Inference and Representation

DS-GA-1005, CSCI-GA.2569

David Sontag

New York University

Lecture 2, Sept. 19, 2016

Today's lecture

- Markov random fields
  1. Formalism
  2. Conditional independence properties
  3. Examples
- Factor graphs
- Bayesian networks $\Rightarrow$ Markov random fields (*moralization*)
- Learning graphical models from data

Bayesian networks

Reminder of first lecture

- A **Bayesian network** is specified by a directed *acyclic* graph $G = (V, E)$ 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
- Corresponds 1-1 with a particular factorization of the joint distribution:

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

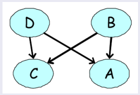
- Powerful framework for designing *algorithms* to perform probability computations

Bayesian networks have limitations

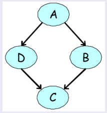
- Recall that G is a **perfect map** for distribution p if $I(G) = I(p)$
- **Theorem:** Not every distribution has a perfect map as a DAG

Proof.

(By counterexample.) There is a distribution on 4 variables where the only independencies are $A \perp C \mid \{B, D\}$ and $B \perp D \mid \{A, C\}$. This cannot be represented by any Bayesian network.



(a)



(b)

Both (a) and (b) encode $(A \perp C|B, D)$, but in both cases $(B \not\perp D|A, C)$. $\square$

Example

- Let's come up with an example of a distribution p satisfying $A \perp C \mid \{B, D\}$ and $B \perp D \mid \{A, C\}$
- A=Alex's hair color (red, green, blue)
  B=Bob's hair color
  C=Catherine's hair color
  D=David's hair color
- Alex and Bob are friends, Bob and Catherine are friends, Catherine and David are friends, David and Alex are friends
- Friends *never* have the same hair color!

Undirected graphical models

- An alternative representation for joint distributions is as an **undirected graphical model**
- As in BNs, 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,

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

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

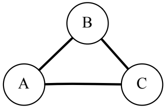
$$Z = \sum_{\hat{x}_1, \dots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

- Like CPD's, $\phi_c(\mathbf{x}_c)$ 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 (potential function on each edge encourages the variables to take the same value):



$$\phi_{A,B}(a,b) = \begin{array}{cc|c|c|} & & \multicolumn{2}{c}{B} \\ & & 0 & 1 \\ \hline A & 0 & 10 & 1 \\ \hline & 1 & 1 & 10 \\ \hline \end{array} \qquad \phi_{B,C}(b,c) = \begin{array}{cc|c|c|} & & \multicolumn{2}{c}{C} \\ & & 0 & 1 \\ \hline B & 0 & 10 & 1 \\ \hline & 1 & 1 & 10 \\ \hline \end{array} \qquad \phi_{A,C}(a,c) = \begin{array}{cc|c|c|} & & \multicolumn{2}{c}{C} \\ & & 0 & 1 \\ \hline A & 0 & 10 & 1 \\ \hline & 1 & 1 & 10 \\ \hline \end{array}$$

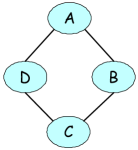
$$p(a, b, c) = \frac{1}{Z} \phi_{A,B}(a, b) \cdot \phi_{B,C}(b, c) \cdot \phi_{A,C}(a, c),$$

where

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

Hair color example as a MRF

- We now have an **undirected** graph:



- The joint probability distribution is parameterized as

$$p(a,b,c,d) = \frac{1}{Z}\phi_{AB}(a,b)\phi_{BC}(b,c)\phi_{CD}(c,d)\phi_{AD}(a,d)\ \phi_A(a)\phi_B(b)\phi_C(c)\phi_D(d)$$

- **Pairwise potentials** enforce that no friend has the same hair color:

$$\phi_{AB}(a,b) = 0 \text{ if } a = b, \quad \text{and 1 otherwise}$$

- **Single-node potentials** specify an affinity for a particular hair color, e.g.

