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 p_{data}









$$\mathbf{x}^{j} \sim p_{data}$$
$$j = 1, 2, \dots |\mathcal{D}|$$

- dataset \mathcal{D}
- data distribution p_{data}
- model parameters $\theta \in \mathcal{M}$

• How to represent (model) a data distribution? It can be an optimization problem:

$$\min_{\theta \in \mathcal{M}} \mathcal{L}(p_{data}, p_{\theta})$$

Why parametric models?

They scale more efficiently with large dataset than non-parametric models.



 p_{data}









$$\mathbf{x}^{j} \sim p_{data}$$
$$j = 1, 2, \dots |\mathcal{D}|$$

- dataset \mathcal{D}
- data distribution p_{data}
- model parameters $\theta \in \mathcal{M}$

- We want to learn a probability distribution p(x) over x
- 1. Generation (sampling): $\mathbf{x}_{new} \sim p(\mathbf{x})$
- **2.** Density Estimation: p(x) high if x looks like a cat
- 3. Unsupervised Representation Learning:

Discovering the underlying structure from the data distribution (e.g., ears, nose, eyes ...)



Recap: Challenges from Lecture 1

Representation ability

How to represent p(x)

For 1-D data x , the probability distribution p(x) is simple, e.g., Gaussian? For high-dimensional data $\mathbf{x}=(x_1,x_2,\dots,x_n)$, how do we learn the joint distribution $p(x_1,x_2,\dots,x_n)$?

Learning method

How do we measure and minimize the distance between the estimated distribution p(x) and the real distribution p_{data} ? we can now perform generative process and density estimation

Inference

How do we perform discriminative task?
i.e., invert the generative process



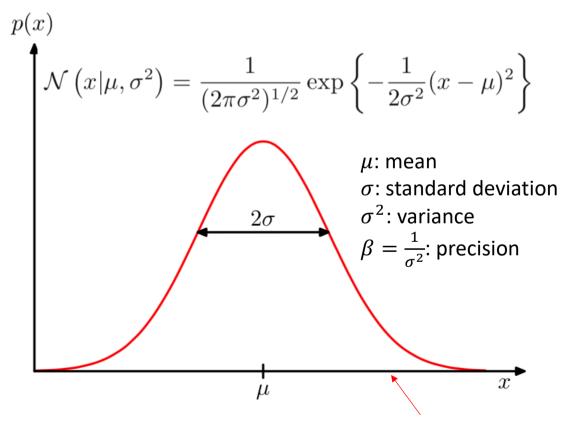
Problem of High-dimensional Data
 Less Parameters: Conditional Independence
 Less Parameters: Bayesian Network
 Naïve Bayes Classifier
 Discriminative vs. Generative Models
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How to represent the age distribution (age from 0 to 99)

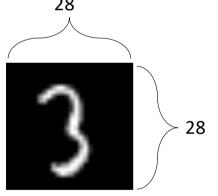


In this case, we have 100 states and we need 2 parameters to represent the probability distribution p(x) μ , σ



• How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$





784 random binary variables

In MNIST, an images have 28 * 28 * 1 = 784 binary values

So... how to represent $p(x_1, x_2, ..., x_{784})$? how many number of parameters?

MNIST dataset



• How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$

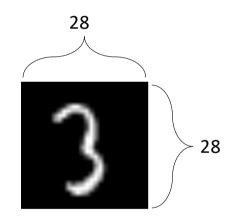


As x can be either 0 or 1, i.e., only 2 states

(Joint distribution)

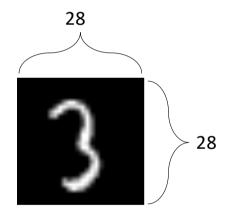
The number of possible state for $p(x_1, x_2, ..., x_n)$ is 2^n which is far larger than the number of data sample

We need a super-large memory to store $p(x_1, x_2, ..., x_n)$ even we have such large memory, we do not have enough data to learn/model it





• How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$



784 random binary variables

$$p(x_1, x_2, ..., x_n)$$
 has 2^n states, then ...

How many number of parameters to model $p(x_1, x_2, ..., x_n)$?

