CENG 796
Deep Generative Models

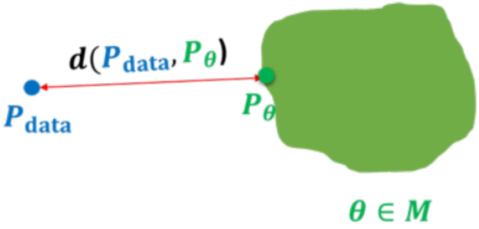
Background Review - B

ORTA DOĞU TEKNİK ÜNİVERSİTESİ
MIDDLE EAST TECHNICAL UNIVERSITY

Learning a generative model

- We are given a training set of examples, e.g., images of dogs

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



- We want to learn a probability distribution $p(x)$ over images x such that
  - **Generation:** If we sample $x_{new} \sim p(x)$, x_{new} should look like a dog (*sampling*)
  - **Density estimation:** $p(x)$ should be high if x looks like a dog, and low otherwise (*anomaly detection*)
  - **Unsupervised representation learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc. (*features*)
- First question: how to represent $p(x)$

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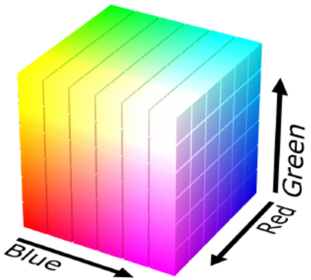
Basic discrete distributions

- Bernoulli distribution: (biased) coin flip
  - $D = \{Heads, Tails\}$
  - Specify $P(X = Heads) = p$. Then $P(X = Tails) = 1 - p$.
  - Write: $X \sim Ber(p)$
  - Sampling: flip a (biased) coin
- Categorical distribution: (biased) m-sided dice
  - $D = \{1, \cdots, m\}$
  - Specify $P(Y = i) = p_i$, such that $\sum p_i = 1$
  - Write: $Y \sim Cat(p_1, \cdots, p_m)$
  - Sampling: roll a (biased) die

Example of joint distribution

Modeling a single pixel's color. Three discrete random variables:

- Red Channel R. $\mathrm{Val}(R) = \{0, \cdots, 255\}$
- Green Channel G. $\mathrm{Val}(G) = \{0, \cdots, 255\}$
- Blue Channel B. $\mathrm{Val}(B) = \{0, \cdots, 255\}$



Sampling from the joint distribution $(r, g, b) \sim p(R, G, B)$ randomly generates a color for the pixel. How many parameters do we need to specify the joint distribution $p(R = r, G = g, B = b)$?

$$256 * 256 * 256 - 1$$

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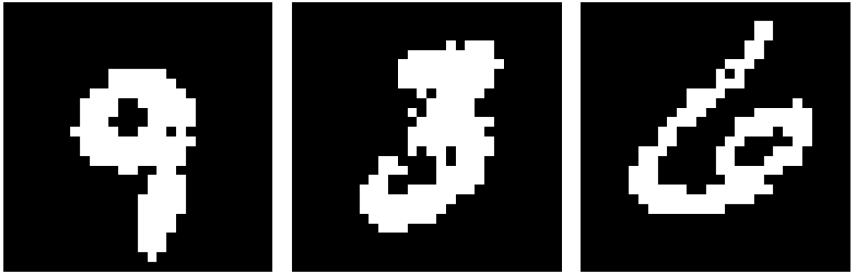
Example of joint distribution



- Suppose $X_1, \ldots, X_n$ are binary (Bernoulli) random variables, i.e., $\mathsf{Val}(X_i) = \{0, 1\} = \{\text{Black}, \text{White}\}$.
- How many possible states?

$$\underbrace{2 \times 2 \times \cdots \times 2}_{n \text{ times}} = 2^n$$

- Sampling from $p(x_1, \ldots, x_n)$ generates an image
- How many parameters to specify the joint distribution $p(x_1, \ldots, x_n)$ over n binary pixels?

$$2^n - 1$$

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Structure through independence

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

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

- How many possible states? 2^n
- How many parameters to specify the joint distribution $p(x_1, \ldots, x_n)$?
  - How many to specify the marginal distribution $p(x_1)$? 1
- 2^n **entries can be described by just** n **numbers** (if $|Val(X_i)| = 2$)!
- Independence assumption is too strong. Model not likely to be useful
  - For example, each pixel chosen independently when we sample from it.

