上海交通大學
SHANGHAI JIAO TONG UNIVERSITY

Machine Learning

Lecture 2

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Bayesian Learning

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London,* **53:370-418**

Your first consulting job

- A billionaire asks you a question:
  - He says: I have a coin, if I flip it, what's the probability it will fall with the head up?
  - You say: Please flip it a few times:

  - You say: The probability is: **3/5**
  - **He says: Why???**
  - You say: Because…

Bernoulli distribution

Data, *D* = 

$$D = \{X_i\}_{i=1}^{n},\ X_i \in \{\mathrm{H}, \mathrm{T}\}$$

- P(Heads) = θ, P(Tails) = 1-θ
- Flips are **i.i.d.**:
  - **Independent** events
  - **Identically distributed** according to Bernoulli distribution

Choose θ that maximizes the probability of observed data

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

MLE of probability of head:

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$ **= 3/5** "Frequency of heads"

Number of heads Number of tails

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$ Independent draws

$$= \arg\max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta)$$ Identically distributed

$$= \arg\max_{\theta} \underbrace{\theta^{\alpha_H}(1-\theta)^{\alpha_T}}_{J(\theta)}$$

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

$$= \arg\max_{\theta} \underbrace{\theta^{\alpha_H}(1-\theta)^{\alpha_T}}_{J(\theta)}$$

$$\frac{\partial J(\theta)}{\partial \theta}\Big|_{\theta=\hat{\theta}_{\mathrm{MLE}}} = 0$$

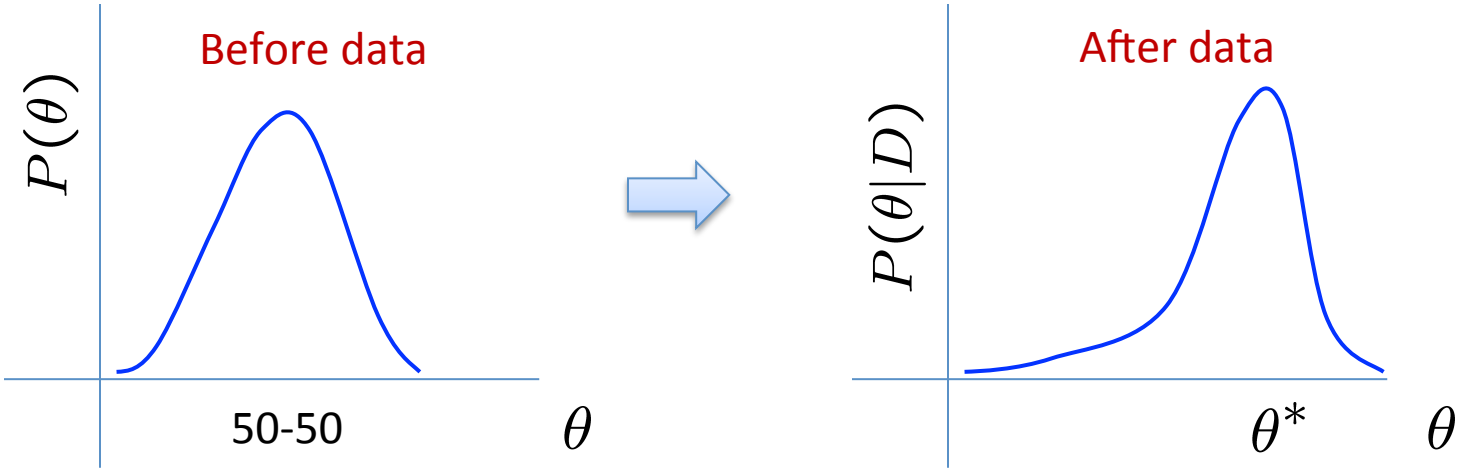
$$\alpha_H(1-\theta) - \alpha_T\theta\big|_{\theta=\hat{\theta}_{\mathrm{MLE}}} = 0$$

$$\boxed{\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}}$$

What about prior knowledge?

- Billionaire says: Wait, I know that the coin is "close" to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way…**

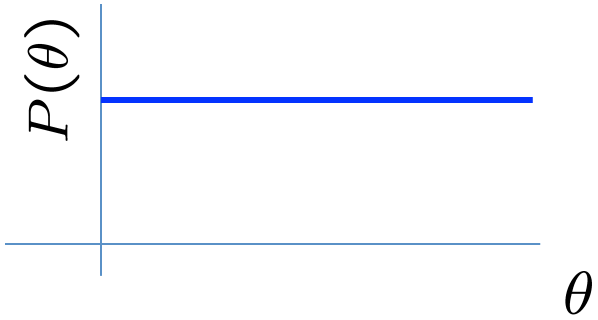
- Rather than estimating a single θ, we obtain a distribution over possible values of θ



