Machine Learning CMSC-471

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Today:
- Naïve Bayes
  - discrete-valued X_i's
  - Document classification
- Gaussian Naïve Bayes
  - real-valued X_i's
  - Brain image classification

Recently:

- Bayes classifiers to learn P(Y|X)
- MLE and MAP estimates for parameters of P
- Conditional independence
- Naïve Bayes → make Bayesian learning practical

Next:

- Text classification
- Naïve Bayes and continuous variables X_i:
  - Gaussian Naïve Bayes classifier
- Learn P(Y|X) directly
  - Logistic regression, Regularization, Gradient ascent
- Naïve Bayes or Logistic Regression?
  - Generative vs. Discriminative classifiers

Discriminative vs Generative Models

Discriminative Models	**Generative Models**
Directly learn the function mapping $h: X \rightarrow y$ **or,** Calculate likelihood $P(y\|X)$	Calculate $P(y\|X)$ **from** $P(X\|y)$ **and** $P(y)$ **But Joint Distribution** $P(X, y) = P(X\|y)\,P(y)$
1. Assume some functional form for $P(y\|X)$ 2. Estimate parameters of $P(y\|X)$ directly from training data	1. Assume some functional form for $P(y), P(X\|y)$ 2. Estimate parameters of $P(X\|y), P(y)$ directly from training data 3. Use Bayes rule to calculate $P(y\|X)$

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

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

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

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 $P(X_1, \ldots X_n \mid Y)$?

$P(X|Y=1)$ ----- $2^n - 1$
$P(X|Y=0)$ ----- $2^n - 1$

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

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

Naïve Bayes uses assumption that the X_i are conditionally independent, given Y

Given this assumption, then:

$$P(X_1, X_2|Y) = P(X_1|X_2, Y)P(X_2|Y) \quad \text{Chain rule}$$
$$= P(X_1|Y)P(X_2|Y) \quad \text{Cond. Indep.}$$

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? $2n + 1$

Naïve Bayes in a Nutshell

Bayes rule:

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

Assuming conditional independence among X_i's:

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

So, classification rule for X^{new} = < $X_1, \ldots, X_n$ > is:

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

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?

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What probability parameters must we estimate?

P(S=1) :
P(D=1 | S=1) :
P(D=1 | S=0) :
P(G=1 | S=1) :
P(G=1 | S=0) :
P(M=1 | S=1) :
P(M=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(M=0 | S=1) :
P(M=0 | S=0) :

Example: Boolean variables A, B, C

A	B	C	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

Example: Live in Sq Hill? P(S|G,D,B) n= 18+33+22+29

- 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) :	5+7+10+4 = 26/102	P(S=0) :	76/102
P(D=1 | S=1) :	3/26	P(D=0 | S=1) :	23/26
P(D=1 | S=0) :	1/76	P(D=0 | S=0) :	
P(G=1 | S=1) :	5+8+4+9/26	P(G=0 | S=1) :	0/26
P(G=1 | S=0) :	7+11+11+8/76	P(G=0 | S=0) :	
P(B=1 | S=1) :	1+2+5+2/26	P(B=0 | S=1) :	16/26
P(B=1 | S=0) :	5+7+8+6/76	P(B=0 | S=0) :	50/76

Tom: D=1, G=0, B=0

P(S=1|D=1,G=0,B=0) =

$$\frac{P(S=1)\, P(D=1|S=1)\, P(G=0|S=1)\, P(B=0|S=1)}{[P(S=1)\, P(D=1|S=1)\, P(G=0|S=1)\, P(B=0|S=1) + P(S=0)\, P(D=1|S=0)\, P(G=0|S=0)\, P(B=0|S=0)]}$$

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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$$P(Y=y|X) \propto P(Y=y)\prod_i P(X_i=x|Y=y)$$

$$P(X_1,\dots,X_n|Y=y)$$

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 $\mathcal{D}$

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Estimating Parameters: Y, X_i discrete-valued

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

MAP estimates (Beta, Dirichlet priors):

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

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

Only difference:
"imaginary" examples

Naïve Bayes: classifying text documents

- Classify which emails are spam?
- Classify which emails promise an attachment?

