# Machine Learning 10-601


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September 27, 2011

Today:
- MAP estimates, Conjugate priors
- Naïve Bayes
  - discrete-valued $X_i$'s
  - Document classification
- Gaussian Naïve Bayes
  - real-valued $X_i$'s
  - Brain image classification

Readings:

Required:
- Mitchell: "Naïve Bayes and Logistic Regression" (available on class website)

Optional
- Bishop 1.2.4
- Bishop 4.2

## Summary: Maximum Likelihood Estimate

- Data:
  - We observed $N$ ***iid*** coin tossing: $D=\{1, 0, 1, \ldots, 0\}$
- Representation:

Binary r.v: $x_n = \{0,1\}$

Bernoulli distribution

- Model:

$$P(x) = \begin{cases} 1-\theta & \text{for } x=0 \\ \theta & \text{for } x=1 \end{cases} \Rightarrow P(x) = \theta^x (1-\theta)^{1-x}$$

- The likelihood of dataset $D=\{x_1, \ldots, x_N\}$:

$$P(x_1, x_2, \ldots, x_N | \theta) = \prod_{i=1}^{N} P(x_i|\theta) = \prod_{i=1}^{N} \left(\theta^{x_i}(1-\theta)^{1-x_i}\right) = \theta^{\sum_{i=1}^{N} x_i} (1-\theta)^{\sum_{i=1}^{N} 1-x_i} = \theta^{\#\text{head}}(1-\theta)^{\#\text{tails}}$$

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(x_1, x_2 \ldots x_n | \theta) = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

# Estimating Parameters

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

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

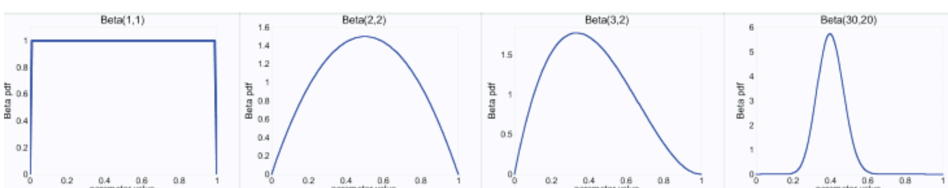
- Maximum a Posteriori (MAP) estimate: choose $\theta$ that is most probable given prior probability and the data

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

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

# Beta prior distribution – P(θ)

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




[C. Guestrin]

## Posterior Distribution: P(Θ | D)

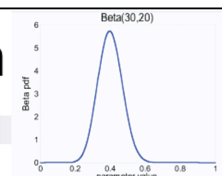
- $$P(\theta) = \frac{\theta^{\beta_H-1}(1-\theta)^{\beta_T-1}}{B(\beta_H,\beta_T)} \sim Beta(\beta_H,\beta_T)$$

- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \;\propto\; P(\mathcal{D} \mid \theta)P(\theta)$

$$\boxed{P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H,\beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H,\beta_T+\alpha_T)}$$

[C. Guestrin]

## MAP for Beta distribution




$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H,\beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H,\beta_T+\alpha_T)$$

- MAP: use most likely parameter:

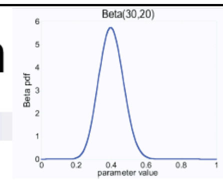
$$\hat{\theta}_{MAP} = \arg\max_{\theta} P(\theta|D) = \frac{\beta_H+\alpha_H-1}{(\beta_H+\alpha_H-1)+(\beta_H+\alpha_T-1)}$$

versus

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta) = \frac{\alpha_H}{\alpha_H+\alpha_T}$$

[C. Guestrin]

# MAP for Beta distribution




$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H, \beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H, \beta_T+\alpha_T)$$

- MAP: use most likely parameter:

$$\hat{\theta}_{MAP} = \arg\max_{\theta} P(\theta|D) = \frac{\beta_H + \alpha_H - 1}{(\beta_H + \alpha_H - 1) + (\beta_H + \alpha_T - 1)}$$

versus

$$\hat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta) = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

- Beta prior equivalent to extra thumbtack flips
- As $N \rightarrow \infty$, prior is "forgotten"
- **But, for small sample size, prior is important!**

[C. Guestrin]

# Conjugate priors

- P(θ) and P(θ|D) have the same form

Eg. 1 Coin flip problem

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

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

**For Binomial, conjugate prior is Beta distribution.**

[A. Singh]

# Conjugate priors

- $P(\theta)$ and $P(\theta|D)$ have the same form

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

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

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

If prior is Dirichlet distribution,

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

Then posterior is Dirichlet distribution

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

**For Multinomial, conjugate prior is Dirichlet distribution.**

[A. Singh]

# Dirichlet distribution

- number of heads in N flips of a two-sided coin
  - follows a binomial distribution
  - Beta is a good prior (conjugate prior for binomial)
- what if it's not two-sided, but k-sided?
  - follows a *multinomial* distribution
  - *Dirichlet* distribution is the conjugate prior

$$P(\theta_1, \theta_2, \dots \theta_K) = \frac{1}{B(\alpha)} \prod_{i}^{K} \theta_i^{(\alpha_1 - 1)}$$

