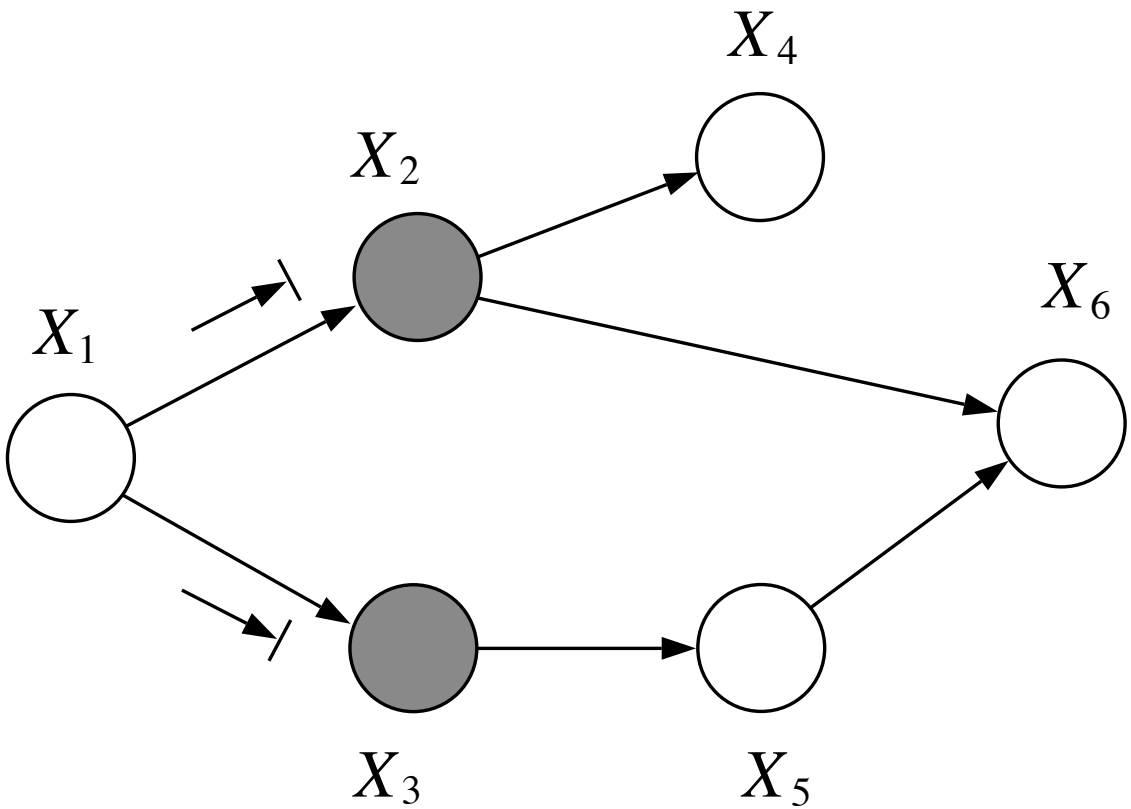


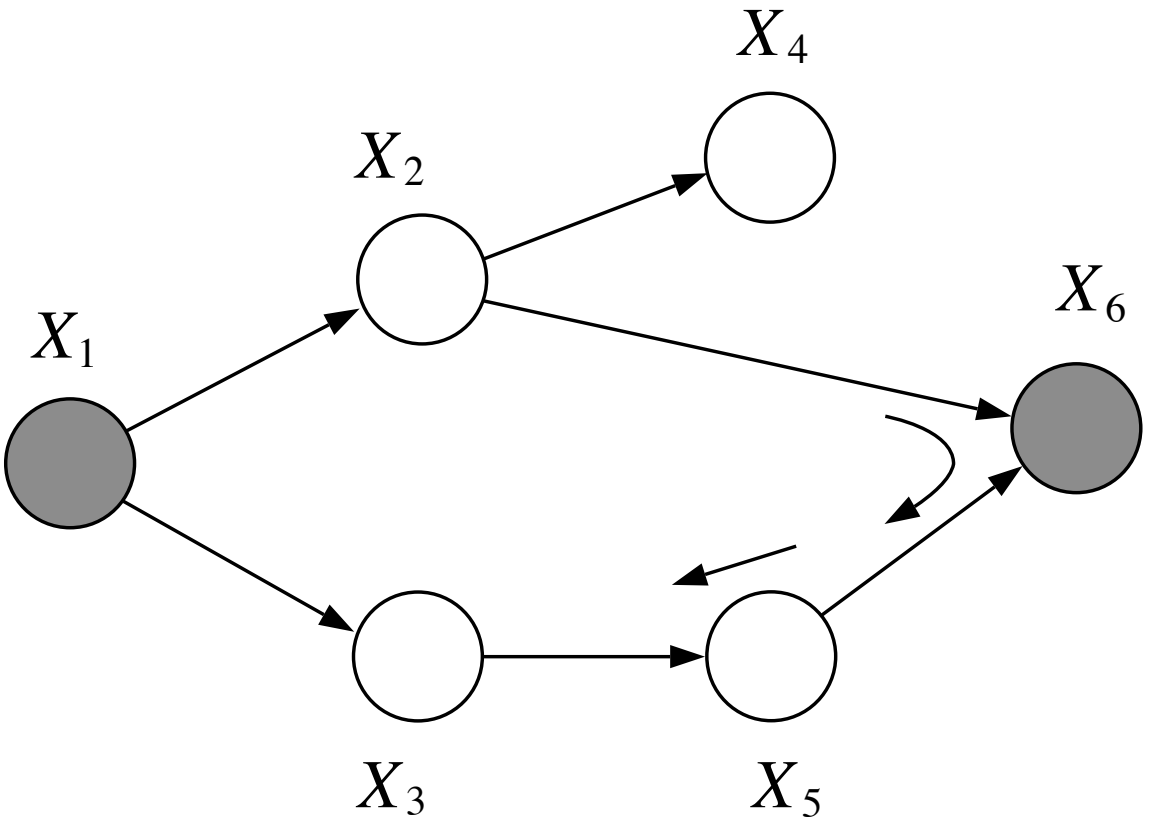
(a) (b)

- If no such path, then X and Z are **d-separated** with respect to $\mathbf{Y}$
- d-separation reduces statistical independencies (hard) to connectivity in graphs (easy)
- Important because it allows us to quickly prune the Bayesian network, finding just the relevant variables for answering a query

