### Machine Learning 10-601 10-301

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

March 31, 2021

#### Today:

- Probabilistic learning
- Joint probabilities
- Estimating parameters
  - MLE
  - MAP

#### Required Reading:

Estimating Probabilities [Mitchell]

#### Optional Probability Review:

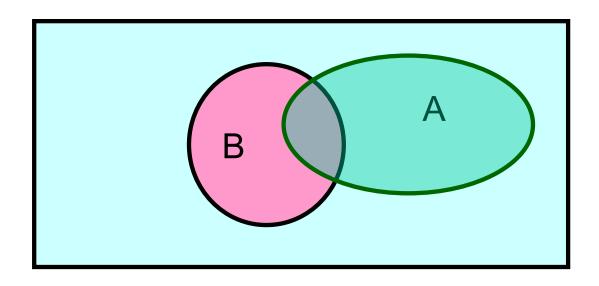
Goodfellow, Ch 3-3.9

some of these slides are derived from William Cohen, Andrew Moore, Aarti Singh, Eric Xing, Carlos Guestrin.
- Thanks!

### probabilistic function approximation:

instead of  $F: X \rightarrow Y$ , learn  $P(Y \mid X)$ 

### Definition of Conditional Probability



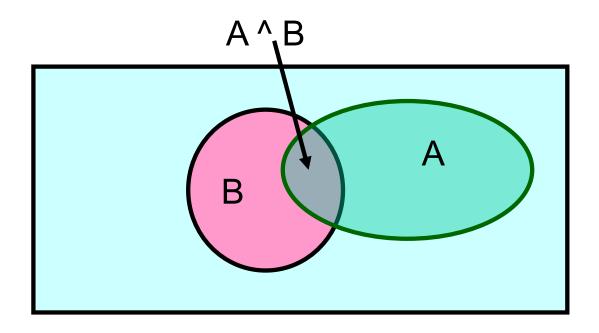
## Definition of Conditional Probability

### Corollary: The Chain Rule

$$P(A \land B) = P(A|B) P(B)$$

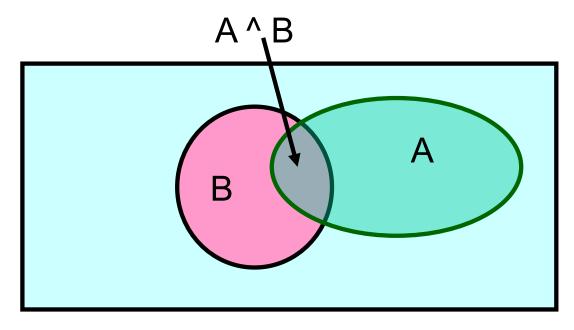
### Bayes Rule

let's write 2 expressions for P(A ^ B)



### Bayes Rule

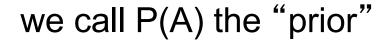
let's write 2 expressions for P(A ^ B)



$$P(A \land B) = P(A|B)P(B) = P(B|A) P(B)$$

implies: 
$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)}$$

$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)}$$
 Bayes' rule



and P(A|B) the "posterior"



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** 

$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)}$$
 Bayes' rule



we call P(A) the "prior"

and P(A|B) the "posterior"

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** 

...by no means merely a curious speculation in the doctrine of chances, but necessary to be solved in order to a sure foundation for all our reasonings concerning past facts, and what is likely to be hereafter.... necessary to be considered by any that would give a clear account of the strength of *analogical* or *inductive reasoning*...

### Other Forms of Bayes Rule

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)}$$

$$P(A|B) = \frac{P(B|A)P(A)}{P(B|A)P(A) + P(B|\sim A)P(\sim A)}$$

$$P(A|B \land X) = \frac{P(B|A \land X)P(A \land X)}{P(B \land X)}$$

### Applying Bayes Rule

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B \mid A)P(A) + P(B \mid \sim A)P(\sim A)}$$

A = you have the flu, B = you just coughed

#### Assume:

$$P(A) = 0.05$$
  
 $P(B|A) = 0.80$ 

$$P(B| \sim A) = 0.2$$

what is  $P(flu \mid cough) = P(A|B)$ ?

# The Awesome Joint Probability Distribution $P(X_1, X_2, ..., X_N)$

from which we can calculate  $P(X_1|X_2...X_N)$ , and <u>every</u> other probability we desire over subsets of  $X_1...X_N$ 

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

Recipe for making a joint distribution of M variables:

 Make a table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2<sup>M</sup> rows).