Prior distribution

- What about prior?
  - Represents expert knowledge
  - Simple posterior form

- Uninformative priors:
  - Uniform distribution



- Conjugate priors:
  - Closed-form representation of posterior
  - P(θ) and P(θ|D) have the same form

Conjugate Prior

- P(θ) and P(θ|D) have the same form

Eg. 1 Coin flip problem

Likelihood is ~ Binomial

$$P(\mathcal{D} \mid \theta) = \binom{n}{\alpha_H} \theta^{\alpha_H} (1-\theta)^{\alpha_T}$$

If prior is Beta distribution,

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$

Then posterior is Beta distribution

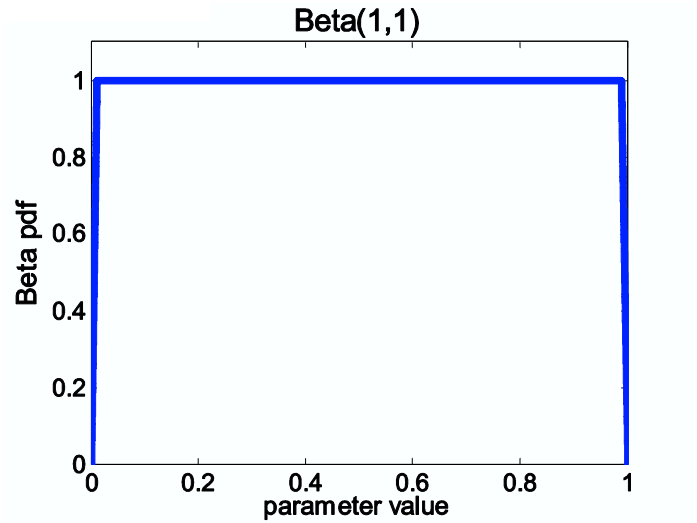
$$P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

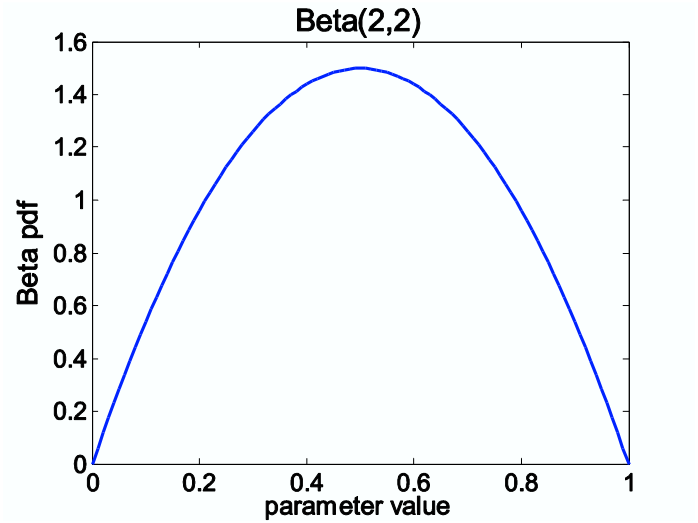
For Binomial, conjugate prior is Beta distribution.

