

# 10-701 INTRODUCTION TO MACHINE LEARNING (PHD)

## LECTURE 4: NAIVE BAYES

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Reading: <http://www.cs.cmu.edu/~tom/mlbook/NBayesLogReg.pdf>  
(<http://www.cs.cmu.edu/~tom/mlbook/NBayesLogReg.pdf>). Generative and Discriminative Classifiers by Tom Mitchell.

### LECTURE OUTCOMES:

- Conditional Independence
- Naïve Bayes, Gaussian Naive Bayes
- Practical Examples

## THE NAÏVE BAYES ALGORITHM

Naïve Bayes assumes conditional independence of the  $X_i$ 's:  $P(X_1, \dots, X_d | Y) = \prod_i P(X_i | Y)$

(more on this assumption soon!)

Using Bayes rule with that assumption:

$$P(Y = y_k | X_1, \dots, X_d) = \frac{P(Y = y_k) \prod_i P(X_i | Y = y_k)}{P(X)}$$

- Train the algorithm (estimate  $P(X_i | Y = y_k)$  and  $P(Y = y_k)$ )
- To classify, pick the most probable  $Y^{\text{new}}$  for a new sample  $X^{\text{new}} = (X_1^{\text{new}}, X_2^{\text{new}}, \dots, X_d^{\text{new}})$  as:

$$Y^{\text{new}} \leftarrow \operatorname{argmax}_{y_k} P(Y = y_k) \prod_i P(X_i^{\text{new}} | Y = y_k)$$

## NAÏVE BAYES - TRAINING AND PREDICTION PHASE - DISCRETE $X_i$

Training:

- Estimate  $\pi_k \equiv P(Y = y_k)$ , get  $\hat{\pi}_k$
- Estimate  $\theta_{ijk} \equiv P(X_i = x_{ij} | Y = y_k)$ , get  $\hat{\theta}_{ijk}$ 
  - $\theta_{ijk}$  is estimate for each label  $y_k$ :
    - For each variable  $X_i$ :
    - For each value  $x_{ij}$  that  $X_i$  can take.

- Prediction: Classify  $Y^{\text{new}}$

$$\begin{aligned} Y^{\text{new}} &= \operatorname{argmax}_{y_k} P(Y = y_k) \prod_i P(X_i^{\text{new}} = x_j^{\text{new}} | Y = y_k) \\ &= \operatorname{argmax}_{y_k} \pi_k \prod_i \theta_{i, X_i^{\text{new}}, k} \end{aligned}$$

But... how do we estimate these parameters?

## NAÏVE BAYES - TRAINING PHASE - DISCRETE $X_i$ - MAXIMUM (CONDITIONAL) LIKELIHOOD ESTIMATION

$P(X|Y = y_k)$  has parameters  $\theta_{ijk}$ , one for each value  $x_{ij}$  of each  $X_i$ .

$P(Y)$  has parameters  $\pi$ .

To follow the MLE principle, we pick the parameters  $\pi$  and  $\theta$  that maximizes the (**conditional**) likelihood of the data given the parameters.

To estimate:

- Compute

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

- For each label  $y_k$ :

- For each variable  $X_i$ :

- For each value  $x_{ij}$  that  $X_i$  can take, compute:

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

.

## NAÏVE BAYES - TRAINING PHASE - DISCRETE $X_i$

### METHOD 1: MAXIMUM (CONDITIONAL) LIKELIHOOD ESTIMATION

$P(X|Y = y_k)$  has parameters  $\theta_{ijk}$ , one for each value  $x_{ij}$  of each  $X_i$ .

To follow the MLE principle, we pick the parameters  $\theta$  that maximizes the **conditional** likelihood of the data given the parameters.

### METHOD 2: MAXIMUM A POSTERIORI PROBABILITY ESTIMATION

To follow the MAP principle, pick the parameters  $\theta$  with maximum posterior probability given the conditional likelihood of the data and the prior on  $\theta$ .

# NAÏVE BAYES - TRAINING PHASE - DISCRETE $X_i$

## METHOD 1: MAXIMUM (CONDITIONAL) LIKELIHOOD ESTIMATION

To estimate:

- Compute

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

- For each label  $y_k$ :

- For each variable  $X_i$ :

- For each value  $x_{ij}$  that  $X_i$  can take, compute:

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

## METHOD 2: MAXIMUM A POSTERIORI PROBABILITY ESTIMATION (BETA OR DIRICHLET PRIORS)

- $K$ : the number of values  $Y$  can take
- $J$ : the number of values  $X$  can take (we assume here that all  $X_j$  have the same number of possible values, but this can be changed)
- Example prior for  $\pi_k$  where  $K > 2$ :
  - Dirichlet( $\beta_\pi, \beta_\pi, \dots, \beta_\pi$ ) prior. (optionally, you can choose different values for each parameter to encode a different weighting).
  - if  $K = 2$  this becomes a Beta prior.
- Example prior for  $\theta_{ijk}$  where  $J > 2$ :
  - Dirichlet( $\beta_\theta, \beta_\theta, \dots, \beta_\theta$ ) prior. (optionally, you can choose different values for each parameter to encode a different weighting, you can choose a different prior per  $X_i$  or even per label  $y_k$ ).
  - if  $J = 2$  this becomes a Beta prior.

## METHOD 2: MAXIMUM A POSTERIORI PROBABILITY ESTIMATION (BETA OR DIRICHLET PRIORS)

- $K$ : the number of values  $Y$  can take
- $J$ : the number of values  $X$  can take

These priors will act as imaginary examples that smooth the estimated distributions and prevent zero values.

To estimate:

- Compute

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

- For each label  $y_k$ :

- For each variable  $X_i$ :

- For each value  $x_{ij}$  that  $X_i$  can take, compute:

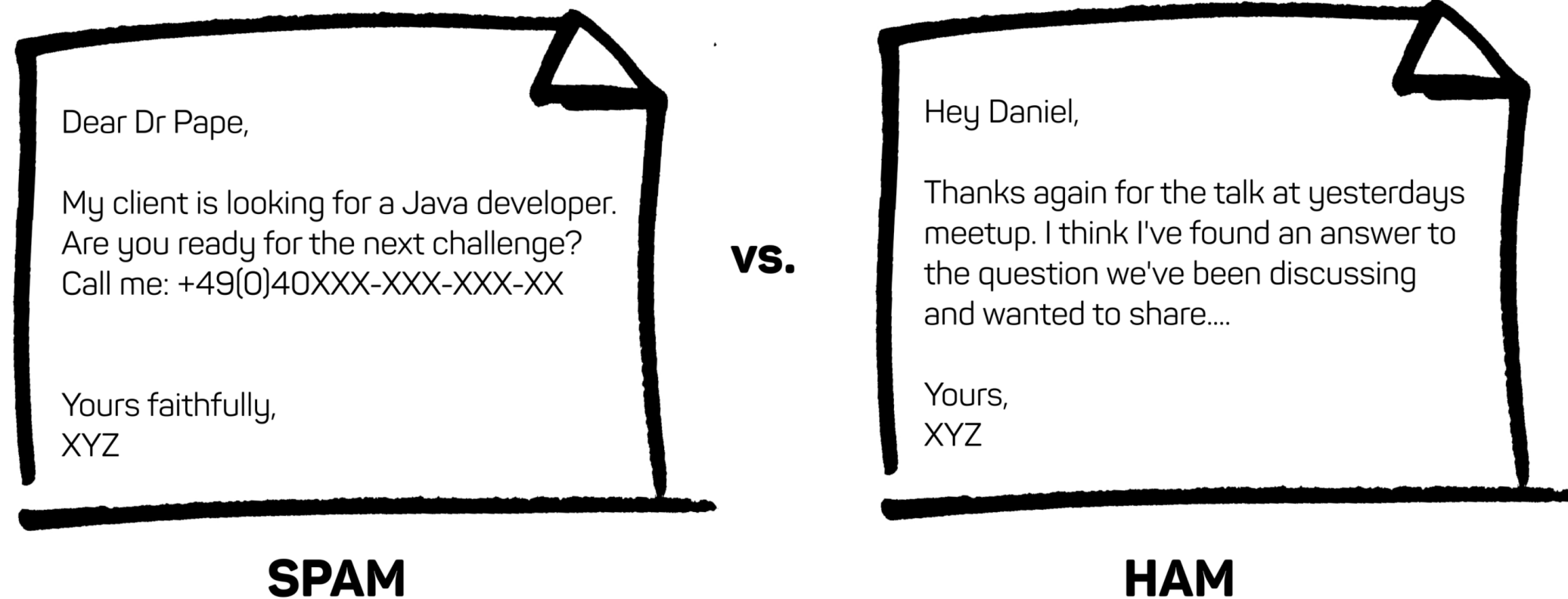
$$\hat{\theta}_{ijk} = \hat{P}(X_i = x_{ij} | Y = y_k) = \frac{\#D(X_i = x_{ij} \wedge Y = y_k) + (\beta_\theta - 1)}{\#D(Y = y_k) + J(\beta_\theta - 1)}$$

.



## EXAMPLE: TEXT CLASSIFICATION

- Classify which emails are spam?



[image by Daniel Pape \(https://blog.codecentric.de/en/2016/06/spam-classification-using-sparks-dataframes-ml-zeppelin-part-1/\)](https://blog.codecentric.de/en/2016/06/spam-classification-using-sparks-dataframes-ml-zeppelin-part-1/)

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

How shall we represent text documents for Naïve Bayes?

## HOW CAN WE EXPRESS X?

- Y discrete valued. e.g., Spam or not
- $X = ?$

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- $X = (X_1, X_2, \dots, X_d)$  with d the number of words in English.
- (This is what we do in homework 2)

What are the limitations with this representation?

## HOW CAN WE EXPRESS X?

- Y discrete valued. e.g., Spam or not
- $X = (X_1, X_2, \dots, X_d)$  with d the number of words in English.
- (This is what we do in homework 2)

What are the limitations with this representation?

- Some words always present
- Some words very infrequent
- Doesn't count how often a word appears
- Conditional independence assumption is false...

## ALTERNATIVE FEATURIZATION

- $Y$  discrete valued. e.g., Spam or not
- $X = (X_1, X_2, \dots, X_d)$  = 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
- $X_i$  represents the  $i$ th word position in document
- $X_1 = \text{"I"}, X_2 = \text{"am"}, X_3 = \text{"pleased"}$

How many parameters do we need to estimate  $P(X|Y)$ ? (say 1000 words per document, 10000 words in english)

## ALTERNATIVE FEATURIZATION

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How many parameters do we need to estimate  $P(X|Y)$ ? (say 1000 words per document, 10000 words in english)

**Conditional Independence Assumption** very useful:

- reduce problem to only computing  $P(X_i|Y)$  for every  $X_i$ .

## “BAG OF WORDS” MODEL

Additional assumption: position doesn't matter!

