Machine Learning 10-601

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Today:

- Bayes Classifiers
- Conditional Independence
- Naïve Bayes

Readings:

Mitchell:

"Naïve Bayes and Logistic Regression"
(available on class website)

Two Principles for Estimating Parameters

- Maximum Likelihood Estimate (MLE): choose θ 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 the data

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

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

Maximum Likelihood Estimate

X=1 X=0

P(X=1) = θ

P(X=0) = 1-θ

(Bernoulli)

- 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 α_1 ones, α_0 zeros

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

$$\hat{\theta}^{MLE} = \arg\max_{\theta} P(D|\theta) = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

Maximum A Posteriori (MAP) Estimate

- Data set D of independent, identically distributed (iid) flips produces α_1 ones, α_0 zeros

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

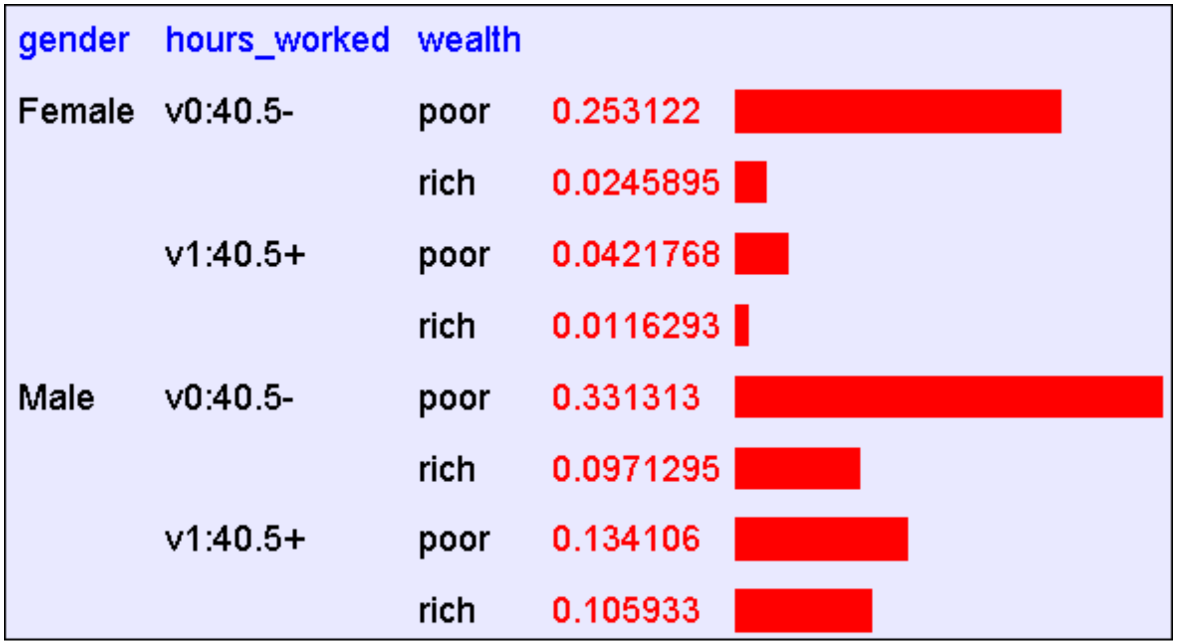
- Assume prior $P(\theta) = Beta(\beta_1, \beta_0) = \frac{1}{B(\beta_1,\beta_0)}\, \theta^{\beta_1 - 1}(1-\theta)^{\beta_0 - 1}$
- Then

$$\hat{\theta}^{MAP} = \arg\max_{\theta} P(D|\theta)P(\theta) = \frac{\alpha_1 + \beta_1 - 1}{(\alpha_1 + \beta_1 - 1) + (\alpha_0 + \beta_0 - 1)}$$

(like MLE, but hallucinating $\beta_1 - 1$ additional heads, $\beta_0 - 1$ additional tails)

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

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

If we have 30 boolean X_i's: $P(Y | X_1, X_2, \ldots X_{30})$

How many parameters must we estimate?

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

$P(Y | X_1, \ldots X_n)$

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

$p + \cancel{p} = 1$

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

2^n

If we have 30 X_i's instead of 2?

$2^{30} \sim$ 1 Billion

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

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

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

How many parameters to define $P(Y)$?

Can we reduce params using Bayes Rule?

Suppose X =<X_1,… X_n>

where X_i and Y are boolean RV's

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

how many params for $P(X_1 \cdots X_n | Y)$ $(2^n - 1) \cdot 2$

how many for $P(Y) = 1$

Naïve Bayes

Naïve Bayes assumes

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

i.e., that X_i and X_j 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:

$$\begin{aligned} P(X_1, X_2|Y) &= P(X_1|X_2, Y)P(X_2|Y) \\ &= P(X_1|Y)P(X_2|Y) \end{aligned}$$

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

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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 uses assumption that the X_i are conditionally independent, given Y

Given this assumption, then:

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

$$= P(X_1|Y)P(X_2|Y)$$ Cond. Indep.

