Lecture 16: Naïve Bayes, Generative Model, EM

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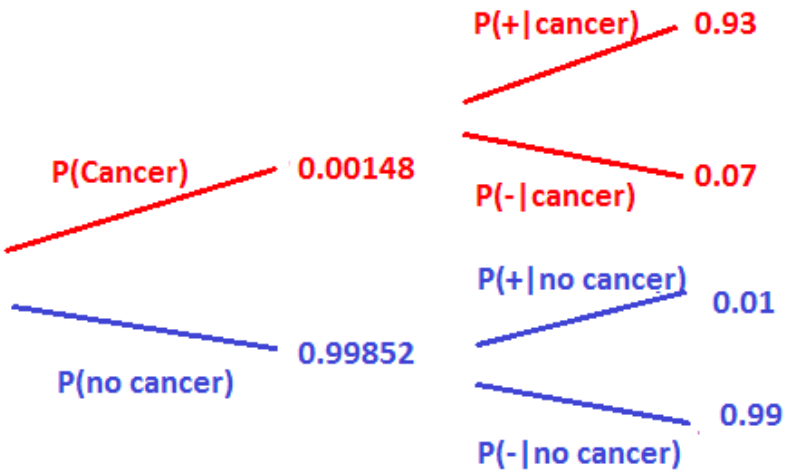
Recap: Bayes Theorem Example

- How likely the patient got cancer if the test is positive?

$$P(\text{CANCER}|+) = \frac{P(cancer\ and +)}{P(cancer\ and +) + P(no\ cancer\ and +)} = 0.12$$



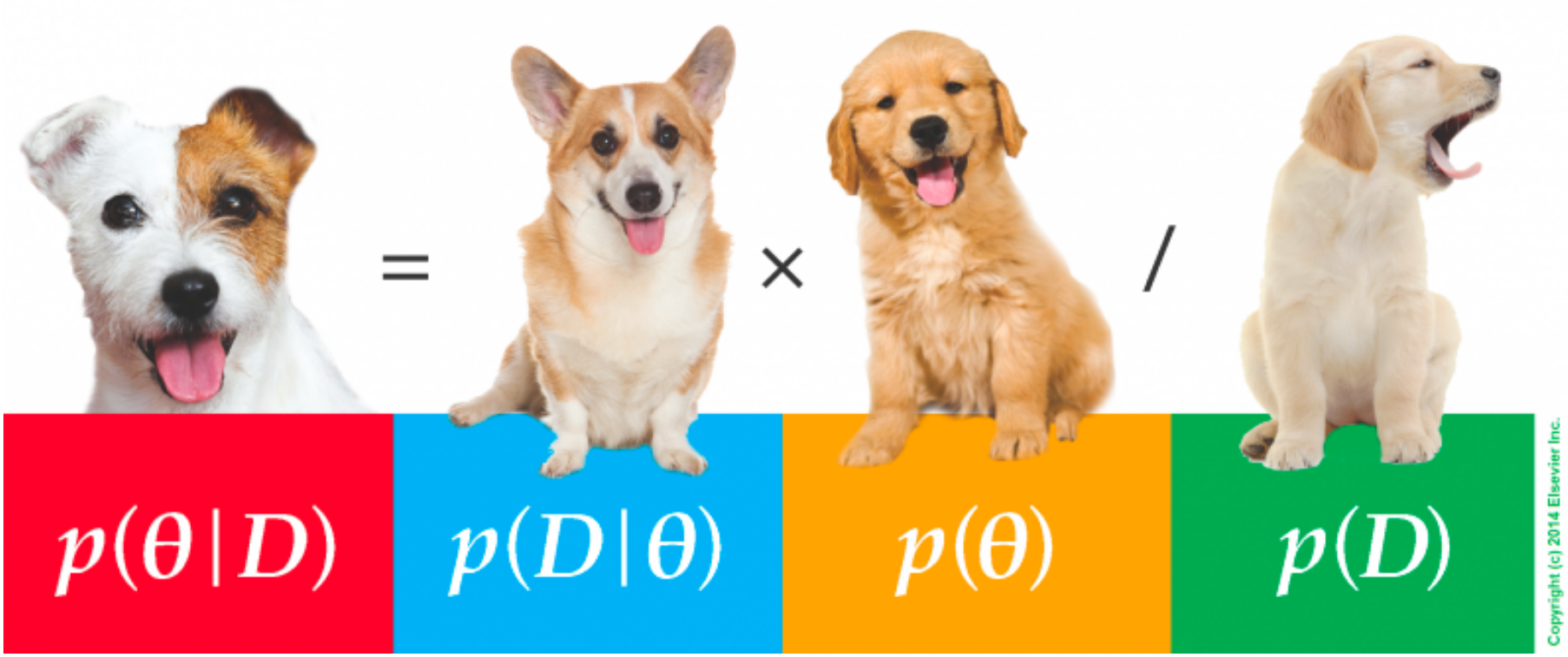
Recap: Bayes Theorem

$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

Short for

$$\forall x, y \quad P(Y = y|X = x) = \frac{P(X = x|Y = y)P(Y = y)}{P(X = x)}$$

Probabilistic models and Bayesian Learning



Probabilistic Learning

Two different notions of probabilistic learning

- Learning probabilistic concepts (P(Y|X))
  - The learned concept is a function c:X→[0,1]
  - c(x) may be interpreted as the probability that the label 1 is assigned to x
  - The learning theory that we have studied before is applicable (with some extensions)

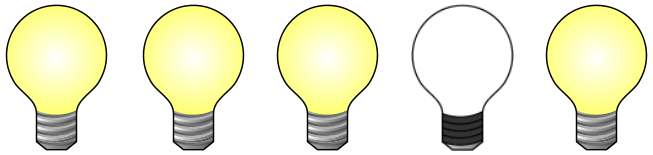
- Bayesian Learning: Use of a probabilistic criterion in selecting a hypothesis (P($\Theta|D$))
  - The hypothesis can be deterministic, a Boolean function
  - The criterion for selecting the hypothesis is probabilistic

Faulty lightbulbs

The experiment:

Try out 100 lightbulbs

80 work, 20 don't



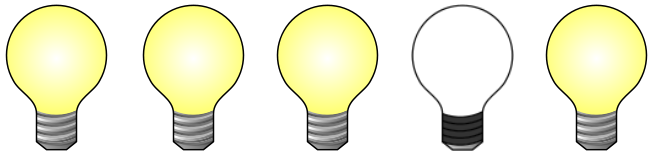
You: The probability is P(failure) = 0.2

CEO: But how do you know?

You: Because…

Bernoulli trials

- P(failure) = p, P(success) = 1 – p



- Each trial is i.i.d
  - Independent and identically distributed

MAP v.s. MLE

- MLE:

$$\underset{p}{\operatorname{argmax}}\, a \log p + b \log(1-p)$$

$$\Rightarrow p_{best} = \frac{a}{a+b}$$

- MAP

$$\underset{p}{\operatorname{argmax}}\ (a+\alpha-1)\log p + (b+\beta-1)\log(1-p)$$

$$\Rightarrow p_{best} = \frac{a+\alpha-1}{a+b+\alpha+\beta-2}$$

Today's lecture

- Naïve Bayes
- Generative Models
- EM

MAP prediction

Don't confuse with *MAP learning*: finds hypothesis by

$$h_{MAP} = \arg\max_{h \in H} P(D|h)P(h)$$

Let's be use the Bayes rule for predicting y given an input $\mathbf{x}$

$$P(Y = y|X = \mathbf{x}) = \frac{P(X = \mathbf{x}|Y = y)P(Y = y)}{P(X = \mathbf{x})}$$

Predict y for the input $\mathbf{x}$ using

$$\arg\max_{y} P(X = \mathbf{x}|Y = y)P(Y = y)$$

MAP prediction

Predict y for the input $\mathbf{x}$ using

$$\arg\max_{y} P(X = \mathbf{x}|Y = y)P(Y = y)$$

Likelihood of observing this input $\mathbf{x}$ when the label is y

Prior probability of the label being y

All we need are these two sets of probabilities

Example: Tennis

Prior

Play tennis	P(Play tennis)
Yes	0.3
No	0.7

Without any other information, what is the prior probability that I should play tennis?

Example: Tennis

Prior

Play tennis	P(Play tennis)
Yes	0.3
No	0.7

Without any other information, what is the prior probability that I should play tennis?

Likelihood

Temperature	Wind	P(T, W |Tennis = Yes)
Hot	Strong	0.15
Hot	Weak	0.4
Cold	Strong	0.1
Cold	Weak	0.35

On days that I do play tennis, what is the probability that the temperature is T and the wind is W?