### Example: Boolean variables A, B, C

A	В	С
0	0	0
0	0	1
0	1	0
0	1	1
1	0	0
1	0	1
1	1	0
1	1	1

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

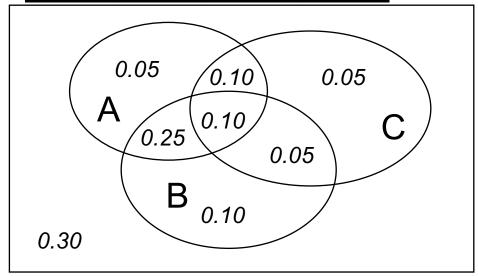
- Make a table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2<sup>M</sup> rows).
- 2. For each combination of values, say how probable it is.

A	В	С	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10

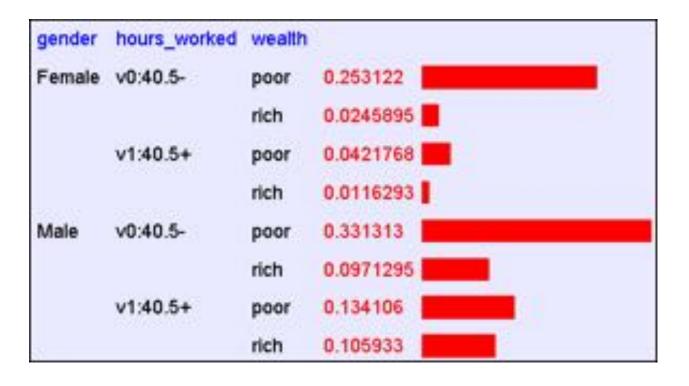
Recipe for making a joint distribution of M variables:

- Make a table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2<sup>M</sup> rows).
- 2. For each combination of values, say how probable it is.
- 3. If you subscribe to the axioms of probability, those numbers must sum to 1.

A	В	С	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



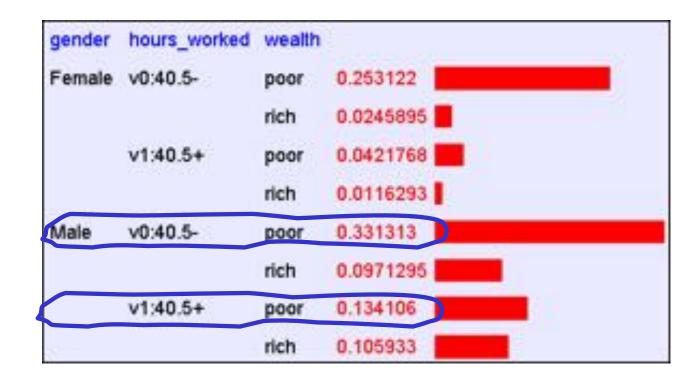
# Using the Joint Distribution



Once you have the JD you can ask for the probability of **any** logical expression involving these variables