(this is not true of language, but can be a useful assumption for building a classifier)

- assume the  $X_i$  are IID:  
$$P(X_i|Y) = P(X_j|Y)(\forall i, j)$$
- we call this "Bag of Words"



Art installation in Gates building (now removed)

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 $P(X_i|Y) = P(X_j|Y)(\forall i, j)$
- we call this "Bag of Words"

Since all  $X_i$ s have the same distribution, we only have to estimate one parameter per word, per class.

$P(X|Y = y_k)$  is a multinomial distribution:

$$P(X|Y = y_k) \propto \theta_{1k}^{\alpha_{1k}} \theta_{2k}^{\alpha_{2k}} \dots \theta_{dk}^{\alpha_{dk}}$$



## REVIEW OF DISTRIBUTIONS

$$P(X_i = w_j) \begin{cases} \theta_1, & \text{if } X_i = w_1 \\ \theta_2, & \text{if } X_i = w_2 \\ \dots & \\ \theta_k, & \text{if } X_i = w_K \end{cases}$$

Probability of observing a document with  $\alpha_1$  count of  $w_1$ ,  $\alpha_2$  count of  $w_2$  ... is a multinomial:

$$\frac{|D|!}{\alpha_1! \dots \alpha_J!} \theta_1^{\alpha_1} \theta_2^{\alpha_2} \theta_3^{\alpha_3} \dots \theta_J^{\alpha_J}$$

# REVIEW OF DISTRIBUTIONS

Dirichlet Prior examples:

- if constant across classes and words:

$$P(\theta) = \frac{\theta^{\beta_\theta} \theta^{\beta_\theta}, \dots, \theta^{\beta_\theta}}{\text{Beta}(\beta_\theta, \beta_\theta, \dots, \beta_\theta)}$$

- if constant across classes but different for different words:

$$P(\theta) = \frac{\theta^{\beta_1} \theta^{\beta_2}, \dots, \theta^{\beta_J}}{\text{Beta}(\beta_1, \beta_2, \dots, \beta_J)}$$

- if different for different classes  $k$  and words:

$$P(\theta_k) = \frac{\theta^{\beta_{1k}} \theta^{\beta_{2k}}, \dots, \theta^{\beta_{Jk}}}{\text{Beta}(\beta_{1k}, \beta_{2k}, \dots, \beta_{Jk})}$$

## MAP ESTIMATES FOR BAG OF WORDS:

(Dirichlet is the conjugate prior for a multinomial likelihood function)

$$\theta_{jk} = \frac{\alpha_{jk} + \beta_{jk} - 1}{\sum_m (\alpha_{mk} + \beta_{mk} - 1)}$$

Again the prior acts like hallucinated examples

What  $\beta$ s should we choose?

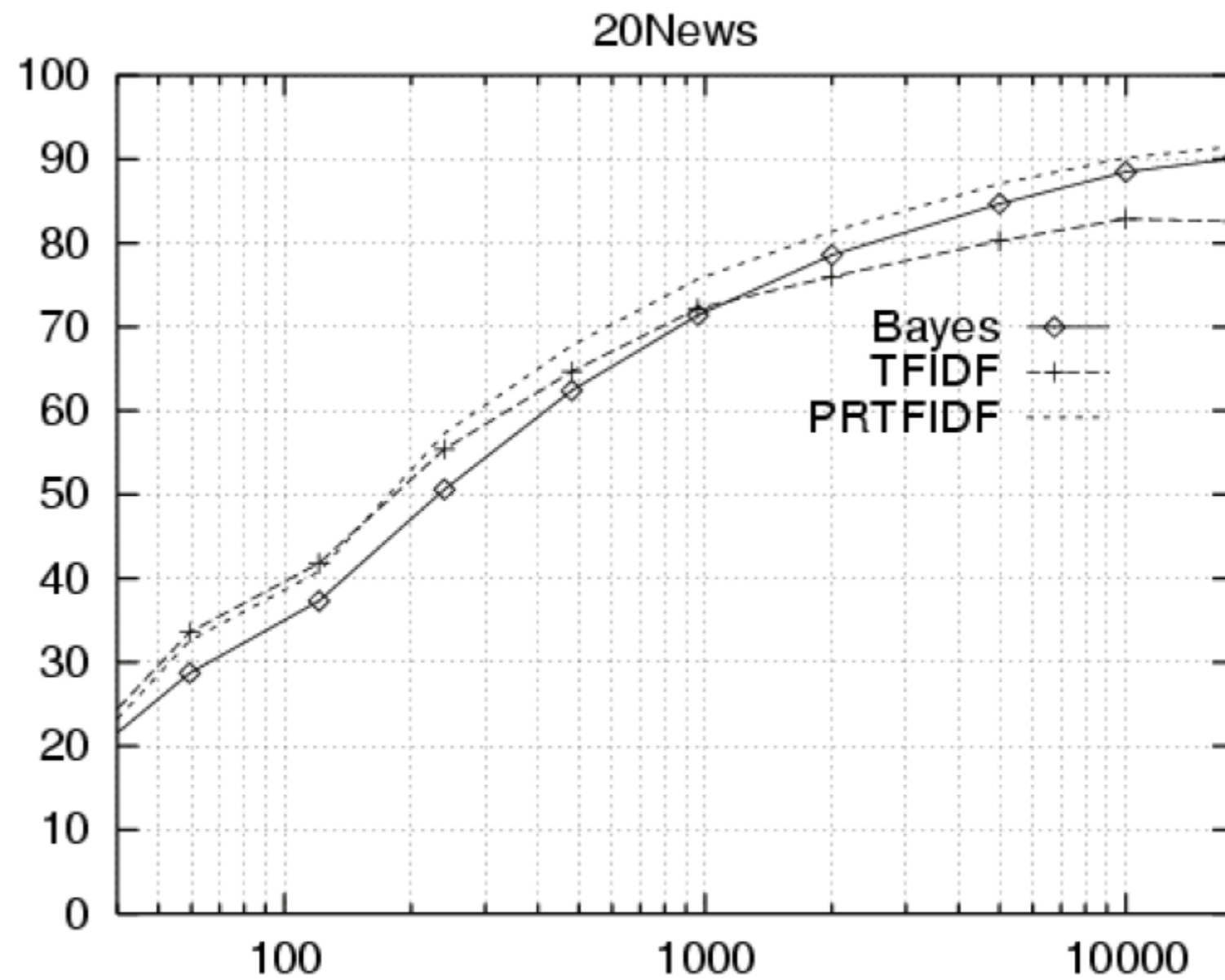
## EXAMPLE: TWENTY NEWSGROUPS

For code and data, see [www.cs.cmu.edu/~tom/mlbook.html](http://www.cs.cmu.edu/~tom/mlbook.html) click on “Software and Data”.

Can group labels into groups that share priors:

- comp.graphics, comp.os.ms-windows.misc, comp.sys.ibm.pc.hardware, comp.sys.max.hardware, comp.windows.x
  - misc.forsale
  - rec.autos, rec.motorcycles, rec.sport.baseball, rec.sport.hockey
  - alt.atheism,
  - soc.religion.christian,
  - talk.religion.misc, talk.politics.mideast, talk.politics.misc, talk.politics.guns,
  - sci.space, sci.crypt, sci.electronics, sci.med
- 
- Naïve Bayes: 89% classification accuracy

## LEARNING CURVE FOR 20 NEWSGROUPS



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

## **EVEN IF INCORRECT ASSUMPTION, PERFORMANCE CAN BE VERY GOOD**

Even when taking half of the email

- Assumption doesn't hurt the particular problem?
- Redundancy?
- Leads less examples to train? Converges faster to asymptotic performance? (Ng and Jordan)

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More recently, algorithms such as LSTMs and Transformers have become very good

- are able to capture the sequential aspect of language and produce more complex representations.
- They do have many parameters, but nowhere as much as we mentioned before ( $10000^{1000}$ ).

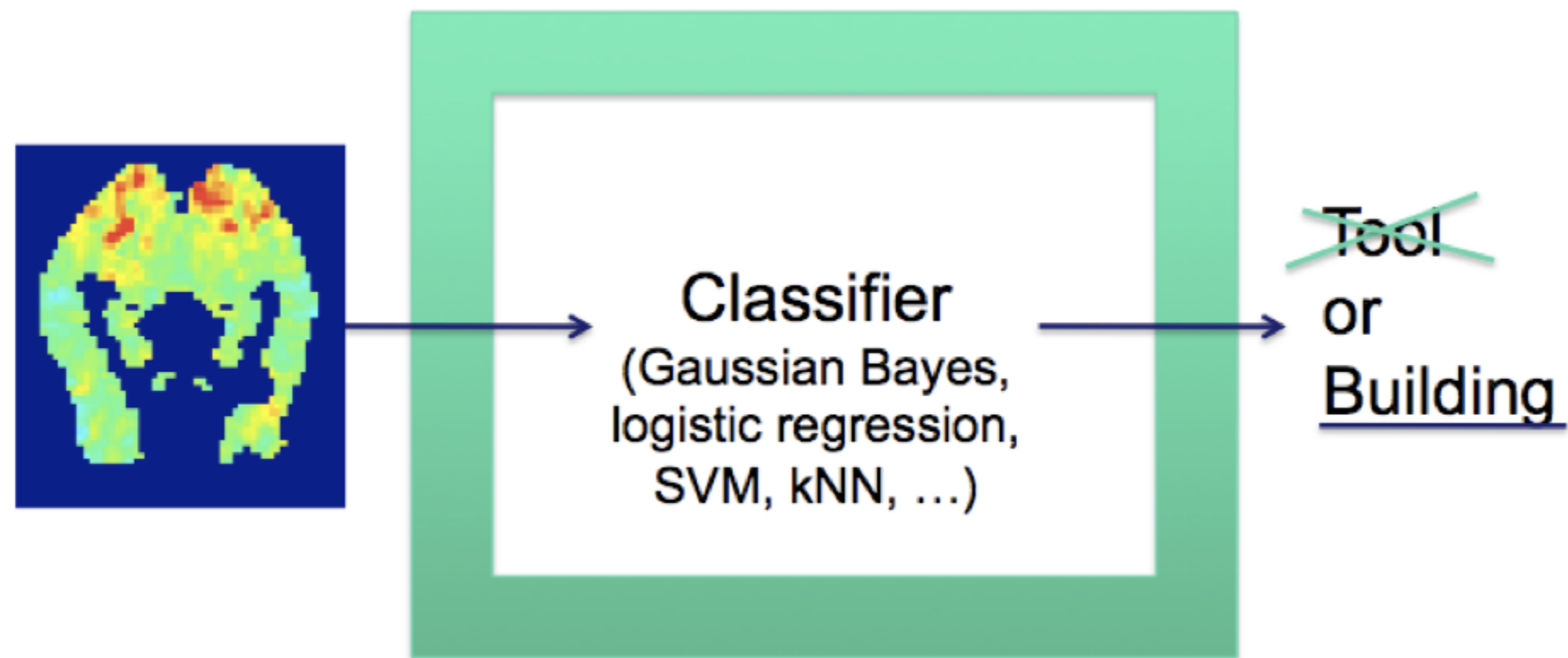
## CONTINUOUS $X_i$ S

What can we do?