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? $2(2^n-1)+1$
- With conditional indep assumption? $2n \quad + 1$

Naïve Bayes in a Nutshell

Bayes rule:

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

Assuming conditional independence among X_i' s:

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

So, to pick most probable Y for $X^{new} = < X_1, \dots, X_n >$

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

Naïve Bayes Algorithm – discrete X_i

- Train Naïve Bayes (examples)

  for each* value y_k

  estimate $\pi_k \equiv P(Y = y_k)$

  for each* value x_{ij} of each attribute X_i

  estimate $\theta_{ijk} \equiv P(X_i = x_{ij} | Y = y_k)$

- Classify (X^{new})

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

$$Y^{new} \leftarrow \arg\max_{y_k} \; \pi_k \prod_i \theta_{ijk}$$

* probabilities must sum to 1, so need estimate only n-1 of these...

Estimating Parameters: Y, X_i discrete-valued

Maximum likelihood estimates (MLE's):

$$\widehat{\pi}_k = \widehat{P}(Y = y_k) = \frac{\#D\{Y = y_k\}}{|D|}$$

$$\widehat{\theta}_{ijk} = \widehat{P}(X_i = x_{ij} | Y = y_k) = \frac{\#D\{X_i = x_{ij} \wedge Y = y_k\}}{\#D\{Y = y_k\}}$$

Number of items in dataset D for which $Y=y_k$

Example: Live in Sq Hill? $P(S|G,D,M)$

80, 8

- S=1 iff live in Squirrel Hill
- G=1 iff shop at SH Giant Eagle
- D=1 iff Drive to CMU
- M=1 iff Rachel Maddow fan

What probability parameters must we estimate?

Example: Live in Sq Hill? P(S|G,D,M)

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- S=1 iff live in Squirrel Hill
- G=1 iff shop at SH Giant Eagle
- D=1 iff Drive to CMU
- M=1 iff Rachel Maddow fan

	D	M	G	$\hat{S}$
S=1	0	0	1	1 ✓
S=0	0	0	1	1 –
S=1	1	1	1	0 –
0	0	0	0	0 ✓
1	0	0	0	0 –
0	0	0	0	0 ✓
1	0	0	1	1 ✓
1	0	0	1	1 ✓

P(S=1) : .4   32/80 = .4

P(D=1 | S=1) : 6/32 = .188

P(D=1 | S=0) : 18/48 = .38

P(G=1 | S=1) : 29/32 = .91

P(G=1 | S=0) : 17/48 = .35

P(M=1 | S=1) : 2/32 = .06

P(M=1 | S=0) : 3/48 = .06

P(S=0) : .6

P(D=0 | S=1) :

P(D=0 | S=0) :

P(G=0 | S=1) :

P(G=0 | S=0) :

P(M=0 | S=1) :

P(M=0 | S=0) : .94

$P(S=1 \mid G\,M\,D) \Rightarrow P(S=1) \cdot P(G=g \mid S=1)\, P(D=d \mid S=1)\, P(M=m \mid S=1)$

$P(S=0) \; (\quad \mid S=0)\, P(M \mid S=0)\, P(\quad \mid S=0)$

Test: S=1 G=1 D=1 M=0

$P(S=1 \mid X^{Test}) \propto .4 \; .91 \; .19 \; .94$

$P(S=0 \mid X^{Test}) = .54$

$\hat{P}(S=0 \mid X^{Test}) \propto .6 \; .35 \; .38 \; .94$

Example: Live in Sq Hill? $P(S|G,D,B)$

- $S=1$ iff live in Squirrel Hill
- $G=1$ iff shop at SH Giant Eagle
- $D=1$ iff Drive or carpool to CMU
- $B=1$ iff Birthday is before July 1

What probability parameters must we estimate?

Example: Live in Sq Hill? P(S|G,D,E)

- S=1 iff live in Squirrel Hill
- G=1 iff shop at SH Giant Eagle
- D=1 iff Drive or Carpool to CMU
- B=1 iff Birthday is before July 1

P(S=1) :

P(D=1 | S=1) :

P(D=1 | S=0) :

P(G=1 | S=1) :

P(G=1 | S=0) :

P(B=1 | S=1) :

P(B=1 | S=0) :

P(S=0) :

P(D=0 | S=1) :

P(D=0 | S=0) :

P(G=0 | S=1) :

P(G=0 | S=0) :

P(B=0 | S=1) :

P(B=0 | S=0) :

Naïve Bayes: Subtlety #1

Often the X_i are not really conditionally independent

- We use Naïve Bayes in many cases anyway, and it often works pretty well
  - often the right classification, even when not the right probability (see [Domingos&Pazzani, 1996])
- What is effect on estimated P(Y|X)?
  - Extreme case: what if we add two copies: $X_i = X_k$

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$$P(Y=y \mid X) \propto P(Y=y) \underbrace{\prod_i P(X_i = x \mid Y=y)}_{P(X_1, \ldots, X_n \mid Y=y)}$$

Naïve Bayes: Subtlety #2

If unlucky, our MLE estimate for $P(X_i \mid Y)$ might be zero.
(for example, X_i = *birthdate.* X_i = *Jan_25_1992*)

- Why worry about just one parameter out of many?