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

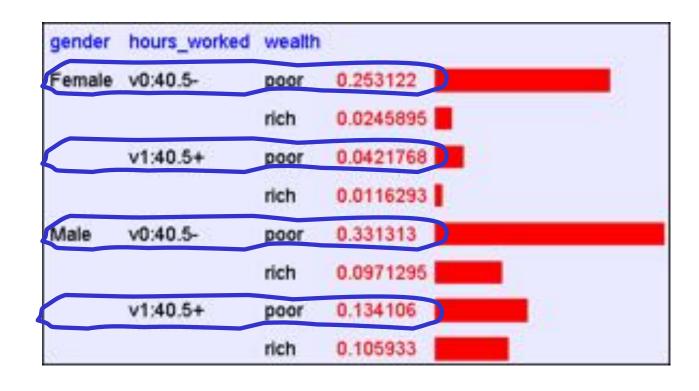
### Using the Joint



$$P(Poor Male) = 0.4654$$

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

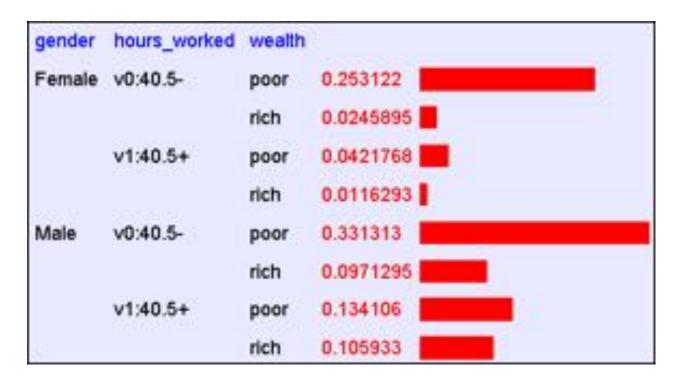
### Using the Joint



$$P(Poor) = 0.7604$$

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

# Using the Joint Distribution



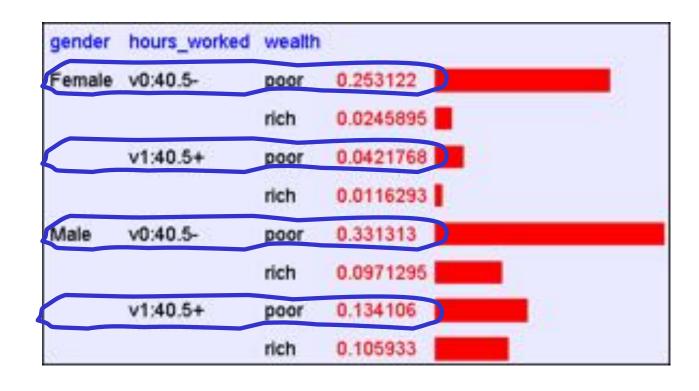
Once you have the JD you can ask for the probability of **any** logical expression involving these variables

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

Poll question 1:

What is P(rich, female)?

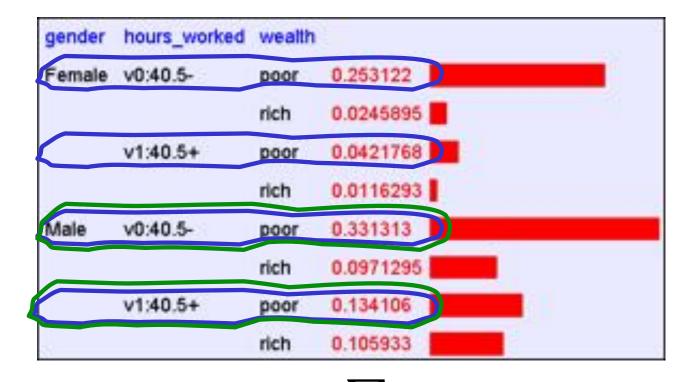
### Using the Joint



$$P(Poor) = 0.7604$$

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

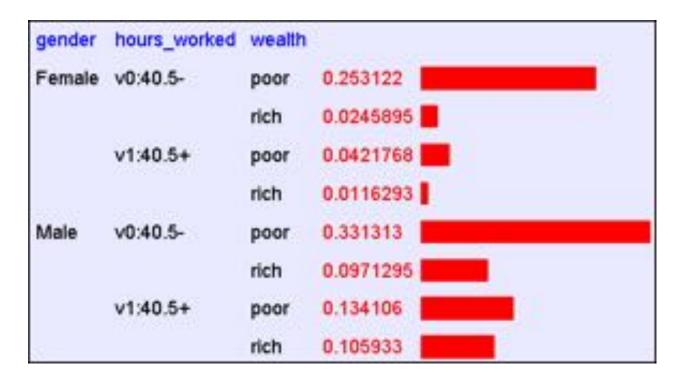
# Inference with the Joint



$$P(E_1 | E_2) = \frac{P(E_1 \land E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2}}{\sum_{\text{rows matching } E_2}} P(\text{row})$$

 $P(Male \mid Poor) = 0.4654 / 0.7604 = 0.612$ 

# Inference with the Joint



$$P(E_1 | E_2) = \frac{P(E_1 \land E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2}}{\sum_{\text{rows matching } E_2}} P(\text{row})$$

#### Poll question 2:

What is P(female | poor, v0:40.5)

## Learning and the Joint Distribution



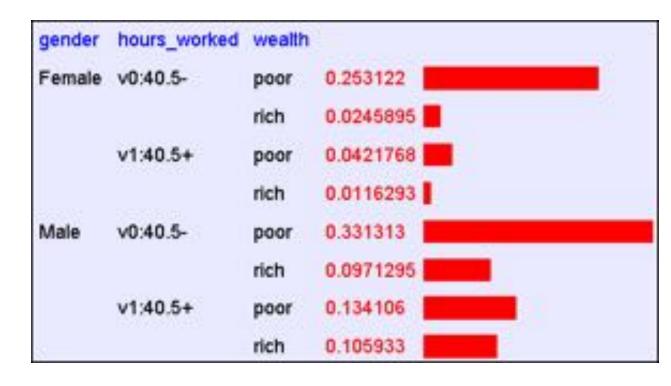
Suppose we want to learn the function f:  $\langle G, H \rangle \rightarrow W$ 

Equivalently, P(W | G, H)

Solution: learn joint distribution from data, calculate P(W | G, H)

e.g.,  $P(W=rich \mid G = female, H = 40.5-) =$ 

## Learning and the Joint Distribution



Suppose we want to learn the function f:  $\langle G, H \rangle \rightarrow W$ 

Equivalently, P(W | G, H)

Solution: learn joint distribution from data, calculate P(W | G, H)

# sounds like the solution to learning F: X → Y, or P(Y | X).

Are we done?