> I am pleased to announce that Bob Frederking of the Language Technologies Institute is our new Associate Dean for Graduate Programs. In this role, he oversees the many issues that arise with our multiple masters and PhD programs. Bob brings to this position considerable experience with the masters and PhD programs in the LTI.
>
> I would like to thank Frank Pfenning, who has served ably in this role for the past two years.
>
> ********************************
>
> Randal E. Bryant
> Dean and University Professor

How shall we represent text documents for Naïve Bayes?

Learning to classify documents: P(Y|X)

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

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- X_i is a random variable describing…

Answer 1: X_i is boolean, 1 if word i is in document, else 0

e.g., $X_{pleased} = 1$

Issues?

Learning to classify documents: P(Y|X)

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

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- X_i is a random variable describing…

Answer 2:

- X_i represents the i^{th} *word position* in document
- X_1 = "I", X_2 = "am", X_3 = "pleased"
- and, let's assume the X_i are iid (indep, identically distributed)

$$P(X_i|Y) = P(X_j|Y) \quad (\forall i, j)$$

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

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

- X_i are iid random variables. Each represents the word at its position i in the document
- Generating a document according to this distribution = rolling a 50,000 sided die, once for each word position in the document

- The observed counts for each word follow a ??? distribution

Multinomial Distribution

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

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

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

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

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

$$\hat{\theta}_i^{MAP} = \hat{P}(X = i) = \frac{\alpha_i + \beta_i - 1}{\sum_{j=1}^{k} (\alpha_j + \beta_j - 1)}$$

Multinomial Distribution

K sides

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

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

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

$\theta_i = P(X = i)$

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

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

$$\hat{\theta}_i^{MAP} = \hat{P}(X = i) = \frac{\alpha_i + \beta_i - 1}{\sum_{j=1}^{k} (\alpha_j + \beta_j - 1)}$$

Dirichlet is a generalization of Beta Distribution

Multinomial Bag of Words

counts / α_i's

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

Bag of Word Model

MAP estimates for bag of words

Map estimate for multinomial

$$\hat{\theta}_i^{MAP} = \hat{P}(X = i) = \frac{\alpha_i + \beta_i - 1}{\sum_{j=1}^{k}(\alpha_j + \beta_j - 1)}$$

$$\hat{\theta}_{aardvark}^{MAP} = P(X = \text{aardvark}) = \frac{\#\text{ observed 'aardvark'} + \#\text{ hallucinated 'aardvark'}}{\#\text{ observed words} + \#\text{ hallucinated words}}$$

What β's should we choose?

MAP estimates for bag of words

Map estimate for multinomial

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What β's should we choose?

- Large document, how many times each word occur
- Uniform distribution

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

  prob that word x_{ij} 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

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

Naïve Bayes Algorithm – discrete X_i

- Train Naïve Bayes (examples)

  for each value y_k

  spam: k=1
  ¬spam: k=0

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

  for each value x_{ij} of each attribute X_i

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

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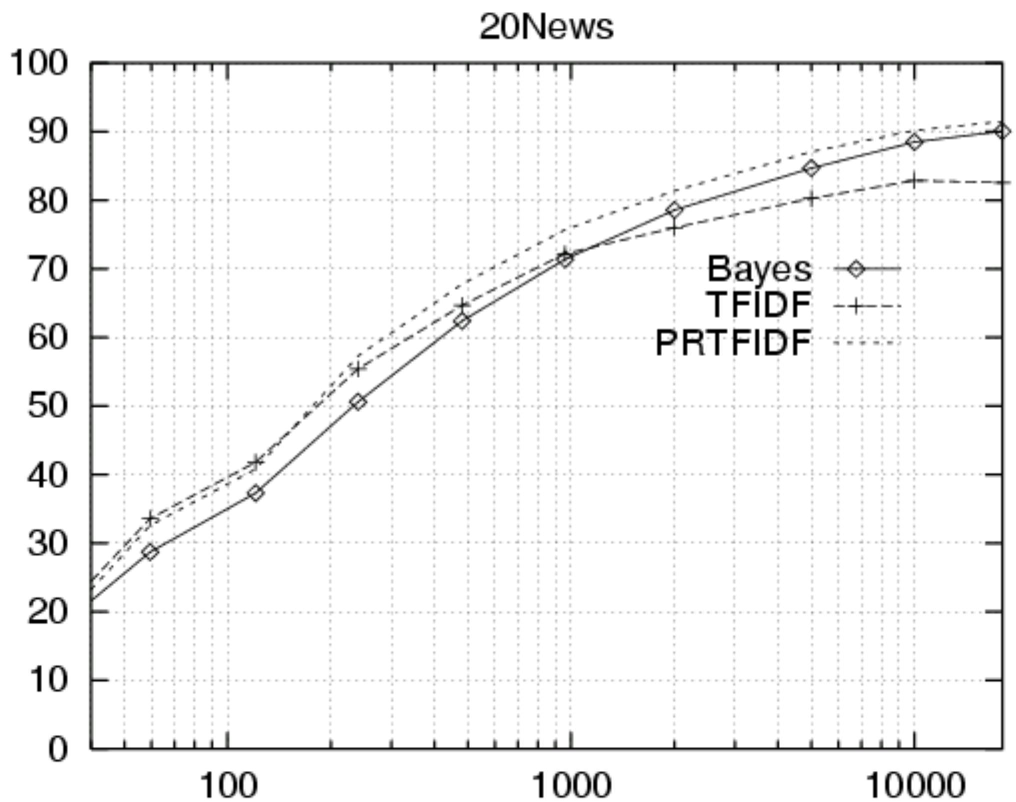
Twenty NewsGroups