Temperature	Wind	P(T, W |Tennis = No)
Hot	Strong	0.4
Hot	Weak	0.1
Cold	Strong	0.3
Cold	Weak	0.2

On days that I don't play tennis, what is the probability that the temperature is T and the wind is W?

Example: Tennis again

Input:
Temperature = Hot (H)
Wind = Weak (W)

Should I play tennis?

Prior

Play tennis	P(Play tennis)
Yes	0.3
No	0.7

Likelihood

Temperature	Wind	P(T, W |Tennis = Yes)
Hot	Strong	0.15
Hot	Weak	0.4
Cold	Strong	0.1
Cold	Weak	0.35

Temperature	Wind	P(T, W |Tennis = No)
Hot	Strong	0.4
Hot	Weak	0.1
Cold	Strong	0.3
Cold	Weak	0.2

Example: Tennis again

Input:
Temperature = Hot (H)
Wind = Weak (W)

Should I play tennis?

Prior

Play tennis	P(Play tennis)
Yes	0.3
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Likelihood

Temperature	Wind	P(T, W |Tennis = Yes)
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Temperature	Wind	P(T, W |Tennis = No)
Hot	Strong	0.4
Hot	Weak	0.1
Cold	Strong	0.3
Cold	Weak	0.2

argmax_y P(H, W | play?) P (play?)

Example: Tennis again

Prior

Play tennis	P(Play tennis)
Yes	0.3
No	0.7

Likelihood

Temperature	Wind	P(T, W |Tennis = Yes)
Hot	Strong	0.15
Hot	Weak	0.4
Cold	Strong	0.1
Cold	Weak	0.35

Temperature	Wind	P(T, W |Tennis = No)
Hot	Strong	0.4
Hot	Weak	0.1
Cold	Strong	0.3
Cold	Weak	0.2

Input:
Temperature = Hot (H)
Wind = Weak (W)

Should I play tennis?

argmax_y P(H, W | play?) P (play?)

P(H, W | Yes) P(Yes) = 0.4 £ 0.3
= 0.12

P(H, W | No) P(No) = 0.1 £ 0.7
= 0.07

MAP prediction = Yes

How hard is it to learn probabilistic models?

Prior P(Y)

- If there are k labels, then k – 1 parameters (why not k?)

Likelihood P(**X** | Y)

- If there are d Boolean features:
  - We need a value for each possible $P(x_1, x_2, \cdots, x_d \mid y)$ for each y
  - $k(2^d - 1)$ parameters

Need a lot of data to estimate these many numbers!

High model complexity

If there is very limited data, high variance in the parameters

How can we deal with this?

Answer: Make independence assumptions

Recall: Conditional independence

Suppose X, Y and Z are random variables

X is *conditionally independent* of Y given Z if the probability distribution of X is independent of the value of Y when Z is observed

$$P(X|Y,Z) = P(X|Z)$$

Or equivalently

$$P(X,Y|Z) = P(X|Z)P(Y|Z)$$

Modeling the features

$P(x_1, x_2, \cdots, x_d|y)$ required k(2^d – 1) parameters

What if all the features were conditionally independent given the label?

The Naïve Bayes Assumption

Modeling the features

$P(x_1, x_2, \cdots, x_d|y)$ required k(2^d – 1) parameters

What if all the features were conditionally independent given the label?

The Naïve Bayes Assumption

That is,

$$P(x_1, x_2, \cdots, x_d|y) = P(x_1|y)P(x_2|y)\cdots P(x_d|y)$$

Requires only d numbers for each label. kd parameters overall. Not bad!

The Naïve Bayes Classifier

Assumption: Features are conditionally independent given the label Y

To predict, we need two sets of probabilities

- Prior P(y)
- For each x_j, we have the likelihood $P(x_j \mid y)$

The Naïve Bayes Classifier

Assumption: Features are conditionally independent given the label Y

To predict, we need two sets of probabilities

- Prior P(y)
- For each x_j, we have the likelihood $P(x_j \mid y)$

Decision rule

$$h_{NB}(\boldsymbol{x}) = \underset{y}{\operatorname{argmax}}\, P(y)P(x_1, x_2, \cdots, x_d|y)$$

The Naïve Bayes Classifier

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Decision rule

$$h_{NB}(\boldsymbol{x}) = \underset{y}{\operatorname{argmax}} P(y)P(x_1, x_2, \cdots, x_d|y)$$

$$= \underset{y}{\operatorname{argmax}} P(y) \prod_j P(x_j|y)$$

Decision boundaries of naïve Bayes

What is the decision boundary of the naïve Bayes classifier?

Consider the two class case. We predict the label to be + if

$$P(y=+)\prod_j P(x_j|y=+) > P(y=-)\prod_j P(x_j|y=-)$$

Decision boundaries of naïve Bayes

What is the decision boundary of the naïve Bayes classifier?

Consider the two class case. We predict the label to be + if

$$P(y=+)\prod_j P(x_j|y=+) > P(y=-)\prod_j P(x_j|y=-)$$

$$\frac{P(y=+)\prod_j P(x_j|y=+)}{P(y=-)\prod_j P(x_j|y=-)} > 1$$

Decision boundaries of naïve Bayes

What is the decision boundary of the naïve Bayes classifier?

Taking log and simplifying, we can show that the decision boundary of naïve Bayes is a linear function

$$\log \frac{P(y = -|\boldsymbol{x})}{P(y = +|\boldsymbol{x})}$$

This is a linear function of the feature space!

Today's lecture

- The naïve Bayes Classifier
- Learning the naïve Bayes Classifier
- Generative model

Let’s learn a naïve Bayes classifier

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

Let’s learn a naïve Bayes classifier

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6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

P(Play = +) = 9/14 P(Play = -) = 5/14

Let's learn a naïve Bayes classifier

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
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6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

P(Play = +) = 9/14 P(Play = -) = 5/14

P(**O** = S | Play = +) = 2/9

Let's learn a naïve Bayes classifier

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
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13	O	H	N	W	+
14	R	M	H	S	-

P(Play = +) = 9/14 P(Play = -) = 5/14

P(**O** = S | Play = +) = 2/9

P(**O** = R | Play = +) = 3/9

Let's learn a naïve Bayes classifier

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

P(Play = +) = 9/14 P(Play = -) = 5/14

P(**O** = S | Play = +) = 2/9

P(**O** = R | Play = +) = 3/9

P(**O** = O | Play = +) = 4/9

And so on, for other attributes and also for Play = -

Learning the naïve Bayes Classifier

- What is the hypothesis function *h* defined by?
  - A collection of probabilities

hypothesis?

Learning the naïve Bayes Classifier

- What is the hypothesis function *h* defined by?
  - A collection of probabilities
    - Prior for each label: $P(y)$
    - Likelihoods for feature x_j given a label: $P(x_j | y)$

hypothesis?

Learning the naïve Bayes Classifier

- What is the hypothesis function *h* defined by?
  - A collection of probabilities
    - Prior for each label: $P(y)$
    - Likelihoods for feature x_j given a label: $P(x_j | y)$

Suppose we have a data set $D = \{(\boldsymbol{x}_i, y_i)\}$ with m examples

A note on convention for this section:

- Examples in the dataset are indexed by the subscript i (e.g. $\boldsymbol{x}_i$)
- Features within an example are indexed by the subscript j
  - The j^{th} feature of the i^{th} example will be x_{ij}

Learning the naïve Bayes Classifier

- What is the hypothesis function *h* defined by?
  - A collection of probabilities
    - Prior for each label: $P(y)$
    - Likelihoods for feature x_j given a label: $P(x_j | y)$

If we have a data set $D = \{(\boldsymbol{x}_i, y_i)\}$ with m examples

And we want to learn the classifier in a probabilistic way

- What is a probabilistic criterion to select the hypothesis?

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_{h \in H} P(D|h)$$

Here h is defined by all the probabilities used to construct the naïve Bayes decision

Maximum likelihood estimation

Given a dataset $D = \{(\boldsymbol{x}_i, y_i)\}$ with m examples

$$h_{ML} = \arg\max_{h \in H} P(D|h)$$

$$h_{ML} = \arg\max_{h} \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h)$$

Each example in the dataset is independent and identically distributed

So we can represent P(D| h) as this product

Maximum likelihood estimation

Given a dataset $D = \{(\boldsymbol{x}_i, y_i)\}$ with m examples

$$h_{ML} = \arg\max_h \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h)$$

Each example in the dataset is independent and identically distributed

So we can represent $\mathrm{P(D|\ h)}$ as this product

Asks "What probability would this particular h assign to the pair $(\mathbf{x}_\mathrm{i}, \mathrm{y}_\mathrm{i})$?"

