

# 10-315 Introduction to Machine Learning (SCS Majors)

## Lecture 6: 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

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- 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  $X_i$ :

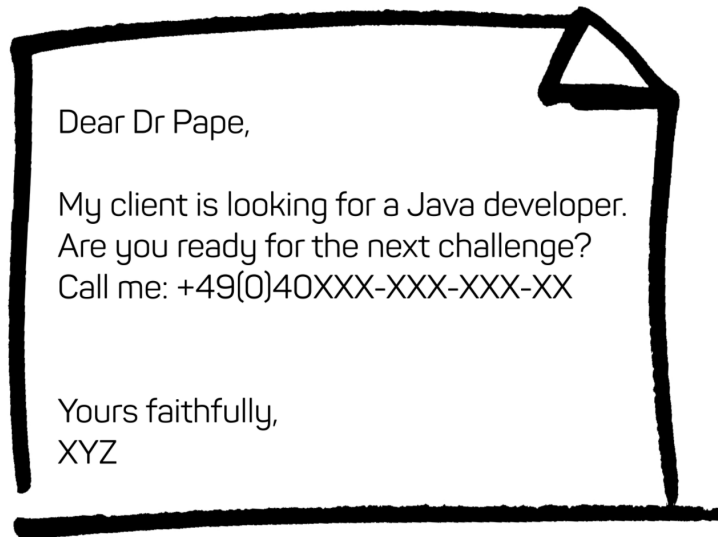
- For each value  $x_{ij}$  that  $X_i$  can take, compute:

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



## Example: Text classification

- Classify which emails are spam?



**SPAM**

**vs.**



**HAM**

[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 $X$ ?

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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
- $X = (X_1, X_2, \dots, X_d) = \text{document}$
- $X_i$  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)

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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)

# "Bag of Words" model

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- assume the  $X_i$  are IID:  
 $P(X_i|Y) = P(X_j|Y)(\forall i, j)$
- 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?