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

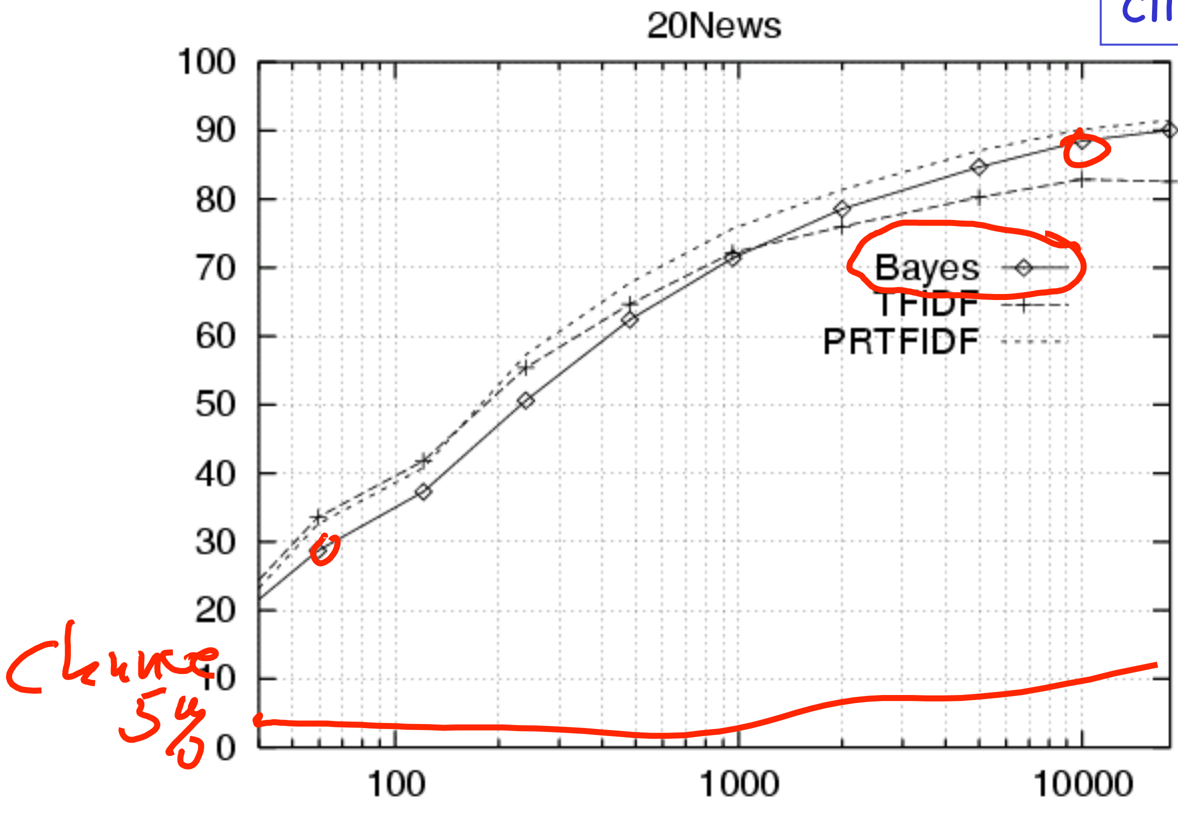
Learning Curve for 20 Newsgroups



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

Learning Curve for 20 Newsgroups

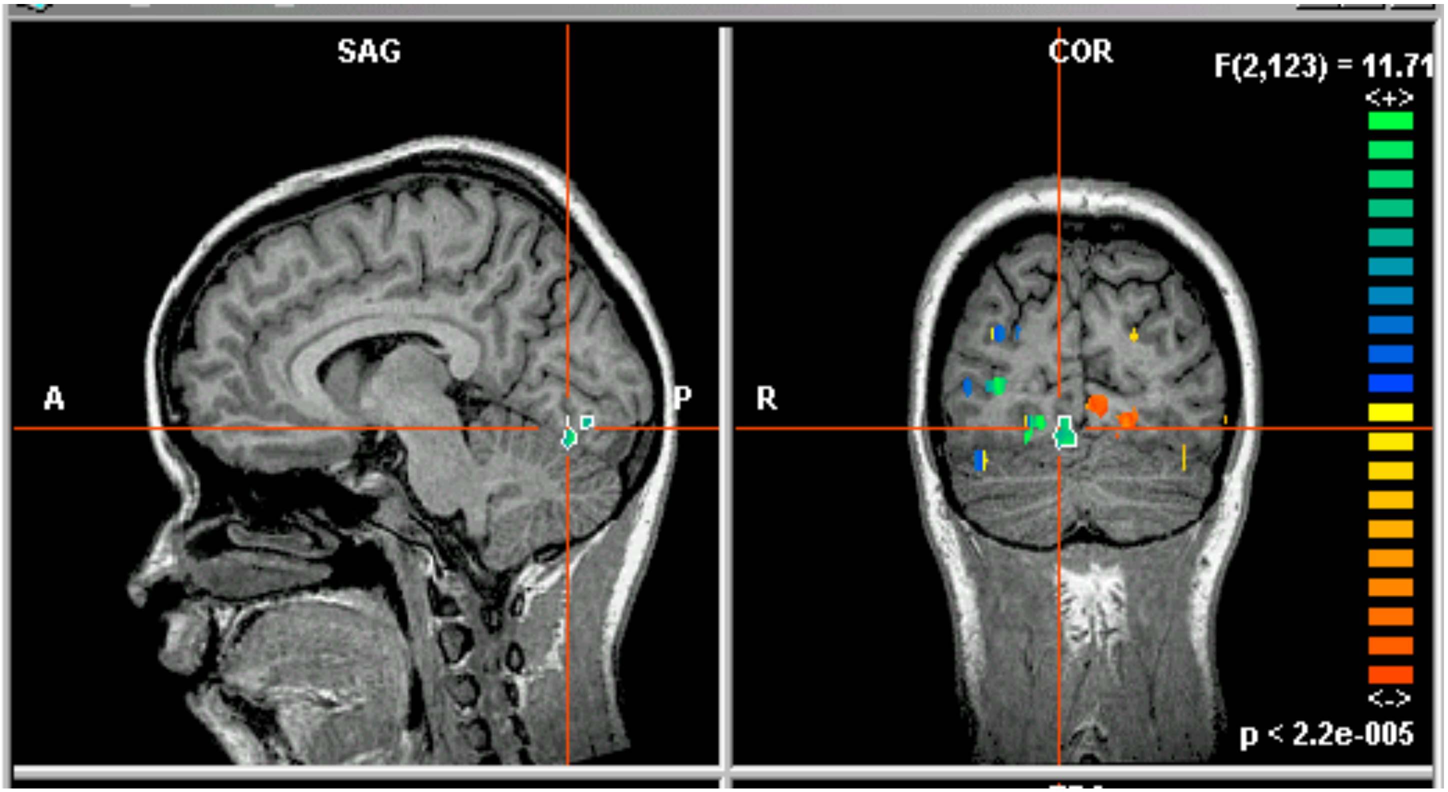
For code and data, see
www.cs.cmu.edu/~tom/mlbook.html
click on "Software and Data"



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

What if we have continuous X_i ?

Eg., image classification: X_i is real-valued ith pixel



What if we have continuous X_i ?