- What can be done to address this?

Naïve Bayes: Subtlety #2

If unlucky, our MLE estimate for $P(X_i \mid Y)$ might be zero. (e.g., X_i = Birthday_Is_January_30_1992)

- Why worry about just one parameter out of many?

$$P(Y|X) \propto P(Y) \prod_i \underbrace{P(X_i = x^{New} | Y)}_{0}$$

- What can be done to address this?

Estimating Parameters

- Maximum Likelihood Estimate (MLE): choose θ 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 the data

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

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

Estimating Parameters: Y, X_i discrete-valued

Maximum likelihood estimates:

$$\widehat{\pi}_k = \widehat{P}(Y = y_k) = \frac{\#D\{Y = y_k\}}{|D|}$$

$$\hat{\theta}_{ijk} = \hat{P}(X_i = x_j | Y = y_k) = \frac{\#D\{X_i = x_j \wedge Y = y_k\}}{\#D\{Y = y_k\}}$$

MAP estimates (Beta, Dirichlet priors):

$$\hat{\pi}_k = \hat{P}(Y = y_k) = \frac{\#D\{Y = y_k\} + (\beta_k - 1)}{|D| + \sum_m (\beta_m - 1)}$$

Only difference:
"imaginary" examples

$$\hat{\theta}_{ijk} = \hat{P}(X_i = x_j | Y = y_k) = \frac{\#D\{X_i = x_j \wedge Y = y_k\} + (\beta_k - 1)}{\#D\{Y = y_k\} + \sum_m (\beta_m - 1)}$$

Learning to classify text documents

- Classify which emails are spam?
- Classify which emails promise an attachment?
- Classify which web pages are student home pages?

How shall we represent text documents for Naïve Bayes?

Baseline: Bag of Words Approach

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

Learning to classify document: P(Y|X) the "Bag of Words" model

- Y discrete valued. e.g., Spam or not
- $X = \langle X_1, X_2, \ldots X_n \rangle$ = document

- X_i is a random variable describing the word at position i in the document
- possible values for X_i : any word w_k in English

- Document = bag of words: the vector of counts for all w_k's
  - like #heads, #tails, but we have many more than 2 values
  - assume word probabilities are position independent (i.i.d. rolls of a 50,000-sided die)

Naïve Bayes Algorithm – discrete X_i

- Train Naïve Bayes (examples)

  for each value y_k

  estimate $\pi_k \equiv P(Y = y_k)$

  for each value x_j of each attribute X_i

  estimate $\theta_{ijk} \equiv P(X_i = x_j | Y = y_k)$

  prob that word x_j appears in position i, given $Y=y_k$

- Classify (X^{new})

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

$$Y^{new} \leftarrow \arg\max_{y_k} \; \pi_k \prod_i \theta_{ijk}$$

* Additional assumption: word probabilities are position independent

$$\theta_{ijk} = \theta_{mjk} \;\; \text{for all } i, m$$

MAP estimates for bag of words

Map estimate for multinomial

$$\theta_i = \frac{\alpha_i + \beta_i - 1}{\sum_{m=1}^{k} \alpha_m + \sum_{m=1}^{k} (\beta_m - 1)}$$

What β' s should we choose?

Twenty NewsGroups

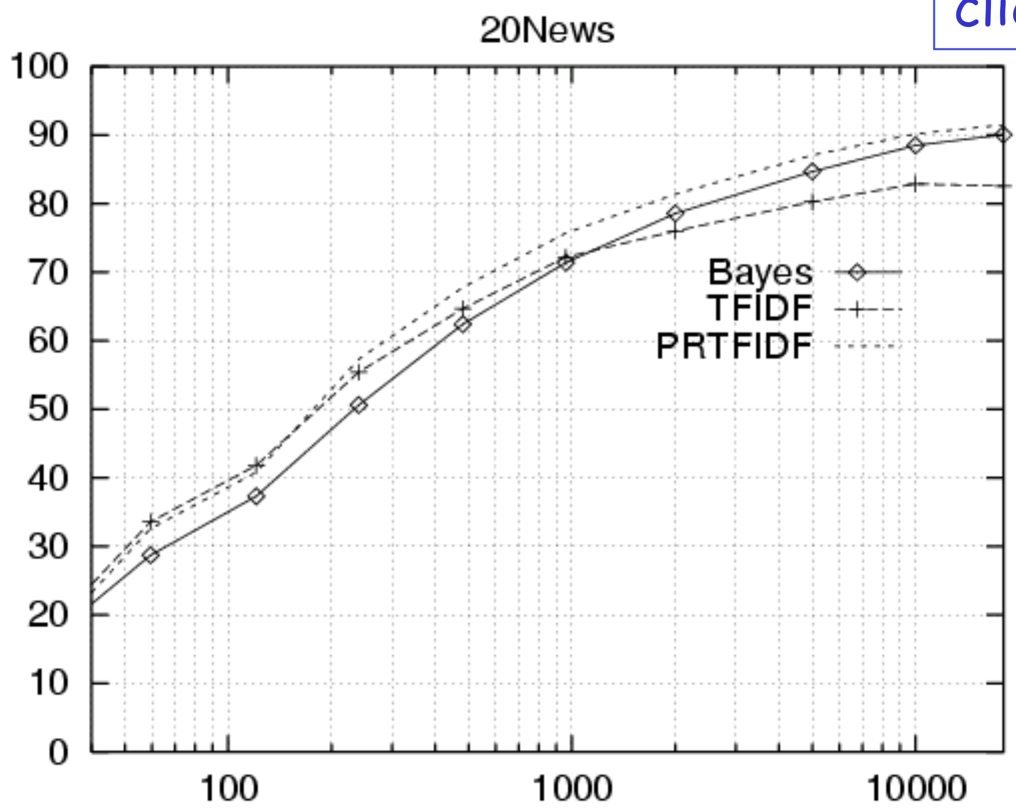
Given 1000 training documents from each group
Learn to classify new documents according to which newsgroup it came from