**Lejeune Dirichlet**

Johann Peter Gustav Lejeune Dirichlet

| | |
|---|---|
| Born | 13 February 1805<br>Düren, French Empire |
| Died | 5 May 1859 (aged 54)<br>Göttingen, Hanover |
| Residence | Germany |
| Nationality | German |
| Fields | Mathematician |
| Institutions | University of Berlin<br>University of Breslau<br>University of Göttingen |
| Alma mater | University of Bonn |
| Doctoral advisor | Simeon Poisson<br>Joseph Fourier |
| Doctoral students | Ferdinand Eisenstein<br>Leopold Kronecker<br>Rudolf Lipschitz<br>Carl Wilhelm Borchardt |
| Known for | Dirichlet function<br>Dirichlet eta function |

## Estimating Parameters

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

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

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

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

Another way to view Naïve Bayes (Boolean Y):
Decision rule: is this quantity greater or less than 1?

$$\frac{P(Y=1|X_1 \ldots X_n)}{P(Y=0|X_1 \ldots X_n)} = \frac{P(Y=1)\prod_i P(X_i|Y=1)}{P(Y=0)\prod_i P(X_i|Y=0)}$$

## 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…

## Learning to classify documents: P(Y|X)

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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
- $X = <X_1, X_2, \ldots X_n>$ = 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

- P(θ) and P(θ|D) have the same form

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

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

**For Multinomial, conjugate prior is Dirichlet distribution.**

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# Multinomial Bag of Words


→

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

## MAP estimates for bag of words

Map estimate for multinomial

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

$$\theta_{aardvark} = P(X_i = \text{aardvark}) = \frac{\#\text{ observed 'aardvark' } + \#\text{ hallucinated 'aardvark'} - 1}{\#\text{ observed words } + \#\text{ hallucinated words} - k}$$

What $\beta$'s should we choose?

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

probability that word $x_{ij}$ appears in document 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

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

## Twenty NewsGroups

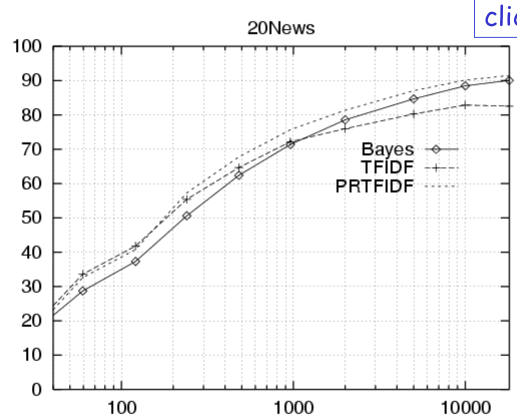
Given 1000 training documents from each group
Learn to classify new documents according to
which newsgroup it came from

| | |
|---|---|
| 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

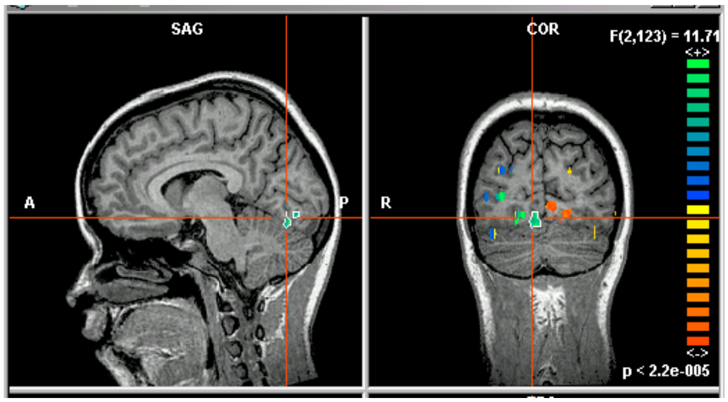
For code and data, see
www.cs.cmu.edu/~tom/mlbook.html
click on "Software and Data"




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

## What if we have continuous $X_i$ ?

Eg., image classification: $X_i$ is real-valued i[th] pixel




## What if we have continuous $X_i$ ?

Eg., image classification: $X_i$ is real-valued i[th] pixel

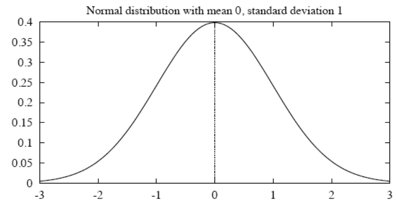
Naïve Bayes requires $P(X_i \mid Y=y_k)$, but $X_i$ is real (continuous)

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

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

## 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 $X$, $\sigma_X$, 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 $\sigma$

- is independent of $Y$ (i.e., $\sigma_i$),
- or independent of $X_i$ (i.e., $\sigma_k$)
- or both (i.e., $\sigma$)

## 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 $P(X_i|Y = y_k)$

  - conditional mean $\mu_{ik}$ , variance $\sigma_{ik}$

- Classify ($X^{new}$)

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

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

Q: how many parameters must we estimate?