Eg., image classification: X_i is real-valued ith pixel

Naïve Bayes requires $P(X_i \mid Y=y_k)$, but X_i is real (continuous)

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

Common approach: assume $P(X_i \mid Y=y_k)$ follows a Normal (Gaussian) distribution

What if we have continuous X_i ?

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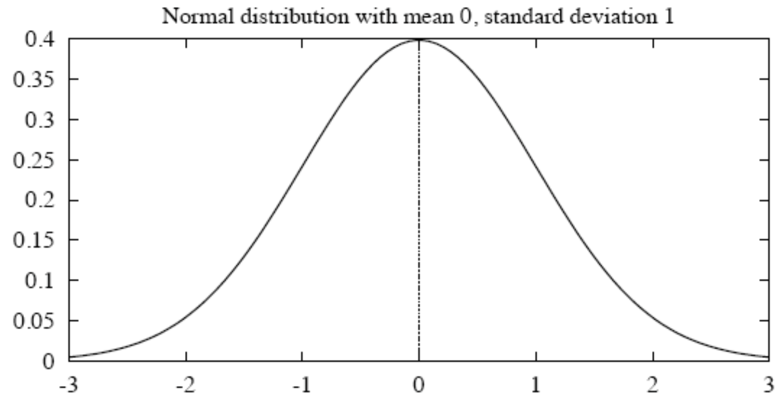
Common approach: assume $P(X_i \mid Y=y_k)$ follows a Normal (Gaussian) distribution

Gaussian Distribution

(also called "Normal")

p(x) is a *probability density function*, whose integral (not sum) is 1



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

The probability that X will fall into the interval (a, b) is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of X, $E[X]$, is

$$E[X] = \mu$$

- Variance of X is

$$Var(X) = \sigma^2$$

- Standard deviation of X, σ_X, is

$$\sigma_X = \sigma$$

What if we have continuous X_i ?

Gaussian Naïve Bayes (GNB): assume

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

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)

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 $P(X_i|Y = y_k)$

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

- Classify (X^{new})

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

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

* 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

$\delta()=1$ if $(Y^j=y_k)$ else 0

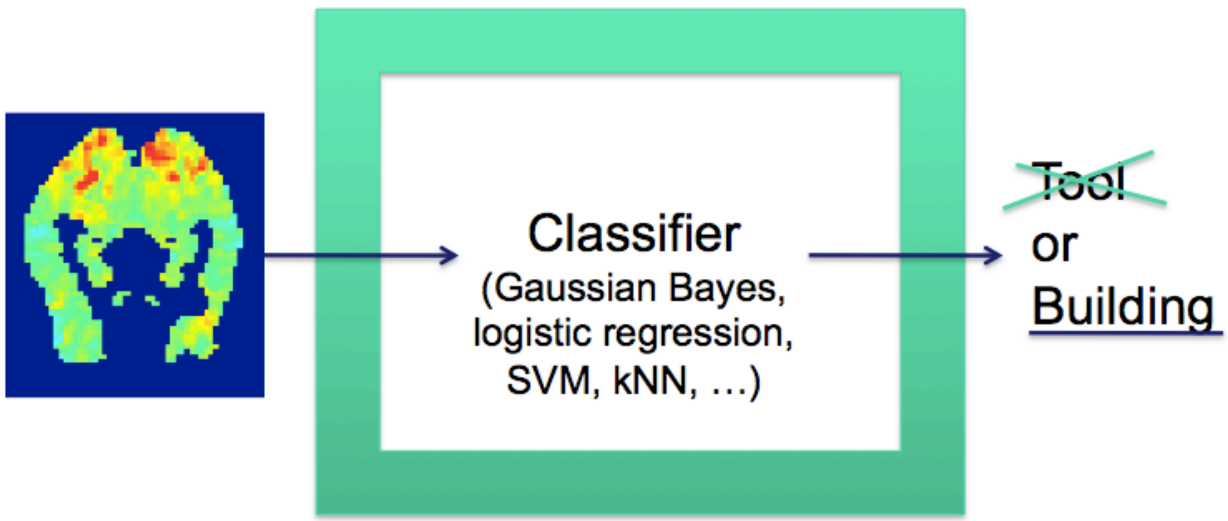
$$\widehat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \widehat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

How many parameters must we estimate for Gaussian Naïve Bayes if Y has k possible values, X=<X1, … Xn>?