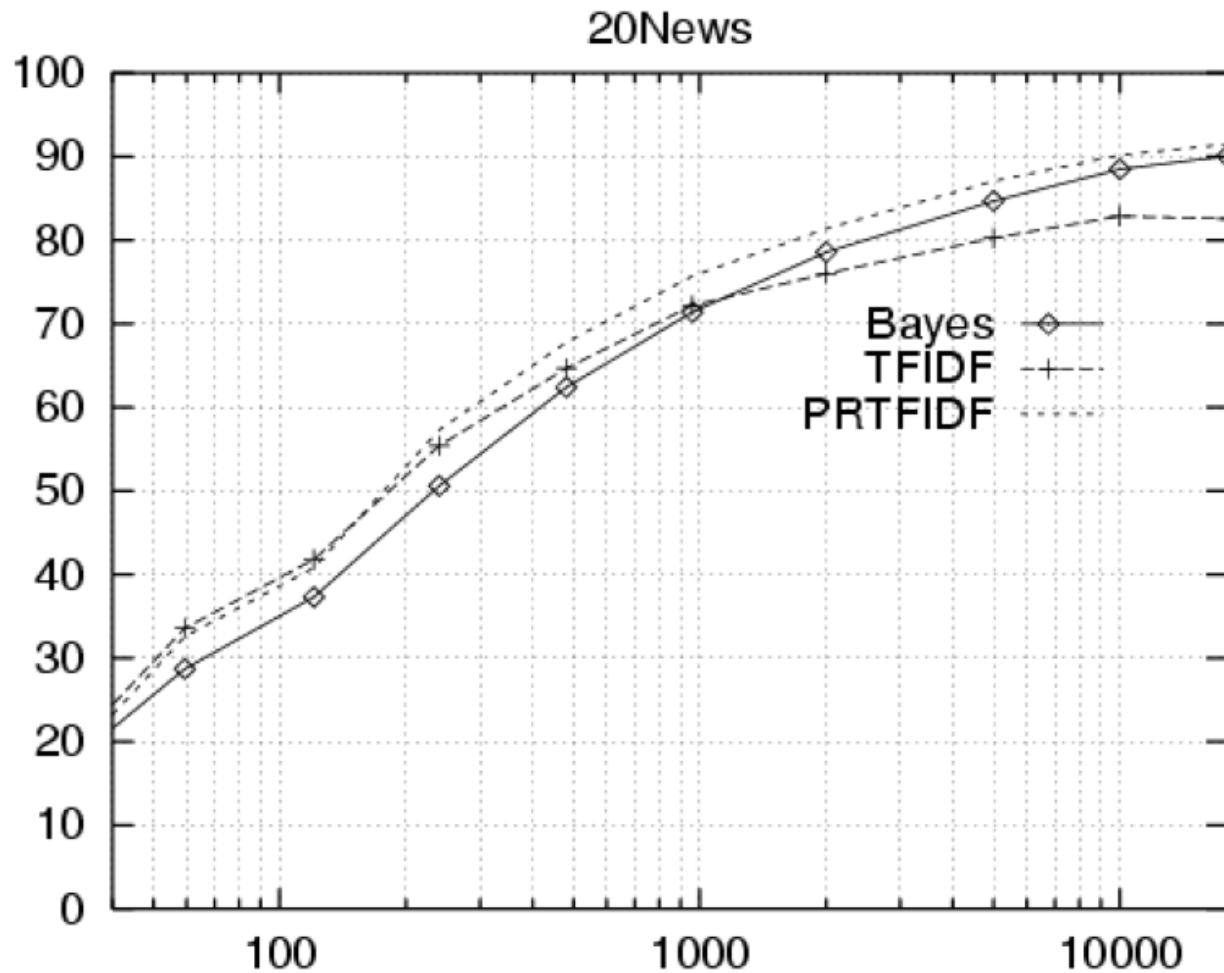
# Example: Twenty NewsGroups

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 ( $10000^{1000}$ ).

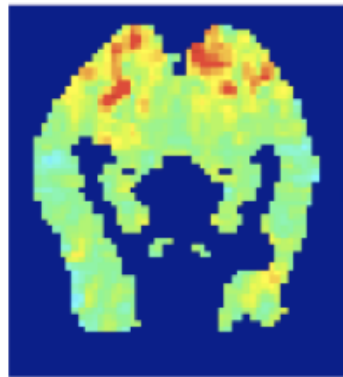
# Continuous $X_i$ s

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?