# sounds like the solution to learning F: X →Y, or P(Y | X).

Main problem: learning P(Y|X) can require more data than we have

consider learning Joint Dist. with 100 attributes # of rows in this table? # of people on earth?

# sounds like the solution to learning F: X →Y, or P(Y | X).

Main problem: learning P(Y|X) can require more data than we have

```
consider learning Joint Dist. with 100 attributes # of rows in this table? 2^{100} > 10^{30} # of people on earth? 10^{10} fraction of rows with 0 training examples? 99.99
```

#### What to do?

- 1. Be smart about how we estimate probabilities from sparse data
  - maximum likelihood estimates
  - maximum a posteriori estimates

- 2. Be smart about how to represent joint distributions
  - Bayes networks, graphical models, conditional independencies

## 1. Be smart about how we estimate probabilities

### **Estimating Probability of Heads**



- I show you the above coin X, and ask you to estimate the probability that it will turn up heads (X=1) or tails (X=0)
- You flip it repeatedly, observing
  - it turns up heads  $\alpha_1$  times
  - it turns up tails  $\alpha_0$  times
- Your estimate for  $\hat{\theta} = \hat{P}(X = 1)$  is ...?

### **Estimating Probability of Heads**



- I show you the above coin X, and ask you to estimate the probability that it will turn up heads (X=1) or tails (X=0)
- You flip it repeatedly, observing
  - it turns up heads  $\alpha_1$  times
  - it turns up tails  $\alpha_0$  times

Algorithm 1 (MLE): 
$$\hat{\theta} = \hat{P}(X = 1) = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

### Estimating $\theta = P(X=1)$



Test A:

100 flips: 51 Heads, 49 Tails

Test B:

3 flips: 2 Heads, 1 Tails

### **Estimating Probability of Heads**



When data sparse, might bring in prior assumptions to bias our estimate

• e.g., represent priors by "hallucinating"  $\gamma_1$  heads, and  $\gamma_0$  tails, to complement sparse observed  $\alpha_1$ ,  $\alpha_0$ 

Alg 2 (MAP): 
$$\hat{\theta} = \hat{P}(X = 1) = \frac{(\alpha_1 + \gamma_1)}{(\alpha_1 + \gamma_1) + (\alpha_0 + \gamma_0)}$$

### **Estimating Probability of Heads**



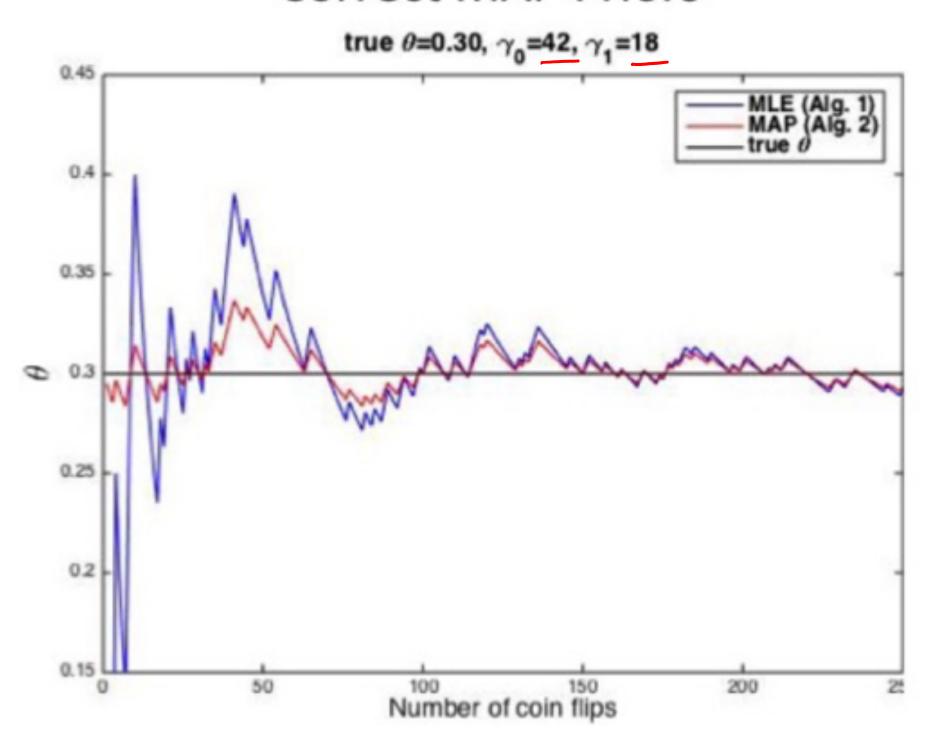
When data sparse, might bring in prior assumptions to bias our estimate