Recap: Product Rule

$$p(x_1, x_2) = p(x_1)p(x_2|x_1)$$

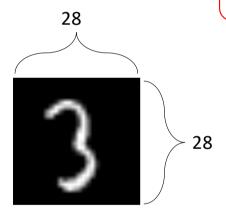
$$p(x_1, x_2, x_3) = p(x_1, x_2)p(x_3|x_1, x_2) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)$$

• • •

$$p(x_1, x_2, ..., x_n) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) ... p(x_n|x_1, ..., x_{n-1})$$



How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$



784 random binary variables

$$p(x_1, x_2, ..., x_n) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) ... p(x_n|x_1, ..., x_{n-1})$$

- $p(x_1)$ need 1 parameter, the probability of x_1 to be 1 (as it is a binary variable)
- $p(x_2|x_1)$ need 2 parameters, i.e., $p(x_2|x_1=0)$ and $p(x_2|x_1=1)$
- $p(x_3|x_1,x_2)$ need 4 parameters, i.e., $p(x_3|x_1=0,x_2=0)$, $p(x_3|x_1=0,x_2=1)$ $p(x_2|x_1=1,x_2=0), p(x_2|x_1=1,x_2=1)$

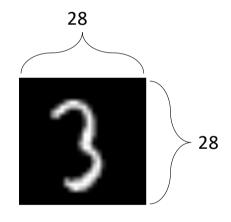
So ... The number of parameters to model $p(x_1, x_2, ..., x_n)$ is: $1 + 2 + 4 + \cdots + 2^{n-1} = 2^n - 1$

$$1 + 2 + 4 + \dots + 2^{n-1} = 2^n - 1$$

(when variables are binary)



• How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$



784 random binary variables

Product Rule:

$$p(x_1, x_2, ..., x_n) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) ... p(x_n|x_1, ..., x_{n-1})$$

$$2^n \text{ states} \qquad \qquad 2^n - 1 \text{ parameters}$$

 $2^n - 1$ is exponential, the product rule does not help to reduce the num of parameters



• How to represent a high-dimensional data $\mathbf{x} = (x_1, x_2, x_3, ..., x_n)$

In practice

- 1) The x can be continuous, i.e., infinite states
- 2) The number of x can be millions

For simplicity

We use binary x and MNIST for demo

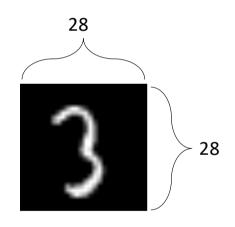


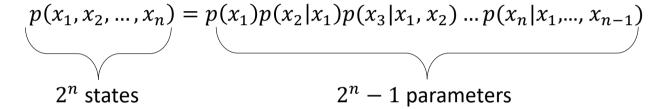
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• How to reduce the number of parameter to represent $p(x_1, x_2, ..., x_n)$?

Product Rule does not help:





784 random binary variables



• How to reduce the number of parameter to represent $p(x_1, x_2, ..., x_n)$?

Recap: If variables x_1, x_2 are conditional independent given variable x_3 , denotes as $x_1 \perp x_2 \mid x_3$

$$p(x_1, x_2 | x_3) = p(x_1 | x_3) p(x_2 | x_3)$$

If not independent:

$$p(x_1, x_2 | x_3) = \frac{p(x_1, x_2, x_3)}{p(x_3)} = \frac{p(x_1, x_2, x_3)}{p(x_2, x_3)} \frac{p(x_2, x_3)}{p(x_3)} = p(x_1 | x_2, x_3) p(x_2 | x_3)$$

so we can have $p(x_1|x_2,x_3)p(x_2|x_3) = p(x_1|x_3)p(x_2|x_3)$ if $x_1 \perp x_2 \mid x_3$



• How to reduce the number of parameter to represent $p(x_1, x_2, ..., x_n)$?

Given product rule: $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$

If
$$x_4 \perp x_2 \mid \{x_1, x_3\}$$
, we can simplify it as:
$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, x_2, x_3)$$

If
$$x_2 \perp \{x_1, x_3\} \mid x_4$$
, we can simplify it as:

$$p(x_1, x_2, x_3, x_4) = p(x_4, x_3, x_2, x_1) = p(x_4)p(x_3|x_4)p(x_2|x_3, x_4)p(x_1|x_2, x_3, x_4)$$

$$= p(x_4)p(x_3|x_4)p(x_2|x_3, x_4)p(x_1|x_2, x_3, x_4)$$



• How to reduce the number of parameter to represent $p(x_1, x_2, ..., x_n)$?