E.g. image classification, where  $X_i$  is real valued

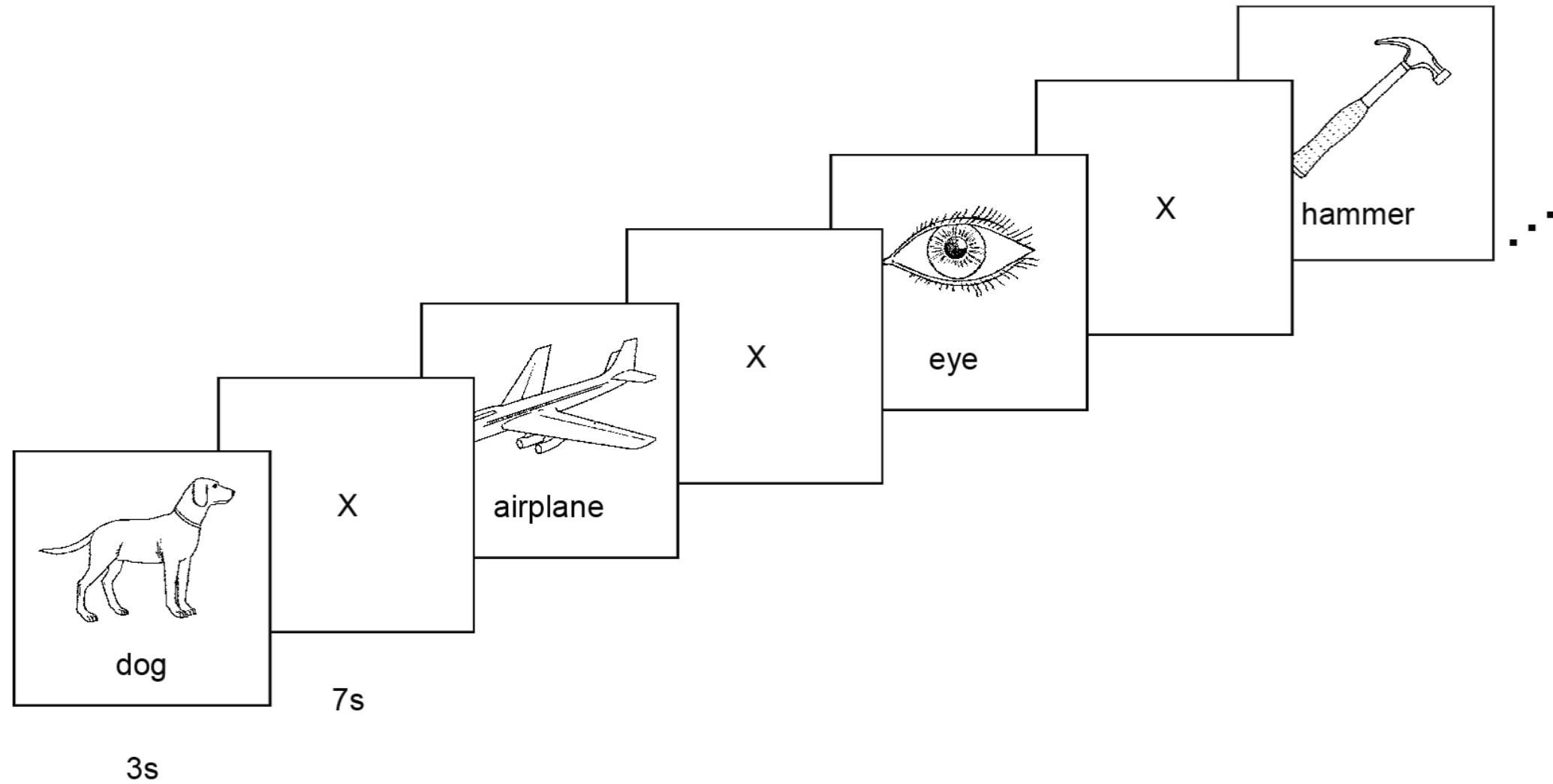
Classify a person's cognitive state, based on brain image

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





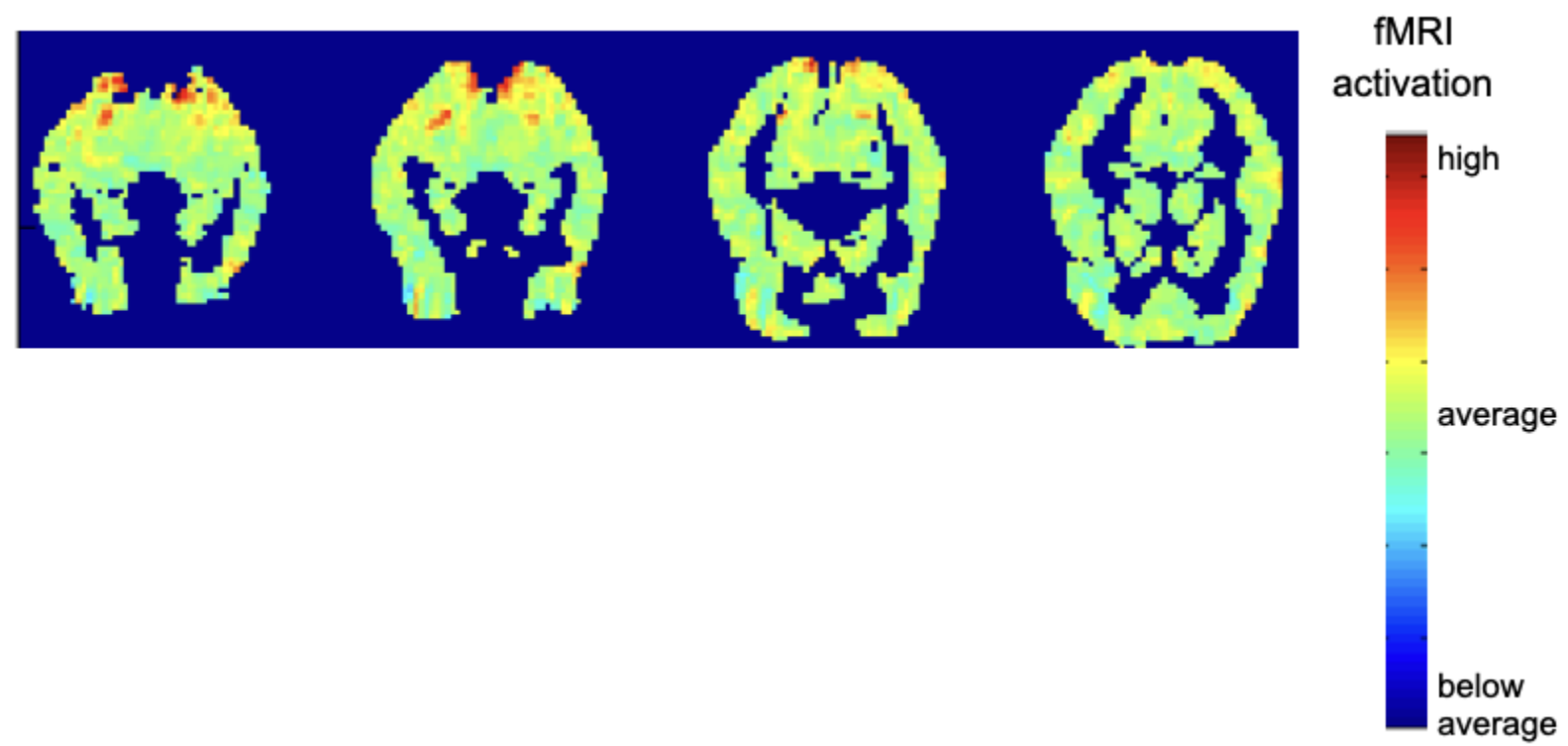
## STIMULUS FOR THE STUDY



60 distinct exemplars, presented 6 times each

Mitchell et al. Science 2008 (<https://science.sciencemag.org/content/320/5880/1191.abstract>), data available [online](https://www.cs.cmu.edu/afs/cs/project/theo-73/www/science2008/data.html) (<https://www.cs.cmu.edu/afs/cs/project/theo-73/www/science2008/data.html>).

CONTINUOUS  $X_i$



$Y$  is the mental state (reading “house” or “bottle”)

$X_i$  are the voxel activities (voxel = volume pixel).

## CONTINUOUS $X_i$

Naïve Bayes requires  $P(X_i|Y = y_k)$  but  $X_i$  is continuous:

$$P(Y = y_k|X_1, \dots, X_d) = \frac{P(Y = y_k) \prod_i P(X_i|Y = y_k)}{\sum_{\ell} P(Y = y_{\ell}) \prod_i P(X_i|Y = y_{\ell})}$$

What can we do?

## CONTINUOUS $X_i$

Naïve Bayes requires  $P(X_i|Y = y_k)$  but  $X_i$  is continuous:

$$P(Y = y_k|X_1, \dots, X_d) = \frac{P(Y = y_k) \prod_i P(X_i|Y = y_k)}{\sum_{\ell} P(Y = y_{\ell}) \prod_i P(X_i|Y = y_{\ell})}$$

What can we do?

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

$$p(X_i = x|Y = y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{ik})^2}{\sigma_{ik}^2}\right)$$

Sometimes assume standard deviation

- 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)

- Training:
  - Estimate  $\pi_k \equiv P(Y = y_k)$
  - Each label  $y_k$ :
    - For each variable  $X_i$  estimate  $P(X_i = x_{ij} | Y = y_k)$ :
    - estimate class conditional mean  $\mu_{ik}$  and standard deviation  $\sigma_{ik}$

- Prediction: Classify  $Y^{\text{new}}$

$$\begin{aligned} Y^{\text{new}} &= \operatorname{argmax}_{y_k} P(Y = y_k) \prod_i P(X_i^{\text{new}} = x_j^{\text{new}} | Y = y_k) \\ &= \operatorname{argmax}_{y_k} \pi_k \prod_i \mathcal{N}(X_i^{\text{new}}; \mu_{ik}, \sigma_{ik}) \end{aligned}$$

