

Bayes Optimal Classifier & Naïve Bayes

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The logo consists of the letters 'ML' in a bold, black, sans-serif font. A thick red horizontal line is positioned directly beneath the 'L'. The background behind the letters is a light gray with abstract, overlapping geometric shapes.

MACHINE LEARNING DEPARTMENT

The logo features a pattern of small, light gray dots arranged in a grid that tapers to the right, creating a sense of depth and movement.

Carnegie Mellon.
School of Computer Science

Classification

Goal: Construct a **predictor** $f : X \rightarrow Y$ to minimize a risk (performance measure) $R(f)$



Features, X



Sports
Science
News

Labels, Y

$$R(f) = P(f(X) \neq Y)$$

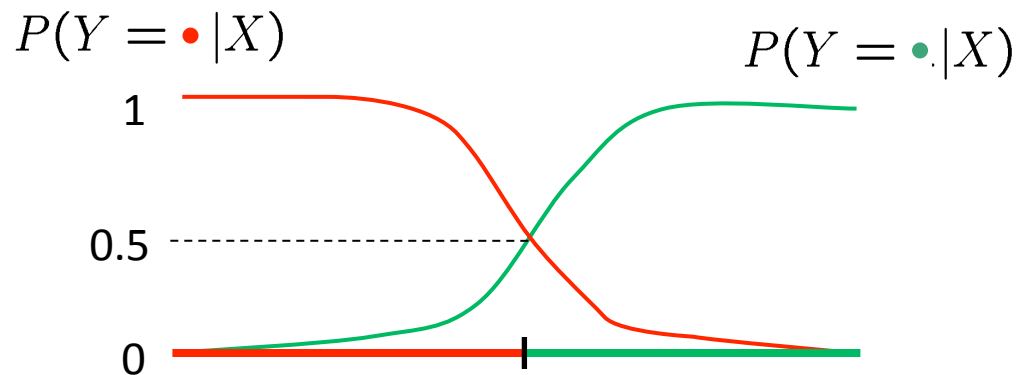
Probability of Error

Optimal Classification

Optimal predictor: $f^* = \arg \min_f P(f(X) \neq Y)$
(Bayes classifier)

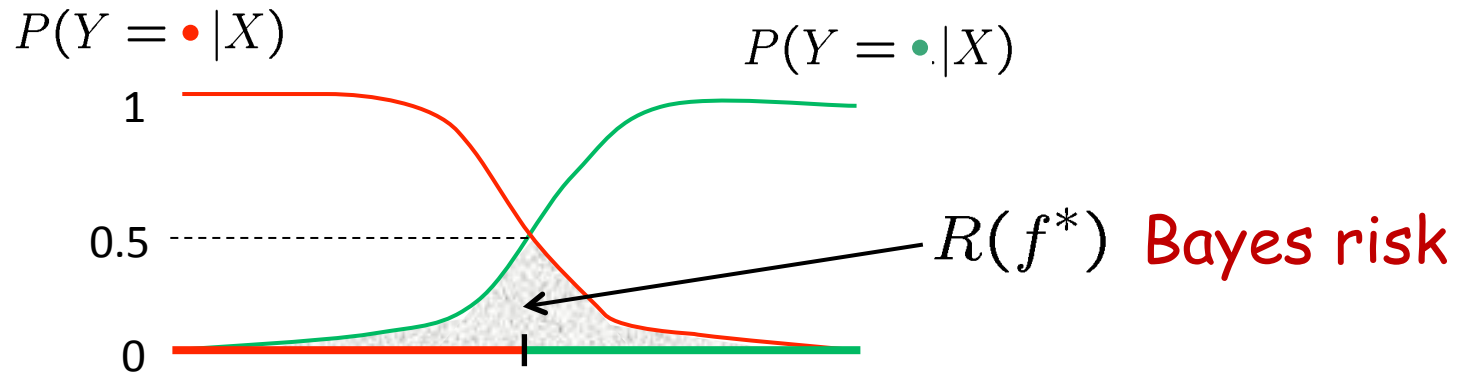
Equivalently,

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



Optimal Classification

Optimal predictor: $f^*(x) = \arg \max_{Y=y} P(Y = y|X = x)$
(Bayes classifier)