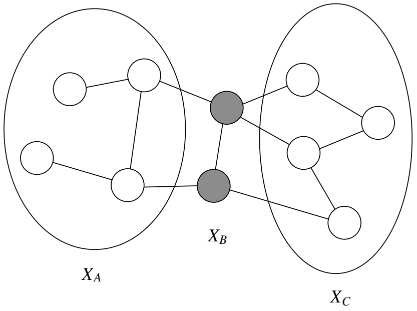
$$\phi_D(\text{“red”}) = 0.6, \quad \phi_D(\text{“blue”}) = 0.3, \quad \phi_D(\text{“green”}) = 0.1$$

  The normalization Z makes the potentials **scale invariant**! Equivalent to

$$\phi_D(\text{“red”}) = 6, \quad \phi_D(\text{“blue”}) = 3, \quad \phi_D(\text{“green”}) = 1$$

Markov network structure implies conditional independencies

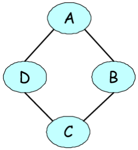
- Let G be the undirected graph where we have one edge for every pair of variables that appear together in a potential
- Conditional independence is given by **graph separation**!



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

Example

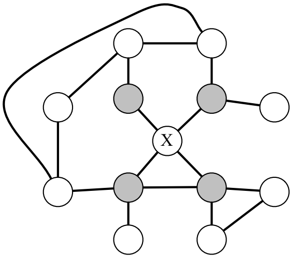
- Returning to hair color example, its undirected graphical model is:



- Since removing A and C leaves no path from D to B, we have $D \perp B \mid \{A, C\}$
- Similarly, since removing D and B leaves no path from A to C, we have $A \perp C \mid \{D, B\}$
- No other independencies implied by the graph

Markov blanket

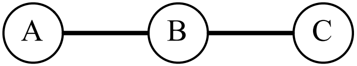
- A set **U** is a **Markov blanket** of X if $X \notin \mathbf{U}$ and if **U** is a minimal set of nodes such that $X \perp (\mathcal{X} - \{X\} - \mathbf{U}) \mid \mathbf{U}$
- In undirected graphical models, the Markov blanket of a variable is precisely its **neighbors** in the graph:



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

Proof of independence through separation

- We will show that $A \perp C \mid B$ for the following distribution:



$$p(a,b,c) = \frac{1}{Z}\phi_{AB}(a,b)\phi_{BC}(b,c)$$

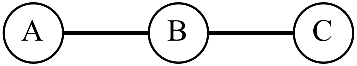
- First, we show that $p(a \mid b)$ can be computed using only $\phi_{AB}(a,b)$:

$$\begin{aligned} p(a \mid b) &= \frac{p(a,b)}{p(b)} \\ &= \frac{\frac{1}{Z}\sum_{\hat{c}} \phi_{AB}(a,b)\phi_{BC}(b,\hat{c})}{\frac{1}{Z}\sum_{\hat{a},\hat{c}} \phi_{AB}(\hat{a},b)\phi_{BC}(b,\hat{c})} \\ &= \frac{\phi_{AB}(a,b)\sum_{\hat{c}} \phi_{BC}(b,\hat{c})}{\sum_{\hat{a}} \phi_{AB}(\hat{a},b)\sum_{\hat{c}} \phi_{BC}(b,\hat{c})} = \frac{\phi_{AB}(a,b)}{\sum_{\hat{a}} \phi_{AB}(\hat{a},b)}. \end{aligned}$$

- More generally, the probability of a variable conditioned on its Markov blanket depends *only* on potentials involving that node

Proof of independence through separation

- We will show that $A \perp C \mid B$ for the following distribution:



$$p(a,b,c) = \frac{1}{Z}\phi_{AB}(a,b)\phi_{BC}(b,c)$$

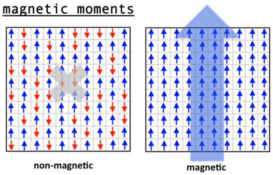
Proof.

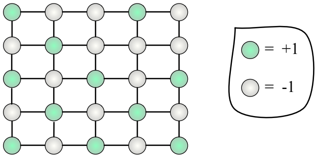
$$\begin{aligned} p(a,c \mid b) = \frac{p(a,c,b)}{\sum_{\hat{a},\hat{c}} p(\hat{a},b,\hat{c})} &= \frac{\phi_{AB}(a,b)\phi_{BC}(b,c)}{\sum_{\hat{a},\hat{c}} \phi_{AB}(\hat{a},b)\phi_{BC}(b,\hat{c})} \\ &= \frac{\phi_{AB}(a,b)\phi_{BC}(b,c)}{\sum_{\hat{a}} \phi_{AB}(\hat{a},b)\sum_{\hat{c}} \phi_{BC}(b,\hat{c})} \\ &= p(a \mid b)p(c \mid b) \end{aligned}$$

$\square$

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 biased by the spins of atoms nearby on the material:

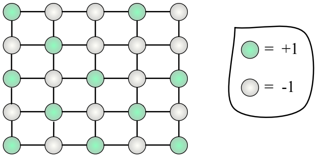




- Each atom $X_i \in \{-1, +1\}$, whose value is the direction of the atom spin
- If a spin at position i is $+1$, what is the probability that the spin at position j is also $+1$?
- Are there phase transitions where spins go from "disorder" to "order"?