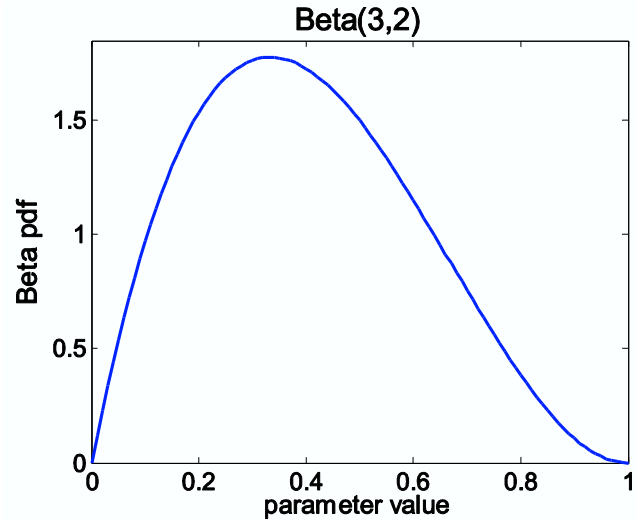
Beta distribution

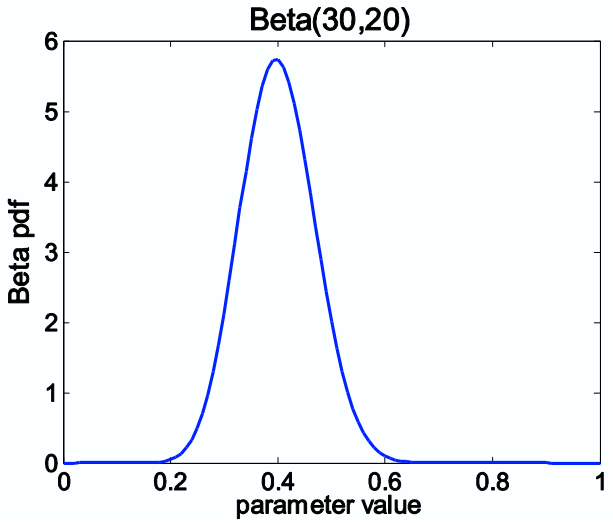
$Beta(\beta_H, \beta_T)$

More concentrated as values of β_H, β_T increase



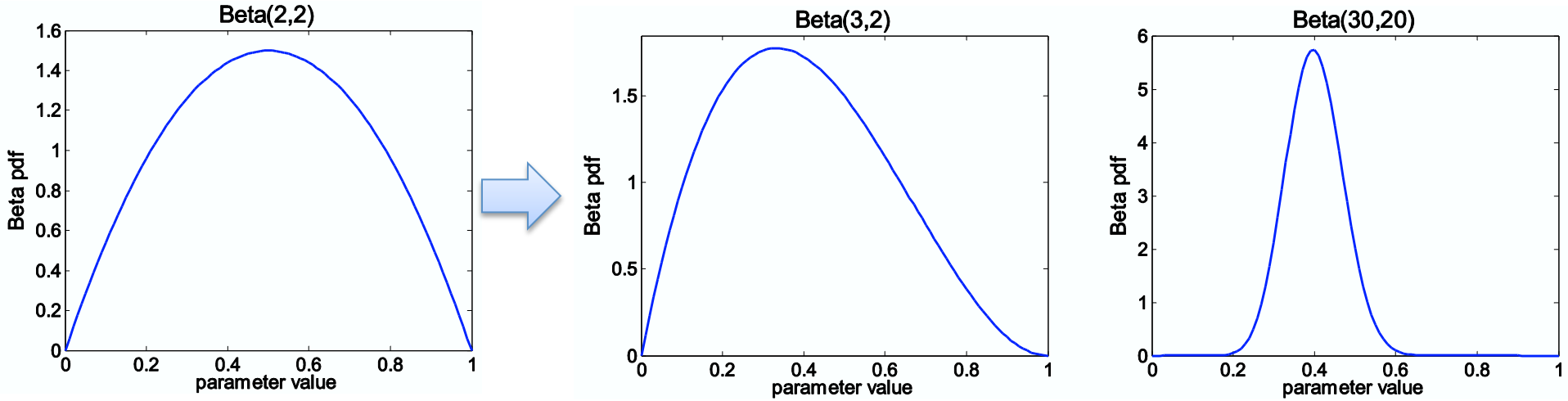






Beta conjugate prior

$$P(\theta) \sim Beta(\beta_H, \beta_T) \qquad P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



As $n = \alpha_H + \alpha_T$ increases

As we get more samples, effect of prior is "washed out"

Conjugate Prior

- P(θ) and P(θ|D) have the same form

Eg. 2 Dice roll problem (6 outcomes instead of 2)

Likelihood is ~ Multinomial(θ = $\{\theta_1, \theta_2, \ldots, \theta_k\}$)

$$P(\mathcal{D} \mid \theta) = \frac{n!}{\alpha_1!\alpha_2!\ldots\alpha_k!}\theta_1^{\alpha_1}\theta_2^{\alpha_2}\ldots\theta_k^{\alpha_k} \quad \sum_{i=1}^{k}\alpha_i = n \quad \sum_{i=1}^{k}\theta_i = 1$$

If prior is Dirichlet distribution,

$$P(\theta) = \frac{\prod_{i=1}^{k}\theta_i^{\beta_i-1}}{B(\beta_1,\ldots,\beta_k)} \sim \text{Dirichlet}(\beta_1,\ldots,\beta_k)$$

Then posterior is Dirichlet distribution

$$P(\theta|D) \sim \text{Dirichlet}(\beta_1+\alpha_1,\ldots,\beta_k+\alpha_k)$$

For Multinomial, conjugate prior is Dirichlet distribution.

Maximum A Posteriori Estimation

Choose θ that maximizes a posterior probability

$$\begin{aligned}\widehat{\theta}_{MAP} &= \arg\max_{\theta} P(\theta \mid D) \\ &= \arg\max_{\theta} P(D \mid \theta) P(\theta)\end{aligned}$$

MAP estimate of probability of head:

$$P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

$$\widehat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

Mode of Beta distribution

MLE vs. MAP

- Maximum Likelihood estimation (MLE)

  Choose value that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$

- Maximum *a posteriori* (MAP) estimation

  Choose value that is most probable given observed data and prior belief

$$\widehat{\theta}_{MAP} = \arg\max_{\theta} P(\theta|D)$$
$$= \arg\max_{\theta} P(D|\theta)P(\theta)$$

When is MAP same as MLE?