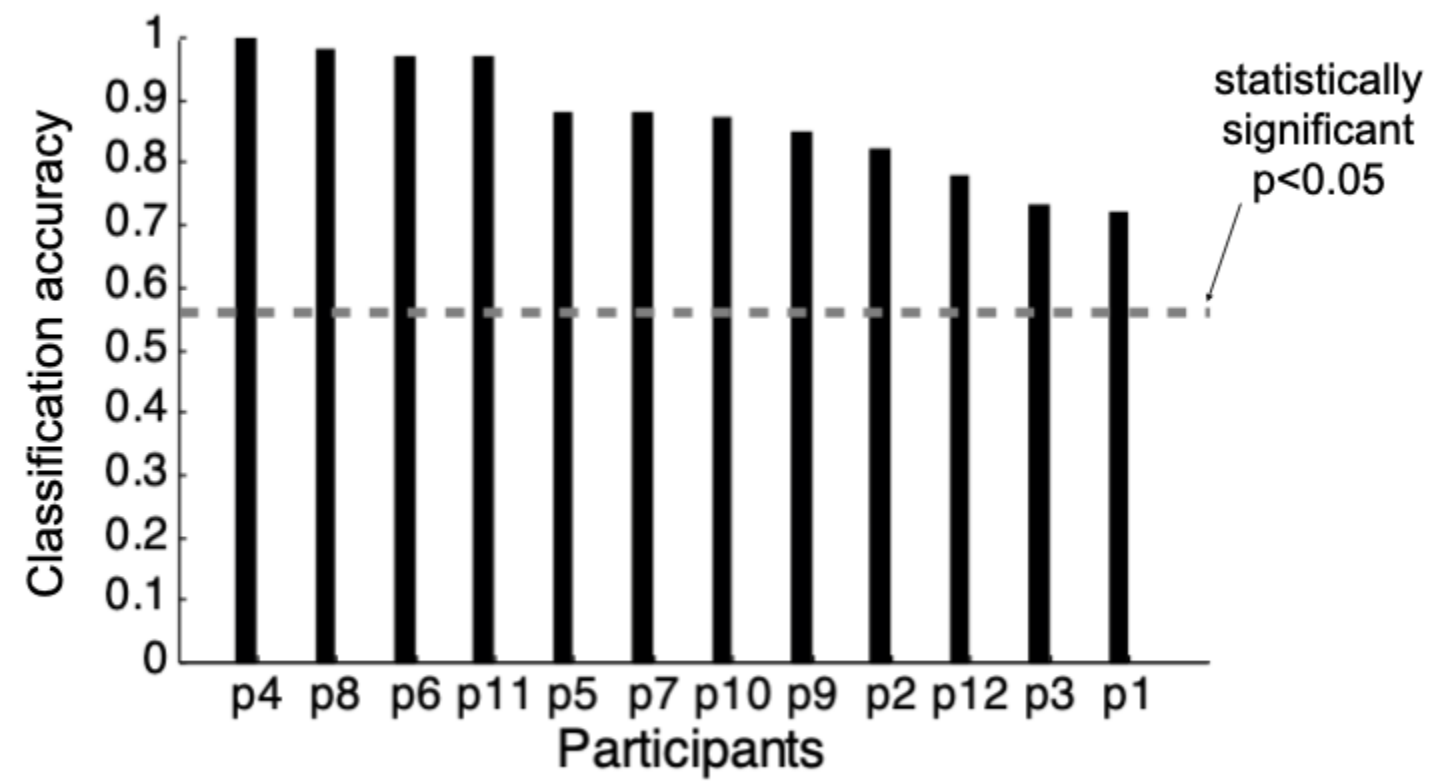
## ESTIMATING PARAMETERS: $Y$ DISCRETE, $X_i$ CONTINUOUS

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

- $i$ : index of feature
- $j$ : index of data point
- $k$ : index of class
- $\delta$  function is 1 if argument is true and 0 otherwise

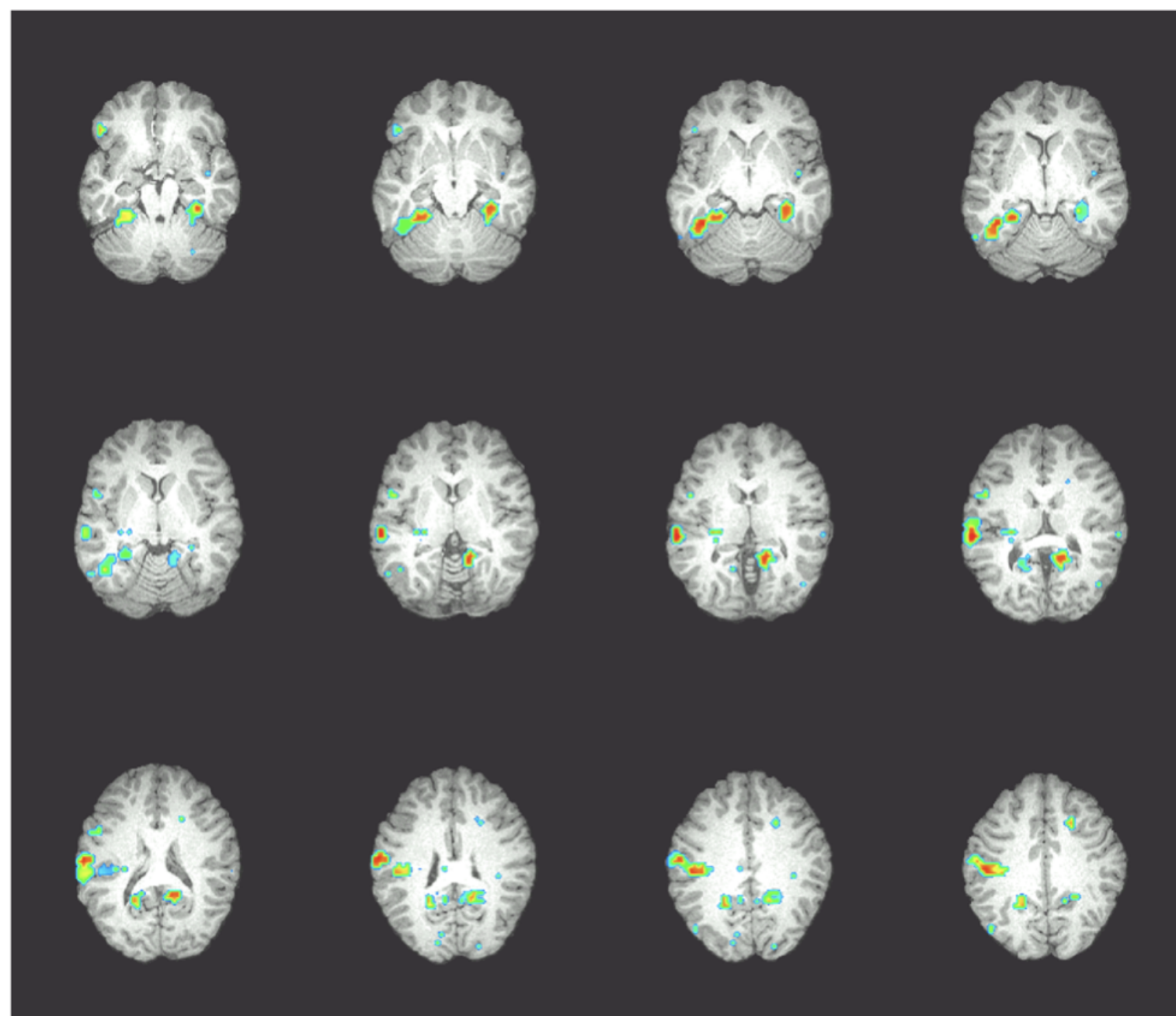
$$\hat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

## 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]





## LET'S SIMULATE THE BEHAVIOR OF GNB!

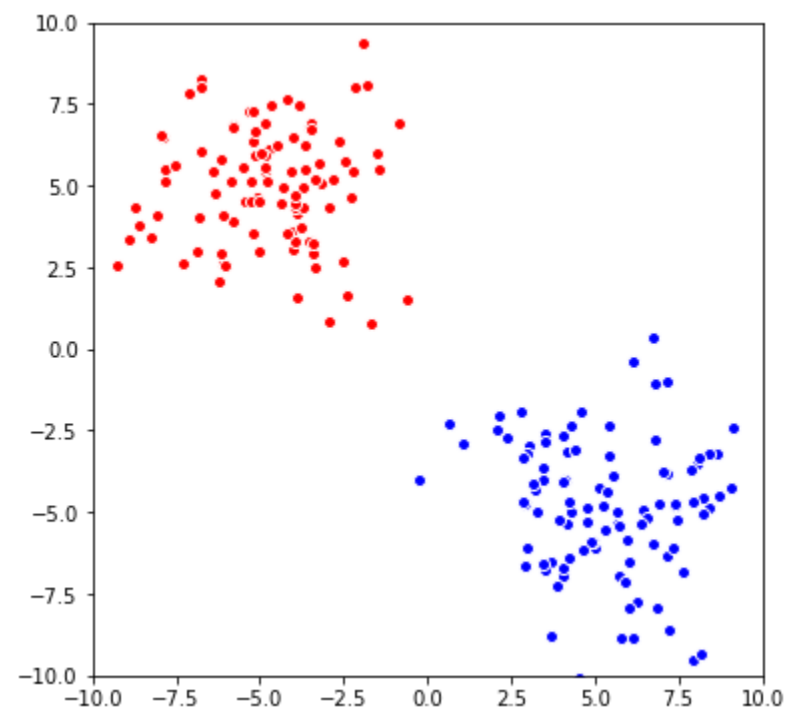
```
In [1]: import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from scipy.stats import norm

x1 = np.linspace(-10,10,1000)
x2 = np.linspace(-10,10,1000)

# Assume I know the true parameters, this is not the case usually!
mu_1_1 = -5; sigma_1_1 = 2
mu_2_1 = 5; sigma_2_1 = 2
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

# Sample data from these distributions
X_positive = norm.rvs(loc=[mu_1_1,mu_2_1], scale=[sigma_1_1, sigma_2_1], size = (100,2))
X_negative = norm.rvs(loc=[mu_1_0,mu_2_0], scale=[sigma_1_0, sigma_2_0], size = (100,2))
```

```
In [16]: plt.figure(figsize=(6,6))
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')
plt.axis([-10,10,-10,10],'equal');
```

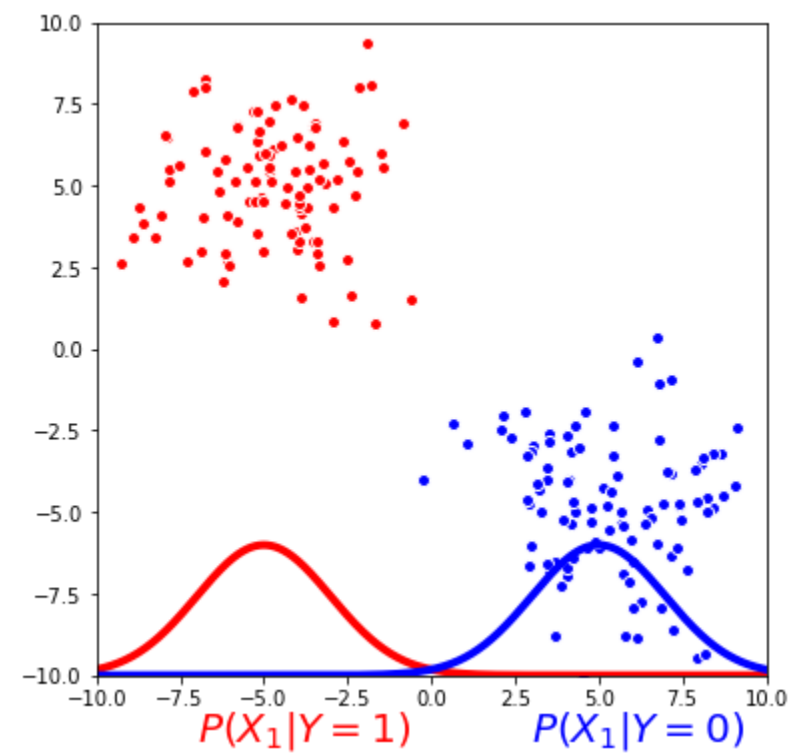


```

In [17]: P_X1_1 = norm.pdf(x1,mu_1_1,sigma_1_1)
P_X2_1 = norm.pdf(x1,mu_2_1,sigma_2_1)
P_X1_0 = norm.pdf(x1,mu_1_0,sigma_1_0)
P_X2_0 = norm.pdf(x1,mu_2_0,sigma_2_0)

plt.figure(figsize=(6,6))
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')
lim_plot = 10
plt.plot(x1,P_X1_1*2*lim_plot-lim_plot,'r',linewidth=4)
plt.text(-7, -12, r'$P(X_1|Y=1)$', color = 'red',fontsize=20)
plt.plot(x1,P_X1_0*2*lim_plot-lim_plot,'b',linewidth=4)
plt.text(3, -12, r'$P(X_1|Y=0)$', color = 'blue',fontsize=20)
plt.axis([-10,10,-10,10],'equal');