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

Learning Curve for 20 Newsgroups

For code and data, see
www.cs.cmu.edu/~tom/mlbook.html
click on “Software and Data”



Accuracy vs. Training set size (1/3 withheld for test)

What you should know:

- Training and using classifiers based on Bayes rule
- Conditional independence
  - What it is
  - Why it's important
- Naïve Bayes
  - What it is
  - Why we use it so much
  - Training using MLE, MAP estimates
  - Discrete variables and continuous (Gaussian)

Questions:

- How can we extend Naïve Bayes if just 2 of the X_i‘s are dependent?

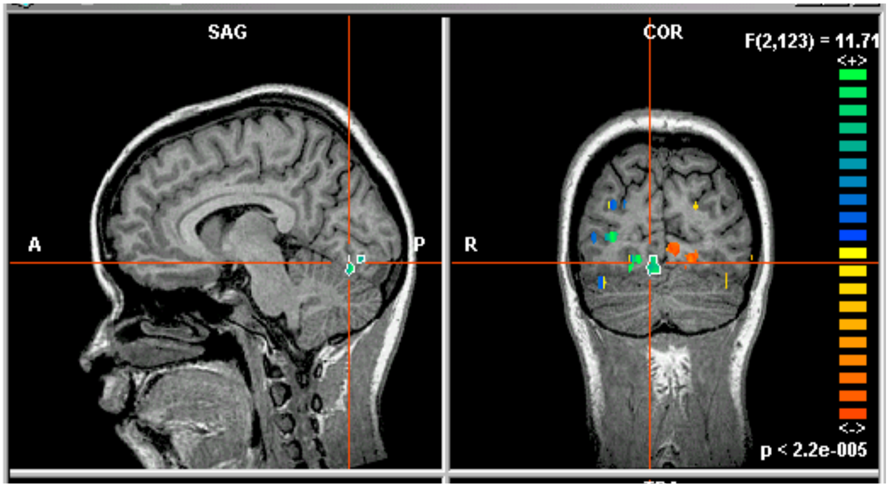
- What does the decision surface of a Naïve Bayes classifier look like?

- What error will the classifier achieve if Naïve Bayes assumption is satisfied and we have infinite training data?

- Can you use Naïve Bayes for a combination of discrete and real-valued X_i?

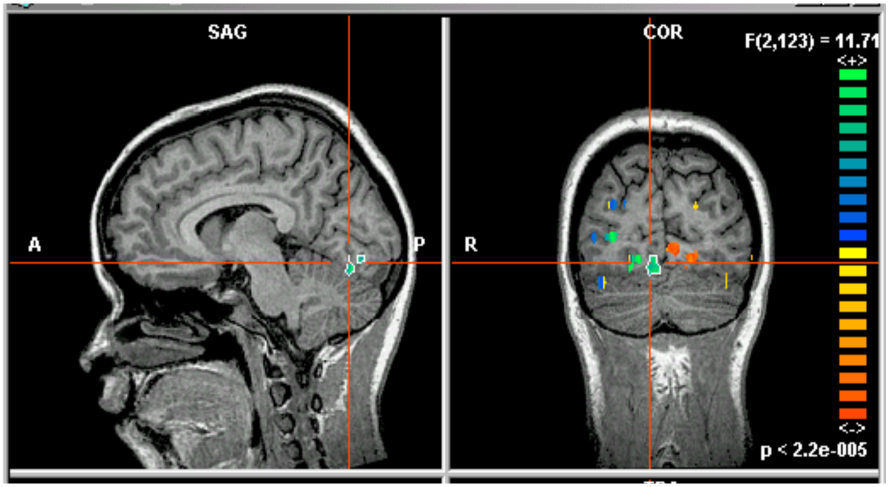
What if we have continuous X_i ?