Maximum likelihood estimation

Given a dataset D = $\{(x_i, y_i)\}$ with m examples

$$
\begin{aligned}
h_{ML} &= \arg\max_h \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h) \\
&= \arg\max_h \prod_{i=1}^{m} P(\mathbf{x}_i|y_i, h) P(y_i|h)
\end{aligned}
$$

Maximum likelihood estimation

Given a dataset D = $\{(x_i, y_i)\}$ with m examples

$$h_{ML} = \arg\max_h \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h)$$

$$= \arg\max_h \prod_{i=1}^{m} P(\mathbf{x}_i|y_i, h) P(y_i|h)$$

$$= \arg\max_h \prod_{i=1}^{m} P(y_i|h) \prod_j P(x_{i,j}|y_i, h)$$

$\mathbf{x}_{ij}$ is the j^{th} feature of $\mathbf{x}_i$

The Naïve Bayes assumption

Maximum likelihood estimation

Given a dataset D = $\{(x_i, y_i)\}$ with m examples

$$
\begin{aligned}
h_{ML} &= \arg\max_h \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h) \\
&= \arg\max_h \prod_{i=1}^{m} P(\mathbf{x}_i|y_i, h) P(y_i|h) \\
&= \arg\max_h \prod_{i=1}^{m} P(y_i|h) \prod_j P(x_{i,j}|y_i, h)
\end{aligned}
$$

How do we proceed?

Maximum likelihood estimation

Given a dataset D = $\{(x_i, y_i)\}$ with m examples

$$
\begin{aligned}
h_{ML} &= \arg\max_h \prod_{i=1}^{m} P((\mathbf{x}_i, y_i)|h) \\
&= \arg\max_h \prod_{i=1}^{m} P(\mathbf{x}_i|y_i, h) P(y_i|h) \\
&= \arg\max_h \prod_{i=1}^{m} P(y_i|h) \prod_j P(x_{i,j}|y_i, h) \\
&= \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)
\end{aligned}
$$

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

What next?

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

For simplicity, suppose there are two labels 1 and 0 and all features are binary

- **Prior**: P(y = 1) = p and P (y = 0) = 1 – p

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

For simplicity, suppose there are two labels 1 and 0 and all features are binary

- **Prior**: P(y = 1) = p and P (y = 0) = 1 – p
- **Likelihood** for each feature given a label
  - $P(x_j = 1 \mid y = 1) = a_j$ and $P(x_j = 0 \mid y = 1) = 1 - a_j$

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

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  - $P(x_j = 1 \mid y = 1) = a_j$ and $P(x_j = 0 \mid y = 1) = 1 - a_j$
  - $P(x_j = 1 \mid y = 0) = b_j$ and $P(x_j = 0 \mid y = 0) = 1 - b_j$

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

- Prior: P(y = 1) = p and P (y = 0) = 1 – p

$$P(y_i|h) = p^{[y_i=1]}(1-p)^{[y_i=0]}$$

[z] is called the indicator function or the Iverson bracket

Its value is 1 if the argument z is true and zero otherwise

Learning the naïve Bayes Classifier

Maximum likelihood estimation

$$h_{ML} = \arg\max_h \sum_{i=1}^{m} \log P(y_i|h) + \sum_i \sum_j \log P(x_{i,j}|y_i, h)$$

Likelihood for each feature given a label

- $P(x_j = 1 \mid y = 1) = a_j$ and $P(x_j = 0 \mid y = 1) = 1 - a_j$
- $P(x_j = 1 \mid y = 0) = b_j$ and $P(x_j = 0 \mid y = 0) = 1 - b_j$

$$P(x_{ij}|y_i, h) = a_j^{[y_i=1, x_{ij}=1]} \times (1 - a_j)^{[y_i=1, x_{ij}=0]} \times b_j^{[y_i=0, x_{ij}=1]} \times (1 - b_j)^{[y_i=0, x_{ij}=0]}$$

Learning the naïve Bayes Classifier

Substituting and deriving the argmax, we get

$$p = \frac{\text{Count}\,(y_i = 1)}{\text{Count}\,(y_i = 1) + \text{Count}\,(y_i = 0)}$$

← P(y = 1) = p

Learning the naïve Bayes Classifier

Substituting and deriving the argmax, we get

$$p = \frac{\text{Count}\,(y_i = 1)}{\text{Count}\,(y_i = 1) + \text{Count}\,(y_i = 0)}$$

← P(y = 1) = p

$$a_j = \frac{\text{Count}\,(y_i = 1, x_{ij} = 1)}{\text{Count}\,(y_i = 1)}$$

← $P(x_j = 1 \mid y = 1) = a_j$

Learning the naïve Bayes Classifier

Substituting and deriving the argmax, we get

$$p = \frac{\text{Count}\,(y_i = 1)}{\text{Count}\,(y_i = 1) + \text{Count}\,(y_i = 0)}$$

← P(y = 1) = p

$$a_j = \frac{\text{Count}\,(y_i = 1, x_{ij} = 1)}{\text{Count}\,(y_i = 1)}$$

← $P(x_j = 1 \mid y = 1) = a_j$

$$b_j = \frac{\text{Count}\,(y_i = 0, x_{ij} = 1)}{\text{Count}\,(y_i = 0)}$$

← $P(x_j = 1 \mid y = 0) = b_j$

Naïve Bayes: Learning and Prediction

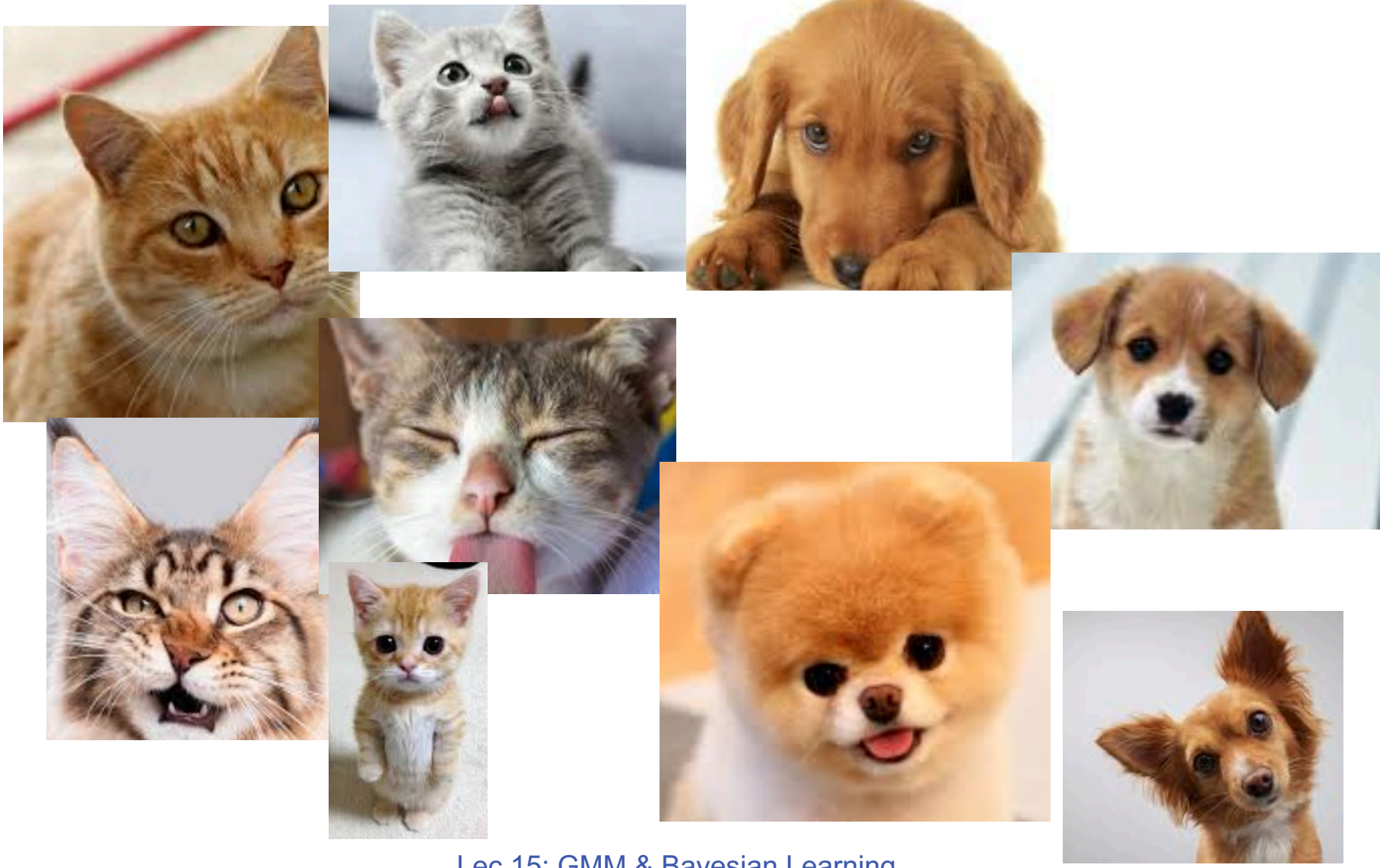
- Learning
  - Count how often features occur with each label. Normalize to get likelihoods
  - Priors from fraction of examples with each label
  - Generalizes to multiclass

- Prediction
  - Use learned probabilities to find highest scoring label

Today's lecture

- The naïve Bayes Classifier
- Learning the naïve Bayes Classifier
- Generative model

How to classify cat and dog?