In an **extreme case**, if $x_{i+1} \perp \{x_1, x_2 \dots x_{i-1}\} \mid x_i$, i.e., the next variable only related to the current variable (Markov model!)

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_4, x_2)p(x_4|x_4, x_2, x_3)$$

$$= p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)$$

If x are binary variables

$$2n-1$$
 parameters $<< 2^n-1$ parameters

So ...

if conditional independencies exist, the number of parameter can be reduced!!



• How to reduce the number of parameter to represent $p(x_1, x_2, ..., x_n)$?

In a MORE extreme case, if x_i are independent identical (IID)

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

$$= p(x_1)p(x_2|x_4)p(x_3|x_4, x_2)p(x_4|x_4, x_2, x_3)$$

$$= p(x_1)p(x_2)p(x_3)p(x_4)$$

However, in practice, there exists "relationship" between variables the independence assumption is not practical...

e.g., the following random samples would not happen







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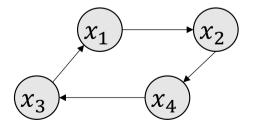
Key idea:

Joint distribution:
$$p(x_1, x_2, ..., x_n) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) ... p(x_n|x_1, ..., x_{n-1})$$

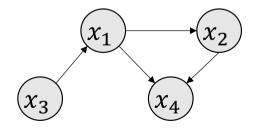
$$2^n - 1 \text{ parameters if } x \text{ are binary variables}$$

use conditional distribution instead of joint distribution to reduce the num of parameters

Bayesian network structure is a **Directed Acyclic Graph**, G = (V, E) where V means vertexes, E means edges



Directed Cycle



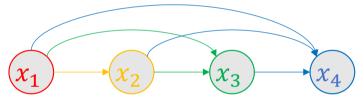
Directed Acyclic Graph



Key idea:

Bayesian network structure is a **Directed Acyclic Graph**, G = (V, E)

Joint distribution: $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$



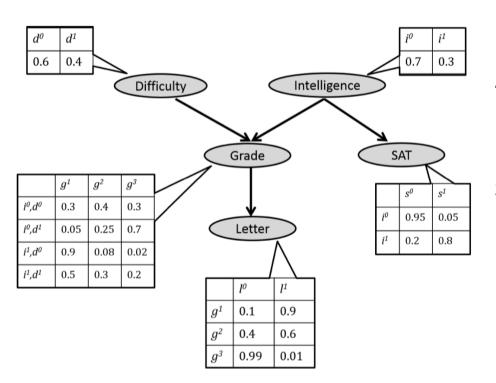
If $x_{i+1} \perp \{x_1, x_2 \dots x_{i-1}\} \mid x_i$ $p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_4, x_2)p(x_4|x_4, x_2, x_3)$ $= p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)$



Less edges == Less parameters



Example



$$p(d,i,g,s,l) = p(d)p(i|d)p(g|d,i)p(s|d,i,g)p(l|d,i,g,s)$$

According to the left Bayesian Net, we have the independencies:

$$d \perp i$$
 $s \perp \{d, g\}$ $l \perp \{d, i, s\}$

So that ..

$$p(d, i, g, s, l) = p(d)p(i)p(g|i, d)p(s|i)p(l|g)$$



- Bayesian Network structure is a **Directed Acyclic Graph**, G = (V, E)
- Bayesian Network is given by (G, P), where P is a set of local conditional probability distributions for each node/vertex of G
- Compute the P using data samples to "learn" the Bayesian Network
- Bayesian Network is also known as Belief Network and Bayes Network

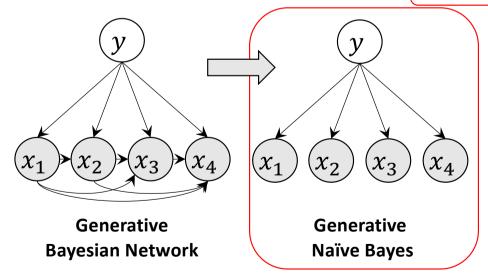


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Naïve Bayes Classifier

- How Bayesian Network performs inferencing? i.e., discriminative tasks?
- Support we have a binary classification problem, label y=0,1, features $\mathbf{x}=(x_1,x_2,x_3,x_4)$
- The probability distribution is $p(y, x_1, x_2, x_3, x_4)$
- Naïve Bayes Classifier assume that $x_i \perp \mathbf{x}_{-i} | y$, so that:



Given Naïve Bayes Assumption:

$$p(y, x_1, x_2, x_3, x_4) = p(y)p(x_1|y)p(x_2|y) p(x_3|y)$$

$$p(\mathbf{x}|y)$$



Naïve Bayes Classifier

$$p(y|\mathbf{x}) = \frac{p(\mathbf{x}, y)}{p(\mathbf{x})} = \frac{p(y)p(\mathbf{x}|y)}{p(\mathbf{x})} \propto p(y)p(x|y)$$

$$\hat{y} = arg \max_{y} p(y|\mathbf{x}) = arg \max_{y} \frac{p(\mathbf{x}, y)}{p(\mathbf{x})} = arg \max_{y} p(y)p(\mathbf{x}|y)$$

Given Naïve Bayes Assumption:

$$p(\mathbf{x}|\mathbf{y}) = p(x_1|\mathbf{y})p(x_2|\mathbf{y}) p(x_3|\mathbf{y})$$



Naïve Bayes Classifier

- Given $p(\mathbf{x}|\mathbf{y}) = p(x_1|\mathbf{y})p(x_2|\mathbf{y}) p(x_3|\mathbf{y})$, how to compute p(Y|X)?
- First, we can **estimate** the parameters from the training set:

| | $x_1 = 0$ | $x_1 = 1$ | $x_2 = 0$ | $x_2 = 1$ | $x_3 = 0$ | $x_3 = 1$ | $x_4 = 0$ | $x_4 = 1$ |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| y = 0 | 3 | 5 | 5 | 2 | 0 | 8 | 7 | 4 |
| y = 1 | 1 | 0 | 3 | 10 | 7 | 4 | 2 | 5 |

•
$$p(Y = 0) = \frac{3+5+5+2+8+7+4}{(3+5+5+2+8+7+4)+(1+3+10+7+4+2+5)}$$

•
$$p(x_1 = 0|Y = 0) = \frac{3}{3+5+5+2+8+7+4}$$

-
- Second, predict the probability of a label given an input with Bayes rule:

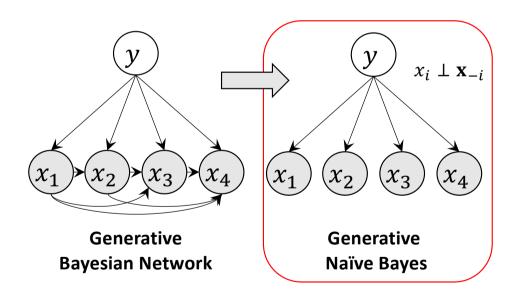
•
$$p(Y = 0 | x_1, x_2, x_3, x_4) = \frac{p(Y=0) \prod_{i=1}^4 p(x_i | Y=0)}{\sum_{y=\{0,1\}} p(Y=y) \prod_{i=1}^4 p(x_i | Y=y)}$$





• Limitation

Are the independence assumptions reasonable ??





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Discriminative vs. Generative Models

- symmetry property p(X,Y) = p(Y,X)

- Given p(Y,X) = p(X|Y)p(Y) = p(Y|X)p(X)
- Discriminative: $X \to Y$, we only need to estimate the conditional distribution P(Y|X) without learning to model P(X) simply input X then output Y



• Generative: $Y \to X$, we need both P(Y) and P(X|Y) to compute p(Y|X) via Bayes (see the Naïve Bayes Classifier as an example)





Discriminative vs. Generative Models

Given a random vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$, the product rules can give us:

$$p(y, \mathbf{x}) = p(y)p(x_1|y)p(x_2|y, x_1) \dots p(x_n|y, x_1, x_2, \dots, x_{n-1})$$

$$p(y, \mathbf{x}) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) \dots p(y|x_1, x_2, \dots, x_{n-1})$$