- Even the optimal classifier makes mistakes $R(f^*) > 0$
- Optimal classifier depends on **unknown** distribution P_{XY}

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:

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

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

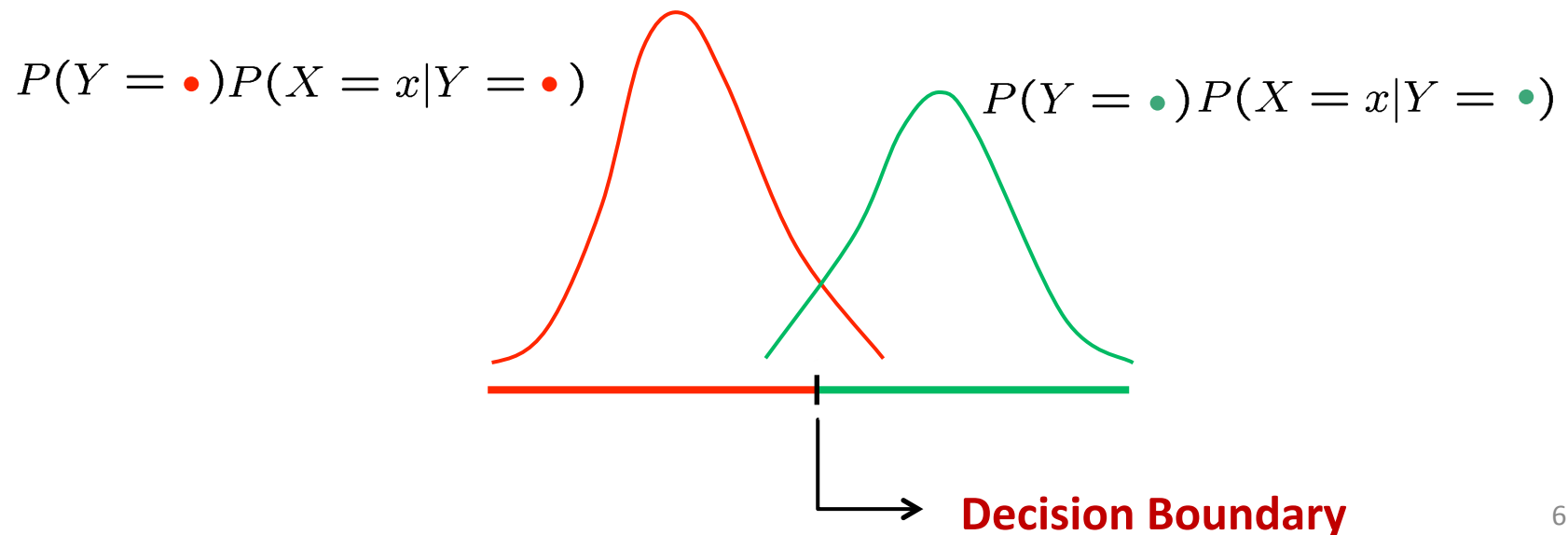
Class conditional density Class prior density