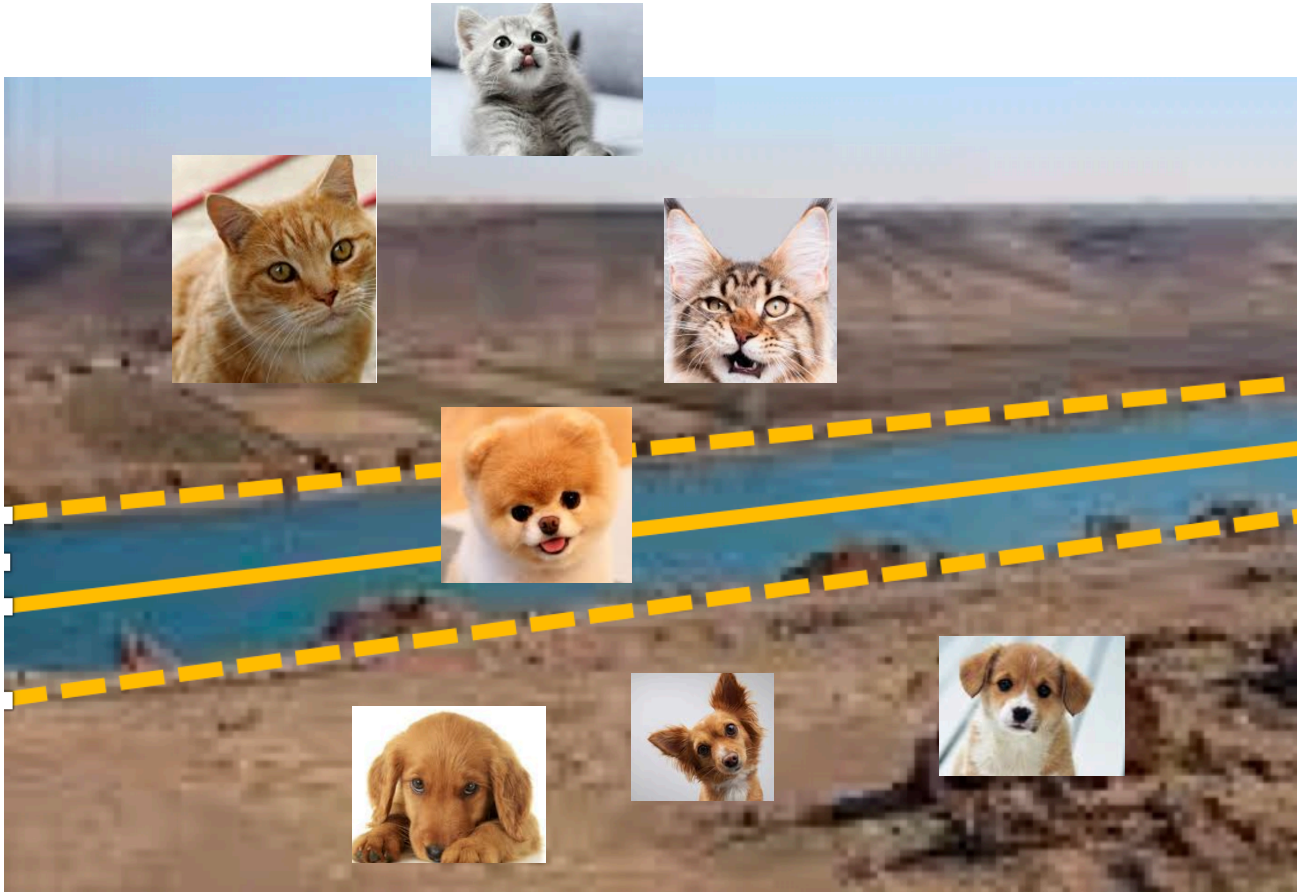
Discriminative models

Goal: learn directly how to make predictions

- Look at many (positive/negative) examples
- Discover regularities in the data
- Use these to construct a prediction policy
- Assumptions come in the form of the hypothesis class

Bottom line: approximating $h : X \rightarrow Y$ is estimating $P(Y|X)$

Discriminative model



margin (upper)

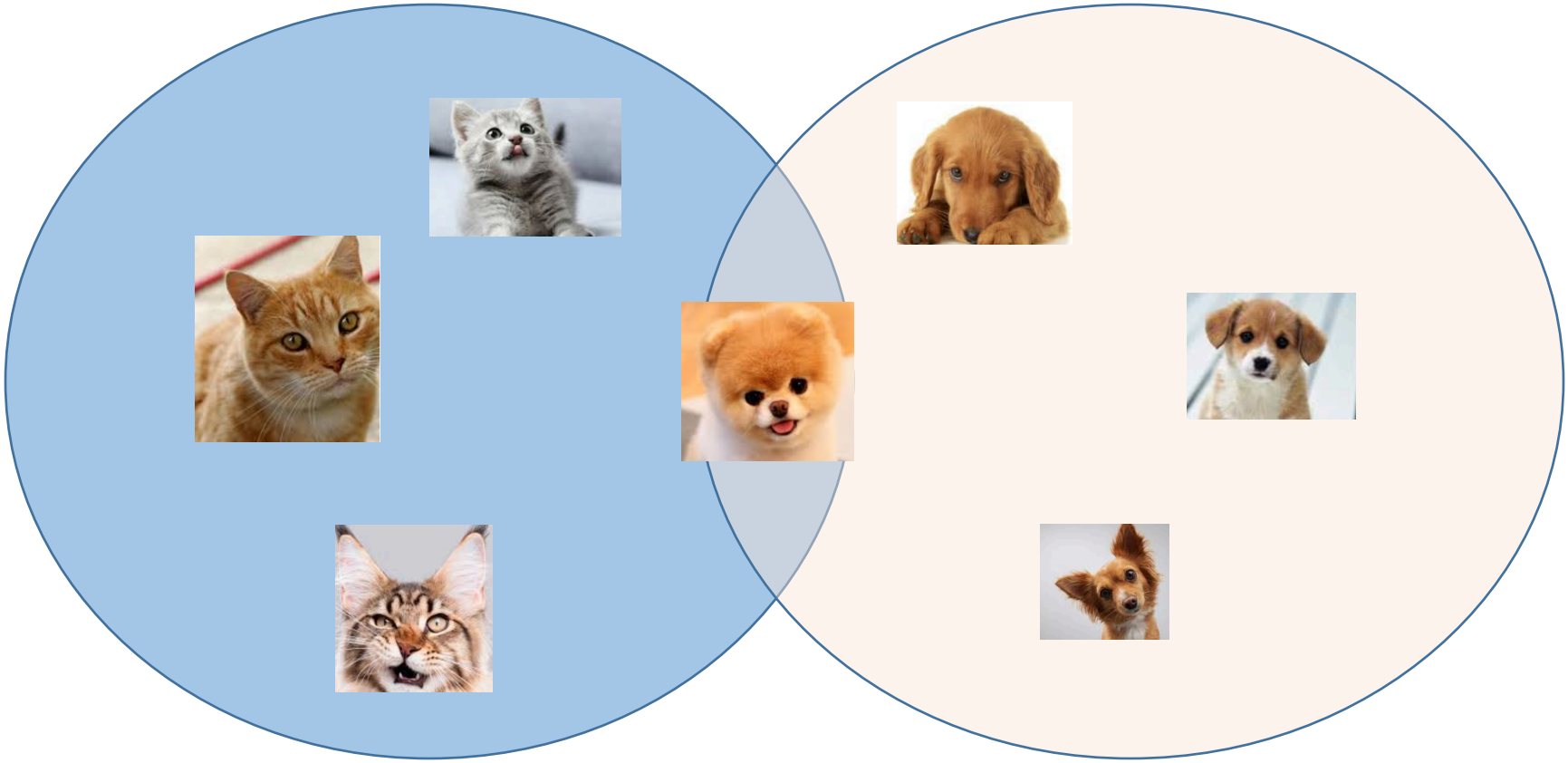
Decision boundary

margin (lower)