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 biased by the spins of atoms nearby on the material:



$$p(x_1, \cdots, x_n) = \frac{1}{Z} \exp\Big(\sum_{i<j} w_{i,j} x_i x_j - \sum_i u_i x_i \Big)$$

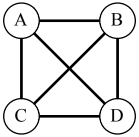
- When $w_{i,j} > 0$, nearby atoms encouraged to have the same spin (called **ferromagnetic**), whereas $w_{i,j} < 0$ encourages $X_i \neq X_j$
- Node potentials $\exp(-u_i x_i)$ encode the bias of the individual atoms
- Scaling the parameters makes the distribution more or less spiky

Higher-order potentials

- The examples so far have all been **pairwise MRFs**, involving only node potentials $\phi_i(X_i)$ and pairwise potentials $\phi_{i,j}(X_i, X_j)$
- Often we need **higher-order** potentials, e.g.

$$\phi(x, y, z) = 1[x + y + z \geq 1],$$

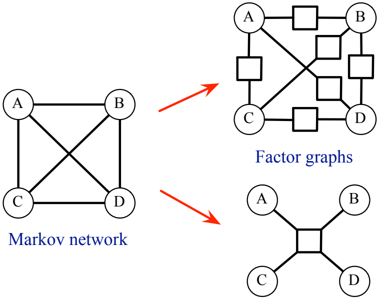
  where X, Y, Z are binary, enforcing that at least one of the variables takes the value 1
- Although Markov networks are useful for understanding independencies, they hide much of the distribution's structure:



Does this have pairwise potentials, or one potential for all 4 variables?

Factor graphs

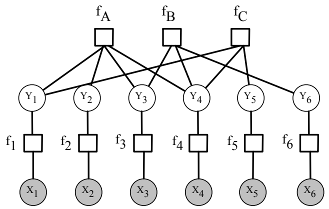
- G does not reveal the structure of the distribution: maximum cliques vs. subsets of them
- A **factor graph** is a bipartite undirected graph with variable nodes and factor nodes. Edges are only between the variable nodes and the factor nodes
- Each factor node is associated with a single potential, whose scope is the set of variables that are neighbors in the factor graph



- The distribution is same as the MRF – this is just a different data structure

Example: Low-density parity-check codes

- Error correcting codes for transmitting a message over a noisy channel (invented by Galleger in the 1960's, then re-discovered in 1996)



- Each of the top row factors enforce that its variables have even parity:

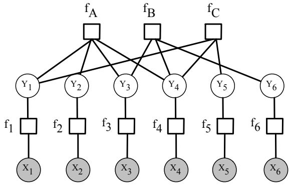
$$f_A(Y_1, Y_2, Y_3, Y_4) = 1 \text{ if } Y_1 \otimes Y_2 \otimes Y_3 \otimes Y_4 = 0, \text{ and } 0 \text{ otherwise}$$

- Thus, the only assignments **Y** with non-zero probability are the following (called **codewords**): *3 bits encoded using 6 bits*

  000000, 011001, 110010, 101011, 111100, 100101, 001110, 010111

- $f_i(Y_i, X_i) = p(X_i \mid Y_i)$, the likelihood of a bit flip according to noise model

Example: Low-density parity-check codes



- The *decoding* problem for LDPCs is to find

$$\mathrm{argmax}_{\mathbf{y}} p(\mathbf{y} \mid \mathbf{x})$$

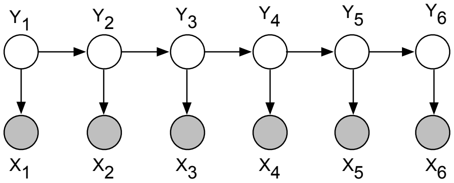
  This is called the **maximum a posteriori** (MAP) assignment
- Since Z and $p(\mathbf{x})$ are constants with respect to the choice of $\mathbf{y}$, can equivalently solve (taking the log of $p(\mathbf{y}, \mathbf{x})$):

$$\mathrm{argmax}_{\mathbf{y}} \sum_{c \in C} \theta_c(\mathbf{y}_c, \mathbf{x}_c),$$

  where $\theta_c(\mathbf{x}_c) = \log \phi_c(\mathbf{y}_c, \mathbf{x}_c)$
- This is a discrete optimization problem!