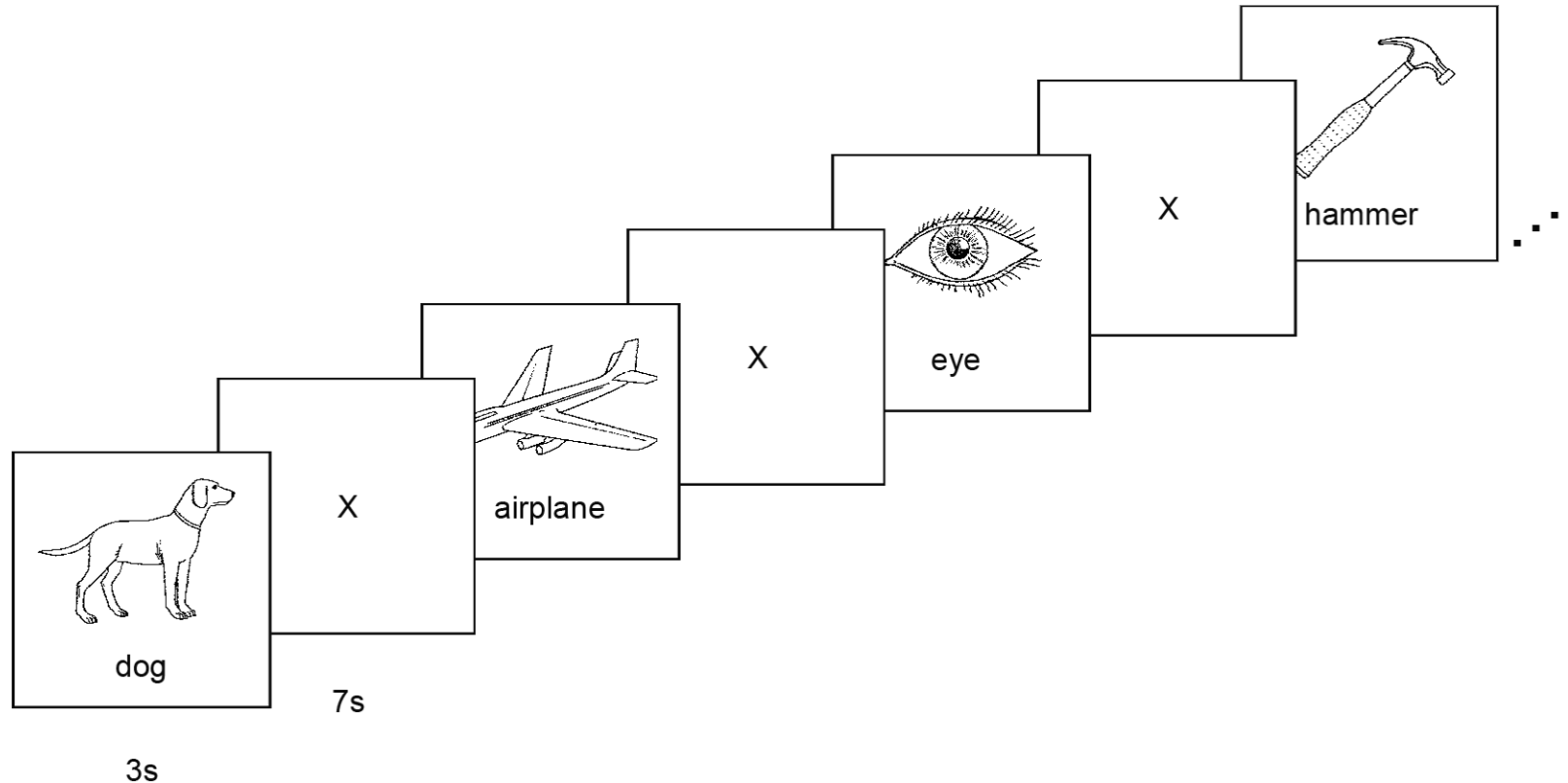


**Classifier**  
(Gaussian Bayes,  
logistic regression,  
SVM, kNN, ...)



~~Tool~~  
or  
Building