Example Decision Boundaries

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

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

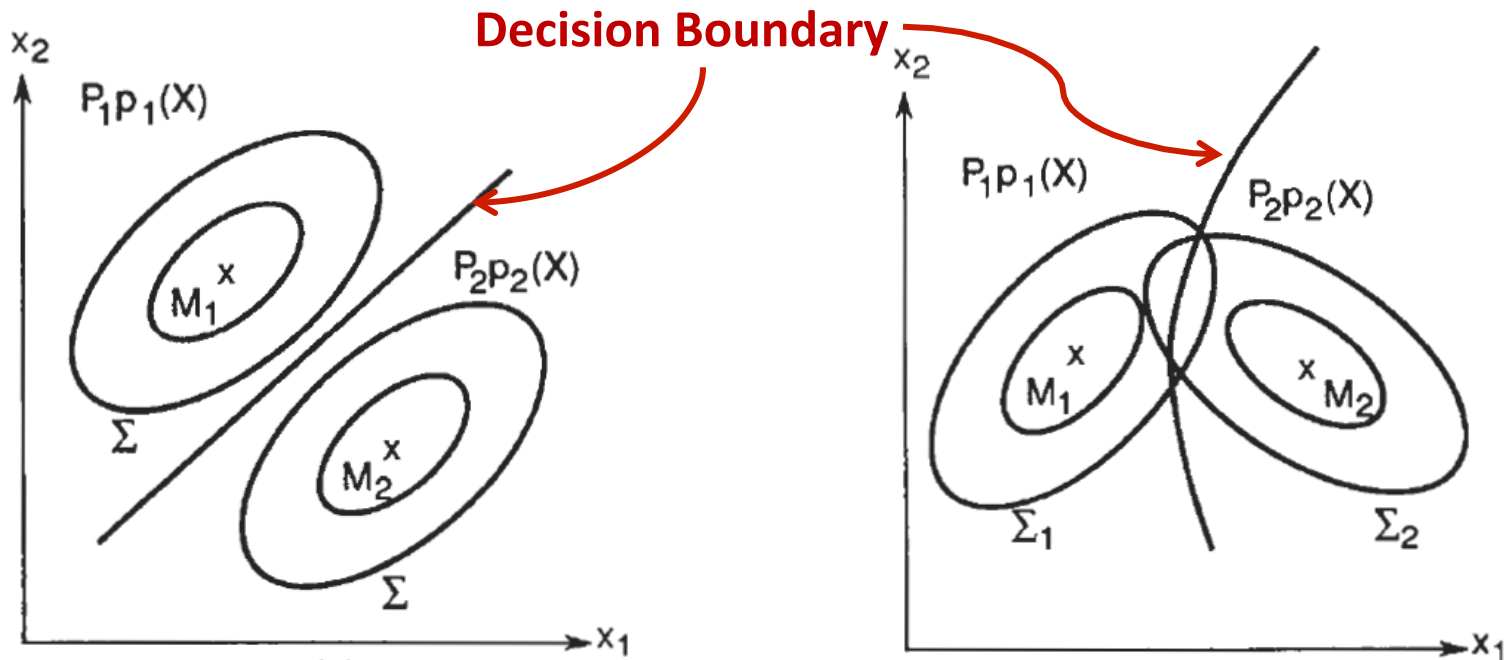
Binary Classification – two classes



Example Decision Boundaries

- Gaussian class conditional densities (2-dimensions/features)

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



Learning the Optimal Classifier

Optimal classifier:

$$\begin{aligned} f^*(x) &= \arg \max_{Y=y} P(Y = y | X = x) \\ &= \arg \max_{Y=y} \underbrace{P(X = x | Y = y)}_{\text{Class conditional density}} \underbrace{P(Y = y)}_{\text{Class prior density}} \end{aligned}$$

Class conditional density Class prior density


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: $X = (X_1 \quad X_2 \quad X_3 \quad \dots \quad \dots \quad X_d) \quad Y$

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

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

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

Need $n \gg 2^d K - 1$ 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:

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

- e.g., $P(\text{Thunder} | \text{Rain}, \text{Lightning}) = P(\text{Thunder} | \text{Lightning})$

Note: does NOT mean Thunder is independent of Rain

Conditional vs. Marginal Independence

- C calls A and B separately and tells them a number $n \in \{1, \dots, 10\}$
- Due to noise in the phone, A and B each imperfectly (and independently) draw a conclusion about what the number was.
- A thinks the number was n_a and B thinks it was n_b .
- Are n_a and n_b marginally independent?
 - No, we expect e.g. $P(n_a = 1 \mid n_b = 1) > P(n_a = 1)$
- Are n_a and n_b conditionally independent given n ?
 - Yes, because if we know the true number, the outcomes n_a and n_b are purely determined by the noise in each phone.

