Inference and Representation

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Today's lecture

- Markov random fields
  1. Factor graphs
  2. Bayesian networks $\Rightarrow$ Markov random fields (*moralization*)
  3. Hammersley-Clifford theorem (conditional independence $\Rightarrow$ joint distribution factorization)

- Conditional models
  3. Discriminative versus generative classifiers
  4. Conditional random fields

- 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:

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

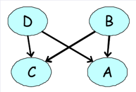
- Powerful framework for designing *algorithms* to perform probability computations

Bayesian networks have limitations

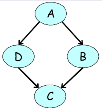
- Recall that G is a **perfect map** for distribution p if $I(G) = I(p)$
- **Theorem:** Not every distribution has a perfect map as a DAG

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)

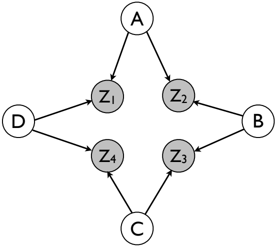
Both (a) and (b) encode $(A \perp C | B, D)$, but in both cases $(B \not\perp D | A, C)$. $\square$

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!

Bayesian networks have limitations

- Although we could represent any distribution as a fully connected BN, this obscures its structure
- Alternatively, we can introduce "dummy" binary variables $\mathbf{Z}$ and work with a **conditional** distribution:



- This satisfies $A \perp C \mid \{B, D, \mathbf{Z}\}$ and $B \perp D \mid \{A, C, \mathbf{Z}\}$
- Returning to the previous example, we would set:

$$p(Z_1 = 1 \mid a, d) = 1 \text{ if } a \neq d, \text{ and } 0 \text{ if } a = d$$

Z_1 is the observation that Alice and David have different hair colors

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:

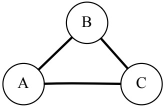
$$Z = \sum_{\hat{x}_1, \dots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

- 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):



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

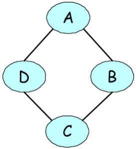
$$p(a,b,c) = \frac{1}{Z} \phi_{A,B}(a,b) \cdot \phi_{B,C}(b,c) \cdot \phi_{A,C}(a,c),$$

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.

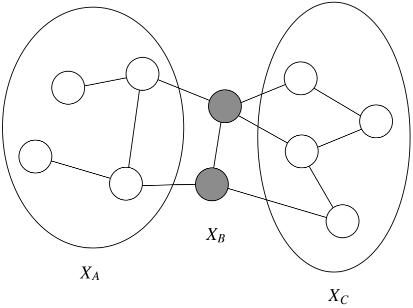
$$\phi_D(\text{“red”}) = 0.6, \quad \phi_D(\text{“blue”}) = 0.3, \quad \phi_D(\text{“green”}) = 0.1$$

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

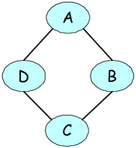
- Let G be the undirected graph where we have one edge for every pair of variables that appear together in a potential
- Conditional independence is given by **graph separation**!



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

Example

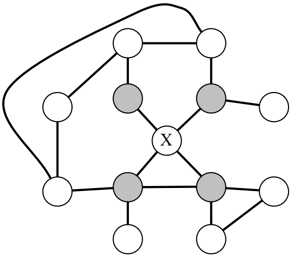
- Returning to hair color example, its undirected graphical model is:



- 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

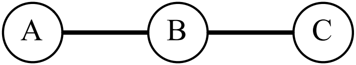
- A set $\mathbf{U}$ is a **Markov blanket** of X if $X \notin \mathbf{U}$ and if $\mathbf{U}$ is a minimal set of nodes such that $X \perp (\mathcal{X} - \{X\} - \mathbf{U}) \mid \mathbf{U}$
- In undirected graphical models, the Markov blanket of a variable is precisely its **neighbors** in the graph:



- 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:



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

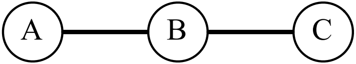
- First, we show that $p(a \mid b)$ can be computed using only $\phi_{AB}(a, b)$:

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

- 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:



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

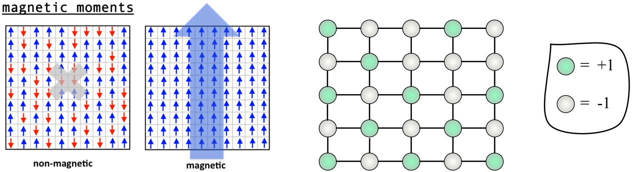
Proof.