```



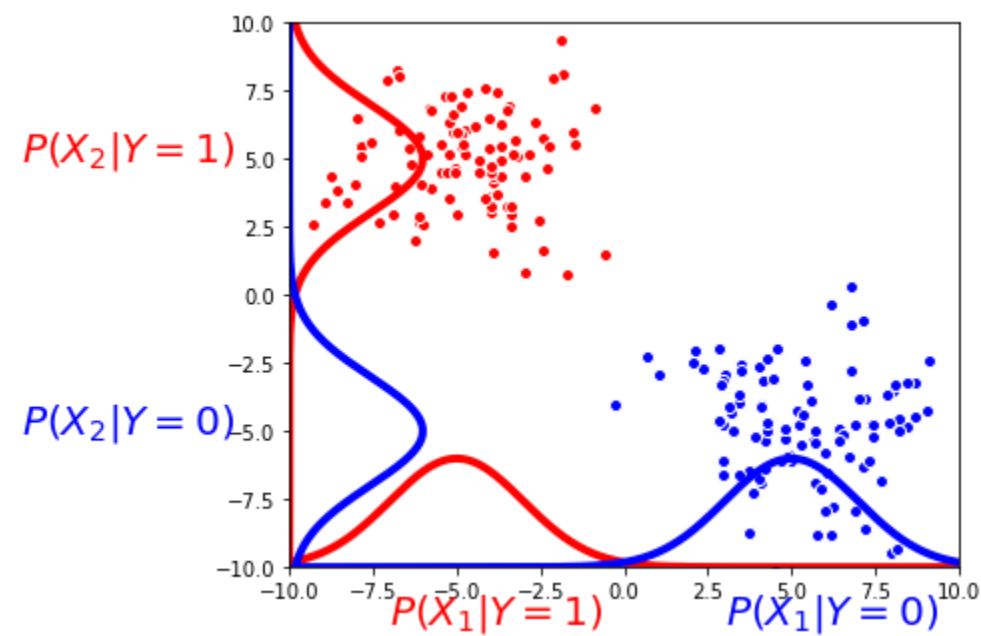
```

In [18]: plt.figure(figsize=(6,5))
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')

lim_plot = 10
plt.plot(x1,P_X1_1*2*lim_plot-lim_plot,'r',linewidth=4)
plt.text(-7, -12, r'$P(X_1|Y=1)$', color = 'red',fontsize=20)
plt.plot(x1,P_X1_0*2*lim_plot-lim_plot,'b',linewidth=4)
plt.text(3, -12, r'$P(X_1|Y=0)$', color = 'blue',fontsize=20)
plt.plot(P_X2_1*2*lim_plot-lim_plot,x1,'r',linewidth=4)
plt.text(-18,5, r'$P(X_2|Y=1)$', color = 'red',fontsize=20)
plt.plot(P_X2_0*2*lim_plot-lim_plot,x1,'b',linewidth=4)
plt.text(-18,-5, r'$P(X_2|Y=0)$', color = 'blue',fontsize=20)
plt.axis([-lim_plot,lim_plot,-lim_plot,lim_plot],'equal')

```

Out[18]: [-10, 10, -10, 10]



```
In [19]: # Compute  $\log( P(Y=1|X) / P(Y=0|X) )$ 
# as  $\log( P(Y=1)P(X1|Y=1)P(X2|Y=1) / P(Y=0|X)P(X1|Y=0)P(X2|Y=0) )$ 
# Using the real parameters. Usually, we have to estimate these!
X1,X2 = np.meshgrid(x1, x2)
def ratio_log(X1,X2):
    pY0 =0.5; pY1 = 1- pY0
    pY1pXY1 = pY1*norm.pdf(X1,mu_1_1,sigma_1_1)*norm.pdf(X2,mu_2_1,sigma_2_1)
    pY0pXY0 = pY0*norm.pdf(X1,mu_1_0,sigma_1_0)*norm.pdf(X2,mu_2_0,sigma_2_0)
    return np.log(pY1pXY1/pY0pXY0)
fX = ratio_log(X1,X2)
```

```

In [20]: plt.figure(figsize=(9,7))

# plot contour plot
cs = plt.contourf(X1, X2, fX,20,cmap='RdBu_r',alpha=0.8);
plt.colorbar()
contours = plt.contour(cs, colors='k',alpha=0.4) # this redraws the lines in black
plt.contour(contours,levels=[0],linewidth=5)      # this makes the 0 line wider

# previous stuff
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w',s=60)
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w',s=60)

lim_plot = 10

plt.plot(x1,P_X1_1*2*lim_plot-lim_plot,'r',linewidth=4)
plt.text(-7, -12, r'$P(X_1|Y=1)$', color = 'red',fontsize=20)

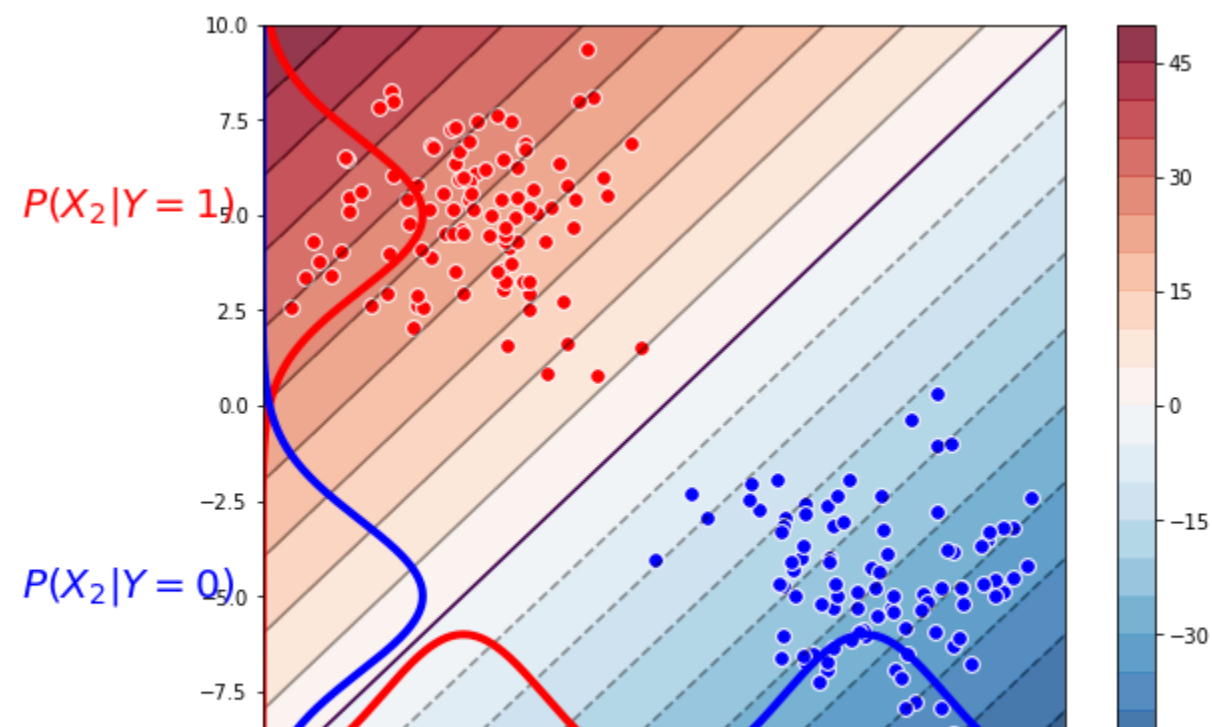
plt.plot(x1,P_X1_0*2*lim_plot-lim_plot,'b',linewidth=4)
plt.text(3, -12, r'$P(X_1|Y=0)$', color = 'blue',fontsize=20)

plt.plot(P_X2_1*2*lim_plot-lim_plot,x1,'r',linewidth=4)
plt.text(-16,5, r'$P(X_2|Y=1)$', color = 'red',fontsize=20)

plt.plot(P_X2_0*2*lim_plot-lim_plot,x1,'b',linewidth=4)
plt.text(-16,-5, r'$P(X_2|Y=0)$', color = 'blue',fontsize=20)

plt.axis([-lim_plot,lim_plot,-lim_plot,lim_plot],'equal');

```



```
In [21]: def ratio_log_updated (X1,X2,params): # just as an example, not used here
          pY0 =0.5; pY1 = 1- pY0
          pY1pXY1 = pY1*norm.pdf(X1,params['mu_1_1'],params['sigma_1_1'])*norm.pdf(X2,params['mu_2_1'],params['sigma_2_1'])
          pY0pXY0 = pY0*norm.pdf(X1,params['mu_1_0'],params['sigma_1_0'])*norm.pdf(X2,params['mu_2_0'],params['sigma_2_0'])
          return np.log(pY1pXY1/pY0pXY0)
```

```

In [23]: def plot_GNB(X_positive,X_negative,params):
    pY0 =0.5; pY1 = 1- pY0
    P_X1_1 = norm.pdf(x1,params['mu_1_1'],params['sigma_1_1'])
    P_X2_1 = norm.pdf(x1,params['mu_2_1'],params['sigma_2_1'])
    P_X1_0 = norm.pdf(x1,params['mu_1_0'],params['sigma_1_0'])
    P_X2_0 = norm.pdf(x1,params['mu_2_0'],params['sigma_2_0'])
    X1,X2 = np.meshgrid(x1, x2)
    # faster way to compute the log ratio, or can use fX = ratio_log_updated(X1,X2,params)
    fX = np.log(pY1/pY0) + np.log(P_X1_1.reshape([1000,1]).dot(P_X2_1.reshape([1,1000]))/
                                   P_X1_0.reshape([1000,1]).dot(P_X2_0.reshape([1,1000])))

    plt.figure(figsize=(10,8))
    # plot contour plot
    cs = plt.contourf(X1, X2, fX,20,cmap='RdBu_r',alpha=0.8);
    plt.colorbar()
    contours = plt.contour(cs, colors='k',alpha=0.4)
    plt.contour(contours,levels=[0],linewidth=5)
    plt.scatter(X_positive[:, 0],X_positive[:, 1],facecolors='r',edgecolors='w',s=60)
    plt.scatter(X_negative[:, 0],X_negative[:, 1],facecolors='b',edgecolors='w',s=60)
    lim_plot = 10
    plt.plot(x1,P_X1_1*2*lim_plot-lim_plot,'r',linewidth=4)
    plt.text(-7, -12, r'$P(X_1|Y=1)$', color = 'red',fontsize=20)
    plt.plot(x1,P_X1_0*2*lim_plot-lim_plot,'b',linewidth=4)
    plt.text(3, -12, r'$P(X_1|Y=0)$', color = 'blue',fontsize=20)
    plt.plot(P_X2_1*2*lim_plot-lim_plot,x1,'r',linewidth=4)
    plt.text(-16,5, r'$P(X_2|Y=1)$', color = 'red',fontsize=20)
    plt.plot(P_X2_0*2*lim_plot-lim_plot,x1,'b',linewidth=4)
    plt.text(-16,-5, r'$P(X_2|Y=0)$', color = 'blue',fontsize=20)
    plt.axis([-lim_plot,lim_plot,-lim_plot,lim_plot],'equal')