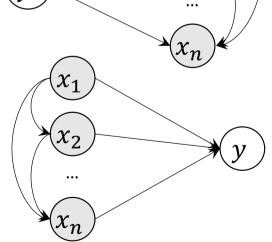
generative

p(y) is simple to estimate

but how to parametrize $p(x_i|y, x_1,...,x_{i-1})$?

discriminative

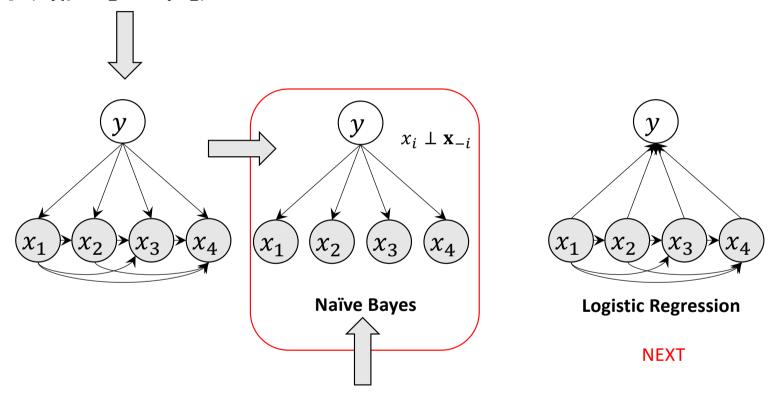
only need to parametrize $p(y|x_1,...,x_{n-1})$





Discriminative vs. Generative Models

parametrize $p(x_i|y, x_1,...,x_{i-1})$ without independent assumptions



parametrize $p(x_i|y, x_1,...,x_{i-1})$ with independent assumptions



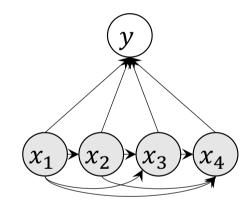
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Logistic Regression

• Parameterize the p(Y|X) without independence assumptions

only need to parametrize $p(y|x_1,...,x_{n-1})$



Logistic Regression

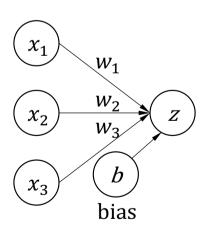


Logistic Regression

• (only need to) parameterize the p(Y|X) without independence assumptions

$$p(Y = 1|\mathbf{x}, \mathbf{w}, b) = f(\mathbf{x}, \mathbf{w}, b)$$

input layer output layer



$$z = x_1 w_1 + x_2 w_2 + x_3 w_3 + b$$

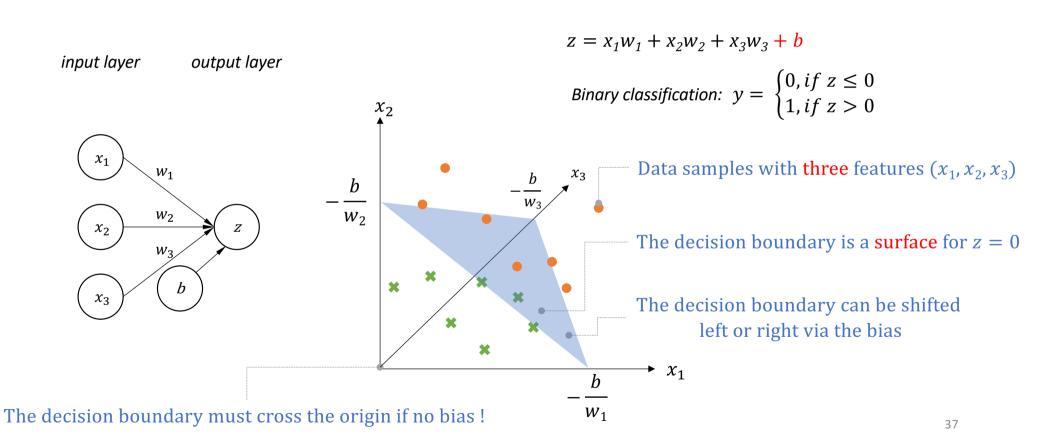
$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

$$z = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b$$

$$z = \begin{bmatrix} w_1 & w_2 & w_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + b$$