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Key notion: conditional independence

- Two events A, B are conditionally independent given event C if

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

- Random variables X, Y are conditionally independent given Z if for all values $x \in \mathrm{Val}(X)$, $y \in \mathrm{Val}(Y)$, $z \in \mathrm{Val}(Z)$

$$p(X = x \cap Y = y | Z = z) = p(X = x|Z = z)p(Y = y|Z = z)$$

- We will also write $p(X, Y|Z) = p(X|Z)p(Y|Z)$. Note the more compact notation.
- Equivalent definition: $p(X|Y, Z) = p(X|Z)$.
- We write $X \perp Y \mid Z$
- Similarly for sets of random variables, $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$

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Two important rules

1. **Chain rule** Let $S_1, \ldots S_n$ be events, $p(S_i) > 0$.

$$p(S_1 \cap S_2 \cap \cdots \cap S_n) = p(S_1)p(S_2 \mid S_1) \cdots p(S_n \mid S_1 \cap \ldots \cap S_{n-1})$$

2. **Bayes' rule** Let S_1, S_2 be events, $p(S_1) > 0$ and $p(S_2) > 0$.

$$p(S_1 \mid S_2) = \frac{p(S_1 \cap S_2)}{p(S_2)} = \frac{p(S_2 \mid S_1)p(S_1)}{p(S_2)}$$

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Structure through conditional independence

- Using Chain Rule

$$p(x_1, \dots, x_n) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2) \cdots p(x_n \mid x_1, \cdots, x_{n-1})$$

- How many parameters? $1 + 2 + \cdots + 2^{n-1} = 2^n - 1$
  - $p(x_1)$ requires 1 parameter
  - $p(x_2 \mid x_1 = 0)$ requires 1 parameter, $p(x_2 \mid x_1 = 1)$ requires 1 parameter Total 2 parameters.
  - $\cdots$
- $2^n - 1$ is still exponential, chain rule does not buy us anything.
- Now suppose $X_{i+1} \perp X_1, \dots, X_{i-1} \mid X_i$, then

$$\begin{aligned} p(x_1, \dots, x_n) &= p(x_1)p(x_2 \mid x_1)p(x_3 \mid \cancel{x_1}, x_2) \cdots p(x_n \mid \cancel{x_1, \cdots}, x_{n-1}) \\ &= p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2) \cdots p(x_n \mid x_{n-1}) \end{aligned}$$

- How many parameters? $2n - 1$. Exponential reduction!

Structure through conditional independence

- Suppose we have 4 random variables $X_1, \cdots, X_4$
- Using Chain Rule we can **always** write

$$p(x_1, \ldots, x_4) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, x_2, x_3)$$

- If $X_4 \perp X_2 \mid \{X_1, X_3\}$, we can simplify as

$$p(x_1, \ldots, x_n) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, \cancel{x_2}, x_3)$$

- Using Chain Rule with a *different ordering* we can **always** also write

$$p(x_1, \ldots, x_4) = p(x_4)p(x_3 \mid x_4)p(x_2 \mid x_3, x_4)p(x_1 \mid x_2, x_3, x_4)$$

- If $X_1 \perp \{X_2, X_3\} \mid X_4$, we can simplify as

$$p(x_1, \ldots, x_4) = p(x_4)p(x_3 \mid x_4)p(x_2 \mid x_3, x_4)p(x_1 \mid \cancel{x_2, x_3}, x_4)$$