Converting BNs to Markov networks

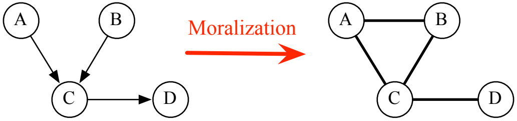
What is the equivalent Markov network for a hidden Markov model?



Many inference algorithms are more conveniently given for undirected models – this shows how they can be applied to Bayesian networks

Moralization of Bayesian networks

- Procedure for converting a Bayesian network into a Markov network
- The **moral graph** $\mathcal{M}[G]$ of a BN $G = (V, E)$ is an undirected graph over V that contains an undirected edge between X_i and X_j if
  1. there is a directed edge between them (in either direction)
  2. X_i and X_j are both parents of the same node

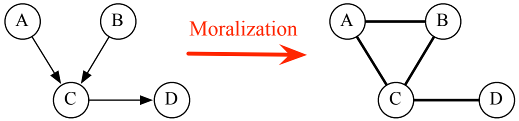


(term historically arose from the idea of "marrying the parents" of the node)

- The addition of the moralizing edges leads to the loss of some independence information, e.g., $A \rightarrow C \leftarrow B$, where $A \perp B$ is lost

Converting BNs to Markov networks

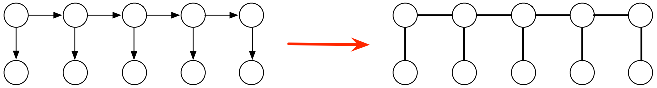
1. Moralize the directed graph to obtain the undirected graphical model:



2. Introduce one potential function for each CPD:

$$\phi_i(x_i, \mathbf{x}_{pa(i)}) = p(x_i \mid \mathbf{x}_{pa(i)})$$

- So, converting a hidden Markov model to a Markov network is simple:



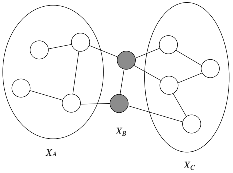
- For variables having > 1 parent, factor graph notation is useful

Factorization implies conditional independencies

- $p(\mathbf{x})$ is a *Gibbs distribution* over G if it can be written as

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

  where the variables in each potential $c \in C$ form a clique in G
- Recall that conditional independence is given by graph separation:



- Theorem (**soundness of separation**): If $p(\mathbf{x})$ is a Gibbs distribution for G, then G is an I-map for $p(\mathbf{x})$, i.e. $I(G) \subseteq I(p)$
  Proof: Suppose **B** separates **A** from **C**. Then we can write

$$p(\mathbf{X_A}, \mathbf{X_B}, \mathbf{X_C}) = \frac{1}{Z} f(\mathbf{X_A}, \mathbf{X_B}) g(\mathbf{X_B}, \mathbf{X_C}).$$

Conditional independencies implies factorization

- Theorem (**soundness of separation**): If $p(\mathbf{x})$ is a Gibbs distribution for G, then G is an I-map for $p(\mathbf{x})$, i.e. $I(G) \subseteq I(p)$
- What about the converse? We need one more assumption:
- A distribution is **positive** if $p(\mathbf{x}) > 0$ for all $\mathbf{x}$
- Theorem (**Hammersley-Clifford**, 1971): If $p(\mathbf{x})$ is a positive distribution and G is an I-map for $p(\mathbf{x})$, then $p(\mathbf{x})$ is a Gibbs distribution that factorizes over G
- Proof is in Koller & Friedman book (as is counter-example for when $p(\mathbf{x})$ is not positive)
- This is important for **learning**:
  - Prior knowledge is often in the form of conditional independencies (i.e., a graph structure G)
  - Hammersley-Clifford tells us that it suffices to search over Gibbs distributions for G – allows us to *parameterize* the distribution