$$P(n_a = 1 \mid n_b = 1, n = 2) = P(n_a = 1 \mid n = 2)$$

Prediction using Conditional Independence

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

parameters needed to learn likelihood given L

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

With conditional independence assumption

$$P(T,R|L) = P(T|L) P(R|L) \quad (2-1)2 + (2-1)2 = 4$$

Naïve Bayes Assumption

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

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

- More generally:

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

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

Naïve Bayes Classifier

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

- Decision rule:

$$\begin{aligned} f_{NB}(\mathbf{x}) &= \arg \max_y P(x_1, \dots, x_d | y) P(y) \\ &= \arg \max_y \prod_{i=1}^d P(x_i | y) P(y) \end{aligned}$$

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

Naïve Bayes Algo – Discrete features

- Training Data $\{(X^{(j)}, Y^{(j)})\}_{j=1}^n$ $X^{(j)} = (X_1^{(j)}, \dots, X_d^{(j)})$

- **Maximum Likelihood Estimates**

- For Class Prior
$$\hat{P}(y) = \frac{\{\#j : Y^{(j)} = y\}}{n}$$

- For Likelihood

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

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

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

Subtlety 1 – Violation of NB Assumption

- Usually, features are not conditionally independent:

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

- Actual probabilities $P(Y | X)$ often biased towards 0 or 1 (Why? Think completely dependent case $X_i = X_j$ or $X_i = 1 - X_j$)
- 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., $Y=\{\text{SpamEmail}\}$, $X_1=\{\text{'Earn'}\}$
 - $P(X_1=a \mid Y=b) = 0$
- Thus, no matter what the values X_2, \dots, X_d take:
 - $P(Y=b \mid X_1=a, X_2, \dots, X_d) = 0$

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

- What now???

MLE vs. MAP

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

What if we toss the coin too few times?

- You say: Probability next toss is a head = 0
- Billionaire says: You're fired! ...with prob 1 😊

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

- Beta prior equivalent to extra coin flips
- As $N \rightarrow 1$, prior is “forgotten”
- **But, for small sample size, prior is important!**

Naïve Bayes Algo – Discrete features

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

$$Q(Y = b)$$

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

MAP Estimate

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

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

Case Study: Text Classification

- Classify e-mails
 - $Y = \{\text{Spam, NotSpam}\}$
- Classify news articles
 - $Y = \{\text{what is the topic of the article?}\}$
- Classify webpages
 - $Y = \{\text{Student, professor, project, ...}\}$
- 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 (opinion)
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 Hrudefy 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

- $P(\mathbf{X}|Y)$ is huge!!!
 - Article at least 1000 words, $\mathbf{X}=\{X_1,\dots,X_{1000}\}$
 - 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

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

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

Bag of words approach

the world of

TOTAL



all about the company

Our energy exploration, production, and distribution operations span the globe, with activities in more than 100 countries.

At TOTAL, we draw our greatest strength from our fast-growing oil and gas reserves. Our strategic emphasis on natural gas provides a strong position in a rapidly expanding market.

Our expanding refining and marketing operations in Asia and the Mediterranean Rim complement already solid positions in Europe, Africa, and the U.S.

Our growing specialty chemicals sector adds balance and profit to the core energy business.

► All About The Company

- Global Activities
- Corporate Structure
- TOTAL's Story
- Upstream Strategy
- Downstream Strategy
- Chemicals Strategy
- TOTAL Foundation
- Homepage



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:

$$\begin{aligned} h_{NB}(\mathbf{x}) &= \arg \max_y P(y) \prod_{i=1}^{LengthDoc} P(x_i|y) \\ &= \arg \max_y P(y) \prod_{w=1}^W P(w|y)^{count_w} \end{aligned}$$

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:

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

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

ith pixel in
jth training image

kth class
jth training image

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

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

Example: GNB for classifying mental states

[Mitchell et al.]