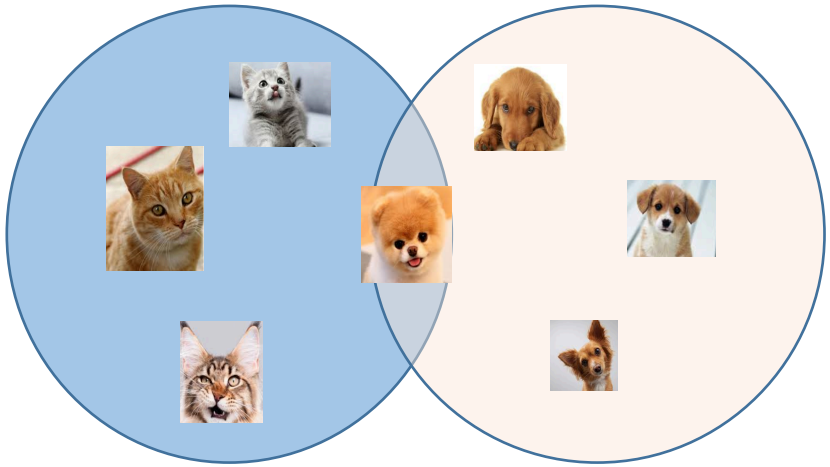
Generative models

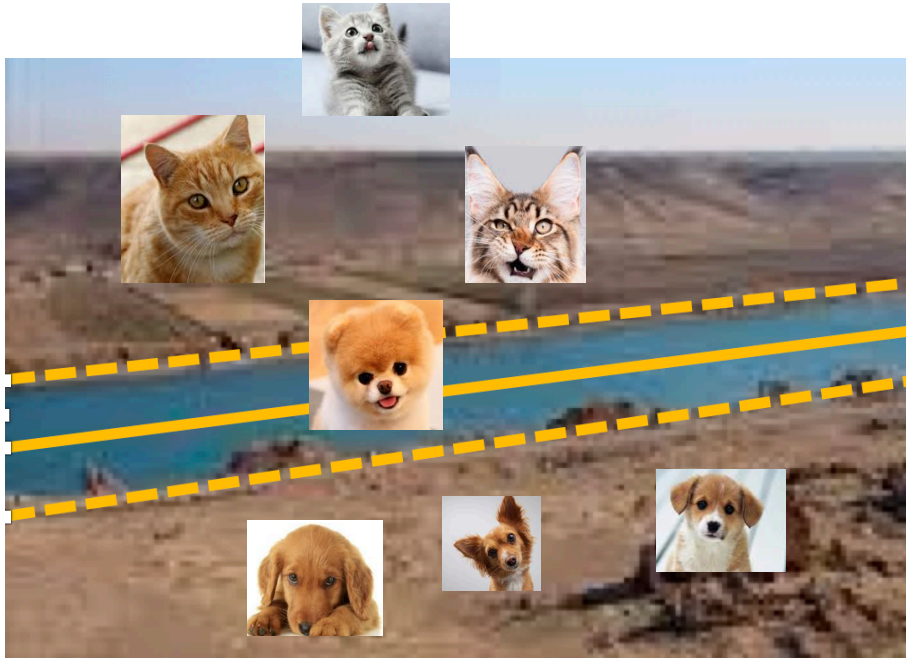
- Explicitly model how instances in each category are generated
- That is, learn P(X | Y) and P(Y)
- We did this for naïve Bayes
  - Naïve Bayes is a generative model
- Predict P(Y | X) using the Bayes rule

Generative model



Generative Model v.s. Discriminative model

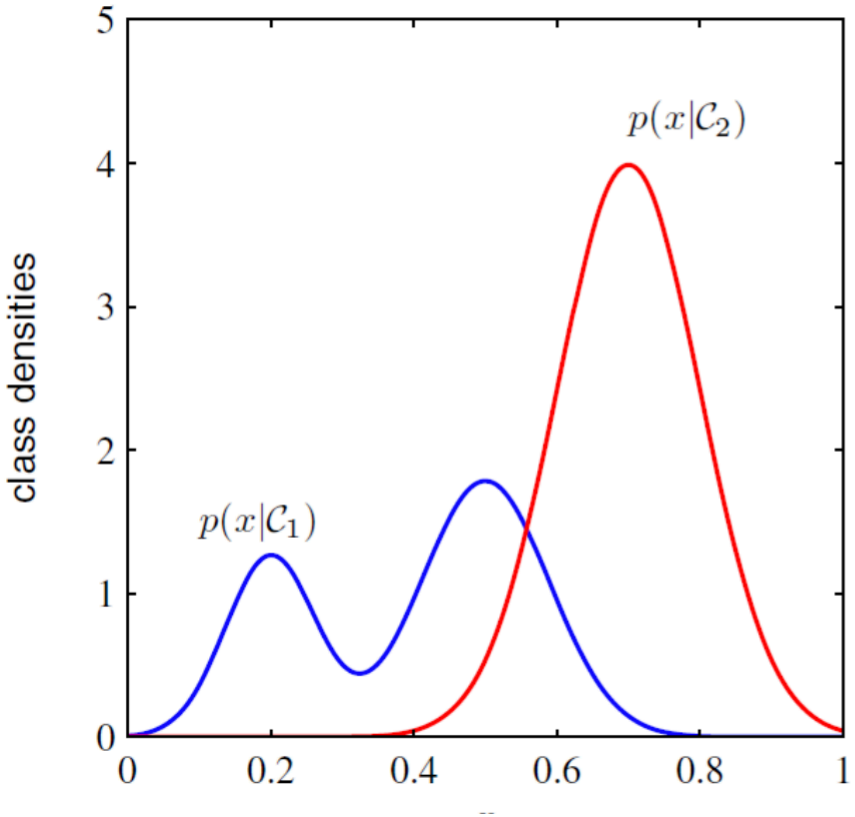




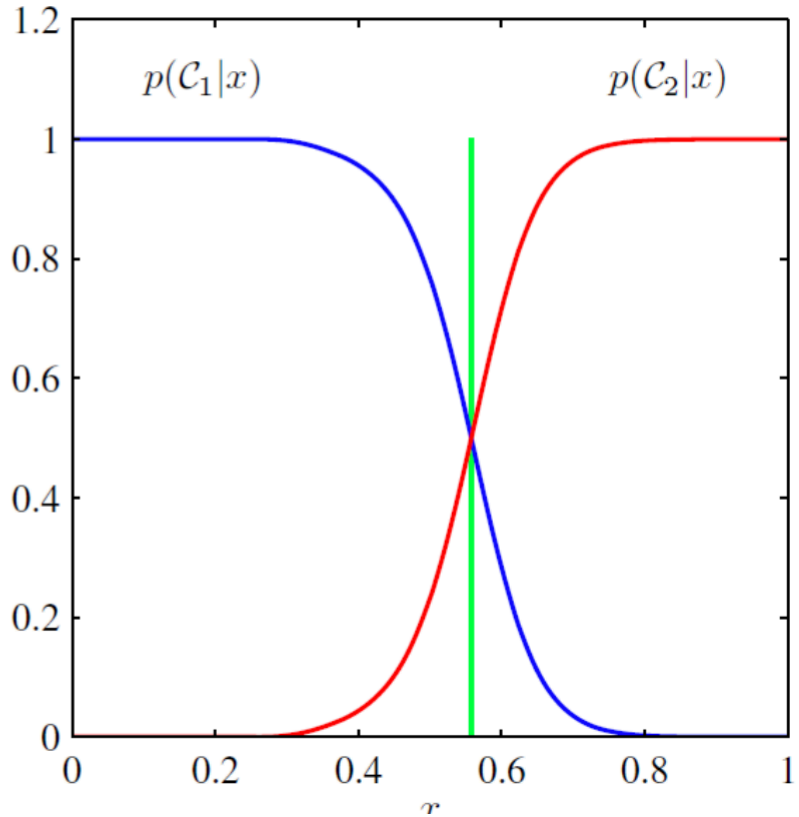
Learn $P(X, Y \mid \Theta)$ or
Learn $P(X \mid Y, \Theta)$ and $P(Y \mid \Theta)$