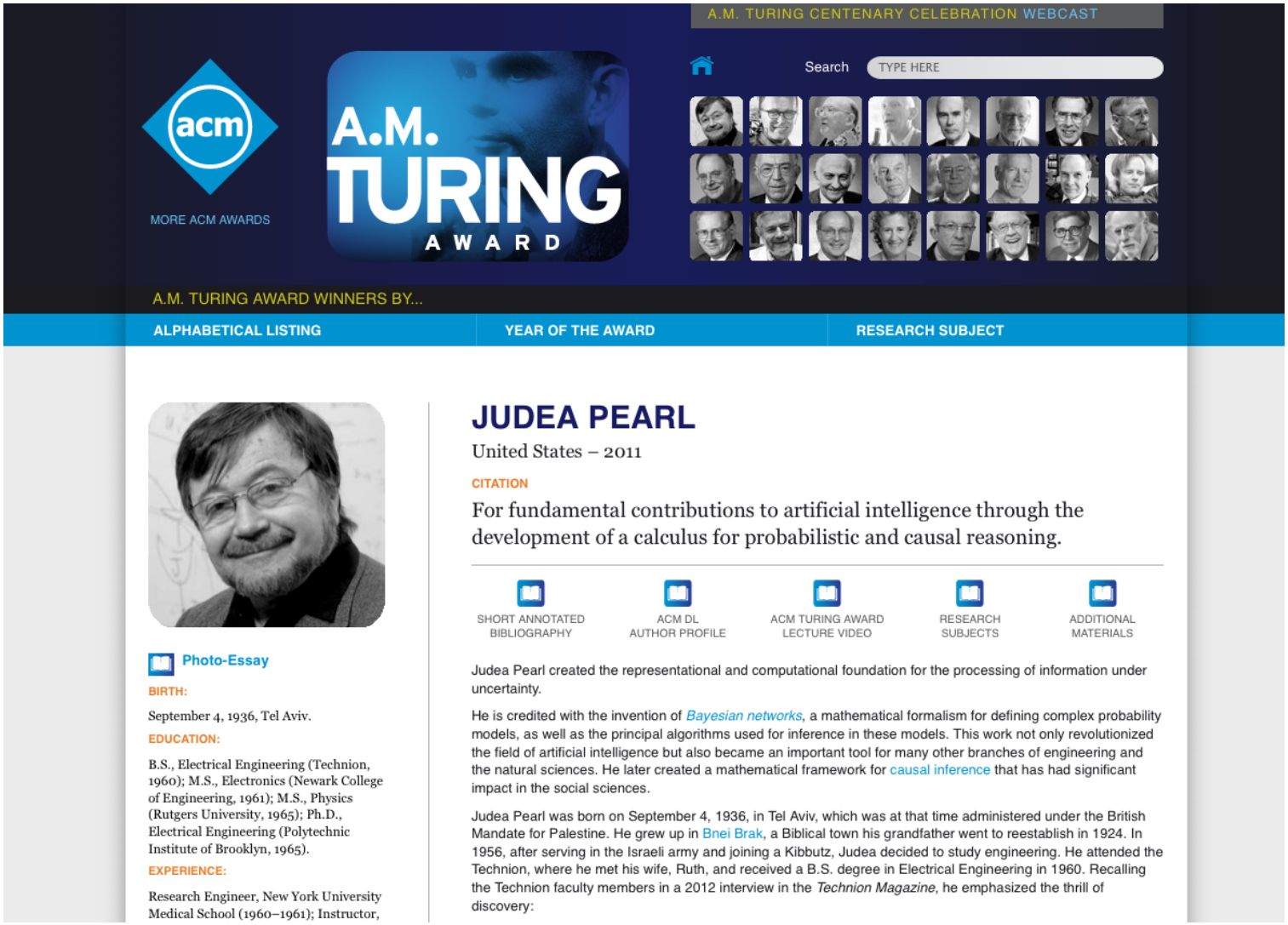
D-separation example 1



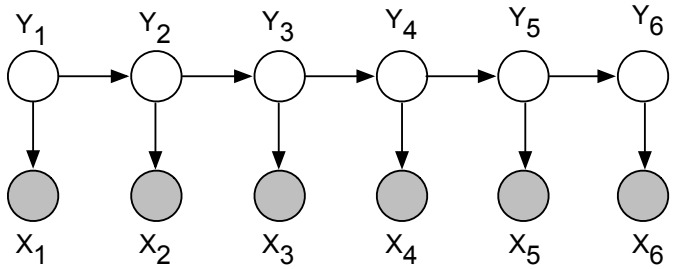
D-separation example 2



2011 Turing Award was for Bayesian networks



Example: hidden Markov model (HMM)

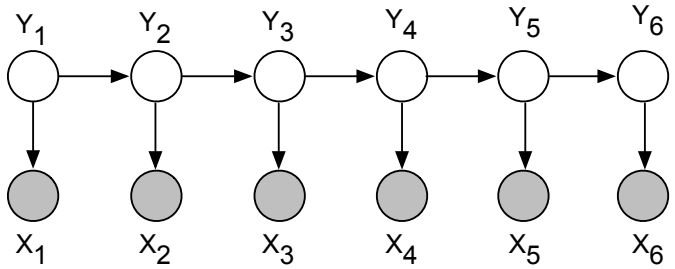


- Frequently used for speech recognition and part-of-speech tagging
- Joint distribution factors as:

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

  - $p(y_1)$ is the initial distribution of the starting state
  - $p(y_t \mid y_{t-1})$ is the transition probability between hidden states
  - $p(x_t \mid y_t)$ is the emission probability
- What are the conditional independencies here?

Example: hidden Markov model (HMM)



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  - $p(x_t \mid y_t)$ is the emission probability
- What are the conditional independencies here?
  Many, e.g. $Y_1 \perp \{Y_3, \ldots, Y_6\} \mid Y_2$

Summary

- A **Bayesian network** specifies the global distribution by a DAG and local conditional probability distributions (CPDs) for each node
- Can interpret as a generative model, where variables are sampled in topological order
- Examples: naive Bayes, hidden Markov models (HMMs), latent Dirichlet allocation
- Conditional independence via d-separation
- Compute the probability of any assignment by multiplying CPDs
- Maximum likelihood learning of CPDs is easy (decomposes, can estimate each CPD separately)

Undirected graphical models

- An alternative representation for a joint distribution is an **undirected graphical model**
- As for directed models, we have one node for each random variable
- Rather than CPDs, we specify (non-negative) **potential functions** over sets of variables associated with cliques C of the graph,

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

Z is the **partition function** and normalizes the distribution:

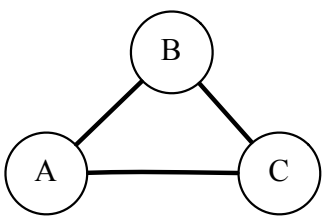
$$Z = \sum_{\hat{x}_1, \ldots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

- Like a CPD, $\phi_c(\mathbf{x}_c)$ can be represented as a table, but it is not normalized
- Also known as **Markov random fields** (MRFs) or Markov networks

Undirected graphical models

$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c), \qquad Z = \sum_{\hat{x}_1, \ldots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

Simple example (each edge potential function encourages its variables to take the same value):



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

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

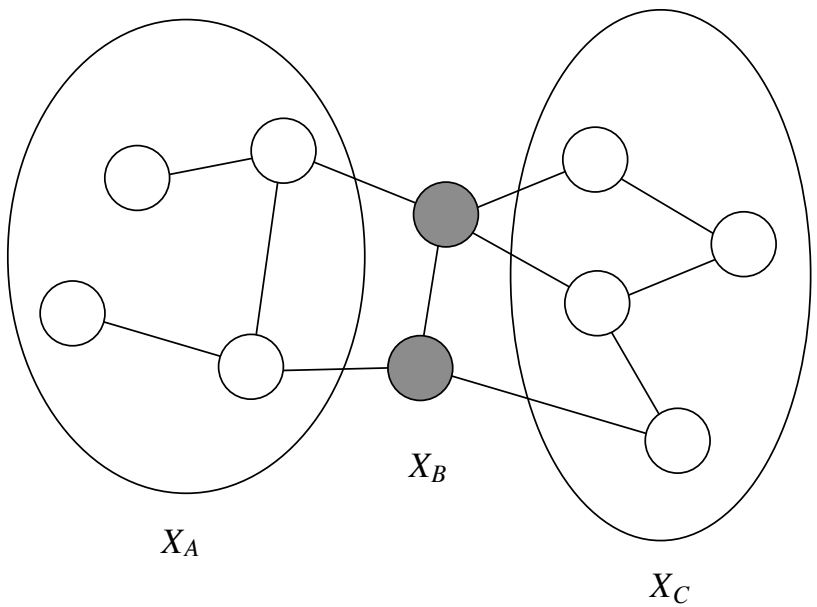
$$p(a,b,c) = \frac{1}{Z} \phi_{A,B}(a,b) \cdot \phi_{B,C}(b,c) \cdot \phi_{A,C}(a,c),$$

where

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

Markov network structure $\Rightarrow$ conditional independencies

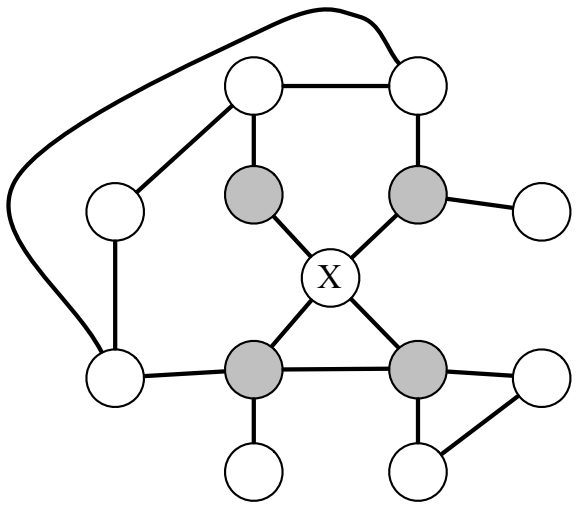
- Let G be the undirected graph where we have one edge for every pair of variables that appear together in a potential
- Conditional independence is given by **graph separation**



- $X_{\mathbf{A}} \perp X_{\mathbf{C}} \mid X_{\mathbf{B}}$ if there is no path from $a \in \mathbf{A}$ to $c \in \mathbf{C}$ after removing all variables in $\mathbf{B}$

Markov blanket

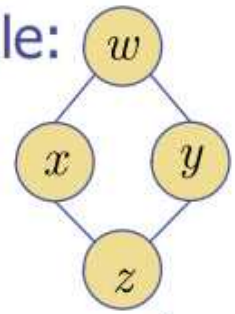
- A set **U** is a **Markov blanket** of X if $X \notin \mathbf{U}$ and if **U** is a minimal set of nodes such that $X \perp (\mathcal{X} - \{X\} - \mathbf{U}) \mid \mathbf{U}$
- In undirected graphical models, the Markov blanket of a variable is precisely its **neighbors** in the graph:



- In other words, X is independent of the rest of the nodes in the graph given its immediate neighbors

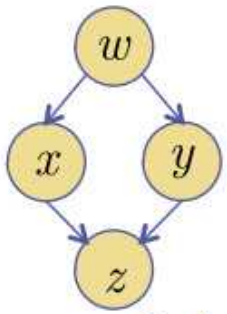
Directed and undirected models are different

- Example:



$$x \perp\!\!\!\perp y \mid \{w, z\}$$

$$w \perp\!\!\!\perp z \mid \{x, y\}$$

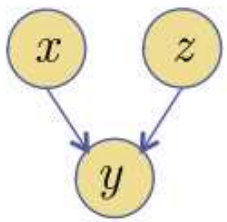


$$x \perp\!\!\!\perp y \mid \{w\}$$

$$x \not\perp\!\!\!\perp y \mid \{w, z\}$$

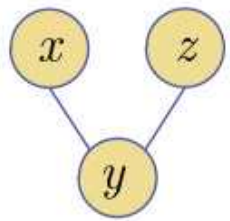
Directed can't do it!
Must be acyclic
Will have at least one V structure and ball goes through

- Example:



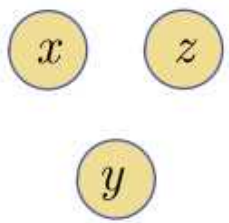
$$x \perp\!\!\!\perp z$$

$$x \not\perp\!\!\!\perp z \mid y$$



Undirected can't do it!

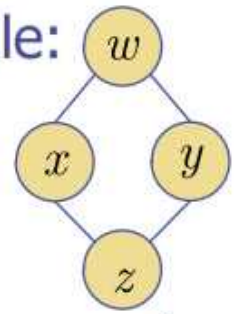
$$x \perp\!\!\!\perp z \mid y$$



$$x \perp\!\!\!\perp z$$

Directed and undirected models are different

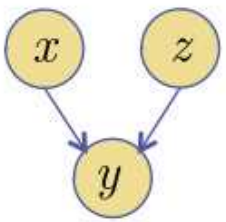
- Example:



$$x \perp\!\!\!\perp y \mid \{w, z\}$$

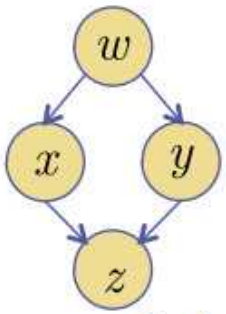
$$w \perp\!\!\!\perp z \mid \{x, y\}$$

- Example:



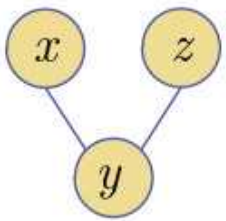
$$x \perp\!\!\!\perp z$$

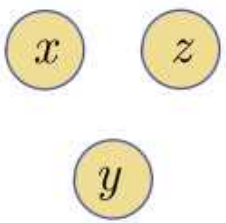
$$x \not\perp\!\!\!\perp z \mid y$$



$$x \perp\!\!\!\perp y \mid \{w\}$$

$$x \not\perp\!\!\!\perp y \mid \{w, z\}$$





Directed can't do it!
Must be acyclic
Will have at least one V structure and ball goes through

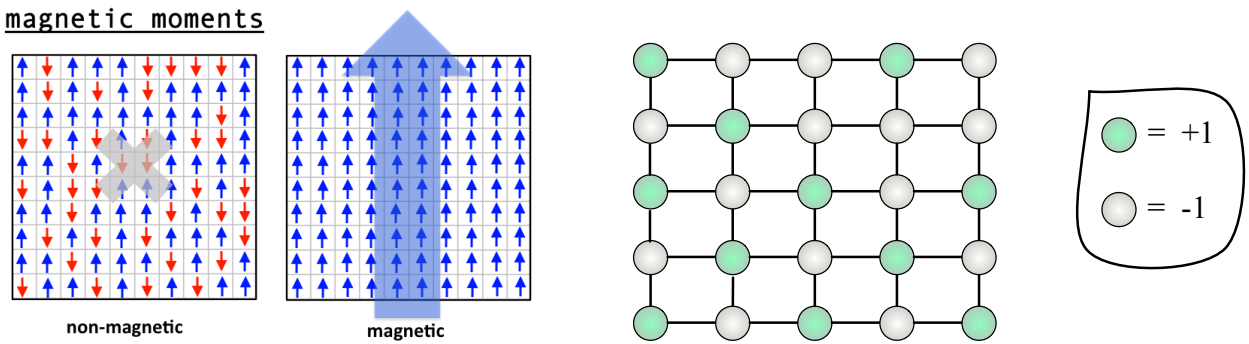
With <3 edges,
Undirected can't do it!