• (only need to) parameterize the p(Y|X) without independence assumptions





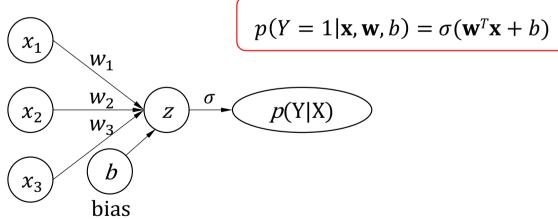
• (only need to) parameterize the p(Y|X) without independence assumptions

$$p(Y = 1|\mathbf{x}, \mathbf{w}, b) = f(\mathbf{x}, \mathbf{w}, b)$$

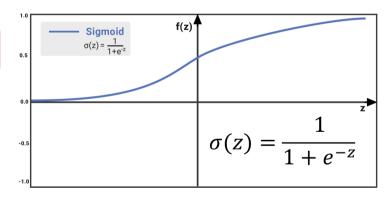
input layer output layer



 $z = \mathbf{w}^T \mathbf{x} + b$



Sigmoid/Logistic function





- Logistic regression does not require independence assumptions $x_i \perp \mathbf{x}_{-i}$, like Naïve Bayes
- Example, in spam classification, $X_1 = 1$ ["bank" exists] and $X_2 = 1$ ["account" exists]

If "bank" and "account" always appear together,

Naïve Bayes will count this evidence twice, $p(X_1|Y) = p(X_2|Y)$

Logistic regressive can set either w_1 or w_2 to **zero** to ignore one of it!!



- Discriminative model is powerful, so what is the advantage of generative model?
 - Discriminative models p(Y|X) require all X are observed, fail to work if some inputs are missing!
 - Generative models $p(Y|X) = \frac{p(Y,X)}{p(X)} = \frac{p(Y)p(X|Y)}{p(X)} \propto p(Y)p(X|Y)$ when some input are unobserved, still allow us to compute p(Y|X)e.g., Naive Bayes

| | $x_1 = 0$ | $x_1 = 1$ | $x_2 = 0$ | $x_2 = 1$ | $x_3 = 0$ | $x_3 = 1$ | $x_4 = 0$ | $x_4 = 1$ |
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| y = 0 | 3 | 5 | 5 | 2 | 0 | 8 | 7 | 4 |
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•
$$p(Y = 0) = \frac{3+5+5+2+8+7+4}{(3+5+5+2+8+7+4)+(1+3+10+7+4+2+5)}$$

• $p(x_1 = 0|Y = 0) = \frac{3}{3+5+5+2+8+7+4}$

•
$$p(x_1 = 0|Y = 0) = \frac{3}{3+5+5+2+8+7+4}$$



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Deep Neural Network

• Logistic regression parameterizes the p(Y|X) without independence assumptions

$$p(Y = 1|\mathbf{x}, \mathbf{w}, b) = f(\mathbf{x}, \mathbf{w}, b)$$

but logistic regression is a **linear dependence** (between input and output)

which might be too simple

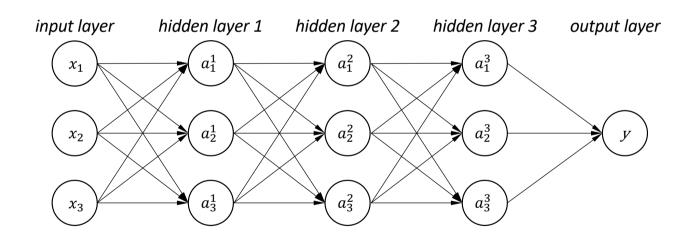
Non-linear dependence is better ...

$$p_{Neural}(Y = 1 | \mathbf{x}, \boldsymbol{\theta}) = f(\mathbf{x}, \boldsymbol{\theta})$$



Deep Neural Network

More parameters and layers, better representation capacity ...