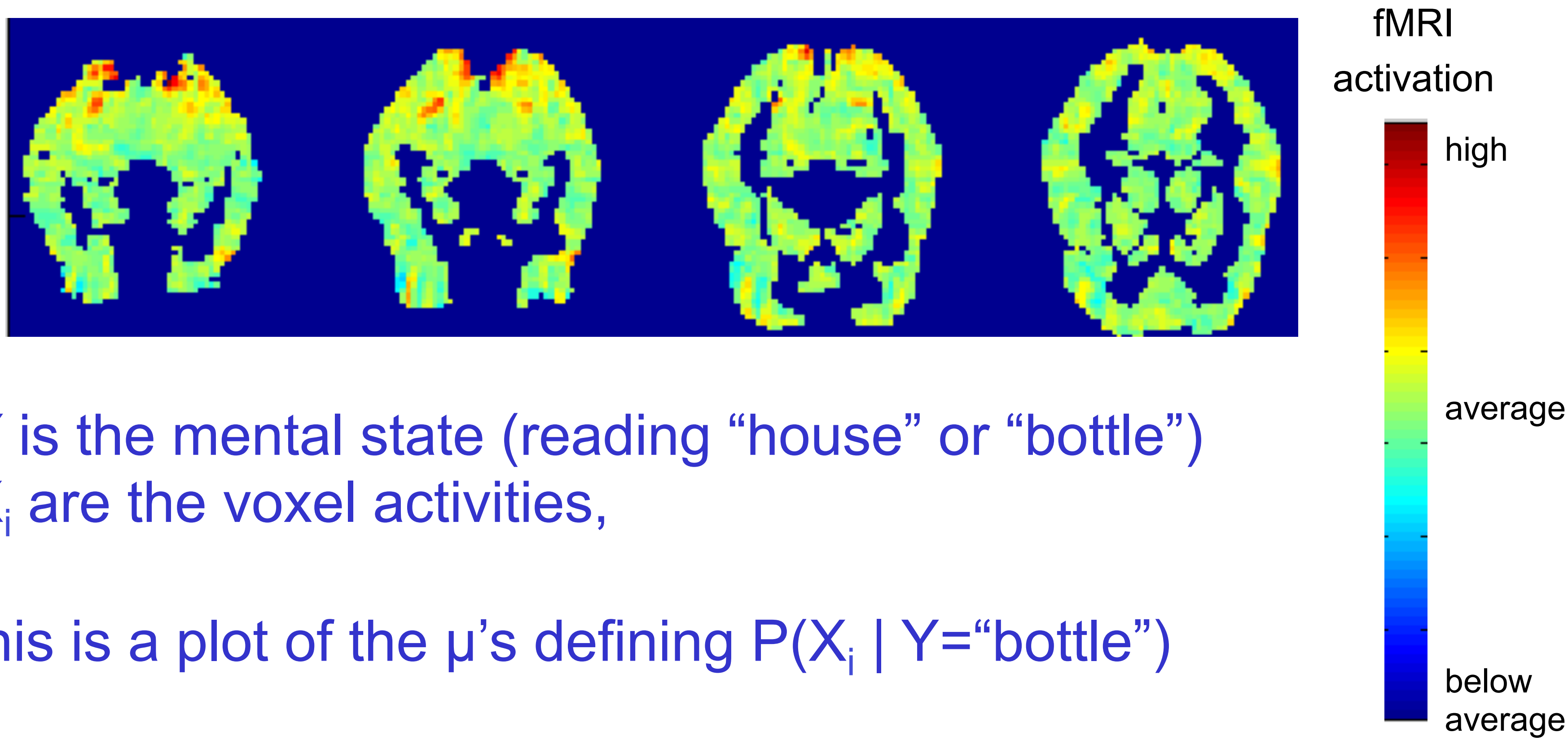
$$p(X_i = x | Y = y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \; e^{-\frac{1}{2}(\frac{x-\mu_{ik}}{\sigma_{ik}})^2}$$

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

- reading a sentence or viewing a picture?
- reading the word describing a "Tool" or "Building"?
- answering the question, or getting confused?