$$x \perp\!\!\!\perp z \mid y$$

$$x \perp\!\!\!\perp z$$

Example: Ising model

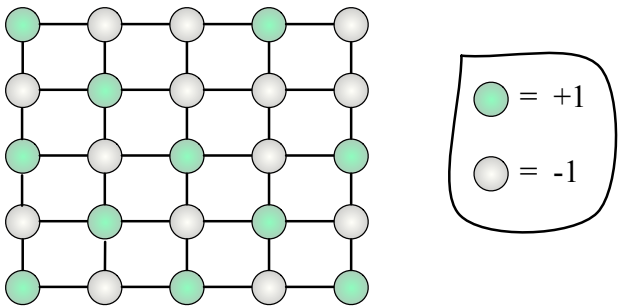
- Invented by the physicist Wilhelm Lenz (1920), who gave it as a problem to his student Ernst Ising
- Mathematical model of ferromagnetism in statistical mechanics
- The spin of an atom is influenced by the spins of atoms nearby on the material:



- Each atom $X_i \in \{-1, +1\}$, whose value is the direction of the atom spin
- If a spin at position i is $+1$, what is the probability that the spin at position j is also $+1$?
- Are there phase transitions where spins go from "disorder" to "order"?

Example: Ising model

- Each atom $X_i \in \{-1, +1\}$, whose value is the direction of the atom spin
- The spin of an atom is influenced by the spins of atoms nearby on the material:



$$p(x_1, \cdots, x_n) = \frac{1}{Z} \exp \frac{1}{T} \left(\sum_{i<j} w_{i,j} x_i x_j + \sum_i \theta_i x_i \right)$$

- When $w_{i,j} > 0$, adjacent atoms encouraged to have the same spin (**attractive** or **ferromagnetic**); $w_{i,j} < 0$ encourages $X_i \neq X_j$
- Node potentials θ_i encode the bias of the individual atoms
- Varying the temperature T makes the distribution more or less spiky

Supplementary material

Extra slides for questions or further explanation

Basic idea

- Suppose we have a simple chain $A \to B \to C \to D$, we want to compute $p(D)$
- $p(D)$ is a **set** of values, $\{p(D = d), d \in \mathrm{Val}(D)\}$. Algorithm computes sets of values at a time – an entire distribution
- The joint distribution factors as

$$p(A, B, C, D) = p(A)p(B \mid A)p(C \mid B)p(D \mid C)$$

- In order to compute $p(D)$, we have to marginalize over A, B, C:

$$p(D) = \sum_{a,b,c} p(A = a, B = b, C = c, D)$$

How can we perform the sum efficiently?

- Our goal is to compute

$$p(D) = \sum_{a,b,c} p(a,b,c,D) = \sum_{a,b,c} p(a)p(b \mid a)p(c \mid b)p(D \mid c)$$
$$= \sum_{c}\sum_{b}\sum_{a} p(D \mid c)p(c \mid b)p(b \mid a)p(a)$$

- We can push the summations inside to obtain:

$$p(D) = \sum_{c} p(D \mid c) \sum_{b} p(c \mid b) \underbrace{\sum_{a} \underbrace{p(b \mid a)p(a)}_{\psi_1(a,b)}}_{\tau_1(b)}$$

- Let's call $\psi_1(A,B) = P(A)P(B|A)$. Then, $\tau_1(B) = \sum_a \psi_1(a,B)$
- Similarly, let $\psi_2(B,C) = \tau_1(B)P(C|B)$. Then, $\tau_2(C) = \sum_b \psi_1(b,C)$
- This procedure is dynamic programming: computation is inside out instead of outside in

Inference in a chain

- Generalizing the previous example, suppose we have a chain $X_1 \to X_2 \to \cdots \to X_n$, where each variable has k states
- For $i = 1$ up to $n - 1$, compute (and cache)

$$p(X_{i+1}) = \sum_{x_i} p(X_{i+1} \mid x_i) p(x_i)$$

- Each update takes k^2 time (why?)
- The total running time is $\mathcal{O}(nk^2)$
- In comparison, naively marginalizing over all latent variables has complexity $\mathcal{O}(k^n)$
- We did inference over the joint without ever explicitly constructing it!