Today's lecture

- Markov random fields
  1. Formalism
  2. Conditional independence properties
  3. Examples
- Factor graphs
- Bayesian networks $\Rightarrow$ Markov random fields (*moralization*)
- Learning graphical models from data

Learning graphical models

- Let's assume that the domain is governed by some underlying distribution p^*, which is induced by some network model $\mathcal{M}^* = (\mathcal{G}^*, \theta^*)$
- We are given a dataset $\mathcal{D}$ of M samples from p^*
- The standard assumption is that the data instances are **independent and identically distributed (IID)**
- We are also given a family of models $\mathcal{M}$, and our task is to learn some model $\hat{\mathcal{M}} \in \mathcal{M}$ (i.e., in this family) that defines a distribution $p_{\hat{\mathcal{M}}}$
- We can learn model parameters for a fixed structure, or both the structure and model parameters

What should our goal be?

- Return a model $\hat{\mathcal{M}}$ that precisely captures the distribution p^* from which our data was sampled
- This is in general not achievable because of
  - computational reasons
  - limited data only provides a rough approximation of the true underlying distribution
- We need to select $\hat{\mathcal{M}}$ to construct the "best" approximation to $\mathcal{M}^*$
- What is "best"?

What is “best”?

This depends on what we want to do

1. Density estimation: we are interested in the full distribution (so later we can compute whatever conditional probabilities we want)
2. Specific prediction tasks: we are using the distribution to make a prediction
   We discuss this in depth in lectures 9 and 10.
3. Structure or knowledge discovery: we are interested in the model itself (often of interest in data science)

Learning for density estimation

- We want to learn the full distribution so that later we can answer *any* probabilistic inference query
- In this setting we can view the learning problem as **density estimation**
- We want to construct $\hat{\mathcal{M}}$ as "close" as possible to p^*
- How do we evaluate "closeness"?
- **KL-divergence** is one possibility:

$$\mathbf{D}(p^*||p_\theta) = \mathbf{E}_{\mathbf{x}\sim p^*}\left[\log\left(\frac{p^*(\mathbf{x})}{p_\theta(\mathbf{x})}\right)\right]$$

- $\mathbf{D}(P^*||\hat{P}) = 0$ iff the two distributions are the same.

Expected log-likelihood

- We can simplify this somewhat:

$$\mathbf{D}(p^*||p_\theta) = \mathbf{E}_{\mathbf{x}\sim p^*}\left[\log\left(\frac{p^*(\mathbf{x})}{p_\theta(\mathbf{x})}\right)\right] = -\mathbf{H}(p^*) - \mathbf{E}_{\mathbf{x}\sim p^*}\left[\log p_\theta(\mathbf{x})\right]$$

- The first term does not depend on θ.
- Then, *minimizing* the KL-divergence from the true distribution is equivalent to *maximizing* the **expected log-likelihood**:

$$\mathbf{E}_{\mathbf{x}\sim p^*}\left[\log p_\theta(\mathbf{x})\right]$$

  - Asks that p_θ assign high probability to instances sampled from p^*, so as to reflect the true distribution
  - Because of log, samples $\mathbf{x}$ where $p_\theta(\mathbf{x}) \approx 0$ weigh heavily in objective
- **Problem:** In general we do not know p^*.

Maximum likelihood

- Approximate the expected log-likelihood

$$\mathbf{E}_{\mathbf{x}\sim p^*}\left[\log p_\theta(\mathbf{x})\right]$$

  with the *empirical log-likelihood*:

$$\mathbf{E}_{\mathcal{D}}\left[\log p_\theta(\mathbf{x})\right] = \frac{1}{|\mathcal{D}|}\sum_{\mathbf{x}\in\mathcal{D}} \log p_\theta(\mathbf{x})$$

- Maximum likelihood learning is then:

$$\max_\theta \quad \frac{1}{|\mathcal{D}|}\sum_{\mathbf{x}\in\mathcal{D}} \log p_\theta(\mathbf{x})$$

How to avoid overfitting?