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

$\square$

Example: Ising model

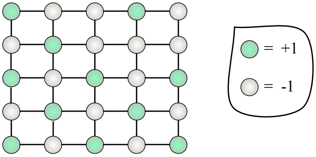
- Invented by the physicist Wilhelm Lenz (1920), who gave it as a problem to his student Ernst Ising
- Mathematical model of ferromagnetism in statistical mechanics
- The spin of an atom is biased by the spins of atoms nearby on the material:



- 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:



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

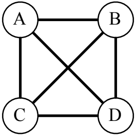
- When $w_{i,j} > 0$, nearby atoms encouraged to have the same spin (called **ferromagnetic**), whereas $w_{i,j} < 0$ encourages $X_i \neq X_j$
- Node potentials $\exp(-u_i x_i)$ encode the bias of the individual atoms
- Scaling the parameters makes the distribution more or less spiky

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.

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

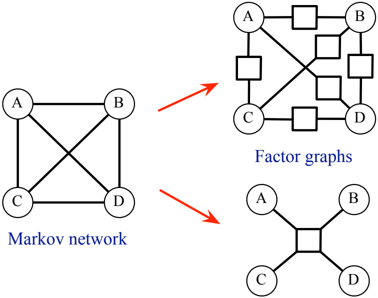
  where X, Y, Z are binary, enforcing that at least one of the variables takes the value 1
- Although Markov networks are useful for understanding independencies, they hide much of the distribution's structure:



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

Factor graphs

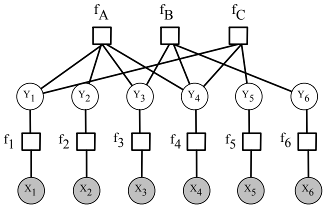
- G does not reveal the structure of the distribution: maximum cliques vs. subsets of them
- A **factor graph** is a bipartite undirected graph with variable nodes and factor nodes. Edges are only between the variable nodes and the factor nodes
- Each factor node is associated with a single potential,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

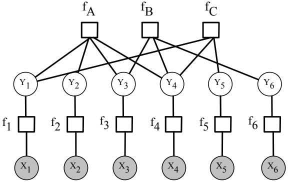
$$f_A(Y_1, Y_2, Y_3, Y_4) = 1 \text{ if } Y_1 \otimes Y_2 \otimes Y_3 \otimes Y_4 = 0, \text{ and } 0 \text{ otherwise}$$

- Thus, the only assignments $\mathbf{Y}$ 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

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

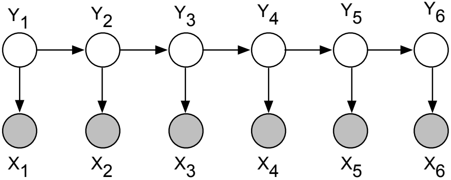
  This is called the **maximum a posteriori** (MAP) assignment
- Since Z and $p(\mathbf{x})$ are constants with respect to the choice of $\mathbf{y}$, can equivalently solve (taking the log of $p(\mathbf{y}, \mathbf{x})$):

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

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

Converting BNs to Markov networks

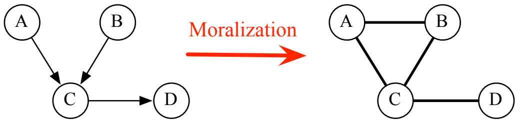
What is the equivalent Markov network for a hidden Markov model?



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

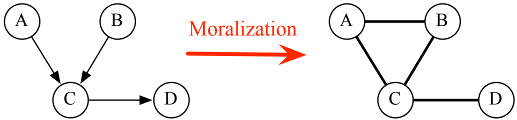


(term historically arose from the idea of "marrying the parents" of the node)

- 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

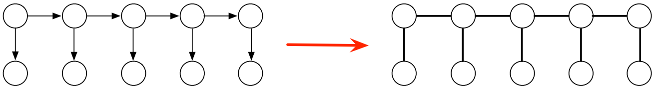
1. Moralize the directed graph to obtain the undirected graphical model:



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:



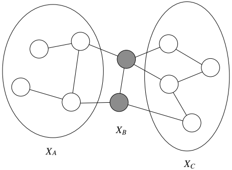
- For variables having > 1 parent, factor graph notation is useful