# Stimulus for the study

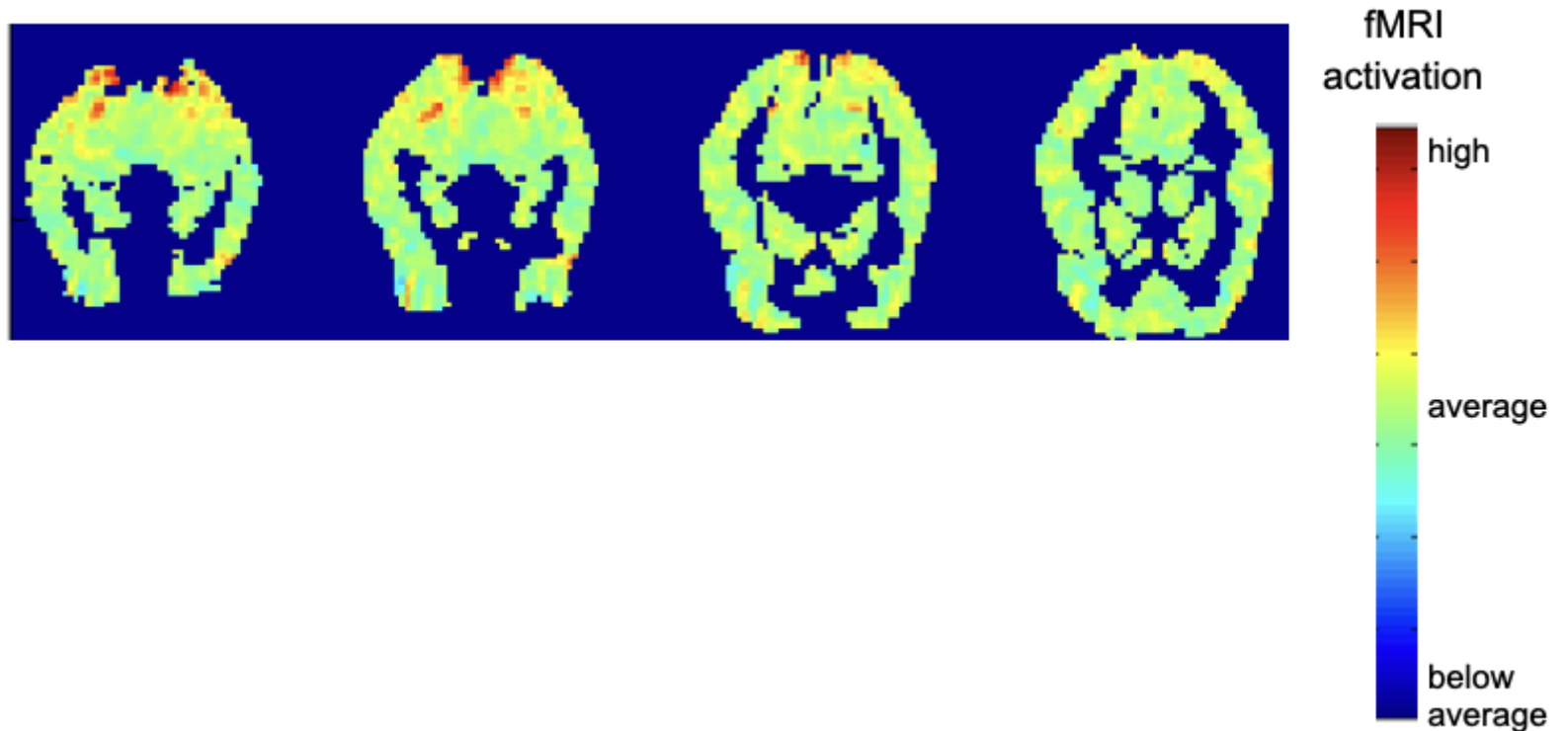


60 distinct exemplars, presented 6 times each

[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  $Y^{\text{new}}$