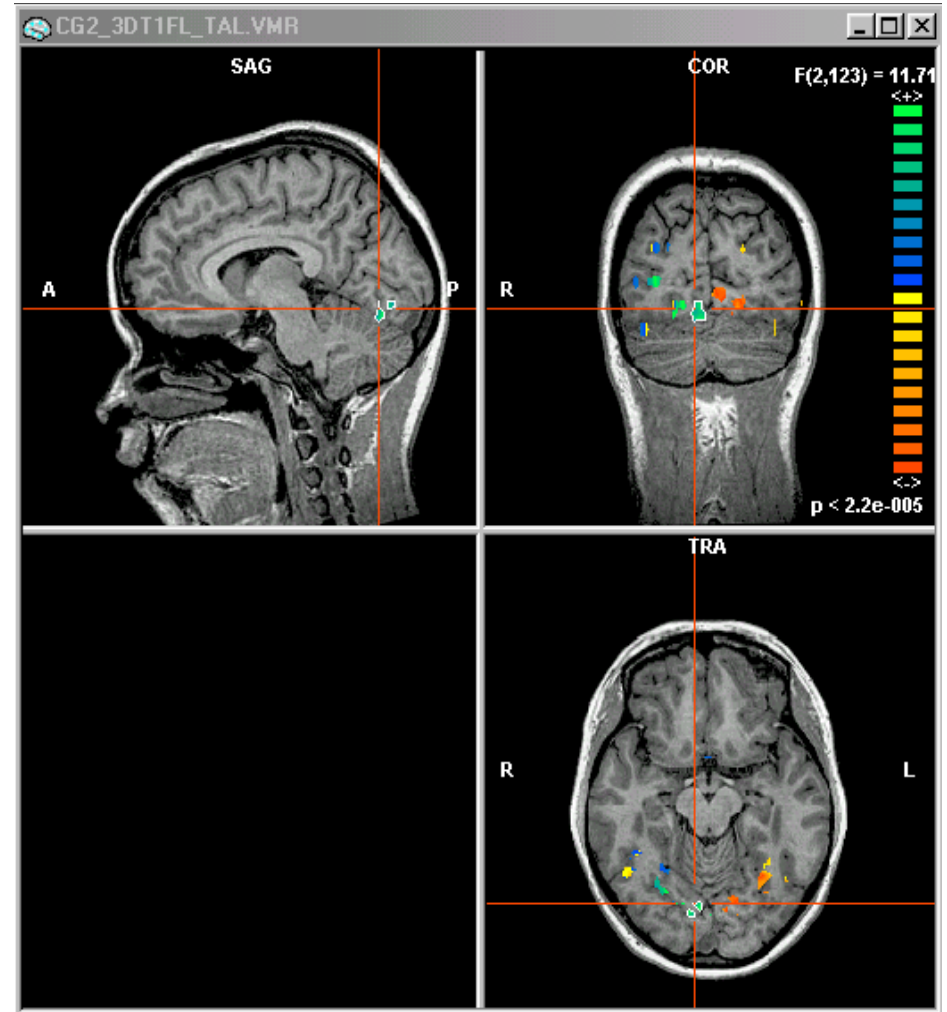
~1 mm resolution

~2 images per sec.