• e.g., represent priors by "hallucinating"  $\gamma_1$  heads, and  $\gamma_0$  tails, to complement sparse observed  $\alpha_1$ ,  $\alpha_0$ 

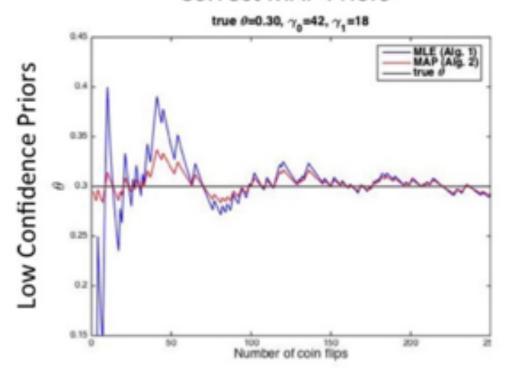
Alg 2 (MAP): 
$$\hat{\theta} = \hat{P}(X = 1) = \frac{(\alpha_1 + \gamma_1)}{(\alpha_1 + \gamma_1) + (\alpha_0 + \gamma_0)}$$

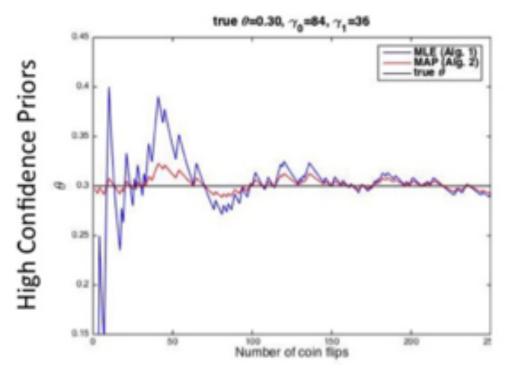
Consider 
$$\gamma_1=1$$
  $\gamma_0=1$  versus  $\gamma_1=1000$   $\gamma_0=1000$  versus  $\gamma_1=500$   $\gamma_0=1500$ 