Learn $P(Y \mid X, \Theta)$

Generative Model's view

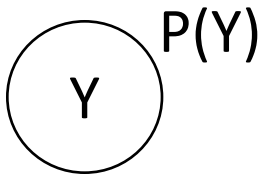


Discriminative Model's view

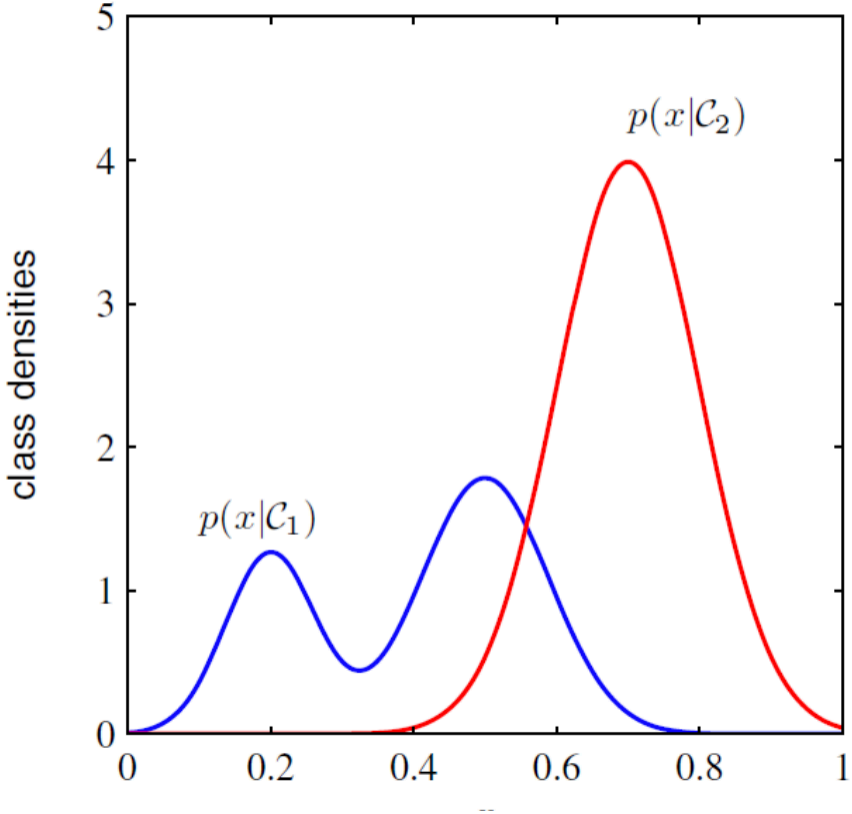


Example: Generative story of naïve Bayes

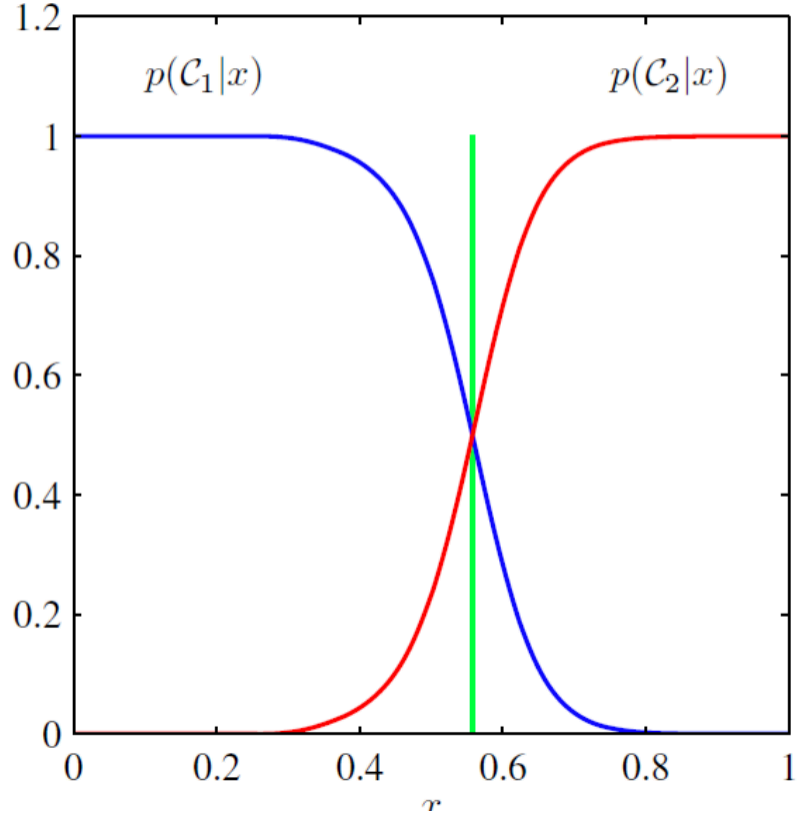
First sample a label



Generative Model's view



Discriminative Model's view

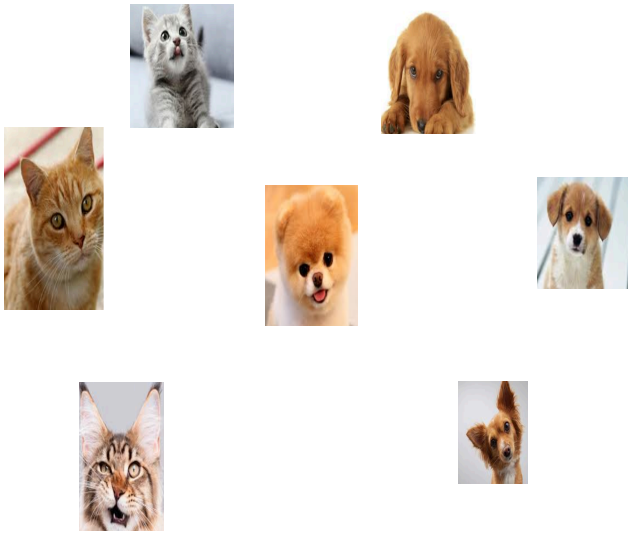


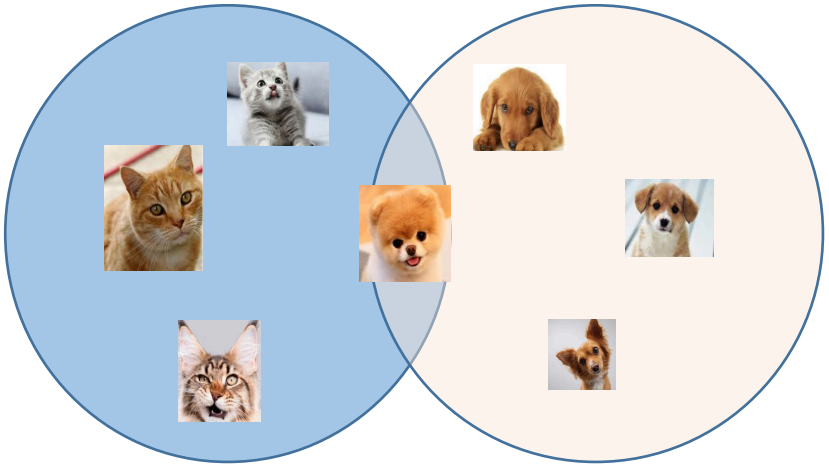
Today's lecture

- The naïve Bayes Classifier
- Learning the naïve Bayes Classifier
- EM

How about unsupervised learning

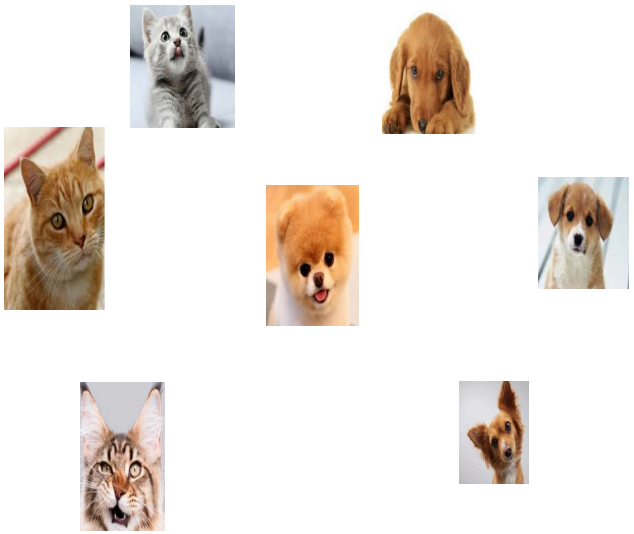
- In unsupervised learning, we only observed input distribution $\tilde{P}(X)$