```

## THE FEATURES $X_1$ AND $X_2$ IN THE SIMULATION WHERE CONDITIONALLY INDEPENDENT

What if:

- we make them dependent (use a non-diagonal covariance matrix to sample multivariate gaussian)
- We still use conditional independence as an assumption for GNB

1st: case where same variance



```
In [ ]: from scipy.stats import multivariate_normal

# Same param as before
mu_1_1 = -5; sigma_1_1 = 2; mu_2_1 = 5; sigma_2_1 = 2
mu_1_0 = 5; sigma_1_0 = 2; mu_2_0 = -5; sigma_2_0 = 2

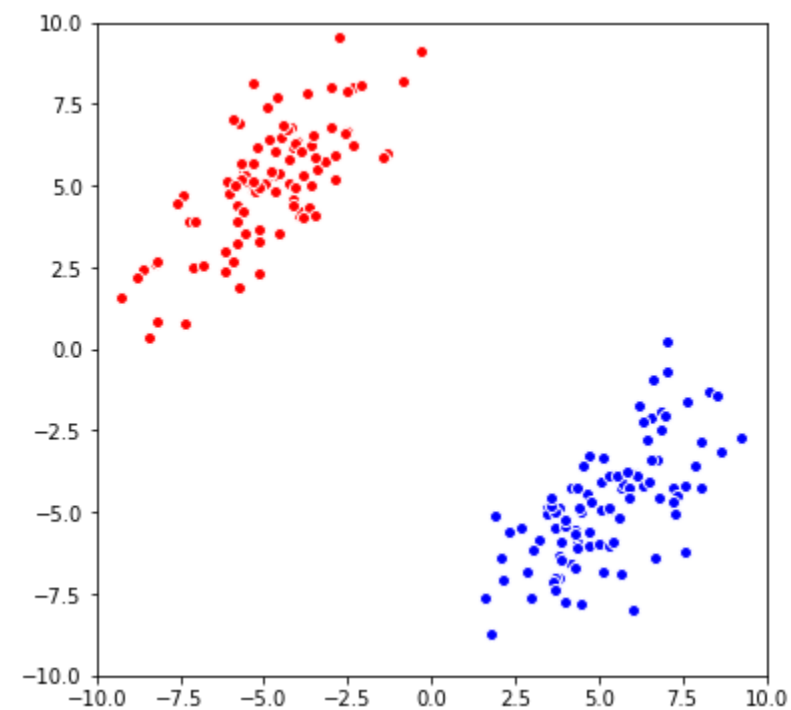
cov_positive = np.array([[sigma_1_1**2,3], [3,sigma_2_1**2]] )
cov_negative = np.array([[sigma_1_0**2,3], [3,sigma_2_0**2]] )

print(cov_positive)

# Sample data from these distributions
X_positive = multivariate_normal.rvs(mean=[mu_1_1,mu_2_1],cov=cov_positive,size=(100))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0],cov=cov_negative,size=(100))
```

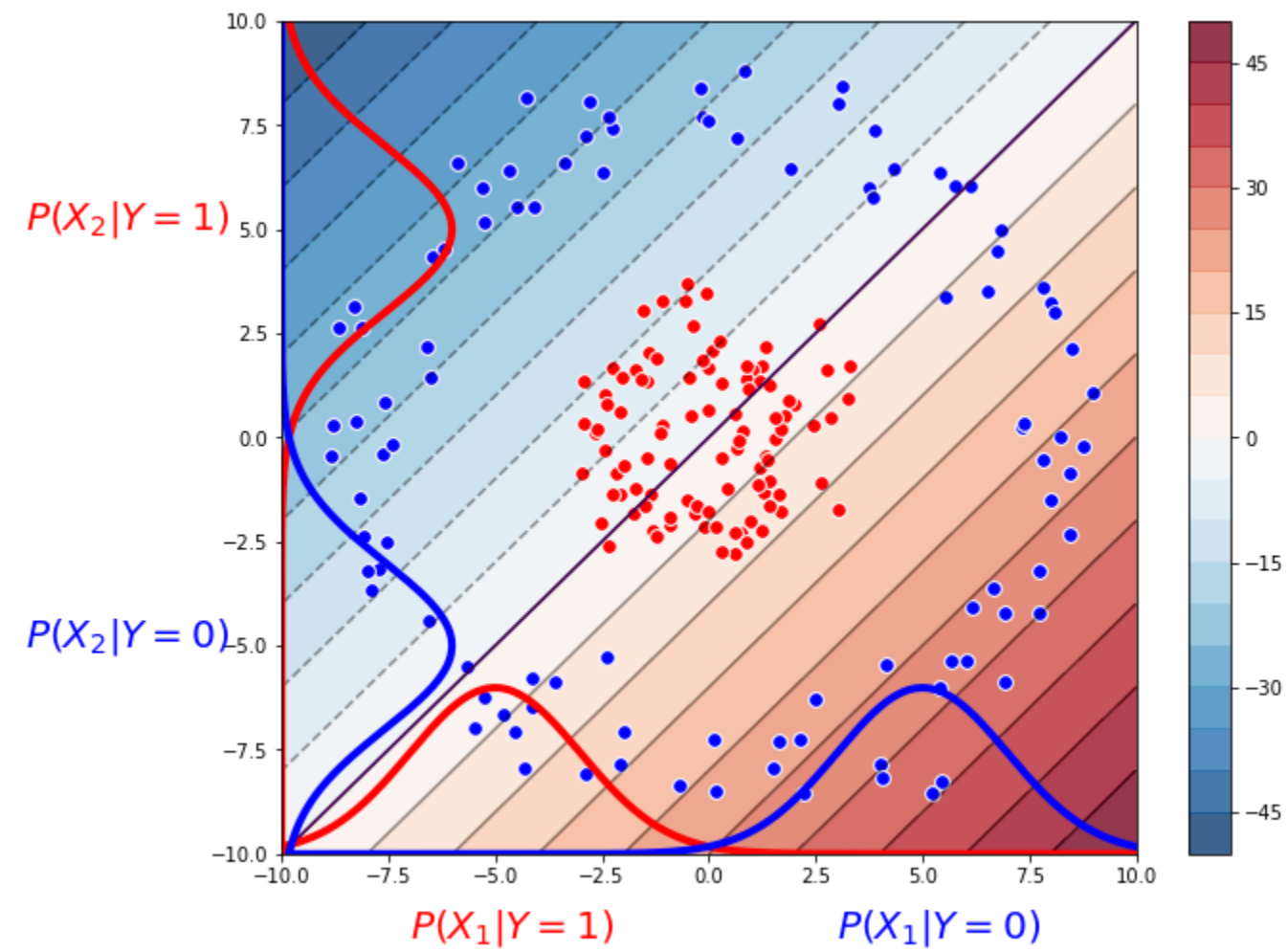
```
In [20]: plt.figure(figsize=(6,6))
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')
plt.axis([-10,10,-10,10],'equal');
```

```
[[4 3]
 [3 4]]
```



```
In [39]: # Assume I perfectly estimate the parameters (not true for limited data!)
params = dict(mu_1_1 = -5, sigma_1_1 = 2, mu_2_1 = 5, sigma_2_1 = 2,
              mu_1_0 = 5, sigma_1_0 = 2, mu_2_0 = -5, sigma_2_0 = 2)

plot_GNB(X_positive, X_negative, params)
```



```
In [22]: # Estimate

mu_1_1, mu_2_1 = np.mean(X_positive,axis=0)
mu_1_0, mu_2_0 = np.mean(X_negative,axis=0)

# Same Variance!

sigma_1_1, sigma_2_1 = np.std(X_positive,axis=0)
sigma_1_0, sigma_2_0 = np.std(X_negative,axis=0)
print(sigma_1_1, sigma_2_1)
print(sigma_1_0, sigma_2_0)

1.7556505128707445 1.830266323858797
1.8626233472002263 1.9122394301165095
```

## IS GNB A LINEAR SEPARATOR?

- It depends on whether we allow it to learn different standard deviations for each class

Decision rule:

$$\ln \frac{P(Y = 1|X_1 \dots X_d)}{P(Y = 0|X_1 \dots X_d)} = \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{P(X_i|Y = 1)}{P(X_i|Y = 0)} \quad > \text{ or } < 0?$$

If  $X_i$ s are  $\mathcal{N}(\mu_{ik}, \sigma_{ik})$ :

$$p(X_i = x|Y = y_k) = \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{ik})^2}{\sigma_{ik}^2}\right)$$

$$\begin{aligned} \ln \frac{P(Y = 1|X_1 \dots X_d)}{P(Y = 0|X_1 \dots X_d)} &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{P(X_i|Y = 1)}{P(X_i|Y = 0)} \\ &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\sigma_{i0}}{\sigma_{i1}} + G(X) \end{aligned}$$

$$\begin{aligned} G(X) &= \sum_i \ln \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{i1})^2}{\sigma_{i1}^2} + \frac{1}{2} \frac{(x_i - \mu_{i0})^2}{\sigma_{i0}^2}\right) \\ &= -\frac{1}{2} \sum_i \left( x_i^2 \left( \frac{1}{\sigma_{i1}^2} - \frac{1}{\sigma_{i0}^2} \right) - 2x_i \left( \frac{\mu_{i1}}{\sigma_{i1}^2} - \frac{\mu_{i0}}{\sigma_{i0}^2} \right) + \left( \frac{\mu_{i1}^2}{\sigma_{i1}^2} - \frac{\mu_{i0}^2}{\sigma_{i0}^2} \right) \right) \end{aligned}$$

What happens if we force  $\sigma_{i0} = \sigma_{i1}$ ?

- We get a linear decision boundary. Otherwise, it's a quadratic decision boundary.