## Estimating Parameters: $Y$ discrete, $X_i$ continuous

Maximum likelihood estimates:

jth training example

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

ith feature

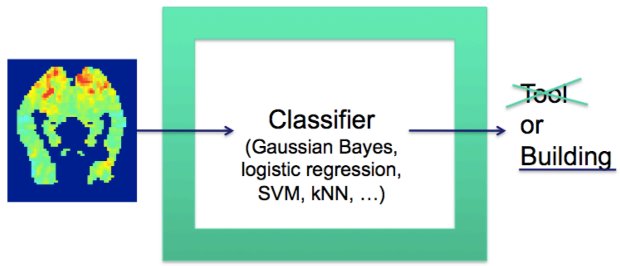
kth class

δ()=1 if ($Y^j$=$y_k$) else 0

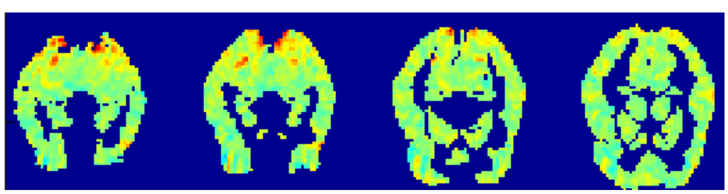
$$\hat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

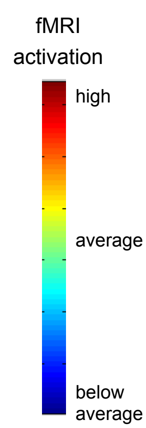
## GNB Example: Classify a person's cognitive state, based on brain image

- 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"

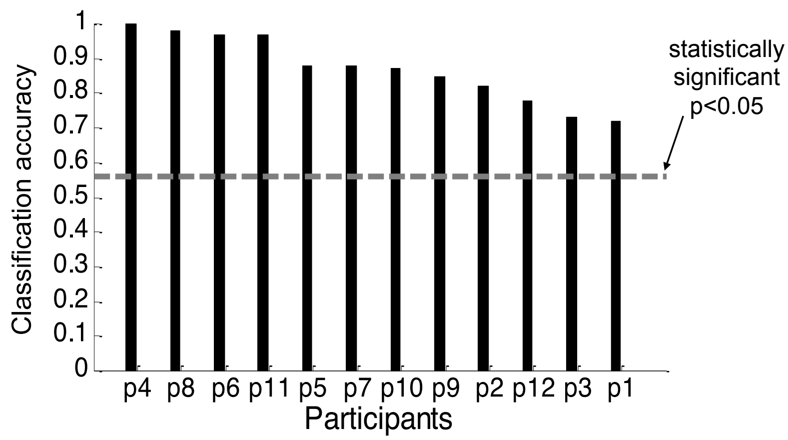





Y is the mental state (reading "house" or "bottle")
$X_i$ are the voxel activities,

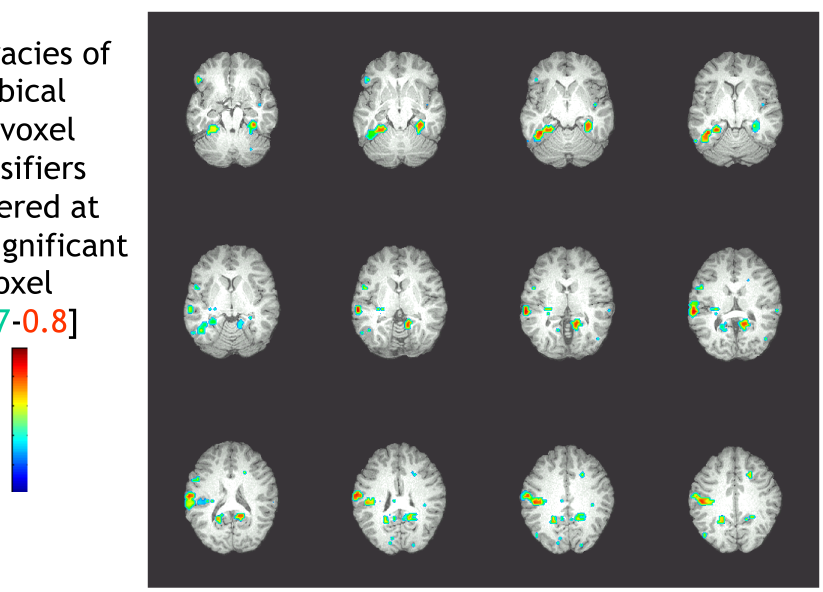
this is a plot of the μ's defining $P(X_i \mid Y=\text{"bottle"})$

## 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?