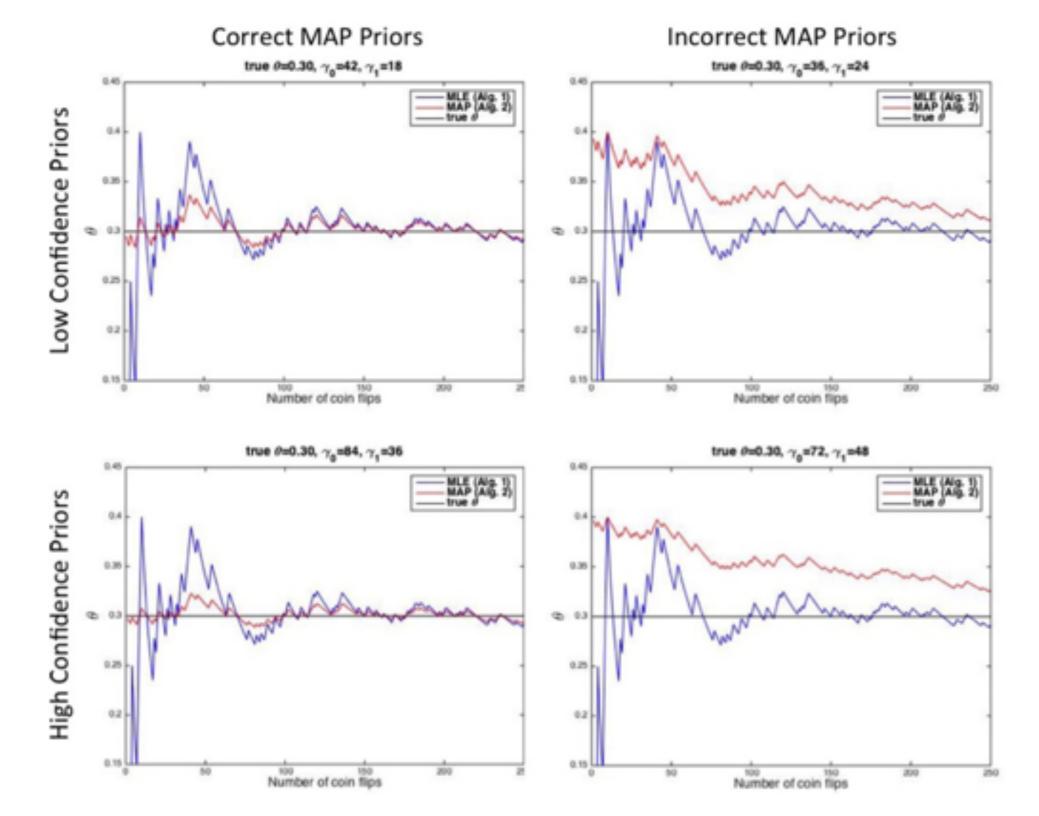
#### Correct MAP Priors



#### Correct MAP Priors







• Maximum Likelihood Estimate (MLE): choose  $\theta$  that maximizes probability of observed data  $\mathcal{D}$ 

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

 Maximum a Posteriori (MAP) estimate: choose θ that is most probable given prior probability and observed data

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

• Maximum Likelihood Estimate (MLE): choose  $\theta$  that maximizes probability of observed data  $\mathcal{D}$ 

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

 Maximum a Posteriori (MAP) estimate: choose θ that is most probable given prior probability and observed data

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

$$= \arg \max_{\theta} \ \frac{P(\mathcal{D} \mid \theta)P(\theta)}{P(\mathcal{D})}$$

$$= \arg \max_{\theta} \ P(\mathcal{D} \mid \theta)P(\theta)$$

#### Principle 1 (maximum likelihood):

- choose parameters θ that maximize P(data | θ)
- result in our case:  $\hat{\theta}^{MLE} = \frac{\alpha_1}{\alpha_1 + \alpha_0}$

Principle 2 (maximum a posteriori probability):

- choose parameters θ that maximize P(θ | data)
- result in our case:

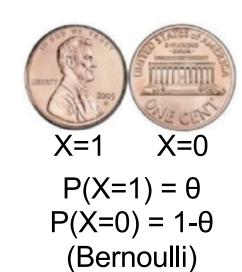
$$\hat{\theta}^{MAP} = \frac{\alpha_1 + \#\text{hallucinated\_1s}}{(\alpha_1 + \#\text{hallucinated\_1s}) + (\alpha_0 + \#\text{hallucinated\_0s})}$$

#### Maximum Likelihood Estimation

given data D, choose  $\theta$  that maximizes P(D |  $\theta$ )

Data D:

$$P(D|\theta) =$$



$$\hat{\theta} = \arg\max_{\theta} \ln P(D|\theta)$$

Set derivative to zero:

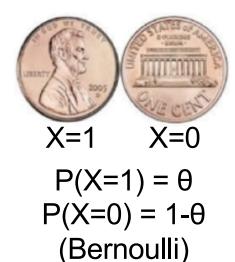
$$\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) = 0$$

$$= \arg \max_{\theta} \ln \left[ \theta^{\alpha_1} (1 - \theta)^{\alpha_0} \right]$$

hint: 
$$\frac{\partial \ln \theta}{\partial \theta} = \frac{1}{\theta}$$

#### Summary:

# Maximum Likelihood Estimate for Bernoulli random variable



Each flip yields boolean value for X

$$X \sim \text{Bernoulli: } P(X) = \theta^X (1 - \theta)^{(1 - X)}$$

• Data set D of independent, identically distributed (iid) flips produces  $\alpha_1$  ones,  $\alpha_0$  zeros (Binomial)

$$P(D|\theta) = P(\alpha_1, \alpha_0|\theta) = \theta^{\alpha_1}(1-\theta)^{\alpha_0}$$

$$\hat{\theta}^{MLE} = \operatorname{argmax}_{\theta} P(D|\theta) = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

Principle 1 (maximum likelihood):

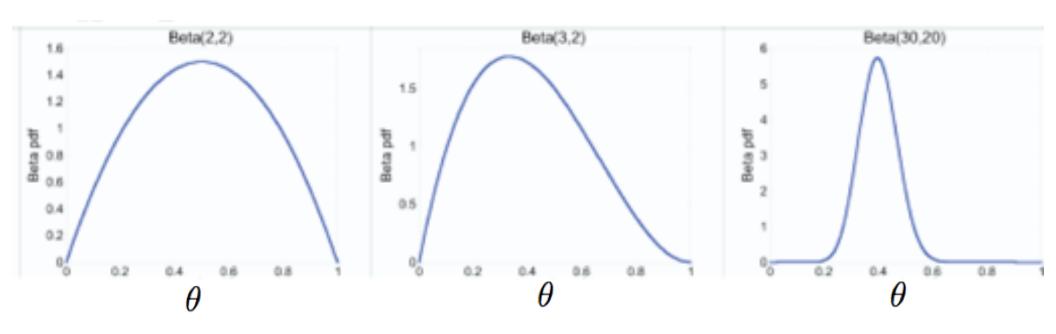
choose parameters θ that maximize
 P(data | θ)