- Bayesian Networks: assume an **ordering** and a set of **conditional independencies** to get compact representation

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Bayes Network: General Idea

- Use conditional parameterization (instead of joint parameterization)
- For each random variable X_i, specify $p(x_i|\mathbf{x}_{\mathbf{A_i}})$ for set $\mathbf{X}_{\mathbf{A_i}}$ of random variables
- Then get joint parametrization as

$$p(x_1, \ldots, x_n) = \prod_i p(x_i|\mathbf{x}_{\mathbf{A_i}})$$

- Need to guarantee it is a *legal* probability distribution. It has to correspond to a chain rule factorization, with factors simplified due to assumed conditional independencies

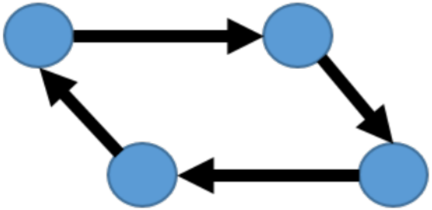
Bayesian networks

- 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
- Graph $G = (V, E)$ is called the structure of the Bayesian Network
- Defines a joint distribution:

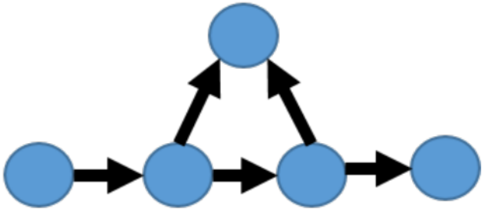
$$p(x_1, \dots x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{\mathrm{Pa}(i)})$$

- Claim: $p(x_1, \dots x_n)$ is a valid probability distribution
- **Economical representation**: exponential in $|\mathrm{Pa}(i)|$, not $|V|$

Example



Directed cycle

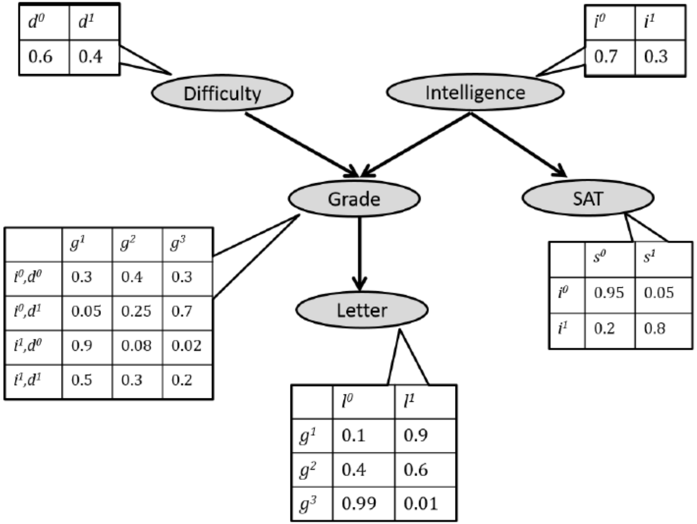


DAG

DAG stands for Directed Acyclic Graph

Example

- 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^1,d^0	0.9	0.08	0.02
i^1,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^3	0.99	0.01

- What is its joint distribution?

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

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

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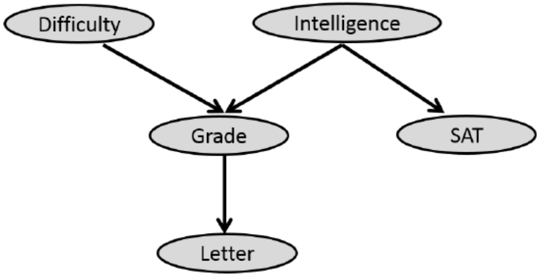
Bayesian network structure implies conditional independencies!