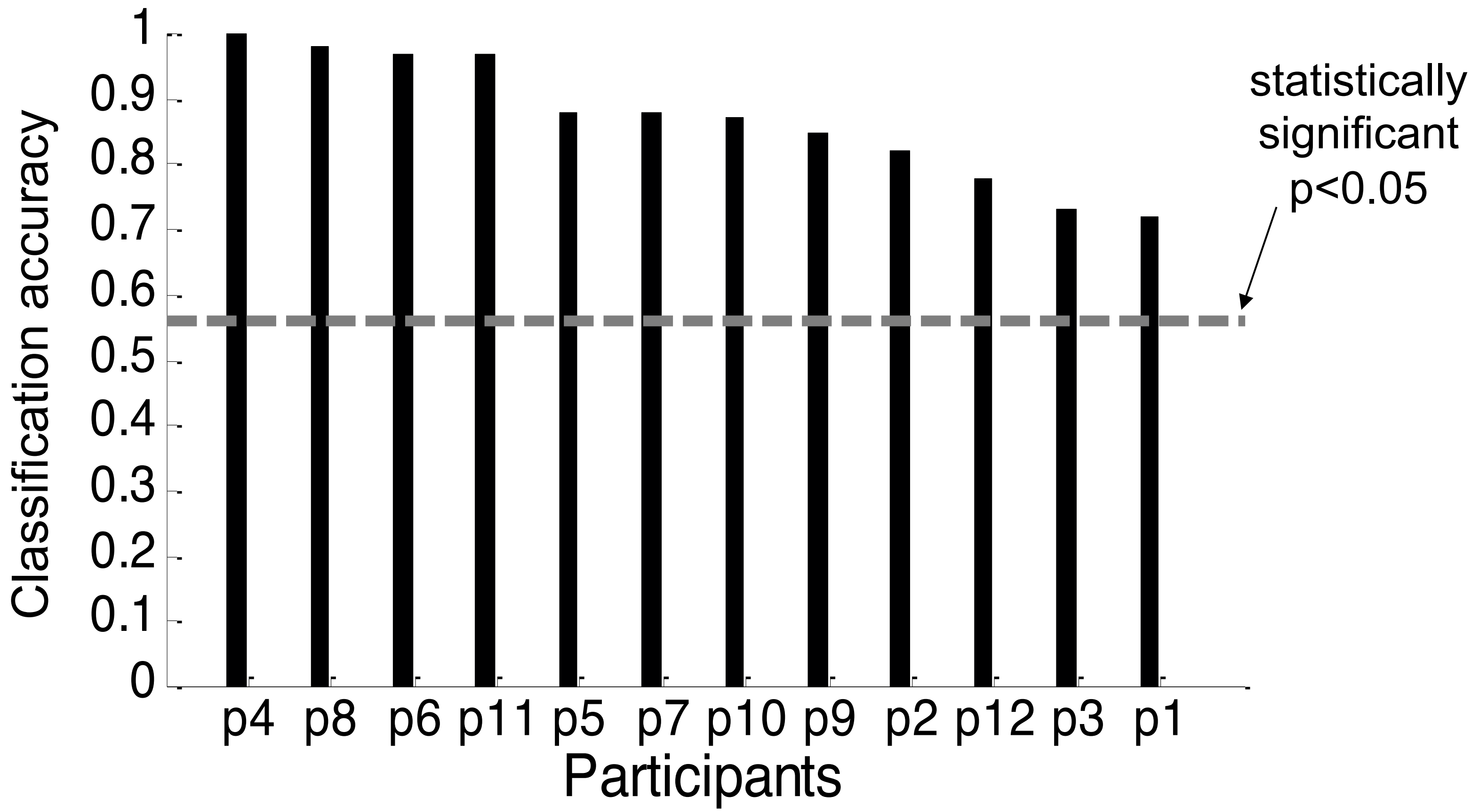
Mean activations over all training examples for Y="bottle"



Y is the mental state (reading "house" or "bottle")
X_i are the voxel activities,