Principle 2 (maximum a posteriori prob.):

• choose parameters  $\theta$  that maximize  $P(\theta \mid data) = P(data \mid \theta) P(\theta)$  P(data)

# Beta prior distribution – $P(\theta)$

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



#### Summary:

# Maximum a Posteriori (MAP) Estimate for Bernoulli random variable

#### Likelihood is ~ Binomial

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

If prior is Beta distribution,

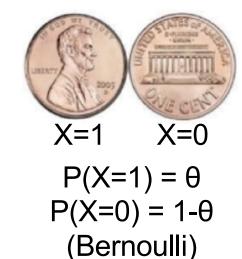
$$P(\theta) = \frac{\theta^{\beta_H - 1} (1 - \theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$

#### Then posterior is Beta distribution

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

and MAP estimate is therefore

$$\hat{\theta}^{MAP} = \frac{\alpha_H + \beta_H - 1}{(\alpha_H + \beta_H - 1) + (\alpha_T + \beta_T - 1)}$$



# Maximum a Posteriori (MAP) Estimate for random variable with k possible outcomes



Likelihood is  $\sim$  Multinomial( $\theta = \{\theta_1, \theta_2, ..., \theta_k\}$ )

$$P(\mathcal{D} \mid \theta) = \theta_1^{\alpha_1} \theta_2^{\alpha_2} \dots \theta_k^{\alpha_k}$$

If prior is Dirichlet distribution,

$$P(\theta) = \frac{\theta_1^{\beta_1 - 1} \, \theta_2^{\beta_2 - 1} \dots \theta_k^{\beta_k - 1}}{B(\beta_1, \dots, \beta_k)} \sim \text{Dirichlet}(\beta_1, \dots, \beta_k)$$

Then posterior is Dirichlet distribution

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

and MAP estimate is therefore

$$\hat{\theta_i}^{MAP} = \frac{\alpha_i + \beta_i - 1}{\sum_{j=1}^k (\alpha_j + \beta_j - 1)}$$

## Some terminology

- Likelihood function: P(data | θ)
- Prior: P(θ)
- Posterior: P(θ | data)
- Conjugate prior: P(θ) is the conjugate prior for likelihood function P(data | θ) if the parametric forms of P(θ) and P(θ | data) are the same.
  - Beta is conjugate prior for Bernoulli, Binomial
  - Dirichlet is conjugate prior for Multinomial

#### You should know

- Probability basics
  - random variables, conditional probs, ...
  - Bayes rule
  - Joint probability distributions
  - calculating probabilities from the joint distribution
- Estimating parameters from data
  - maximum likelihood estimates
  - maximum a posteriori estimates
  - distributions Bernoulli, Binomial, Beta, Dirichlet, ...
  - conjugate priors
  - regularization is a form of MAP estimation

### Extra slides

### Independent Events

- Definition: two events A and B are independent if P(A ^ B)=P(A) P(B)
- Intuition: knowing A tells us nothing about the value of B (and vice versa)

## **Expected values**

Given a discrete random variable X, the expected value

of X, written E[X] is

Probability-weighted average over all possible values of X

$$E[X] = \sum_{x \in \mathcal{X}} x P(X = x)$$

Example:

X	P(X)
0	0.3
1	0.2
2	0.5

$$E[X] =$$

### **Expected values**

Given discrete random variable X, the expected value of X, written E[X] is

$$E[X] = \sum_{x \in \mathcal{X}} x P(X = x)$$

We also can talk about the expected value of functions of X

$$E[f(X)] = \sum_{x \in \mathcal{X}} f(x)P(X = x)$$

#### Covariance

Given two discrete r.v.'s X and Y, we define the covariance of X and Y as

$$Cov(X,Y) = E[(X - E(X))(Y - E(Y))]$$

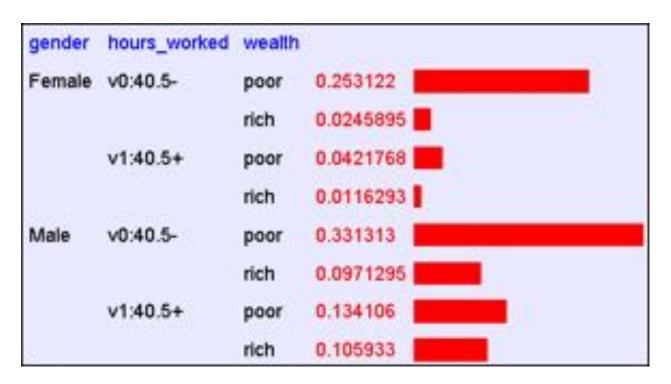
e.g., X=GENDER, Y=PLAYS\_FOOTBALL or X=GENDER, Y=LEFT\_HANDED