MLE vs. MAP

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

What if we toss the coin too few times?

- You say: Probability next toss is a head = 0
- Billionaire says: You're fired!

$$\widehat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

- Beta prior equivalent to extra coin flips
- As $n \rightarrow$ infinity, prior is "forgotten"
- **But, for small sample size, prior is important!**

Bayesians vs. Frequentists

You are no good when sample is small

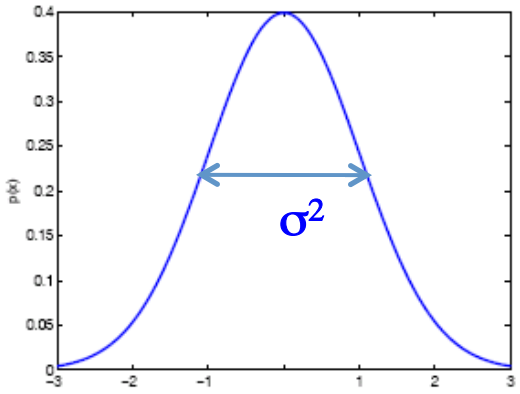
You give a different answer for different priors

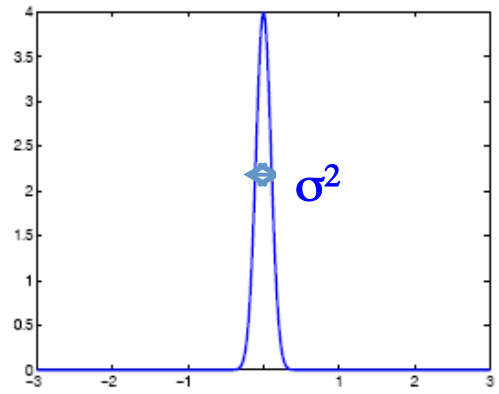
What about continuous variables?

- Billionaire says: If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians…**

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

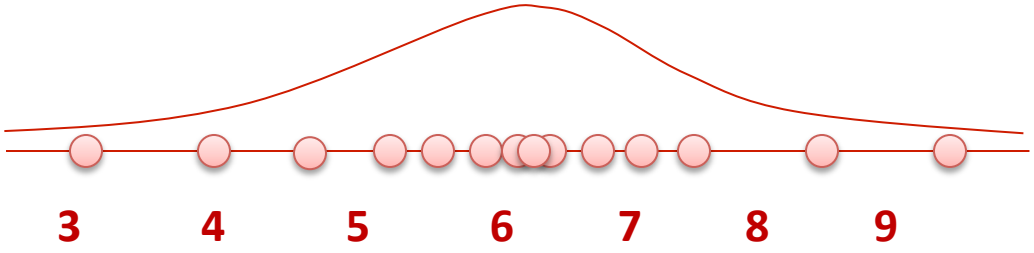
= $N(\mu,\sigma^2)$





Gaussian distribution

Data, D =



- Parameters: μ – mean, σ^2 - variance
- Sleep hrs are **i.i.d.**:
  - **Independent** events
  - **Identically distributed** according to Gaussian distribution

Properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
  - $X \sim N(\mu,\sigma^2)$
  - $Y = aX + b \Rightarrow Y \sim N(a\mu+b,a^2\sigma^2)$

- Sum of Gaussians
  - $X \sim N(\mu_X,\sigma^2_X)$
  - $Y \sim N(\mu_Y,\sigma^2_Y)$
  - $Z = X+Y \Rightarrow Z \sim N(\mu_X+\mu_Y, \sigma^2_X+\sigma^2_Y)$

MLE for Gaussian mean and variance

Choose $\theta = (\mu, \sigma^2)$ that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$

MLE for Gaussian mean and variance

$$\widehat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{n}\sum_{i=1}^{n} (x_i - \widehat{\mu})^2$$

Note: MLE for the variance of a Gaussian is **biased**

- Expected result of estimation is **not** true parameter!
- Unbiased variance estimator:

$$\widehat{\sigma}^2_{unbiased} = \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \widehat{\mu})^2$$

MAP for Gaussian mean and variance

- Conjugate priors
  - Mean: Gaussian prior
  - Variance: Wishart Distribution

- Prior for mean:

$$P(\mu \mid \eta, \lambda) = \frac{1}{\lambda\sqrt{2\pi}} e^{\frac{-(\mu-\eta)^2}{2\lambda^2}}$$

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Bayes Optimal Classifier
& Naive Bayes