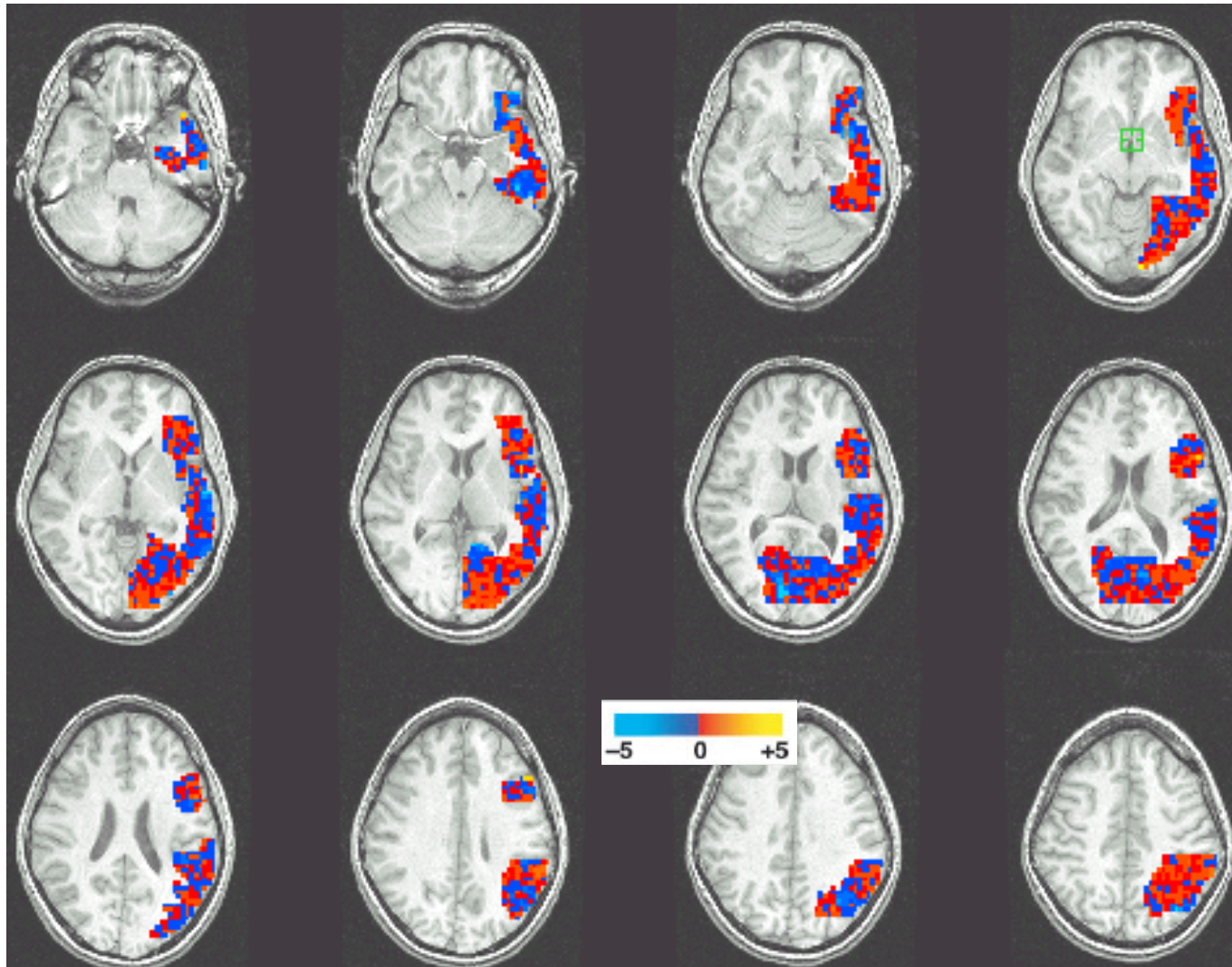
15,000 voxels/image

non-invasive, safe

measures Blood Oxygen Level Dependent (BOLD) response



Gaussian Naïve Bayes: Learned $\mu_{\text{voxel},\text{word}}$



[Mitchell et al.]

15,000 voxels
or features

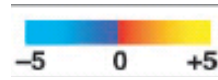
10 training
examples or
subjects per
class

Learned Naïve Bayes Models – Means for $P(\text{BrainActivity} \mid \text{WordCategory})$