Remember: 
$$E[X] = \sum_{x \in \mathcal{X}} x P(X = x)$$

# **NAÏVE BAYES**

### Let's learn classifiers by learning P(Y|X)

Consider Y=Wealth, X=<Gender, HoursWorked>



Gender	HrsWorked	P(rich   G,HW)	P(poor   G,HW)
F	<40.5	.09	.91
F	>40.5	.21	.79
M	<40.5	.23	.77
M	>40.5	.38	.62

#### How many parameters must we estimate?

Suppose  $X = \langle X_1, ..., X_n \rangle$ where  $X_i$  and Y are boolean RV's

Gender	HrsWorked	P(rich   G,HW)	P(poor   G,HW)
F	<40.5	.09	.91
F	>40.5	.21	.79
M	<40.5	.23	.77
M	>40.5	.38	.62

To estimate  $P(Y|X_1, X_2, ..., X_n)$ 

If we have 100 boolean  $X_i$ 's:  $P(Y \mid X_1, X_2, ..., X_{100})$ 

# Bayes Rule

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

#### Which is shorthand for:

$$(\forall i, j) P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{P(X = x_j)}$$

#### **Equivalently:**

$$(\forall i, j) P(Y = y_i | X = x_j) = \frac{P(X = x_j | Y = y_i) P(Y = y_i)}{\sum_k P(X = x_j | Y = y_k) P(Y = y_k)}$$

### Can we reduce params using Bayes Rule?

Suppose X =1,... X<sub>n</sub>> 
$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$
 where X<sub>i</sub> and Y are boolean RV's

How many parameters to define  $P(X_1,...,X_n \mid Y)$ ?

How many parameters to define P(Y)?

# Naïve Bayes

#### Naïve Bayes assumes

$$P(X_1 \dots X_n | Y) = \prod_i P(X_i | Y)$$

i.e., that X<sub>i</sub> and X<sub>j</sub> are conditionally independent given Y, for all i≠j

## Conditional Independence

Definition: X is <u>conditionally independent</u> of Y given Z, if the probability distribution governing X is independent of the value of Y, given the value of Z

$$(\forall i, j, k) P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k)$$

Which we often write

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

E.g.,

P(Thunder|Rain, Lightning) = P(Thunder|Lightning)

Naïve Bayes uses assumption that the  $X_i$  are conditionally independent, given Y. E.g.,  $P(X_1|X_2,Y) = P(X_1|Y)$ 

Given this assumption, then:

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

Naïve Bayes uses assumption that the  $X_i$  are conditionally independent, given Y. E.g.,  $P(X_1|X_2,Y) = P(X_1|Y)$ 

Given this assumption, then:

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

in general: 
$$P(X_1...X_n|Y) = \prod_i P(X_i|Y)$$

Naïve Bayes uses assumption that the  $X_i$  are conditionally independent, given Y. E.g.,  $P(X_1|X_2,Y)=P(X_1|Y)$ 

Given this assumption, then:

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

in general: 
$$P(X_1...X_n|Y) = \prod_i P(X_i|Y)$$

How many parameters to describe  $P(X_1...X_n|Y)$ ? P(Y)?

- Without conditional indep assumption?
- With conditional indep assumption?

# Naïve Bayes in a Nutshell

#### Bayes rule:

$$P(Y = y_k | X_1 ... X_n) = \frac{P(Y = y_k) P(X_1 ... X_n | Y = y_k)}{\sum_j P(Y = y_j) P(X_1 ... X_n | Y = y_j)}$$

Assuming conditional independence among X<sub>i</sub>'s:

$$P(Y = y_k | X_1 ... X_n) = \frac{P(Y = y_k) \prod_i P(X_i | Y = y_k)}{\sum_j P(Y = y_j) \prod_i P(X_i | Y = y_j)}$$

So, to pick most probable Y for  $X^{new} = \langle X_1, ..., X_n \rangle$ 

$$Y^{new} \leftarrow \arg\max_{y_k} P(Y = y_k) \prod_i P(X_i^{new} | Y = y_k)$$