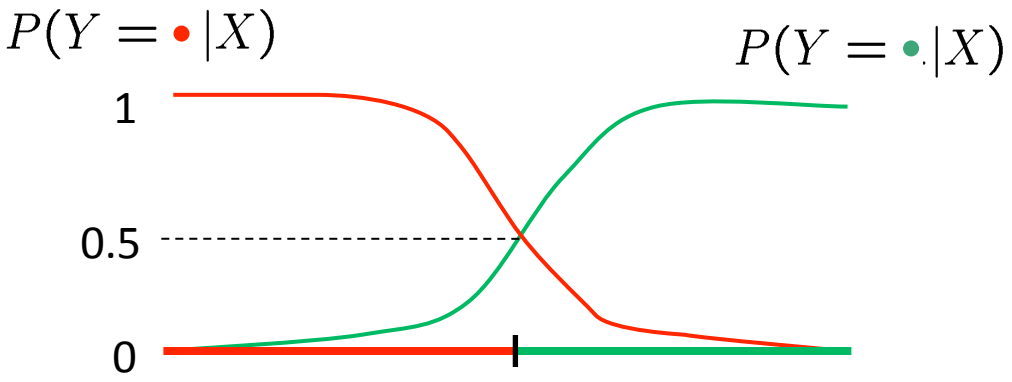
Optimal Classification

Optimal predictor: (Bayes classifier)

$$f^* = \arg\min_f P(f(X) \neq Y)$$

Equivalently,

$$f^*(x) = \arg\max_{Y=y} P(Y = y|X = x)$$



Optimal Classifier

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

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

Optimal classifier:

$$f^*(x) = \arg\max_{Y=y} P(Y = y|X = x)$$

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

Class conditional density

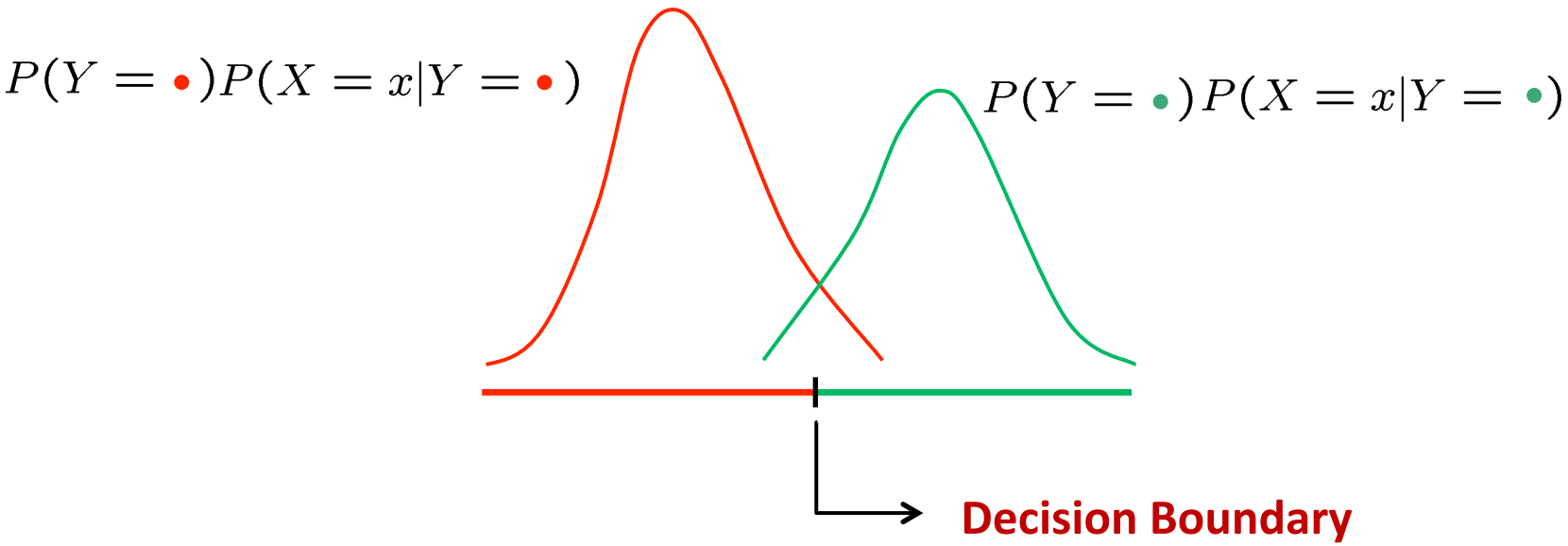
Class prior

Example Decision Boundaries

- Gaussian class conditional densities (1-dimension/feature)

$$P(X = x|Y = y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x-\mu_y)^2}{2\sigma_y^2}\right)$$

Binary Classification – two classes



Learning the Optimal Classifier

Optimal classifier:

$$f^*(x) = \arg\max_{Y=y} P(Y = y|X = x)$$

$$= \arg\max_{Y=y} \underbrace{P(X = x|Y = y)}_{\text{Class conditional density}} \underbrace{P(Y = y)}_{\text{Class prior}}$$

Need to know Prior P(Y = y) for all y

Likelihood P(X=x|Y = y) for all x,y

Learning the Optimal Classifier

Task: Predict whether or not a picnic spot is enjoyable

Training Data: $X = (X_1 \quad X_2 \quad X_3 \quad \ldots \quad \ldots \quad X_d) \quad Y$

n rows

Sky	Temp	Humid	Wind	Water	Forecst	EnjoySpt
Sunny	Warm	Normal	Strong	Warm	Same	Yes
Sunny	Warm	High	Strong	Warm	Same	Yes
Rainy	Cold	High	Strong	Warm	Change	No
Sunny	Warm	High	Strong	Cool	Change	Yes

Lets learn P(Y|X) – how many parameters?