More powerful than logistic regression



Deep Neural Network

Naïve Bayes

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

$$\approx p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

$$\approx p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)$$

Deep Neural Network

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

$$\approx p(x_1)p(x_2|x_1)p_{Neural}(x_3|x_1, x_2)pN_{eural}(x_4|x_1, x_2, x_3)$$

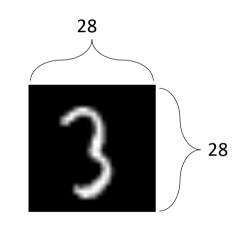


- Problem of High-dimensional Data
- Less Parameters: Conditional Independence
- Less Parameters: Bayesian Network
- Naïve Bayes Classifier
- Discriminative vs. Generative Models
- Logistic Regression
- Deep Neural Networks
- Continuous Variables

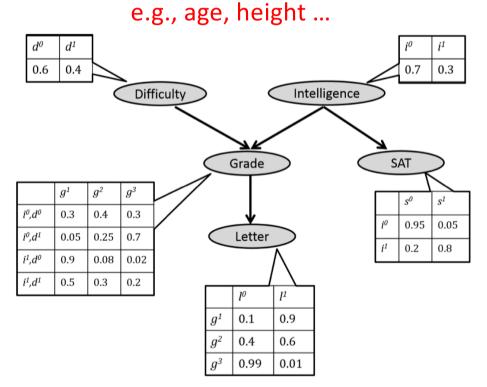


Discrete Variables

The below examples both use discrete variables, but there are many variables are continuous!



784 random binary variables





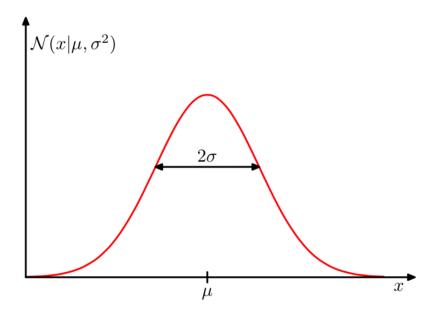
• Represent Continuous Variables

If x is a continuous variable, we can represent it with its **probability density function (PDF)** instead of a **table** anymore ..



• Represent Continuous Variables

Consider x is a random **float-point** variable to represent "age", we can use 1-D Gaussian to parameterized the density.



$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$
$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

 μ : mean

 σ : standard deviation

 σ^2 : variance

$$\beta = \frac{1}{\sigma^2}$$
: precision

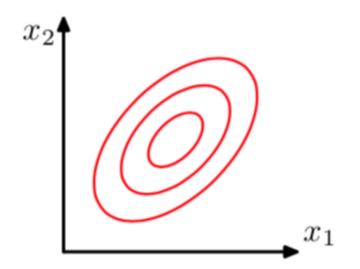


Represent Continuous Variables

Consider x is a random float-point vector to represent "age", "height", "weight" it can be a **joint probability density function**

we can use **D-dimensional Gaussian** to parameterize it

(a.k.a Multivariable Gaussian)



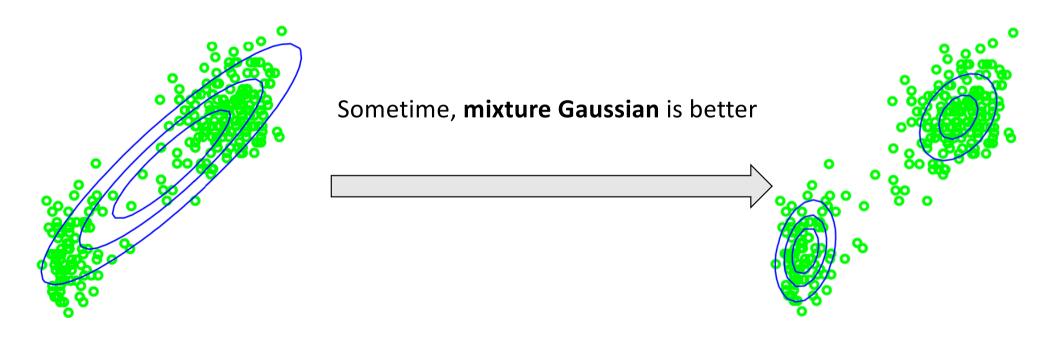
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$

 μ is called the mean, the D × D matrix Σ is called the covariance $|\Sigma|$ denotes the determinant of Σ



• Represent Continuous Variables

Consider x is a random float-point vector to represent "age", "height", "weight"





Data Representation

Problem of High-dimensional Data
 Less Parameters: Conditional Independence
 Less Parameters: Bayesian Network
 Naïve Bayes Classifier
 Discriminative vs. Generative Models
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 Continuous Variables



Thanks