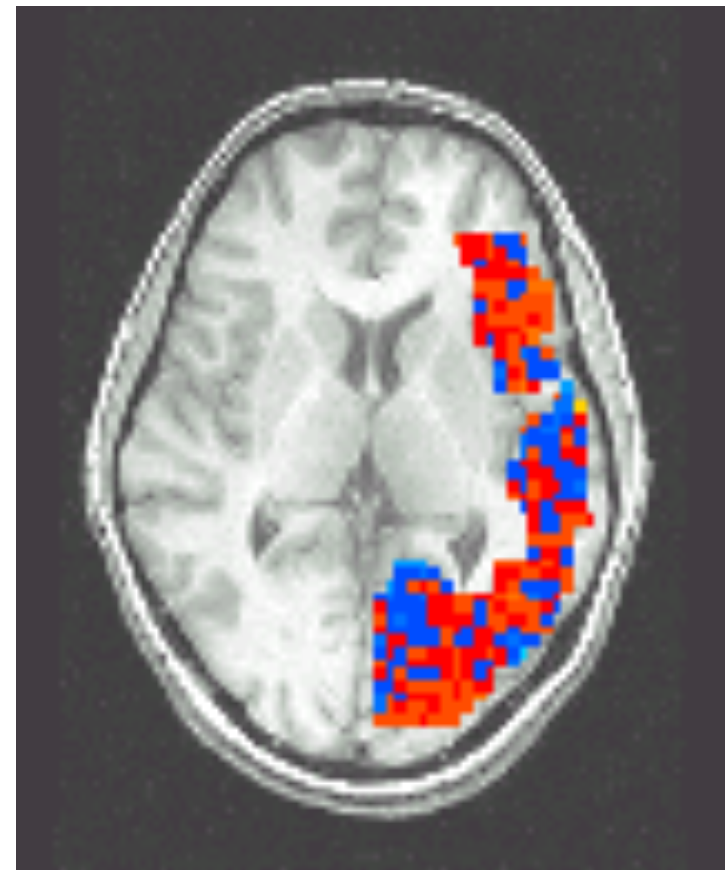
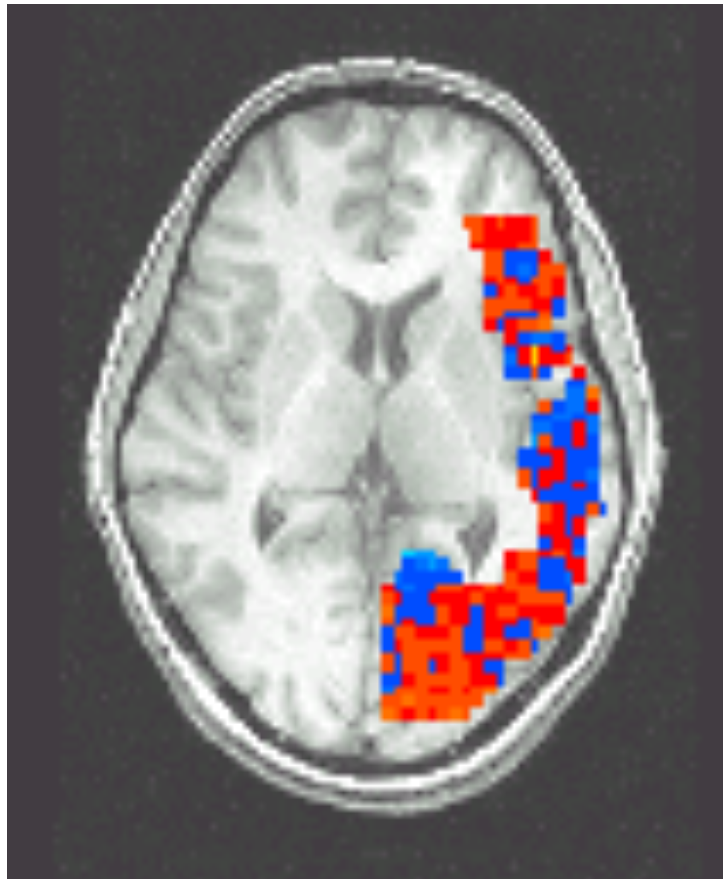
Pairwise classification accuracy: 85%

[Mitchell et al.]

People words



Animal words



What you should know...

- Optimal decision using Bayes Classifier
- Naïve Bayes classifier
 - What's the assumption
 - Why we use it
 - How do we learn it
 - Why is Bayesian (MAP) estimation important
- Text classification
 - Bag of words model
- Gaussian NB
 - Features are still conditionally independent
 - Each feature has a Gaussian distribution given class