Prior: P(Y = y) for all y **K-1 if K labels**

Likelihood: P(X=x|Y = y) for all x,y **$(2^d - 1)K$ if d binary features**

Learning the Optimal Classifier

Task: Predict whether or not a picnic spot is enjoyable

Training Data: $X = (X_1 \quad X_2 \quad X_3 \quad \ldots \quad \ldots \quad X_d) \quad Y$

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Sunny	Warm	High	Strong	Warm	Same	Yes
Rainy	Cold	High	Strong	Warm	Change	No
Sunny	Warm	High	Strong	Cool	Change	Yes

Lets learn P(Y|X) – how many parameters?

$2^dK - 1$ (K classes, d binary features)

Need $n >> 2^dK - 1$ number of training data to learn all parameters

Conditional Independence

- X is **conditionally independent** of Y given Z:

  probability distribution governing X is independent of the value of Y, given the value of Z

$$(\forall x, y, z) P(X = x | Y = y, Z = z) = P(X = x | Z = z)$$

- Equivalent to:

$$P(X, Y \mid Z) = P(X \mid Z) P(Y \mid Z)$$

- e.g., $P(Thunder | Rain, Lightning) = P(Thunder | Lightning)$

  Note: does NOT mean Thunder is independent of Rain

Prediction using Conditional Independence

- Predict Lightening
- From two **conditionally Independent** features
  - Thunder
  - Rain

parameters needed to learn likelihood given L

P(T,R|L) $(2^2-1)2 = 6$

With conditional independence assumption

P(T,R|L) = P(T|L) P(R|L) **(2-1)2 + (2-1)2 = 4**

Naïve Bayes Assumption

- Naïve Bayes assumption:
  - Features are conditionally independent given class:

$$P(X_1, X_2|Y) = P(X_1|X_2, Y)P(X_2|Y)$$
$$= P(X_1|Y)P(X_2|Y)$$

  - More generally:

$$P(X_1 \ldots X_d|Y) = \prod_{i=1}^{d} P(X_i|Y)$$

- How many parameters now? **(2-1)dK vs. (2^d-1)K**
  - Suppose **X** is composed of *d* binary features

Naïve Bayes Classifier

- Given:
  - Class Prior P(Y)
  - *d* conditionally independent features **X** given the class Y
  - For each X_i, we have likelihood $P(X_i|Y)$

- Decision rule:

$$f_{NB}(\mathbf{x}) = \arg\max_y P(x_1, \ldots, x_d \mid y)P(y)$$

$$= \arg\max_y \prod_{i=1}^{d} P(x_i|y)P(y)$$

- If conditional independence assumption holds, NB is optimal classifier! But worse otherwise.

Naïve Bayes Algo – Discrete features

- Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$ $X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)})$
- Maximum Likelihood Estimates
  - For Class Prior

$$\widehat{P}(y) = \frac{\{\#j : Y^{(j)} = y\}}{n}$$

  - For Likelihood

$$\frac{\widehat{P}(x_i, y)}{\widehat{P}(y)} = \frac{\{\#j : X_i^{(j)} = x_i, Y^{(j)} = y\}/n}{\{\#j : Y^{(j)} = y\}/n}$$

- NB Prediction for test data $X = (x_1, \ldots, x_d)$

$$Y = \arg\max_y \widehat{P}(y) \prod_{i=1}^{d} \frac{\widehat{P}(x_i, y)}{\widehat{P}(y)}$$

Subtlety 1 – Violation of NB Assumption

- Usually, features are not conditionally independent:

$$P(X_1 \ldots X_d | Y) \neq \prod_i P(X_i | Y)$$

- Nonetheless, NB is the single most used classifier out there
  - NB often performs well, even when assumption is violated
  - [Domingos & Pazzani '96] discuss some conditions for good performance

Subtlety 2 – Insufficient training data

- What if you never see a training instance where X_1=a when Y=b?
  - e.g., Y={SpamEmail}, X_1={'Earn'}
  - $P(X_1=a \mid Y=b) = 0$
- Thus, no matter what the values $X_2,\ldots,X_d$ take:
  - $P(Y=b \mid X_1=a,X_2,\ldots,X_d) = 0$

$$P(X_1 = a, X_2 \ldots X_n | Y) = P(X_1 = a | Y) \prod_{i=2}^{d} P(X_i | Y)$$

- What now???