- Hard constraints, e.g. by selecting a less expressive hypothesis class:
  - Bayesian networks with at most d parents
  - Bayesian networks with parametric conditional probability distributions (e.g. logistic, noisy-or, neural networks)
  - Pairwise MRFs (instead of arbitrary higher-order potentials)
- Augment the learning objective function with **regularization**:

$$\mathit{objective}(\mathbf{x}, \mathcal{M}) = \mathit{loss}(\mathbf{x}, \mathcal{M}) + R(\mathcal{M})$$

(often equivalent to MAP estimation where we put a prior over parameters θ and maximize $\log p(\theta \mid \mathbf{x}) = \log p(\mathbf{x}; \theta) + \log p(\theta) - \mathrm{constant}$)

ML estimation in Bayesian networks

- Suppose that we know the Bayesian network structure G
- Let $\theta_{x_i|\mathbf{x}_{pa(i)}}$ be the parameter giving the value of the CPD $p(x_i \mid \mathbf{x}_{pa(i)}; \theta)$
- Maximum likelihood estimation corresponds to solving:

$$\max_{\theta} \sum_{n=1}^{N} \log p(\mathbf{x}^n; \theta) = \max_{\theta} \ell(\theta; \mathcal{D})$$

  subject to the non-negativity and normalization constraints
- This is equal to:

$$\begin{aligned}\max_{\theta} \sum_{n=1}^{N} \log p(\mathbf{x}^n; \theta) &= \max_{\theta} \sum_{n=1}^{N} \sum_{i=1}^{|V|} \log p(x_i^n \mid \mathbf{x}_{pa(i)}^n; \theta) \\ &= \max_{\theta} \sum_{i=1}^{|V|} \sum_{n=1}^{N} \log p(x_i^n \mid \mathbf{x}_{pa(i)}^n; \theta)\end{aligned}$$

- The optimization problem decomposes into an independent optimization problem for each CPD!

ML estimation in Bayesian networks

$$
\begin{aligned}
\ell(\theta;\mathcal{D}) = \log p(\mathcal{D};\theta) &= \sum_{i=1}^{|V|}\sum_{n=1}^{N} \log p(x_i^n \mid \mathbf{x}_{pa(i)}^n;\theta) \\
&= \sum_{i=1}^{|V|}\sum_{\mathbf{x}_{pa(i)}}\sum_{\mathbf{x}_i} \sum_{\substack{\hat{\mathbf{x}}\in\mathcal{D}:\\ \hat{\mathbf{x}}_i,\hat{\mathbf{x}}_{pa(i)}=\mathbf{x}_i,\mathbf{x}_{pa(i)}}} \log p(x_i \mid \mathbf{x}_{pa(i)};\theta) \\
&= \sum_{i=1}^{|V|}\sum_{\mathbf{x}_{pa(i)}}\sum_{\mathbf{x}_i} N_{x_i,\mathbf{x}_{pa(i)}} \log \theta_{x_i|\mathbf{x}_{pa(i)}},
\end{aligned}
$$

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

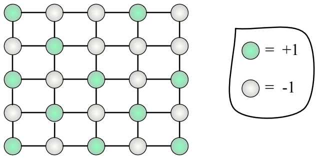
- We have the closed form ML solution:

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

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

ML estimation in Markov networks

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



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

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

Bayesian network structure learning

- Purpose: *knowledge discovery*. We hope that looking at the learned model we can discover something about p^*, e.g.
  - Nature of the dependencies, e.g., positive or negative correlation
  - What are the direct and indirect dependencies
- Simple statistical models (e.g., looking at correlations) can be used for the first
- But the learned network gives us much more information, e.g. conditional independencies, causal relationships
- In this setting we care about discovering the correct model $\mathcal{M}^*$, rather than a different model $\hat{\mathcal{M}}$ that induces a distribution similar to $\mathcal{M}^*$.
- Metric is in terms of the differences between $\mathcal{M}^*$ and $\hat{\mathcal{M}}$.

This is not always achievable

- The true model might not be identifiable
  - e.g., Bayesian network with several I-equivalent structures.
  - In this case the best we can hope is to discover an I-equivalent structure.
  - Problem is worse when the amount of data is limited and the relationships are weak.