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

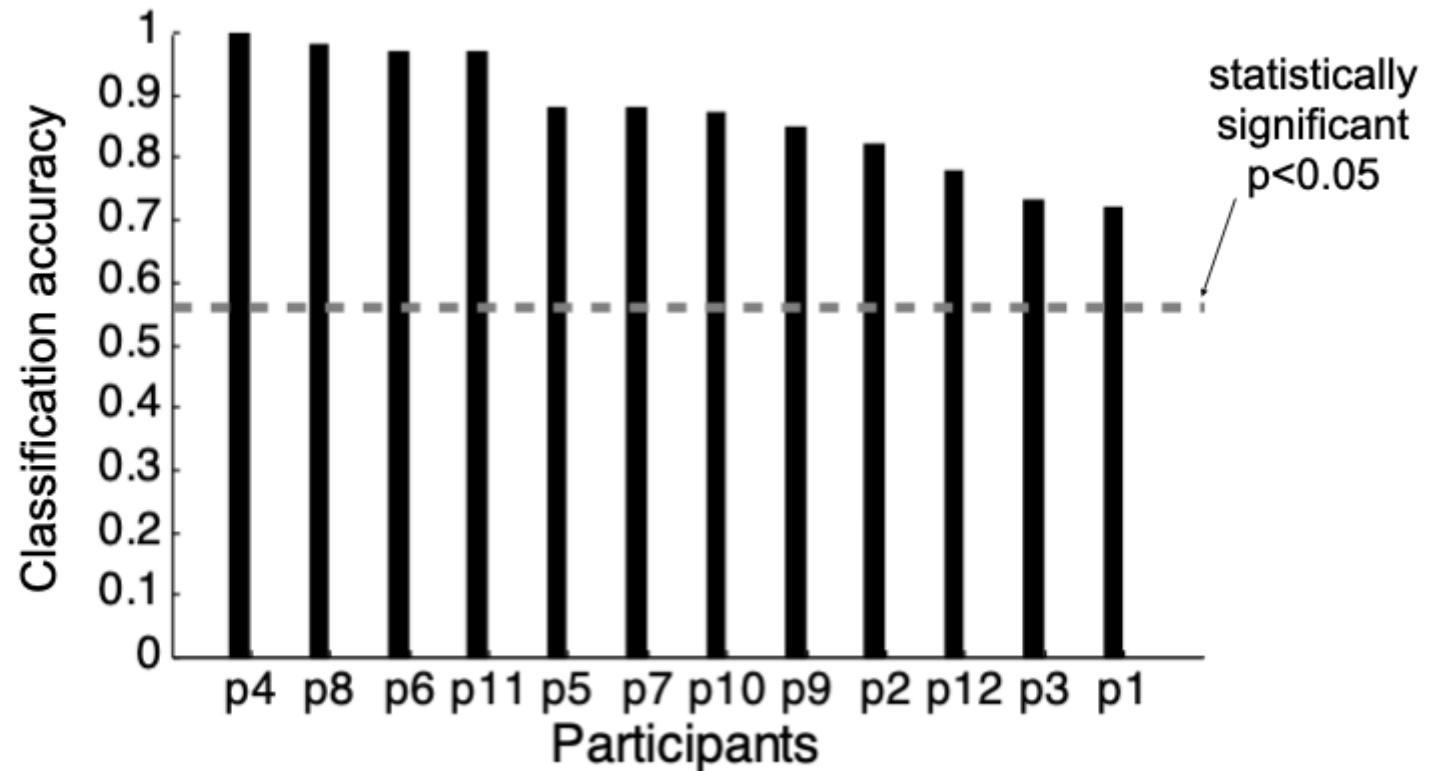
## Estimating Parameters: $Y$ discrete, $X_i$ continuous