Naïve Bayes Algo – Discrete features

- Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$ $X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)})$
- Maximum A Posteriori Estimates – add m "virtual" examples

  Assume priors

$$Q(Y = b) \qquad Q(X_i = a, Y = b)$$

  MAP Estimate

$$\widehat{P}(X_i = a | Y = b) = \frac{\{\#j : X_i^{(j)} = a, Y^{(j)} = b\} + mQ(X_i = a, Y = b)}{\{\#j : Y^{(j)} = b\} + \underbrace{mQ(Y = b)}_{\text{\# virtual examples with Y = b}}}$$

Now, even if you never observe a class/feature posterior probability never zero.

Case Study: Text Classification

- Classify e-mails
  - Y = {Spam,NotSpam}
- Classify news articles
  - Y = {what is the topic of the article?}
- Classify webpages
  - Y = {Student, professor, project, …}

- What about the features **X**?
  - The text!

Features X are entire document – X_i for i^{th} word in article

Article from rec.sport.hockey

```
Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.e
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinic
Date: 5 Apr 93 09:53:39 GMT

I can only comment on the Kings, but the most
obvious candidate for pleasant surprise is Alex
Zhitnik. He came highly touted as a defensive
defenseman, but he's clearly much more than that.
Great skater and hard shot (though wish he were
more accurate). In fact, he pretty much allowed
the Kings to trade away that huge defensive
liability Paul Coffey. Kelly Hrudey is only the
biggest disappointment if you thought he was any
good to begin with. But, at best, he's only a
mediocre goaltender. A better choice would be
Tomas Sandstrom, though not through any fault of
his own, but because some thugs in Toronto decided
```

NB for Text Classification

- P(**X**|Y) is huge!!!
  - Article at least 1000 words, **X**={X_1,…,X_{1000}}
  - X_i represents i^{th} word in document, i.e., the domain of X_i is entire vocabulary, e.g., Webster Dictionary (or more), 10,000 words, etc.

- NB assumption helps a lot!!!
  - P(X_i=x_i|Y=y) is just the probability of observing word x_i at the i^{th} position in a document on topic y

$$h_{NB}(\mathbf{x}) = \arg\max_y P(y) \prod_{i=1}^{LengthDoc} P(x_i|y)$$

Bag of words model

- Typical additional assumption – **Position in document doesn't matter**: $P(X_i=x_i|Y=y) = P(X_k=x_i|Y=y)$
  - "Bag of words" model – order of words on the page ignored
  - Sounds really silly, but often works very well!

$$\prod_{i=1}^{LengthDoc} P(x_i|y) = \prod_{w=1}^{W} P(w|y)^{count_w}$$

When the lecture is over, remember to wake up the person sitting next to you in the lecture room.

Bag of words model

- Typical additional assumption – **Position in document doesn't matter**: $P(X_i=x_i|Y=y) = P(X_k=x_i|Y=y)$
  - "Bag of words" model – order of words on the page ignored
  - Sounds really silly, but often works very well!

$$\prod_{i=1}^{LengthDoc} P(x_i|y) = \prod_{w=1}^{W} P(w|y)^{count_w}$$

in is lecture lecture next over person remember room sitting the the the to to up wake when you

Bag of words approach

aardvark	0
about	2
all	2
Africa	1
apple	0
anxious	0
...	
gas	1
...	
oil	1
…	
Zaire	0

NB with Bag of Words for text classification

- Learning phase: using multiple training documents
  - Class Prior P(Y)
  - $P(X_i|Y)$
- Test phase:
  - For each test document, use naïve Bayes decision rule:

$$h_{NB}(\mathbf{x}) = \arg\max_y P(y) \prod_{i=1}^{LengthDoc} P(x_i|y)$$

$$= \arg\max_y P(y) \prod_{w=1}^{W} P(w|y)^{count_w}$$

Twenty news groups results

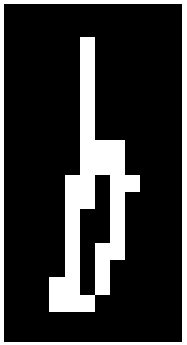
Given 1000 training documents from each group
Learn to classify new documents according to
which newsgroup it came from

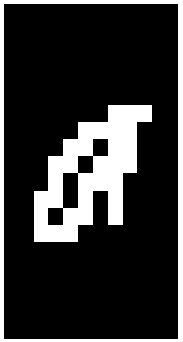
comp.graphics	misc.forsale
comp.os.ms-windows.misc	rec.autos
comp.sys.ibm.pc.hardware	rec.motorcycles
comp.sys.mac.hardware	rec.sport.baseball
comp.windows.x	rec.sport.hockey
alt.atheism	sci.space
soc.religion.christian	sci.crypt
talk.religion.misc	sci.electronics
talk.politics.mideast	sci.med
talk.politics.misc	
talk.politics.guns	

Naive Bayes: 89% classification accuracy

What if features are continuous?