- The joint distribution corresponding to the above BN factors as

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

- However, by the chain rule, *any* distribution can be written as

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

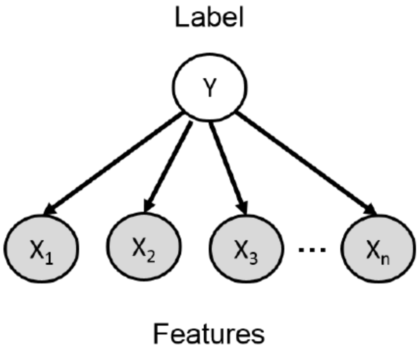
- Thus, we are assuming the following additional independencies:
$D \perp I, \qquad S \perp \{D, G\} \mid I, \qquad L \perp \{I, D, S\} \mid G.$

Summary

- **Bayesian networks** given by (G, P) where P is specified as a set of local **conditional probability distributions** associated with G's nodes
- Efficient representation using a graph-based data structure
- Computing the probability of any assignment is obtained by multiplying CPDs
- Can identify some conditional independence properties by looking at graph properties
- Next: generative vs. discriminative; functional parameterizations

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:



- Then

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

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Example: naive Bayes for classification

- 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 $p(Y, X_1, \ldots, X_n)$
- Suppose that the words are conditionally independent given Y. Then,

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

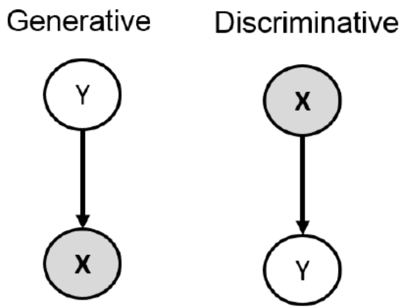
Estimate parameters from training data. **Predict** with Bayes rule:

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

- Are the independence assumptions made here reasonable?
- Philosophy: Nearly all probabilistic models are "wrong", but many are nonetheless useful

Discriminative versus generative models

- Using chain rule $p(Y, \mathbf{X}) = p(\mathbf{X} \mid Y)p(Y) = p(Y \mid \mathbf{X})p(\mathbf{X})$. Corresponding Bayesian networks:



- However, suppose all we need for prediction is $p(Y \mid \mathbf{X})$
- In the left model, we need to specify/learn *both* $p(Y)$ and $p(\mathbf{X} \mid Y)$, then compute $p(Y \mid \mathbf{X})$ via Bayes rule
- In the right model, it suffices to estimate just the **conditional distribution** $p(Y \mid \mathbf{X})$
  - We never need to model/learn/use $p(\mathbf{X})$!
  - Called a **discriminative** model because it is only useful for discriminating Y's label when given $\mathbf{X}$

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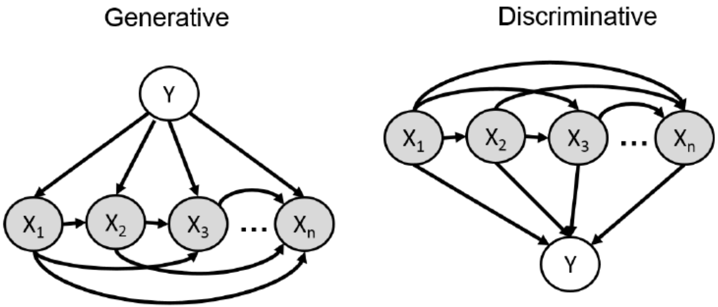
Discriminative versus generative models

- Since $\mathbf{X}$ is a random vector, chain rules will give
  - $p(Y, \mathbf{X}) = p(Y)p(X_1 \mid Y)p(X_2 \mid Y, X_1) \cdots p(X_n \mid Y, X_1, \cdots, X_{n-1})$
  - $p(Y, \mathbf{X}) = p(X_1)p(X_2 \mid X_1)p(X_3 \mid X_1, X_2) \cdots p(Y \mid X_1, \cdots, X_{n-1}, X_n)$



We must make the following choices:

1. In the generative model, $p(Y)$ is simple, but how do we parameterize $p(X_i \mid \mathbf{X}_{pa(i)}, Y)$?
2. In the discriminative model, how do we parameterize $p(Y \mid \mathbf{X})$? Here we assume we don't care about modeling $p(\mathbf{X})$ because $\mathbf{X}$ is always given to us in a classification problem

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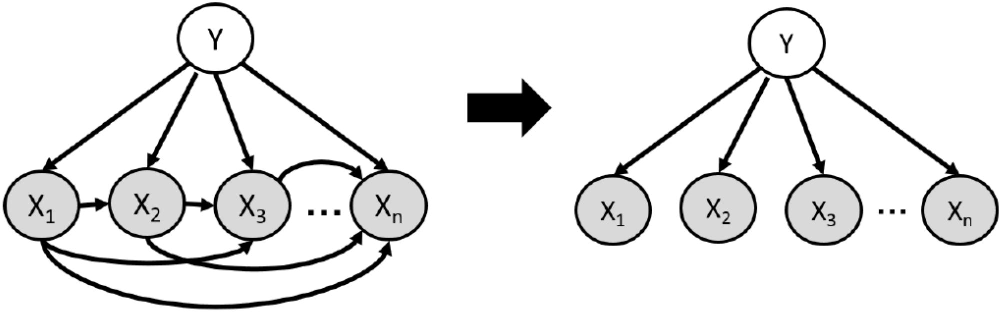
Naive Bayes

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



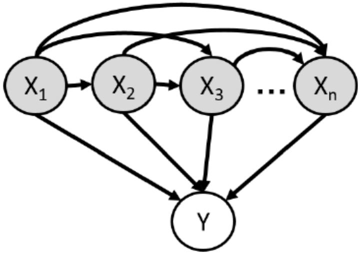
Logistic regression

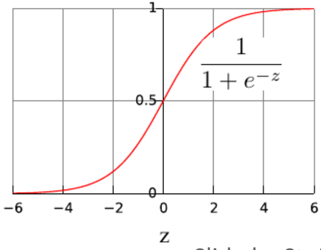
1. For the discriminative model, assume that

$$p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = f(\mathbf{x}, \boldsymbol{\alpha})$$

2. Not represented as a table anymore. It is a parameterized function of $\mathbf{x}$ (regression)
   - Has to be between 0 and 1
   - Depend in some *simple* but reasonable way on $x_1, \cdots, x_n$
   - Completely specified by a vector $\boldsymbol{\alpha}$ of $n+1$ parameters (**compact representation**)

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





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Logistic regression

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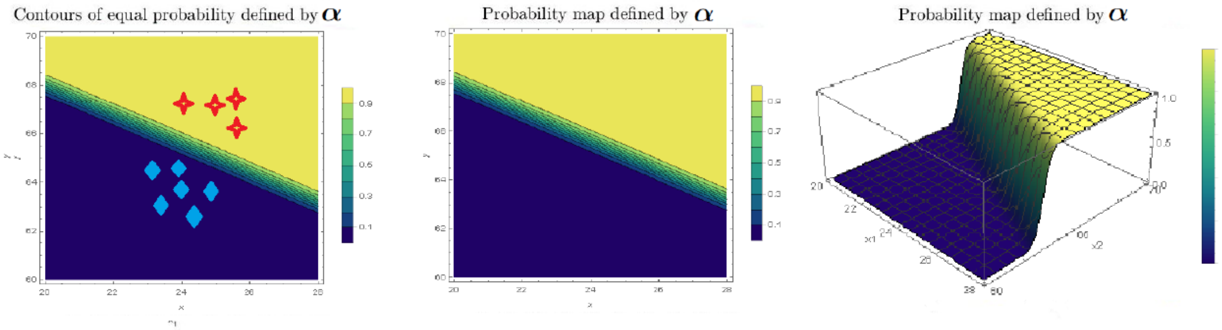
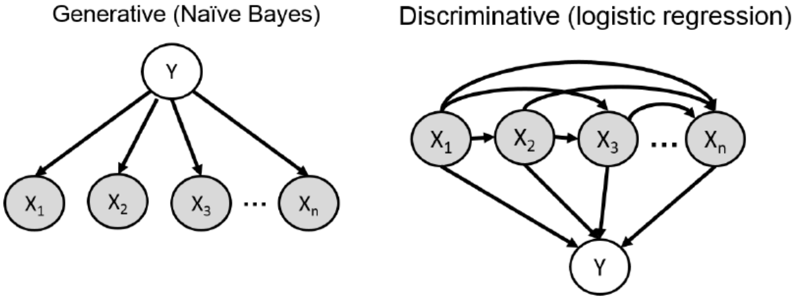