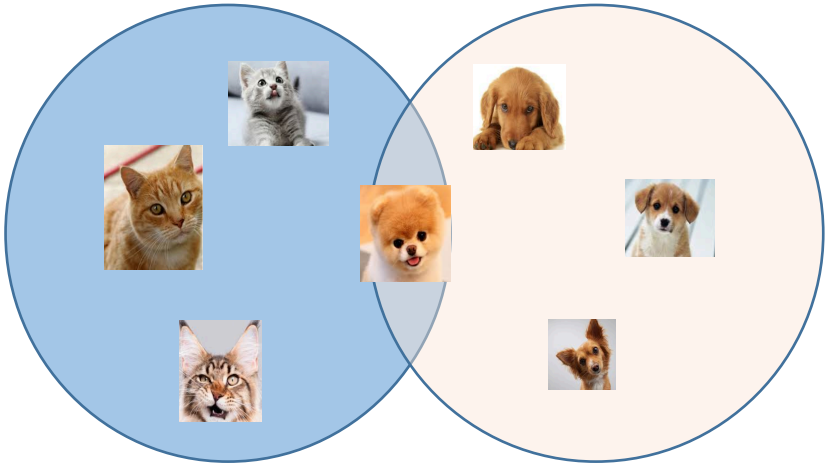




MLE in unsupervised learning

- We only have observation of $\tilde{P}(X)$
- In generative model, we have $P(X, Y \mid \Theta)$
- In discriminative model, we have $P(Y \mid \Theta, X)$
- Which model is more suitable for unsupervised learning?





MLE in unsupervised learning

- We only have observation of $\tilde{P}(X)$
- In generative model, we have $P(X, Y \mid \Theta)$
- We know $P(X \mid \Theta) = \sum_Y P(X, Y \mid \Theta)$
- Therefore, MLE is
  $\text{argmax}_\Theta P(X \mid \Theta) =$
  $\text{argmax}_\Theta \sum_Y P(X, Y \mid \Theta)$

EM algorithm

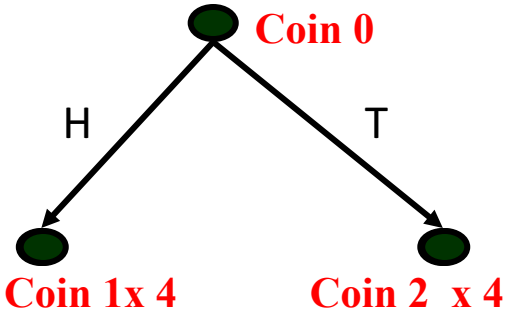
- EM algorithm solves $\text{argmax}_\Theta \sum_Y P(X, Y \mid \Theta)$ by iteratively updating Θ
- In general, known to converge to a local maximum of the maximum likelihood function

Three Coins Example

- We observe a series of coin tosses generated in the following way:
- A person has three coins.
  - Coin 0: probability of Head is α
  - Coin 1: probability of Head p
  - Coin 2: probability of Head q

- Consider the following coin-tossing scenarios:

Scenario I



- Toss coin 0.
  If Head – toss coin 1; o/w – toss coin 2

Observing the sequence
HHHHT, THTHT, HHHHT, HHTTH

produced by Coin 0 , Coin1 and Coin2

Question: Estimate most likely values for p, q (the probability of H in each coin) and the probability to use each of the coins (a)

Scenario I

Supervised Learning

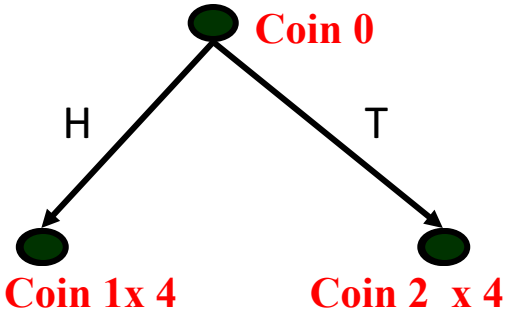
- Toss coin 0.
  If Head – toss coin 1; o/w – toss coin 2

  Observing the sequence
  HHHHT, THTHT, HHHHT, HHTTH

  produced by Coin 0 , Coin1 and Coin2

  Question: Estimate most likely values for p, q (the probability of H in each coin) and the probability to use each of the coins (a)

Scenario II



- Toss coin 0.
  If Head – toss coin 1; o/w – toss coin 2

Observing the sequence
HHHT, HTHT, HHHT, HTTH

produced by ~~Coin 0~~, Coin1 and/or Coin2

Question: Estimate most likely values for p, q (the probability of H in each coin) and the probability to use each of the coins (a)

Intuition of EM algorithm

- Use an iterative approach for estimating the parameters:
  - Guess the probability that a given data point came from Coin 1 or 2; Generate fictional labels, weighted according to this probability.
  - Now, compute the most likely value of the parameters. [recall the scenario I]
  - Compute the likelihood of the data given this model.
  - Re-estimate the initial parameter setting: set them to maximize the likelihood of the data.

Step 1: initialization

Coin 0: probability of Head is α
Coin 1: probability of Head p
Coin 2: probability of Head q

- Guess the probability that a given data point came from Coin 1 or 2; Generate fictional labels, weighted according to this probability.

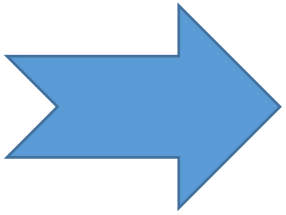
	coin 1=H	coin 1=T
HHHT	100%	0 %
HTHT	100%	0%
HHHT	100%	0%
HTTH	0%	100%

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α
Coin 1: probability of Head p
Coin 2: probability of Head q

- Now, compute the most likely value of the parameters. [recall the scenario I]

	coin 1=H	coin 1=T
HHHT	100%	0 %
HTHT	100%	0%
HHHT	100%	0%
HTTH	0%	100%



HHHHT
HHTHT
HHHHT
THTTH

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α
Coin 1: probability of Head p
Coin 2: probability of Head q

- Now, compute the most likely value of the parameters. [recall the scenario I]

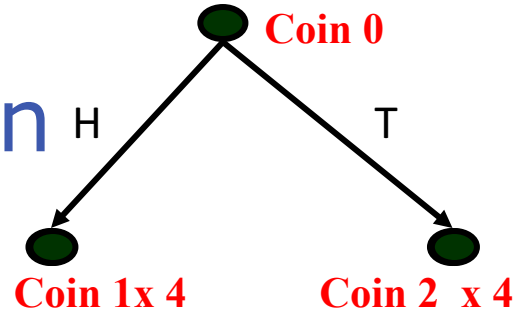
HHHHT
HHTHT
HHHHT
THTTH

$$\alpha_1 = \frac{3}{3+1} = \frac{3}{4}$$

$$p_1 = \frac{8}{8+4} = \frac{2}{3}$$

$$q_1 = \frac{2}{2+2} = \frac{1}{2}$$

Step3: Likelihood Estimation



- Compute the likelihood of the data given this model

$\alpha_1 p_1^{\#H}(1-p_1)^{\#T}$ $\quad$ $(1-\alpha_1)q_1^{\#H}(1-q_1)^{\#T}$

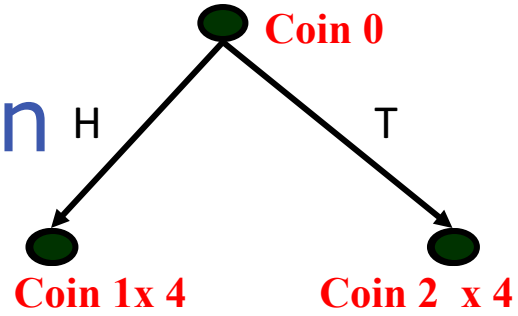
	coin 1=H	coin 1=T
HHHT	$\frac{3}{4}\left(\frac{2}{3}\right)^3\frac{1}{3}$	$\frac{1}{4}\left(\frac{1}{2}\right)^3\frac{1}{2}$
HTHT	$\frac{3}{4}\left(\frac{2}{3}\right)^2\left(\frac{1}{3}\right)^2$	$\frac{1}{4}\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2$
HHHT	$\frac{3}{4}\left(\frac{2}{3}\right)^3\frac{1}{3}$	$\frac{1}{4}\left(\frac{1}{2}\right)^3\frac{1}{2}$
HTTH	$\frac{3}{4}\left(\frac{2}{3}\right)^2\left(\frac{1}{3}\right)^2$	$\frac{1}{4}\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2$