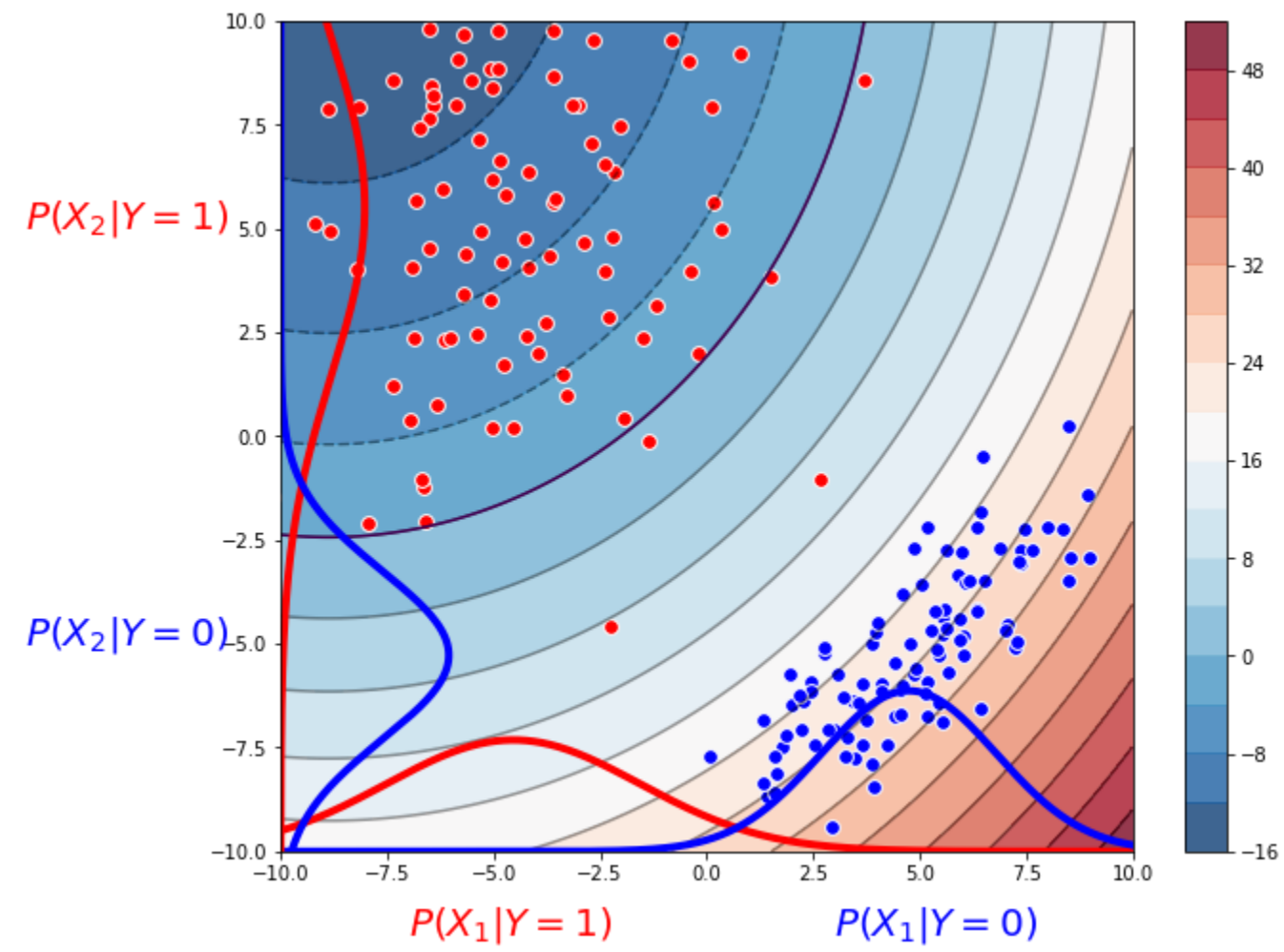
```
In [ ]: # Same param as before
mu_1_1 = -5; sigma_1_1 = 2
mu_2_1 = 5; sigma_2_1 = 2
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

cov_positive = np.array([[sigma_1_1**2,3], [3,sigma_2_1**2]] )
cov_negative = np.array([[sigma_1_0**2,3], [3,sigma_2_0**2]] )

# Sample data from these distributions
X_positive = multivariate_normal.rvs(mean=[mu_1_1,mu_2_1], cov=cov_positive, size = (100))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0], cov=cov_negative, size = (100))
```

```
In [28]: params = dict()
# Estimate - Different variance because of limited sample size
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)
```

```
In [29]: plot_GNB(X_positive,X_negative,params)
```



```
In [40]: # Let's set up another example in which the variances are actually different
mu_1_1 = -5; sigma_1_1 = 3
mu_2_1 = 5; sigma_2_1 = 4
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

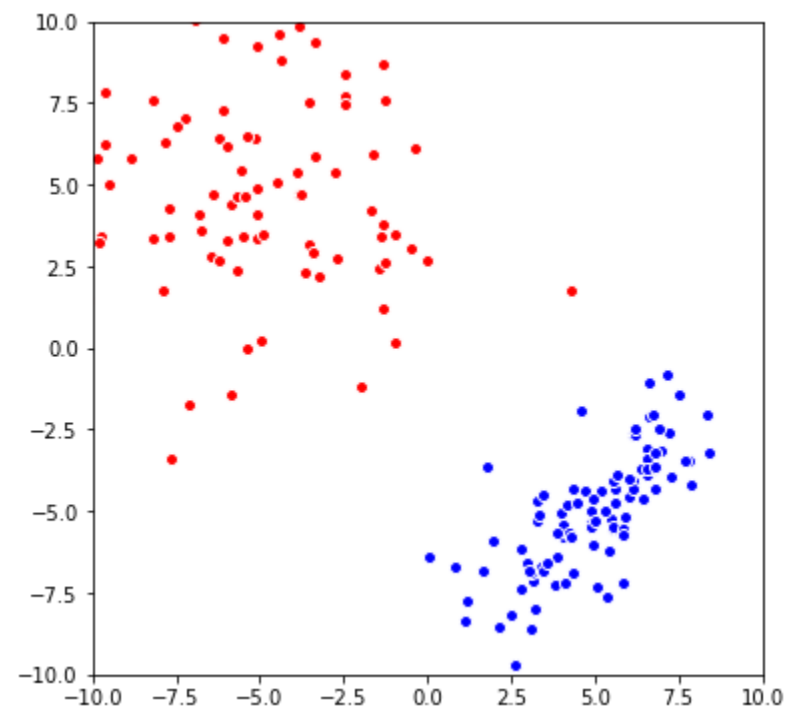
cov_positive = np.array([[sigma_1_1**2,3], [3,sigma_2_1**2]] )
cov_negative = np.array([[sigma_1_0**2,3], [3,sigma_2_0**2]] )

# Sample data from these distributions
X_positive = multivariate_normal.rvs(mean=[mu_1_1,mu_2_1],cov=cov_positive,size=(100))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0],cov=cov_negative,size=(100))

plt.figure(figsize=(6,6))

plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')
plt.axis([-10,10,-10,10],'equal')
```

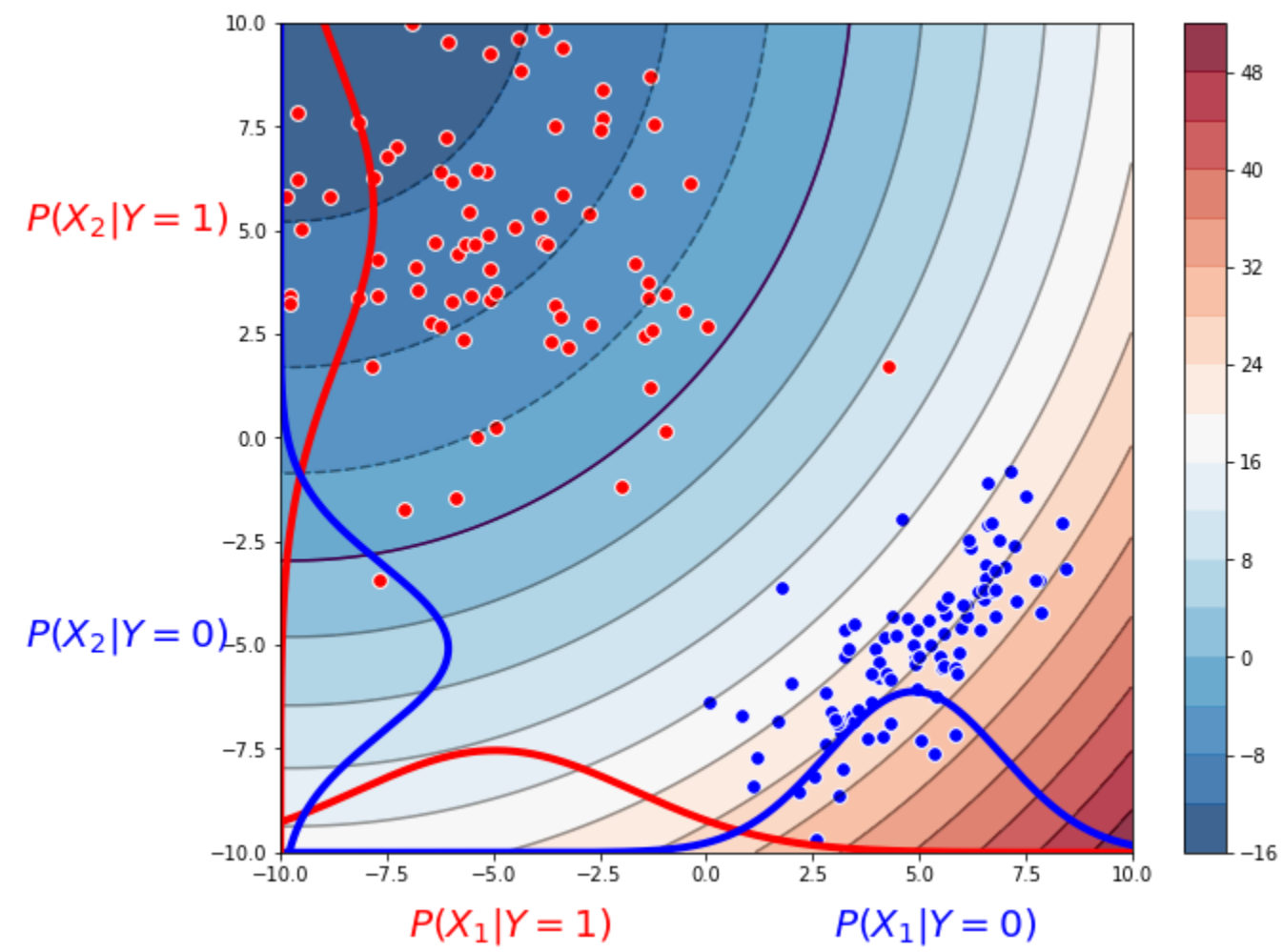
Out[40]: [-10, 10, -10, 10]





```
In [41]: params = dict()
# Estimate - Different variance
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)
```

```
In [42]: plot_GNB(X_positive,X_negative,params)
```



```
In [43]: from sklearn import datasets

plt.figure(figsize=(5,5))
X, y = datasets.make_circles(n_samples=200, factor=.25,noise=.1)

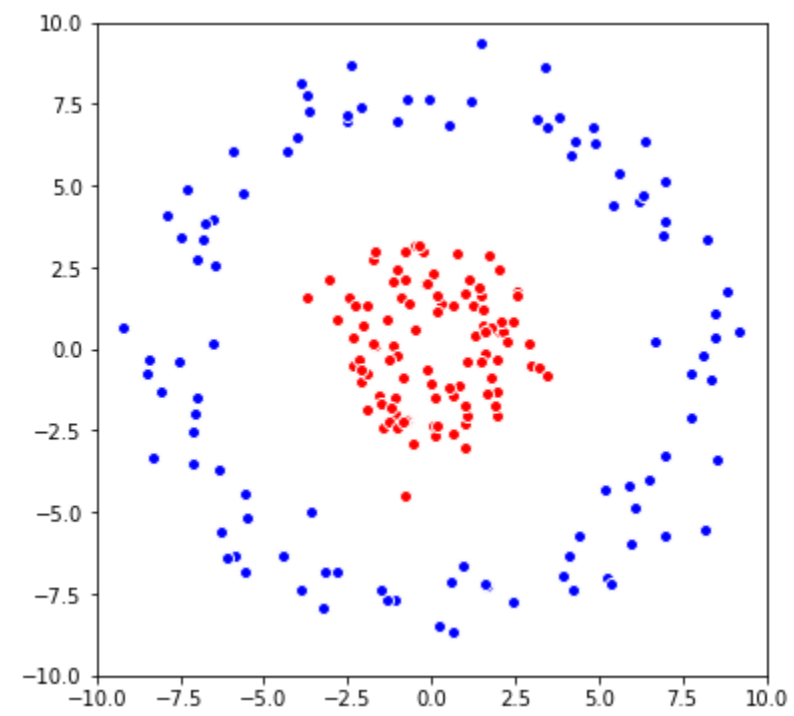
# scale
X_positive = X[y==1]*8
X_negative = X[y==0]*8
```