ML learning in Bayesian networks

- Maximum likelihood learning: $\max_\theta \ell(\theta; \mathcal{D})$, where

$$\begin{aligned}\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}; \theta) &= \sum_{\mathbf{x} \in \mathcal{D}} \log p(\mathbf{x}; \theta) \\ &= \sum_i \sum_{\hat{\mathbf{x}}_{pa(i)}} \sum_{\substack{\mathbf{x} \in \mathcal{D}: \\ \mathbf{x}_{pa(i)} = \hat{\mathbf{x}}_{pa(i)}}} \log p(x_i \mid \hat{\mathbf{x}}_{pa(i)})\end{aligned}$$

- In Bayesian networks, we have the closed form ML solution:

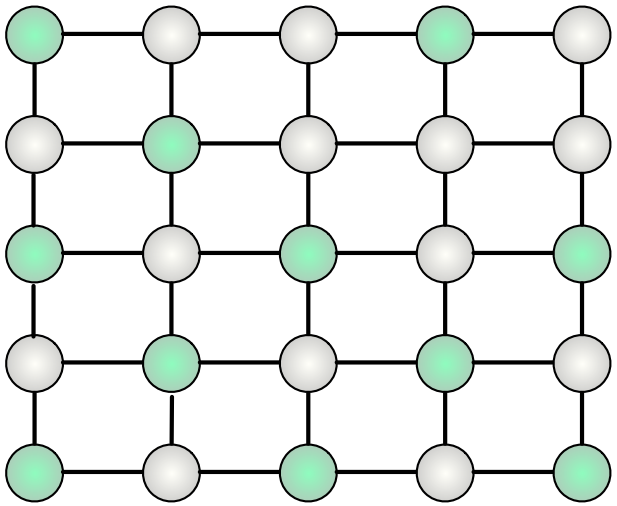
$$\theta^{ML}_{x_i|\mathbf{x}_{pa(i)}} = \frac{N_{x_i, \mathbf{x}_{pa(i)}}}{\sum_{\hat{x}_i} N_{\hat{x}_i, \mathbf{x}_{pa(i)}}}$$

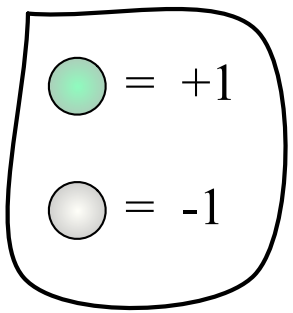
  where $N_{x_i, \mathbf{x}_{pa(i)}}$ is the number of times that the (partial) assignment $x_i, \mathbf{x}_{pa(i)}$ is observed in the training data

- We can estimate each CPD independently because the objective **decomposes** by variable and parent assignment

Parameter learning in Markov networks

- How do we learn the parameters of an Ising model?





$$p(x_1, \cdots, x_n) = \frac{1}{Z} \exp\left(\sum_{i<j} w_{i,j} x_i x_j + \sum_i \theta_i x_i\right)$$

Bad news for Markov networks

- The global normalization constant $Z(\theta)$ kills decomposability:

$$\begin{aligned}
\theta^{ML} &= \arg\max_{\theta} \log \prod_{\mathbf{x} \in \mathcal{D}} p(\mathbf{x}; \theta) \\
&= \arg\max_{\theta} \sum_{\mathbf{x} \in \mathcal{D}} \left(\sum_{c} \log \phi_c(\mathbf{x}_c; \theta) - \log Z(\theta) \right) \\
&= \arg\max_{\theta} \left(\sum_{\mathbf{x} \in \mathcal{D}} \sum_{c} \log \phi_c(\mathbf{x}_c; \theta) \right) - |\mathcal{D}| \log Z(\theta)
\end{aligned}$$

- The log-partition function prevents us from decomposing the objective into a sum over terms for each potential
- Solving for the parameters becomes much more complicated