Factorization implies conditional independencies

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

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

  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

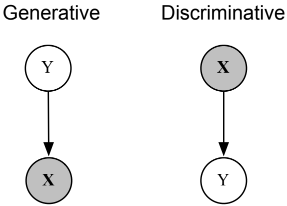
- Theorem (**soundness of separation**): If $p(\mathbf{x})$ is a Gibbs distribution for G, then G is an I-map for $p(\mathbf{x})$, i.e. $I(G) \subseteq I(p)$
- What about the converse? We need one more assumption:
- A distribution is **positive** if $p(\mathbf{x}) > 0$ for all $\mathbf{x}$
- Theorem (**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. Factor graphs
  2. Bayesian networks $\Rightarrow$ Markov random fields (*moralization*)
  3. Hammersley-Clifford theorem (conditional independence $\Rightarrow$ joint distribution factorization)
- Conditional models
  3. Discriminative versus generative classifiers
  4. Conditional random fields

Conditional models

- There is often significant flexibility in choosing the structure and parameterization of a graphical model

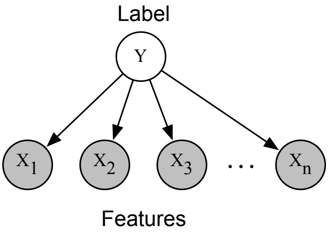


It is important to understand the trade-offs

- In the next few slides, we will study this question in the context of e-mail classification

From lecture 1... naive Bayes for single label prediction

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

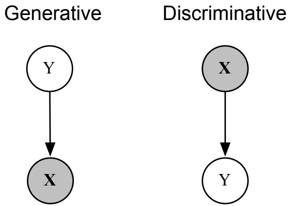


- Prediction given by:

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

Discriminative versus generative models

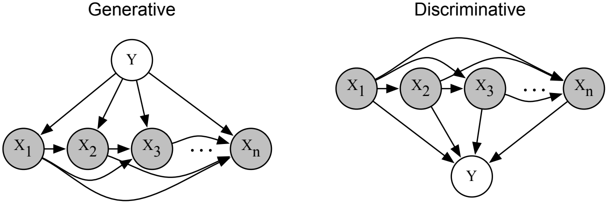
- Recall that these are **equivalent** models of $p(Y, \mathbf{X})$:



- However, suppose all we need for prediction is $p(Y \mid \mathbf{X})$
- In the left model, we need to estimate *both* $p(Y)$ and $p(\mathbf{X} \mid Y)$
- In the right model, it suffices to estimate just the **conditional distribution** $p(Y \mid \mathbf{X})$
  - We never need to estimate $p(\mathbf{X})$!
  - Would need $p(\mathbf{X})$ if $\mathbf{X}$ is only partially observed
  - Called a **discriminative** model because it is only useful for discriminating Y's label

Discriminative versus generative models

- Let's go a bit deeper to understand what are the trade-offs inherent in each approach
- Since $\mathbf{X}$ is a random vector, for $Y \rightarrow \mathbf{X}$ to be equivalent to $\mathbf{X} \rightarrow Y$, we must have:



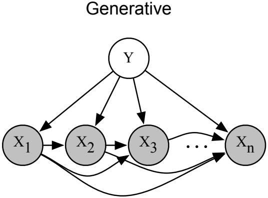
We must make the following choices:

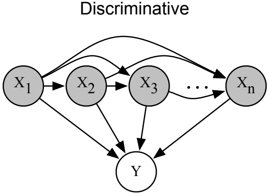
1. In the generative model, how do we parameterize $p(X_i \mid \mathbf{X}_{pa(i)}, Y)$?
2. In the discriminative model, how do we parameterize $p(Y \mid \mathbf{X})$?

Discriminative versus generative models

We must make the following choices:

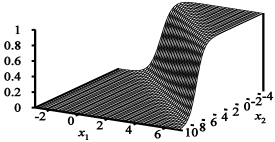
1. In the generative model, how do we parameterize $p(X_i \mid \mathbf{X}_{pa(i)}, Y)$?
2. In the discriminative model, how do we parameterize $p(Y \mid \mathbf{X})$?