1. Decision boundary $p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) > 0.5$ is linear in $\mathbf{x}$
2. Equal probability contours are straight lines
3. Probability rate of change has very specific form (third plot)

Discriminative models are powerful



- Logistic model does *not* assume $X_i \perp \mathbf{X}_{-i} \mid Y$, unlike naive Bayes
- This can make a big difference in many applications
- For example, in spam classification, let $X_1 = 1[\text{"bank" in e-mail}]$ and $X_2 = 1[\text{"account" in e-mail}]$
- Regardless of whether spam, these always appear together, i.e. $X_1 = X_2$
- Learning in naive Bayes results in $p(X_1 \mid Y) = p(X_2 \mid Y)$. Thus, naive Bayes **double counts the evidence**
- Learning with logistic regression sets $\alpha_1 = 0$ or $\alpha_2 = 0$, in effect ignoring it

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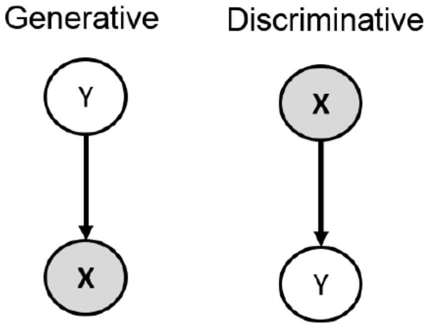
Generative models are still very useful

Using chain rule $p(Y, \mathbf{X}) = p(\mathbf{X} \mid Y)p(Y) = p(Y \mid \mathbf{X})p(\mathbf{X})$. Corresponding Bayesian networks:



1. Using a conditional model is only possible when $\mathbf{X}$ is always observed
   - When some X_i variables are unobserved, the generative model allows us to compute $p(Y \mid \mathbf{X}_{evidence})$ by marginalizing over the unseen variables

Neural Models

1. In discriminative models, we assume that

$$p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = f(\mathbf{x}, \boldsymbol{\alpha})$$

2. **Linear** dependence:
   - let $z(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i$.
   - $p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = \sigma(z(\boldsymbol{\alpha}, \mathbf{x}))$, where $\sigma(z) = 1/(1 + e^{-z})$ is the **logistic function**
   - Dependence might be too simple
3. **Non-linear** dependence: let $\mathbf{h}(A, \mathbf{b}, \mathbf{x}) = f(A\mathbf{x} + \mathbf{b})$ be a non-linear transformation of the inputs (*features*).
   $p_{\text{Neural}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}, A, \mathbf{b}) = \sigma(\alpha_0 + \sum_{i=1}^{h} \alpha_i h_i)$
   - More flexible
   - More parameters: $A, \mathbf{b}, \boldsymbol{\alpha}$