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

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

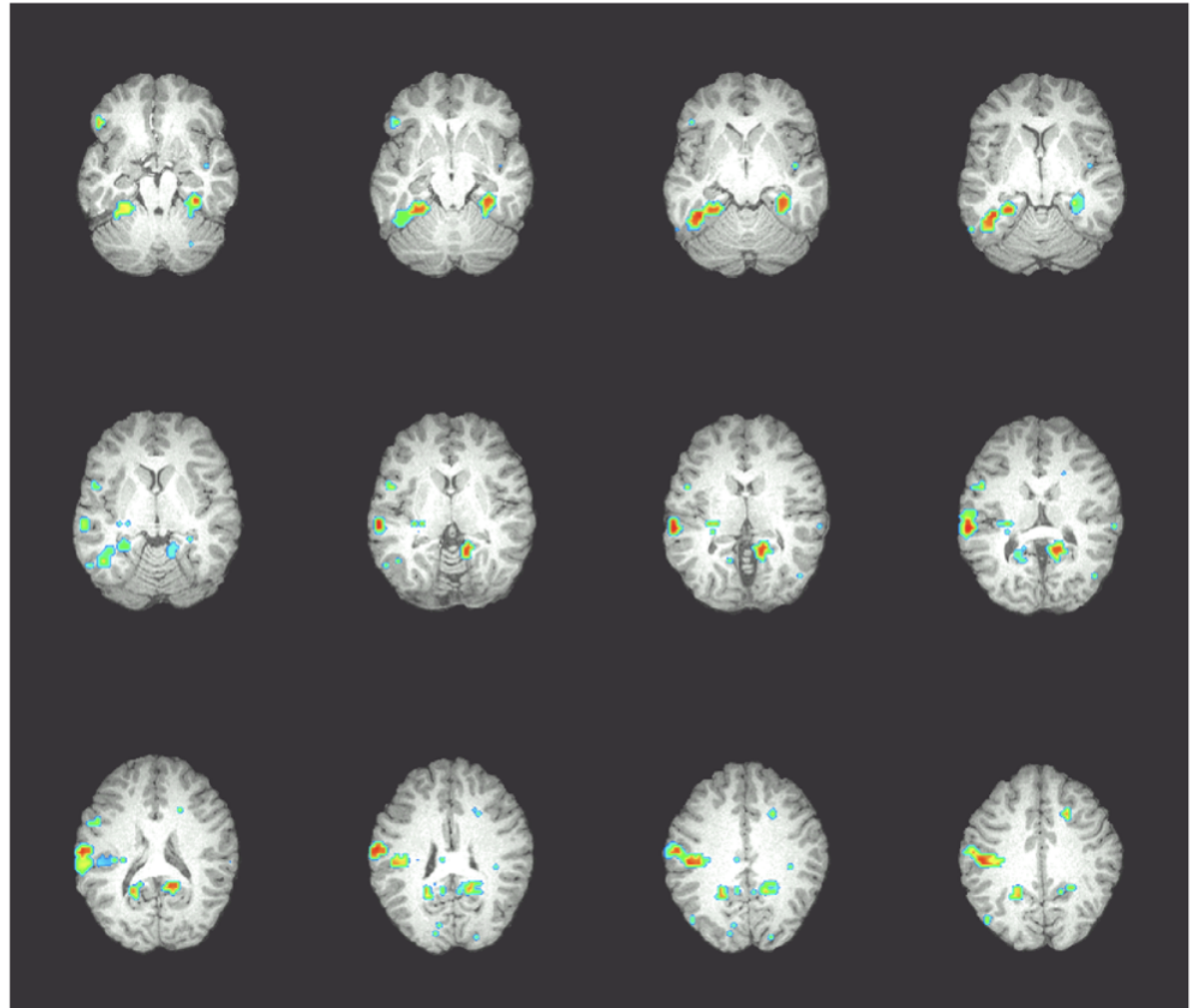
$$\hat{\sigma}_{ik}^2 = \frac{1}{\sum_j \delta(Y^j = y_k)} \sum_j (X_i^j - \hat{\mu}_{ik})^2 \delta(Y^j = y_k)$$

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 [3]: 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))

plt.figure(figsize=(8,8))

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[3]: [-10, 10, -10, 10]
```

```

In [7]: 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=(8,7))

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=24)

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=24)

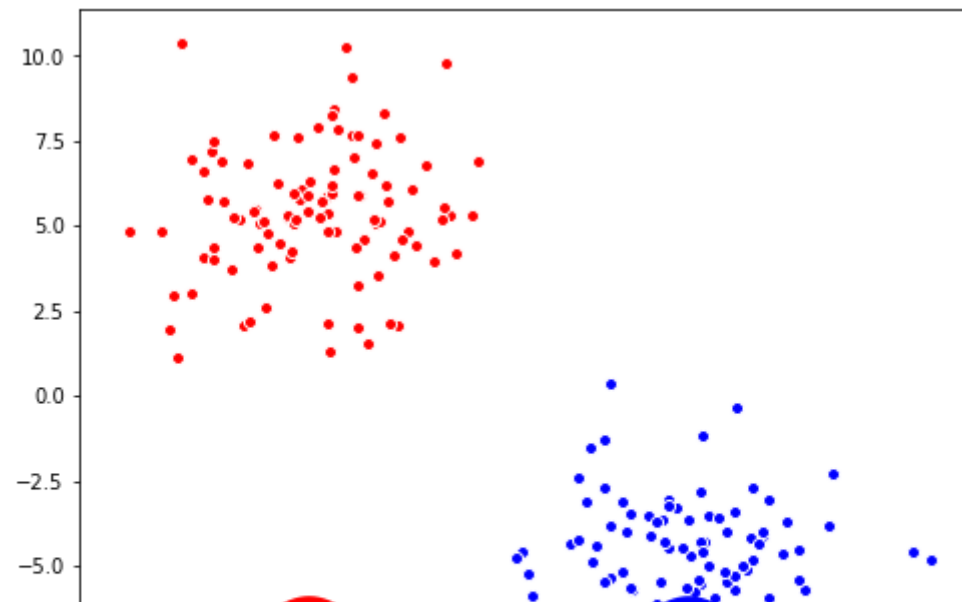
plt.figure(figsize=(8,8))