Eg., image classification: X_i is ith pixel



What if we have continuous X_i ?

image classification: X_i is i[th] pixel, Y = mental state



Still have:

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

Just need to decide how to represent $P(X_i \mid Y)$

What if we have continuous X_i ?

Eg., image classification: X_i is i[th] pixel

Gaussian Naïve Bayes (GNB): assume

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

Sometimes assume σ_{ik}

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

Gaussian Naïve Bayes Algorithm – continuous X_i (but still discrete Y)

- Train Naïve Bayes (examples)

  for each value y_k

  estimate* $\pi_k \equiv P(Y = y_k)$

  for each attribute X_i estimate

  class conditional mean μ_{ik}, variance σ_{ik}

- Classify (X^{new})

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

$$Y^{new} \leftarrow \arg\max_{y_k} \; \pi_k \prod_i Normal(X_i^{new}, \mu_{ik}, \sigma_{ik})$$

* probabilities must sum to 1, so need estimate only n-1 parameters...

Estimating Parameters: Y discrete, X_i continuous

Maximum likelihood estimates:

jth training example

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

ith feature

kth class

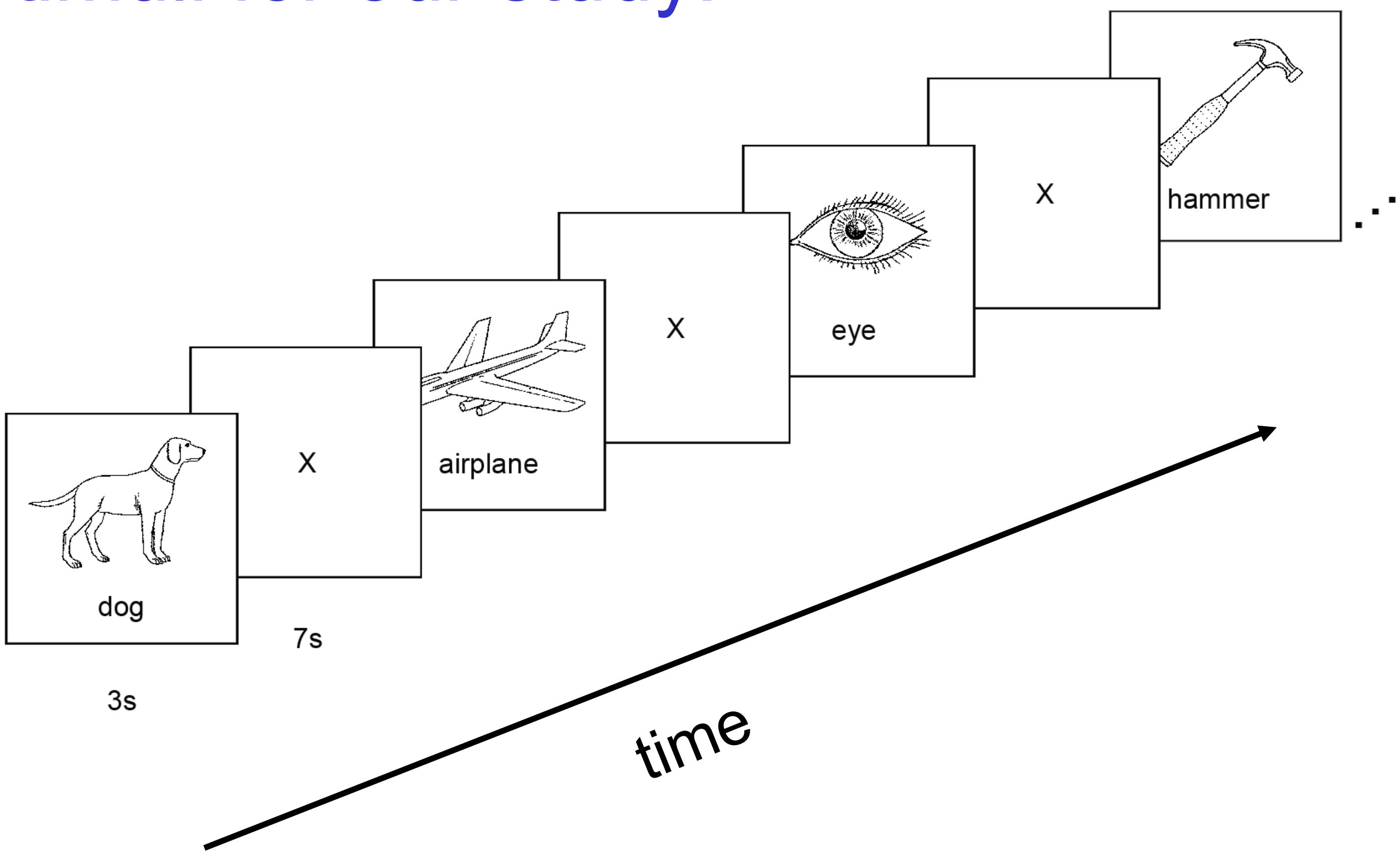
δ(z)=1 if z true, else 0

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

GNB Example: Classify a person's cognitive activity, based on brain image

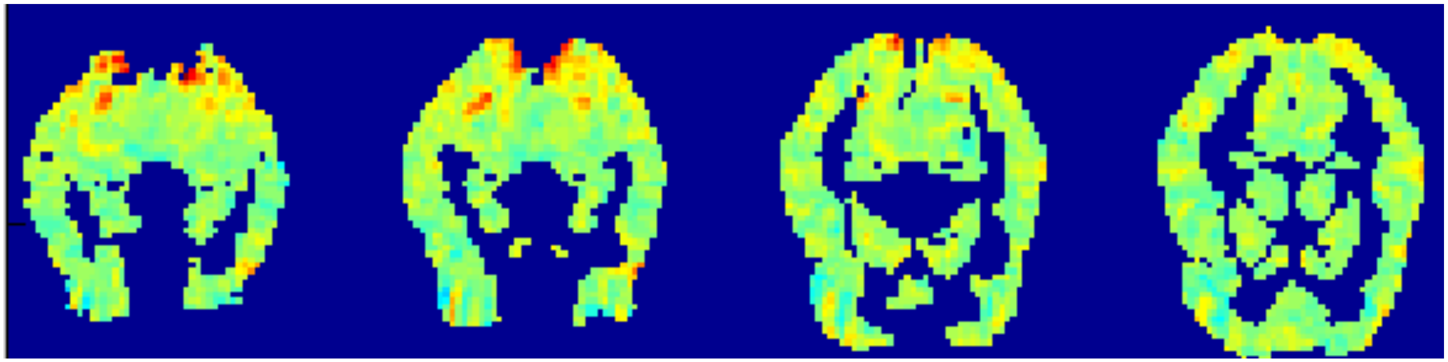
- are they reading a sentence or viewing a picture?
- reading the word "Hammer" or "Apartment"
- viewing a vertical or horizontal line?
- answering the question, or getting confused?

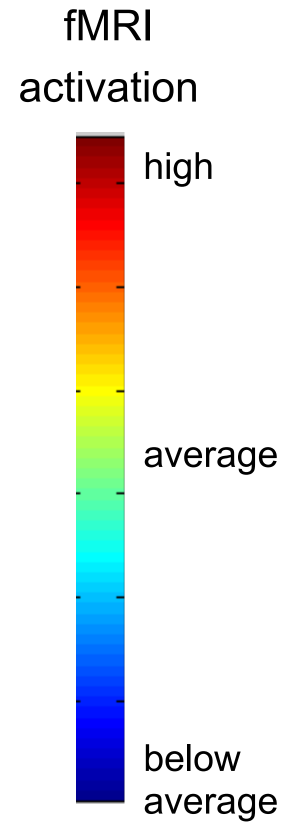
Stimuli for our study:



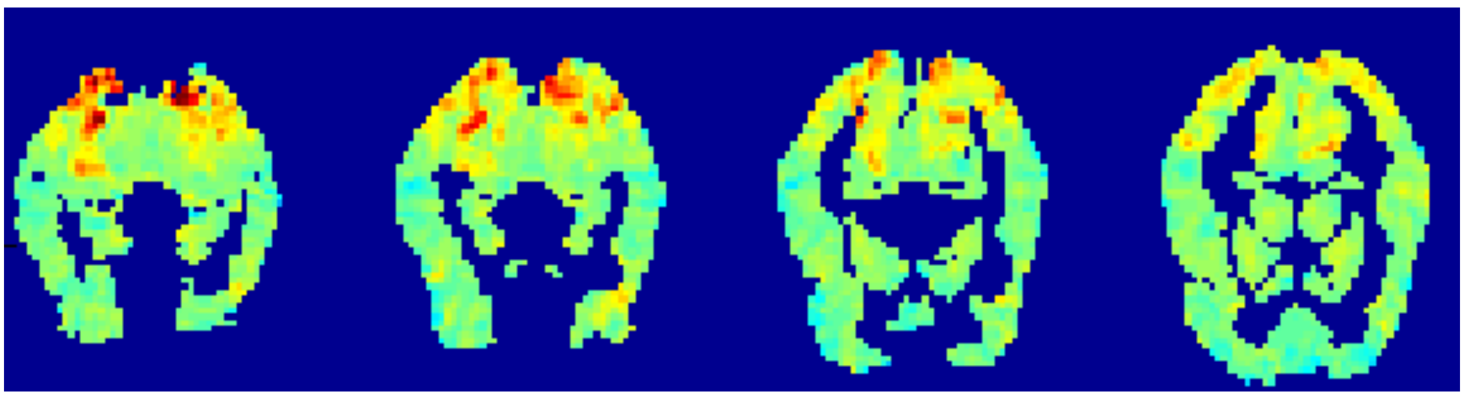
60 distinct exemplars, presented 6 times each

fMRI voxel means for “bottle”: means defining P(Xi | Y=“bottle)