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Neural Models

1. In discriminative models, we assume that

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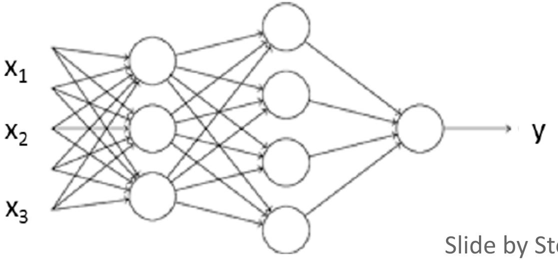
   $p_{\mathrm{Neural}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}, A, \mathbf{b}) = f(\alpha_0 + \sum_{i=1}^{h} \alpha_i h_i)$
   - More flexible
   - More parameters: $A, \mathbf{b}, \boldsymbol{\alpha}$
   - Can repeat multiple times to get a neural network



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Bayesian networks vs neural models

- Using Chain Rule

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, x_2, x_3)$$

Fully General

- Bayes Net

$$p(x_1, x_2, x_3, x_4) \approx p(x_1)p(x_2 \mid x_1)p(x_3 \mid \cancel{x_1}, x_2)p(x_4 \mid x_1, \cancel{x_2, x_3})$$

Assumes conditional independencies

- Neural Models

$$p(x_1, x_2, x_3, x_4) \approx p(x_1)p(x_2 \mid x_1)p_{\mathrm{Neural}}(x_3 \mid x_1, x_2)p_{\mathrm{Neural}}(x_4 \mid x_1, x_2, x_3)$$

Assume specific functional form for the conditionals. A sufficiently deep neural net can approximate any function.

Continuous variables

- If X is a continuous random variable, we can usually represent it using its **probability density function** $p_X : \mathbb{R} \to \mathbb{R}^+$. However, we cannot represent this function as a table anymore. Typically consider parameterized densities:
  - Gaussian: $X \sim \mathcal{N}(\mu, \sigma)$ if $p_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$
  - Uniform: $X \sim \mathcal{U}(a, b)$ if $p_X(x) = \frac{1}{b-a} 1[a \leq x \leq b]$
  - Etc.
- If $\boldsymbol{X}$ is a continuous random vector, we can usually represent it using its **joint probability density function**:
  - Gaussian: if $p_X(x) = \frac{1}{\sqrt{(2\pi)^n|\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(x-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(x-\boldsymbol{\mu})\right)$
- Chain rule, Bayes rule, etc all still apply. For example,

$$p_{X,Y,Z}(x, y, z) = p_X(x) p_{Y|X}(y \mid x) p_{Z|\{X,Y\}}(z \mid x, y)$$

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Continuous variables

- This means we can still use Bayesian networks with continuous (and discrete) variables. Examples:
- **Mixture of 2 Gaussians**: Network $Z \to X$ with factorization $p_{Z,X}(z,x) = p_Z(z)p_{X|Z}(x \mid z)$ and
  - $Z \sim Bernoulli(p)$
  - $X \mid (Z=0) \sim \mathcal{N}(\mu_0, \sigma_0)$, $X \mid (Z=1) \sim \mathcal{N}(\mu_1, \sigma_1)$
  - The parameters are $p, \mu_0, \sigma_0, \mu_1, \sigma_1$
- Network $Z \to X$ with factorization $p_{Z,X}(z,x) = p_Z(z)p_{X|Z}(x \mid z)$
  - $Z \sim \mathcal{U}(a,b)$
  - $X \mid (Z=z) \sim \mathcal{N}(z, \sigma)$
  - The parameters are a, b, σ
- **Variational autoencoder**: Network $Z \to X$ with factorization $p_{Z,X}(z,x) = p_Z(z)p_{X|Z}(x \mid z)$ and
  - $Z \sim \mathcal{N}(0,1)$
  - $X \mid (Z=z) \sim \mathcal{N}(\mu_\theta(z), e^{\sigma_\phi(z)})$ where $\mu_\theta : \mathbb{R} \to \mathbb{R}$ and σ_ϕ are neural networks with parameters (weights) θ, ϕ respectively
  - **Note**: Even if μ_θ, σ_ϕ are very deep (flexible), functional form is still Gaussian