Eg., character recognition: X_i is intensity at i^{th} pixel





Gaussian Naïve Bayes (GNB):

$$P(X_i = x \mid Y = y_k) = \frac{1}{\sigma_{ik}\sqrt{2\pi}} \; e^{\frac{-(x-\mu_{ik})^2}{2\sigma_{ik}^2}}$$

Different mean and variance for each class k and each pixel i.

Sometimes assume variance

- is independent of Y (i.e., σ_i),
- or independent of X_i (i.e., σ_k)
- or both (i.e., σ)

Estimating parameters: Y discrete, X_i continuous

Maximum likelihood estimates:

$$\hat{\mu}_{MLE} = \frac{1}{N}\sum_{j=1}^{N} x_j$$

$$\hat{\mu}_{ik} = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j X_i^j \delta(Y^j = y_k)$$

k^{th} class

j^{th} training image

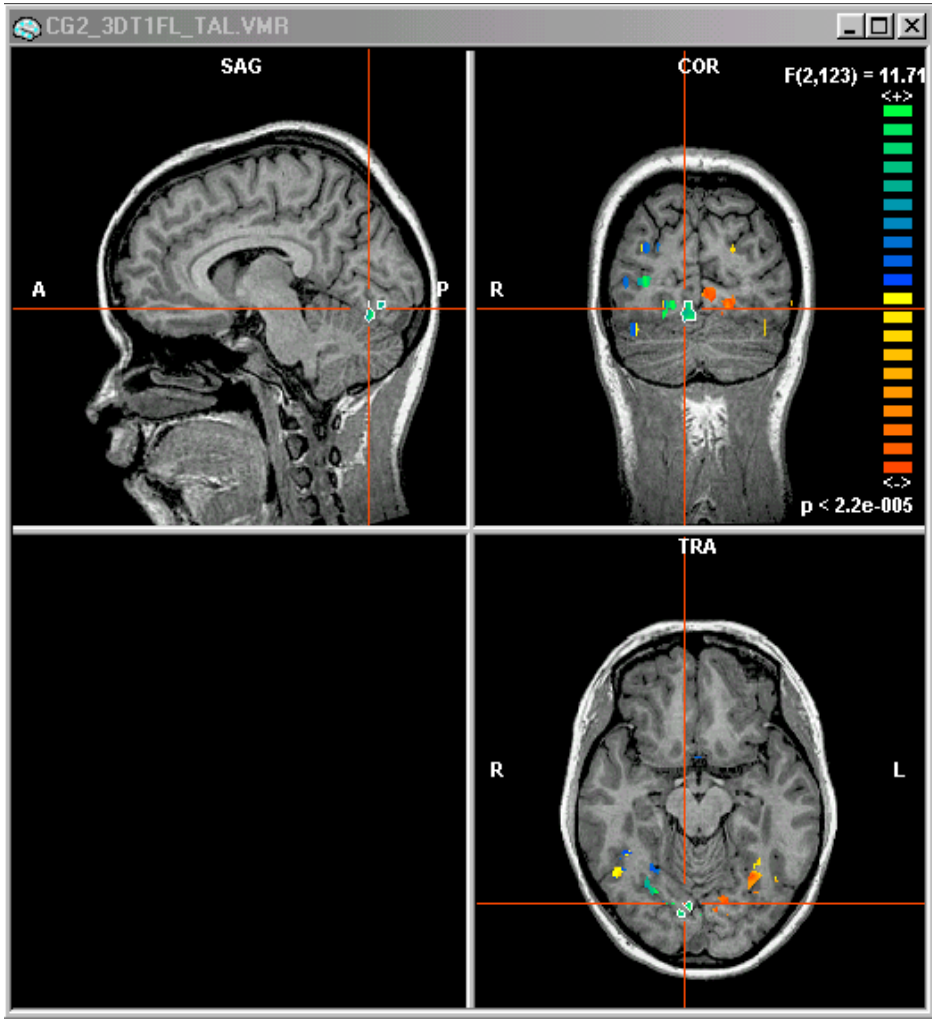
i^{th} pixel in j^{th} training image

$$\hat{\sigma}^2_{unbiased} = \frac{1}{N-1}\sum_{j=1}^{N} (x_j - \hat{\mu})^2$$

$$\hat{\sigma}^2_{ik} = \frac{1}{\sum_j \delta(Y^j = y_k) - 1} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

Example: GNB for classifying mental states

[Mitchell et al.]



~1 mm resolution

~2 images per sec.

15,000 voxels/image

non-invasive, safe

measures Blood Oxygen Level Dependent (BOLD) response