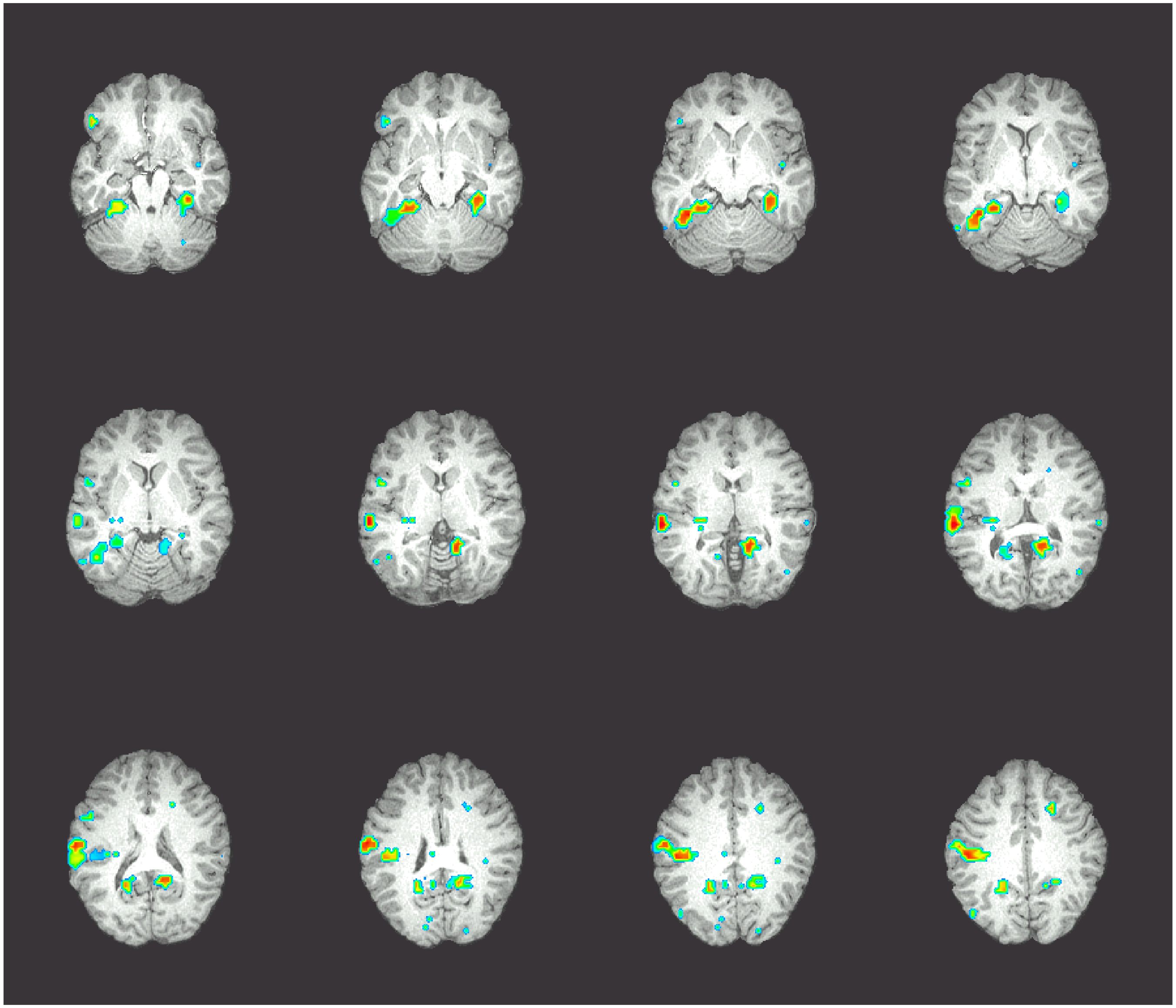
this is a plot of the μ's defining $P(X_i \mid Y=\text{"bottle"})$

Classification task: is person viewing a "tool" or "building"?



Where is information encoded in the brain?

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



Naïve Bayes: What you should know

- Designing classifiers based on Bayes rule

- Conditional independence
  - What it is
  - Why it's important

- Naïve Bayes assumption and its consequences
  - Which (and how many) parameters must be estimated under different generative models (different forms for P(X|Y))
    - and why this matters

- How to train Naïve Bayes classifiers
  - MLE and MAP estimates
  - with discrete and/or continuous inputs X_i

Questions to think about:

- Can you use Naïve Bayes for a combination of discrete and real-valued X_i?
- How can we easily model just 2 of n attributes as dependent?
- What does the decision surface of a Naïve Bayes classifier look like?
- How would you select a subset of X_i's?