<Figure size 360x360 with 0 Axes>

```
In [44]: plt.figure(figsize=(6,6))

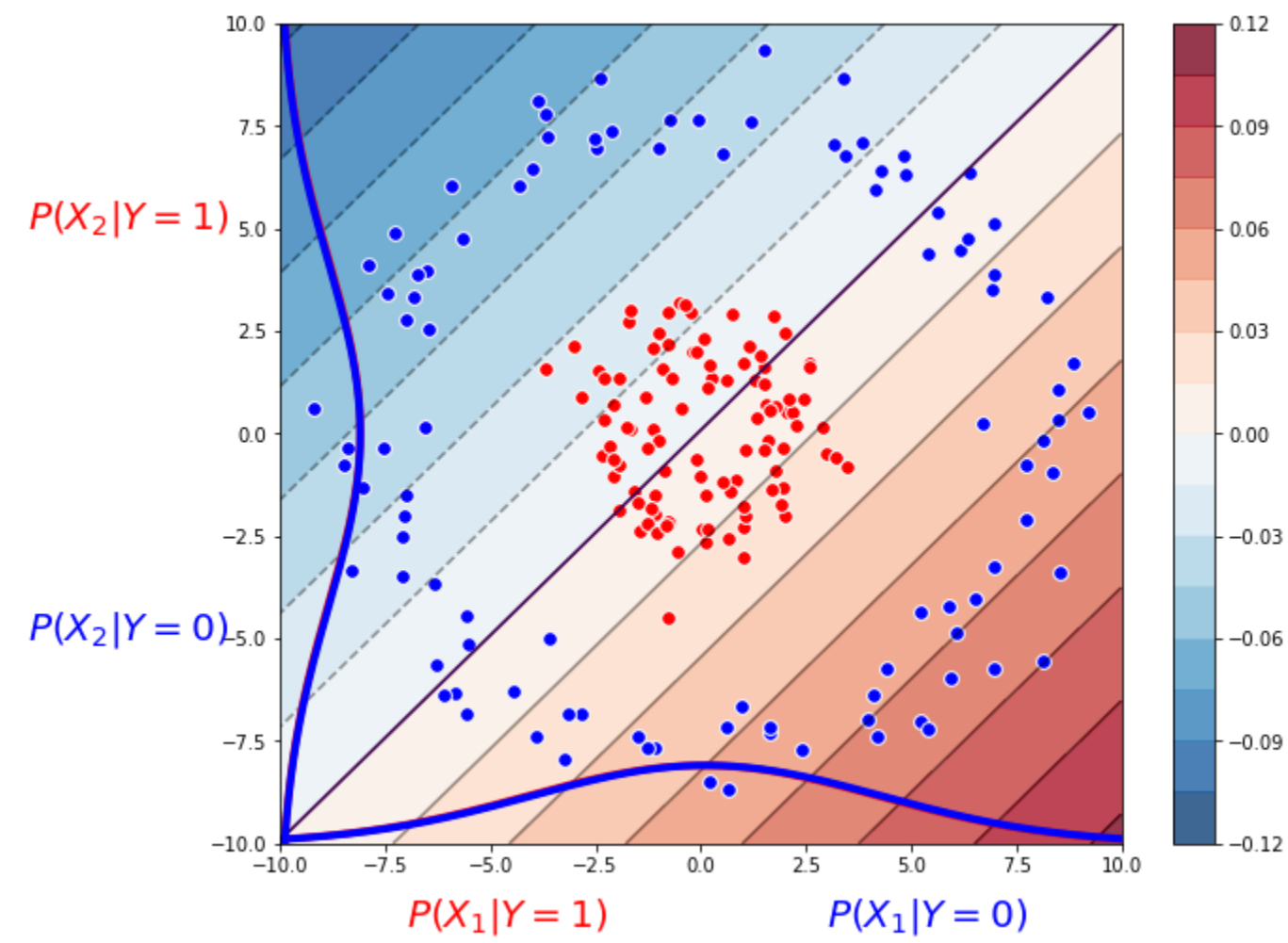
plt.scatter(X_positive[:, 0], X_positive[:, 1],facecolors='r', edgecolors='w')
plt.scatter(X_negative[:, 0], X_negative[:, 1],facecolors='b', edgecolors='w')
plt.axis([-10,10,-10,10],'equal')
```

Out[44]: [-10, 10, -10, 10]



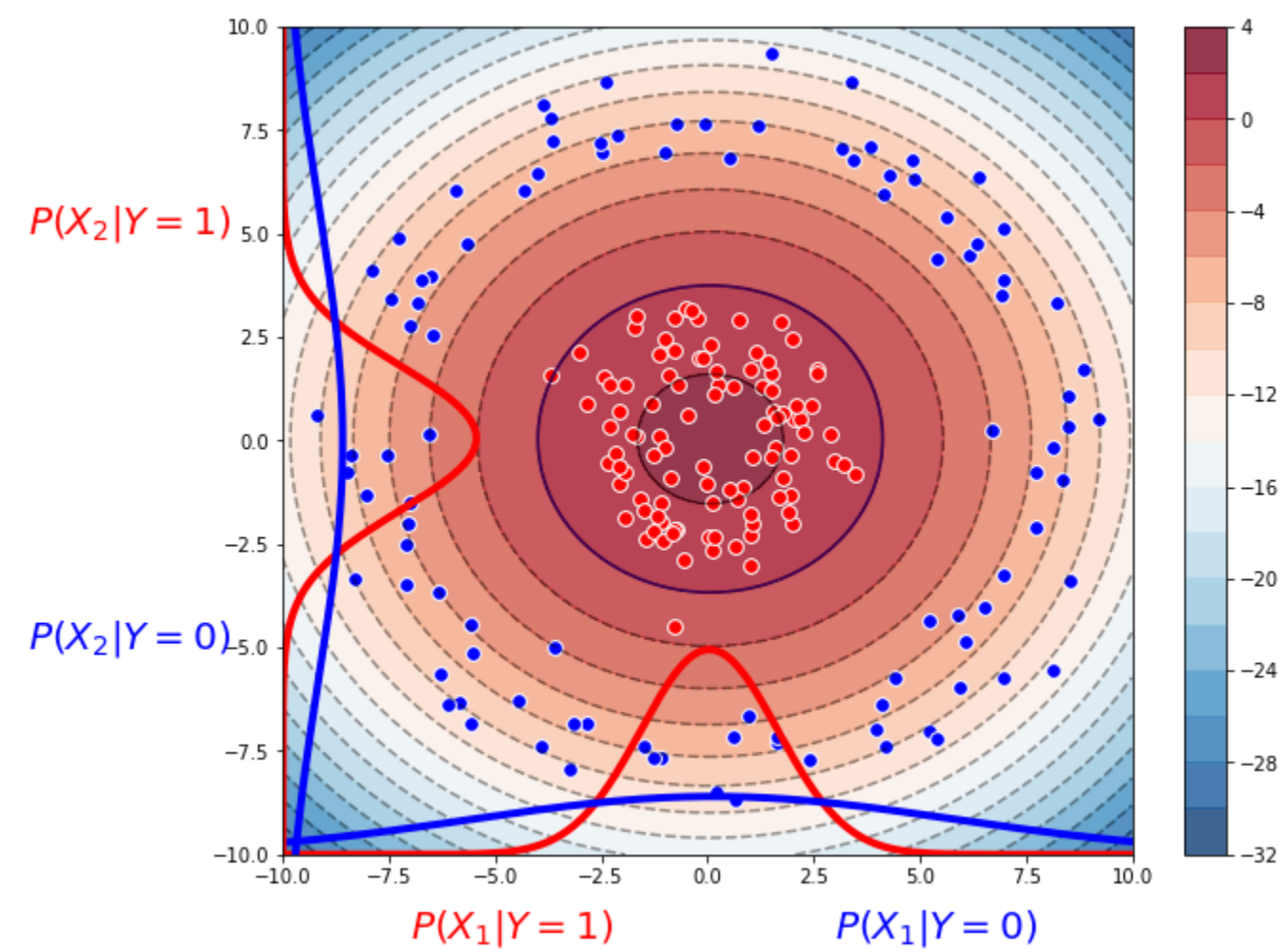
```
In [45]: params = dict()
# Artificially force same variances
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(np.vstack([X_positive,X_negative]),axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(np.vstack([X_positive,X_negative]),axis=0)
```

```
In [46]: plot_GNB(X_positive,X_negative,params)
```



```
In [47]: params = dict()
# Estimate - Different variance
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)
```

```
In [48]: plot_GNB(X_positive,X_negative,params)
```





## THE LAST EXAMPLE IS A CASE WHERE THE CONDITIONAL INDEPENDENCE ASSUMPTION IS INCORRECT

- but GNB does very well

# WHAT YOU SHOULD KNOW

## Naïve Bayes classifier

- What's the assumption
- Why we use it
- How do we learn it
- The different observations we made about it
- Why is Bayesian estimation important