1. For the generative model, assume that $X_i \perp \mathbf{X}_{-i} \mid Y$ (**naive Bayes**)
2. For the discriminative model, assume that

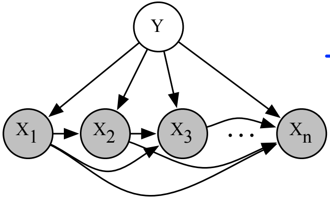
$$p(Y = 1 \mid \mathbf{x}; \alpha) = \frac{1}{1 + e^{-\alpha_0 - \sum_{i=1}^{n} \alpha_i x_i}}$$

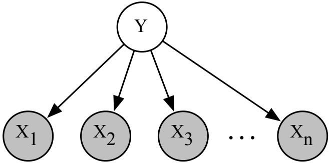


This is called **logistic regression**. *(To simplify the story, we assume $X_i \in \{0, 1\}$)*

Naive Bayes

1. For the generative model, assume that $X_i \perp \mathbf{X}_{-i} \mid Y$ (**naive Bayes**)





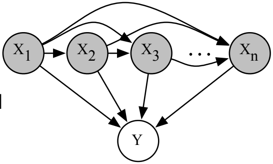
Logistic regression

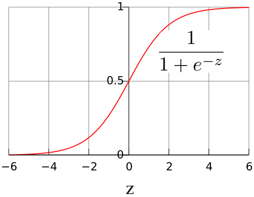
2. For the discriminative model, assume that

$$p(Y = 1 \mid \mathbf{x}; \alpha) = \frac{e^{\alpha_0 + \sum_{i=1}^{n} \alpha_i x_i}}{1 + e^{\alpha_0 + \sum_{i=1}^{n} \alpha_i x_i}} = \frac{1}{1 + e^{-\alpha_0 - \sum_{i=1}^{n} \alpha_i x_i}}$$

Let $z(\alpha, \mathbf{x}) = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i$. Then, $p(Y = 1 \mid \mathbf{x}; \alpha) = f(z(\alpha, \mathbf{x}))$, where $f(z) = 1/(1 + e^{-z})$ is called the **logistic function**:

Same graphical model





Discriminative versus generative models

1. For the generative model, assume that $X_i \perp \mathbf{X}_{-i} \mid Y$ (**naive Bayes**)
2. For the discriminative model, assume that

$$p(Y = 1 \mid \mathbf{x}; \alpha) = \frac{e^{\alpha_0 + \sum_{i=1}^{n} \alpha_i x_i}}{1 + e^{\alpha_0 + \sum_{i=1}^{n} \alpha_i x_i}} = \frac{1}{1 + e^{-\alpha_0 - \sum_{i=1}^{n} \alpha_i x_i}}$$

- Last semester, in problem set 6, you showed **assumption** 1 $\Rightarrow$ **assumption** 2
- Thus, every conditional distribution that can be represented using naive Bayes can *also* be represented using the logistic model
- What can we conclude from this?

With a large amount of training data, logistic regression will perform at least as well as naive Bayes!

Conditional random fields (CRFs)

- **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**
- We typically show the graphical model using just the $\mathbf{Y}$ variables
- Potentials are a function of $\mathbf{X}$ and $\mathbf{Y}$

Formal definition

- A CRF is a Markov network on variables $\mathbf{X} \cup \mathbf{Y}$, which specifies the conditional distribution

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

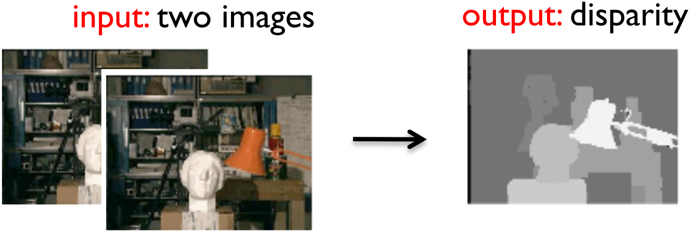
  with partition function

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

- As before, two variables in the graph are connected with an undirected edge if they appear together in the scope of some factor
- The only difference with a standard Markov network is the normalization term – before marginalized over $\mathbf{X}$ and $\mathbf{Y}$, now only over $\mathbf{Y}$

CRFs in computer vision

- Undirected graphical models very popular in applications such as computer vision: segmentation, stereo, de-noising
- Grids are particularly popular, e.g., pixels in an image with 4-connectivity



- Not encoding $p(\mathbf{X})$ is the main strength of this technique, e.g., if $\mathbf{X}$ is the image, then we would need to encode the distribution of natural images!
- Can encode a rich set of features, without worrying about their distribution