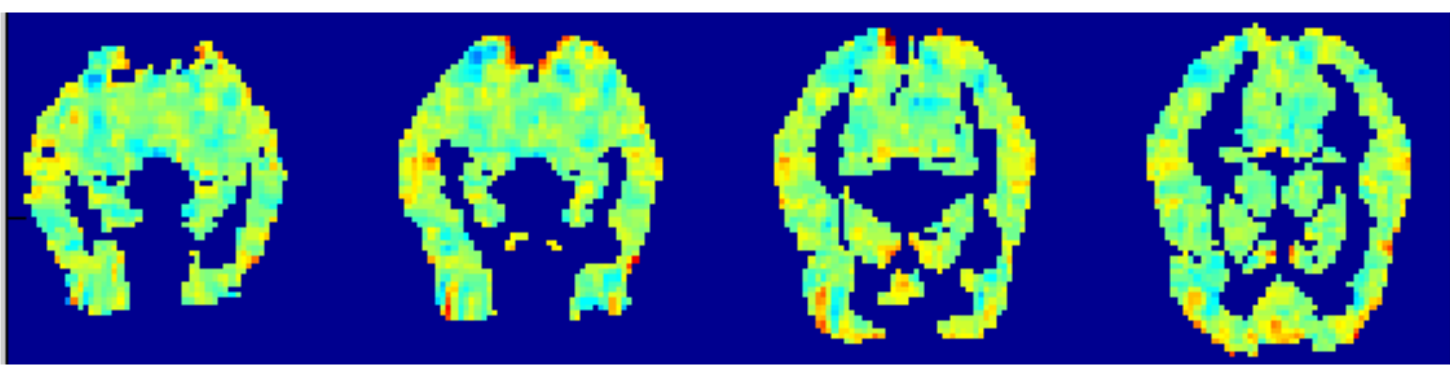




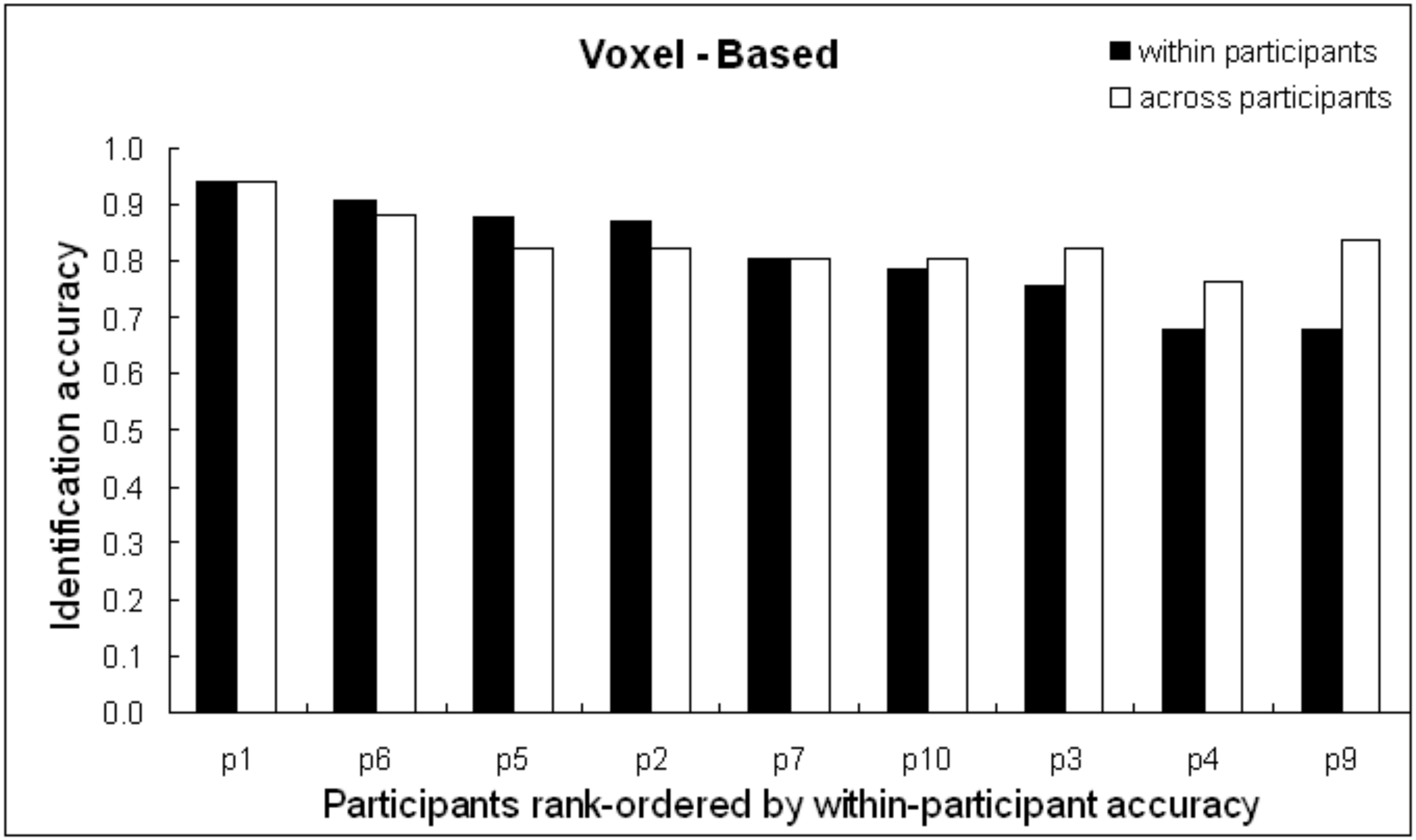
Mean fMRI activation over all stimuli:



“bottle” minus mean activation:

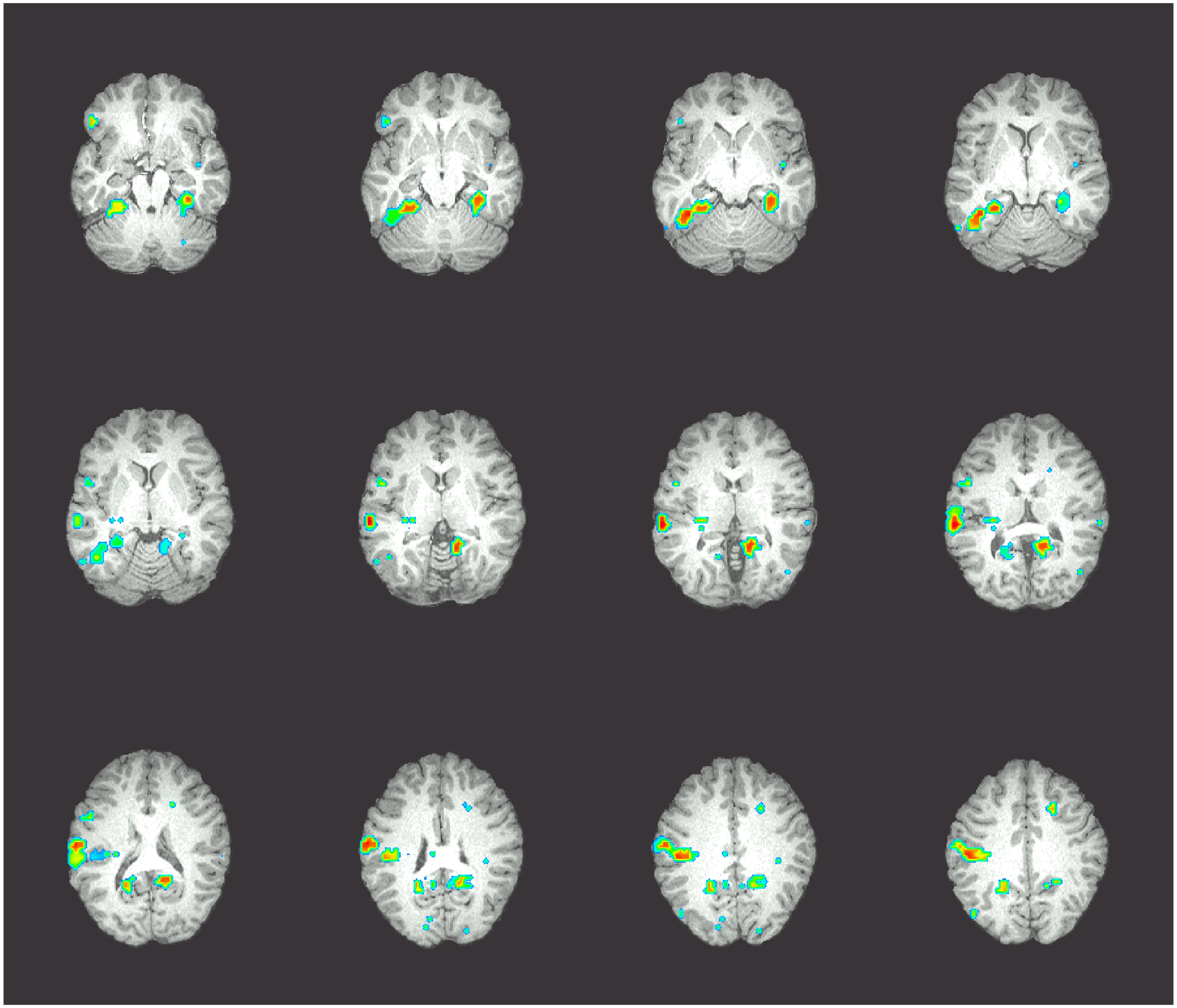


Rank Accuracy Distinguishing among 60 words



Tools vs Buildings: where does brain encode their word meanings?

Accuracies of cubical 27-voxel Naïve Bayes classifiers centered at each voxel [0.7-0.8]



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 random vars 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=playsFootball

or X=gender, Y=leftHanded

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