$$\alpha_1 = \frac{3}{4}$$

$$p_1 = \frac{2}{3}$$

$$q_1 = \frac{1}{2}$$

Step3: Likelihood Estimation



- Compute the likelihood of the data given this model

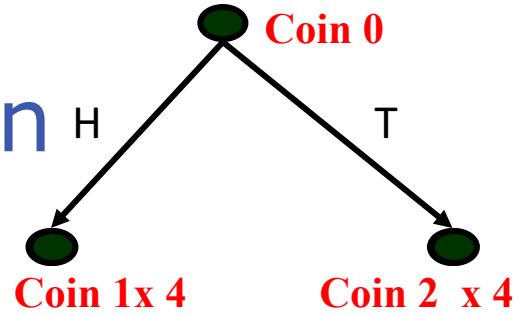
	$\alpha_1 p_1^{\#H}(1-p_1)^{\#T}$ coin 1=H	$(1-\alpha_1)q_1^{\#H}(1-q_1)^{\#T}$ coin 1=T
HHHT	0.074	0.0156
HTHT	0.037	0.0156
HHHT	0.074	0.0156
HTTH	0.037	0.0156

$$\alpha_1 = \frac{3}{4}$$

$$p_1 = \frac{2}{3}$$

$$q_1 = \frac{1}{2}$$

Step3: Likelihood Estimation



- Compute the likelihood of the data given this model

$\alpha_1 p_1^{\#H}(1-p_1)^{\#T}$ $(1-\alpha_1) q_1^{\#H}(1-q_1)^{\#T}$

	coin 1=H	coin 1=T
HHHT	82.6%	17.4%
HTHT		29.7%
HHHT	82.6%	17.4%
HTTH	*70.3%*	29.7%

$$\alpha_1 = \frac{3}{4}$$

$$p_1 = \frac{2}{3}$$

$$q_1 = \frac{1}{2}$$

e.g., $\frac{0.074}{0.074+0.0156} = 82.6\%$

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α
Coin 1: probability of Head p
Coin 2: probability of Head q

- Now, compute the most likely value of the parameters. [recall the scenario I]

	coin 1=H	coin 1=T
HHHT	82.6%	17.4%
HTHT		29.7%
HHHT	82.6%	17.4%
HTTH	*70.3%*	29.7%

HHHHT 82.6%
THHHT 17.4%
HHTHT 70.3%
THTHT 29.7%
HHHHT 82.6%
THHHT 17.4%
HHTTH 70.3%
THTTH 29.7%

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α
Coin 1: probability of Head p
Coin 2: probability of Head q

- Now, compute the most likely value of the parameters. [recall the scenario I]

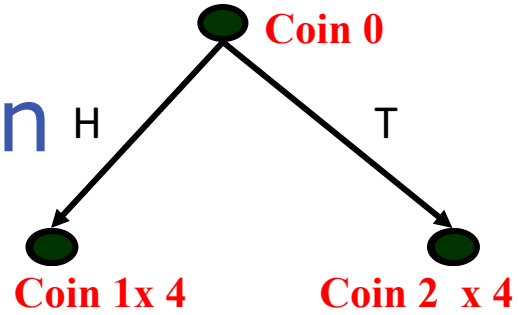
HHHHT 82.6%
HHTHT 70.3%
HHHHT 82.6%
HHTTH 70.3%
THHHT 17.4%
THTHT 29.7%
THHHT 17.4%
THTTH 29.7%

$$\alpha_2 = \frac{82.6\times 2 + 70.3\times 2}{400} = 76.5\%$$

$$p_2 = \frac{82.6\times 6 + 70.3\times 4}{82.6\times 8 + 70.3\times 8} = 63.5\%$$

$$q_2 = \frac{17.4\times 6 + 29.7\times 4}{17.4\times 8 + 29.7\times 8} = 59.2\%$$

Step3: Likelihood Estimation



- Compute the likelihood of the data given this model

$\alpha_2 p_2^{\#H}(1-p_2)^{\#T}$ coin 1=H

$(1-\alpha_2)q_2^{\#H}(1-q_2)^{\#T}$ coin 1=T

HHHT
HTHT
HHHT
HTTH

$$\alpha_2 = 76.5\%$$

$$p_2 = 63.5\%$$

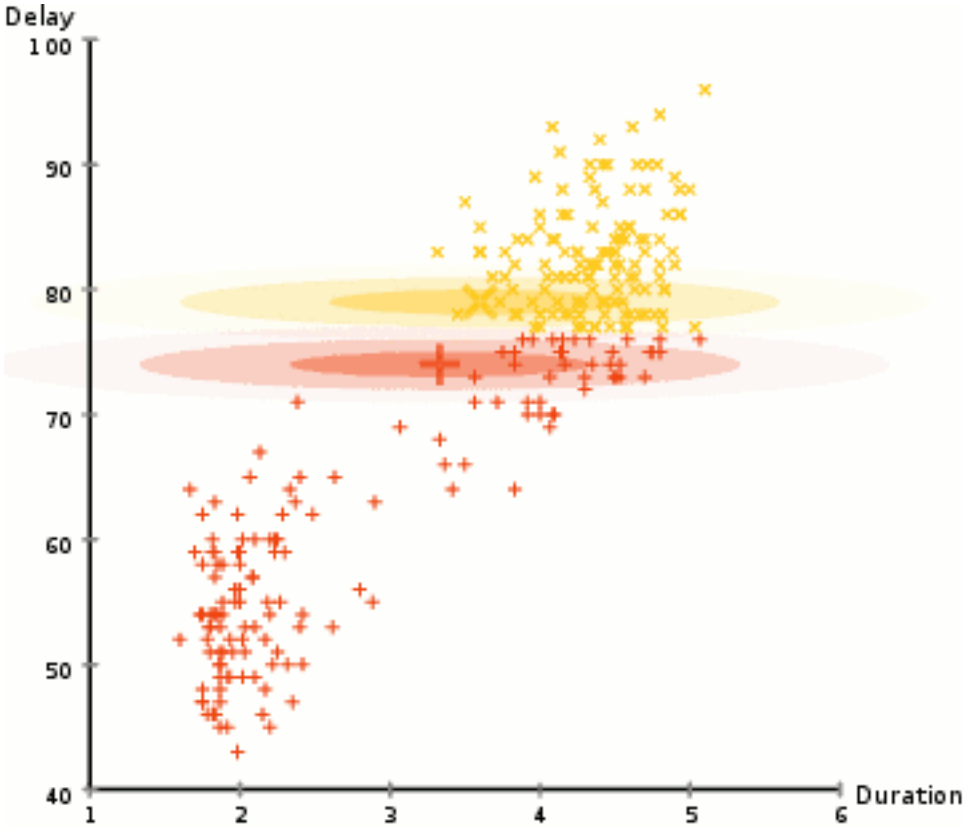
$$q_2 = 59.2\%$$

Intuition of EM algorithm

- Use an iterative approach for estimating the parameters:
  - Guess the probability that a given data point came from Coin 1 or 2; Generate fictional labels, weighted according to this probability.
  - Now, compute the most likely value of the parameters. [recall the scenario I]
  - Compute the likelihood of the data given this model.
  - Re-estimate the initial parameter setting: set them to maximize the likelihood of the data.

Real world Example

GMM clustering of Old Faithful eruption data



GMM as the marginal distribution P(x) of a joint distribution P(x, z)

- Remember, in GMM, we model the marginal probability as

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$\omega_k = p(z = k)$$

Iterative procedure

- LetType equation here. θ represent all parameters $\{\omega_k, \mu_k, \Sigma_k\}$

Step 0: initialize $\boldsymbol{\theta}$ with some values (random or otherwise)

Step 1: compute γ_{nk} using the current $\boldsymbol{\theta}$

Step 2: update $\boldsymbol{\theta}$ using the just computed γ_{nk}

Step 3: go back to Step 1

γ_{nk}: given a data point x_n how likely it belongs to k^{th} cluster

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

Since γ_{nk} is binary, the previous solution is nothing but

- For ω_k: count the number of data points whose z_n is k and divide by the total number of data points (note that $\sum_k \sum_n \gamma_{nk} = N$)
- For $\boldsymbol{\mu}_k$: get all the data points whose z_n is k, compute their mean
- For $\boldsymbol{\Sigma}_k$: get all the data points whose z_n is k, compute their covariance matrix

Estimate γ_{nk}

- γ_{nk} the assignment of instance n to cluster k, can be defined as $\gamma_{nk} = P(z_n = k|x_n)$
- Can be computed vis the posterior probability

$$p(z_n = k|\boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')}$$

$N(x|\mu_k, \Sigma_k)$ ω_k

Parameter estimation for GMMs

- If cluster assignments are observed $\{z_n\}$ are given
  - We know the cluster of each point
  - Let $\gamma_{nk} = 1$ if instance n belongs to cluster k, otherwise $\gamma_{nk} = 0$
- Then the maximum likelihood estimation is

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$