Structure learning using maximum likelihood

- Recall that for Bayesian networks we have decomposability of the likelihood:

$$\log p(\mathcal{D};\theta) = \sum_{i=1}^{|V|} \sum_{\mathbf{x}_{pa(i)}} \sum_{\mathbf{x}_i} N_{x_i,\mathbf{x}_{pa(i)}} \log p(x_i \mid \mathbf{x}_{pa(i)};\theta)$$

- Given a candidate structure $G = (V, E)$, the maximum likelihood parameters are given by: $\theta^{ML}_{x_i|\mathbf{x}_{pa(i)}} = \frac{N_{x_i,\mathbf{x}_{pa(i)}}}{\sum_{\hat{x}_i} N_{\hat{x}_i,\mathbf{x}_{pa(i)}}} = \hat{p}(x_i \mid \mathbf{x}_{pa(i)})$
- Putting these together, maximum likelihood structure learning reduces to:

$$\max_G \sum_{i=1}^{|V|} \mathrm{score}(i \mid pa_i, \mathcal{D}), \qquad \text{where}$$

$$\mathrm{score}(i \mid pa_i, \mathcal{D}) \;=\; \sum_{\mathbf{x}_{pa(i)}} \sum_{\mathbf{x}_i} N_{x_i,\mathbf{x}_{pa(i)}} \log p(x_i \mid \mathbf{x}_{pa(i)}; \theta^{ML}_{x_i|\mathbf{x}_{pa(i)}})$$

Structure learning using maximum likelihood

- Simplifying further, we get:

$$\begin{aligned}
\mathrm{score}(i \mid pa_i, \mathcal{D}) &= N \sum_{\mathbf{x}_{pa(i)}} \frac{N_{\mathbf{x}_{pa(i)}}}{N} \sum_{\mathbf{x}_i} \frac{N_{x_i, \mathbf{x}_{pa(i)}}}{N_{\mathbf{x}_{pa(i)}}} \log \hat{p}(x_i \mid \mathbf{x}_{pa(i)}) \\
&= N \sum_{\mathbf{x}_{pa(i)}} \hat{p}(\mathbf{x}_{pa(i)}) \sum_{\mathbf{x}_i} \hat{p}(x_i \mid \mathbf{x}_{pa(i)}) \log \hat{p}(x_i \mid \mathbf{x}_{pa(i)}) \\
&= -N \sum_{\mathbf{x}_{pa(i)}} \hat{p}(\mathbf{x}_{pa(i)}) \sum_{\mathbf{x}_i} \hat{p}(x_i \mid \mathbf{x}_{pa(i)}) \log \frac{1}{\hat{p}(x_i \mid \mathbf{x}_{pa(i)})} \\
&= -N \cdot \hat{H}(X_i \mid X_{pa(i)}).
\end{aligned}$$

- We see that the maximum likelihood structure problem is equivalent to

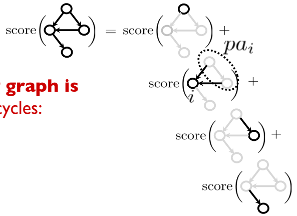
$$\min_G \sum_{i=1}^{N} \hat{H}(X_i \mid X_{pa(i)}),$$

i.e. choose a graph structure which minimizes the entropy of each individual variable.

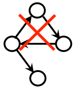
Structure learning: score-based approaches

- Q: What is the maximum likelihood graph?
  - A: The complete graph! Because $H(X \mid Y) \leq H(X)$ **always**.
  - Must *regularize* to recover a sparse graph and have any hope of recoverying true structure
  - Common approaches such as BIC and BDe (Bayesian Dirichlet score) are also decomposable
- Obtain a combinatorial optimization problem over acyclic graphs:

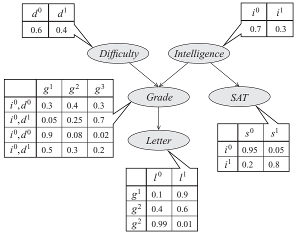
$$\text{score}(G; D) = \sum_{i=1}^{n} \text{score}(i|pa_i, D)$$



Finding highest scoring graph is NP-hard – must disallow cycles:



Independence tests



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

The network structure implies several conditional independence statements:

$$D \perp I$$
$$G \perp S \mid I$$
$$D \perp L \mid G$$
$$L \perp S \mid G$$
$$L \perp S \mid I$$
$$D \perp S$$

If two variables are (conditionally) independent, structure has no edge between them

- Must make assumption that data is drawn from an I-map of the graph
- Possible to learn structure with polynomial number of data points and polynomial computation time (e.g., the SGS algorithm from Spirtes, Glymour, & Scheines '01)
- Very brittle: if we say that $X_i \perp X_j | X_\mathbf{v}$ and they in fact are not, the resulting structure can be very off