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([-lim_plot,lim_plot,-lim_plot,lim_plot],'equal');

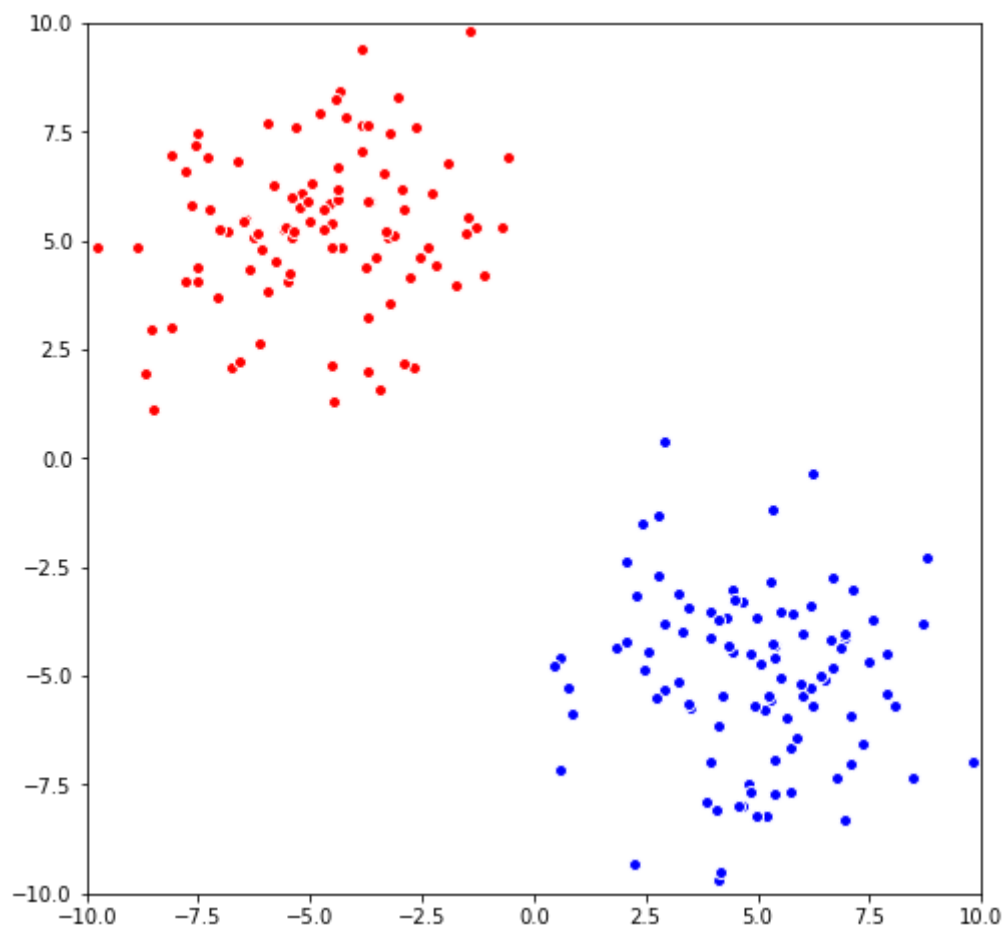
plt.axis([-10,10,-10,10],'equal')

```

Out[7]: [-10, 10, -10, 10]







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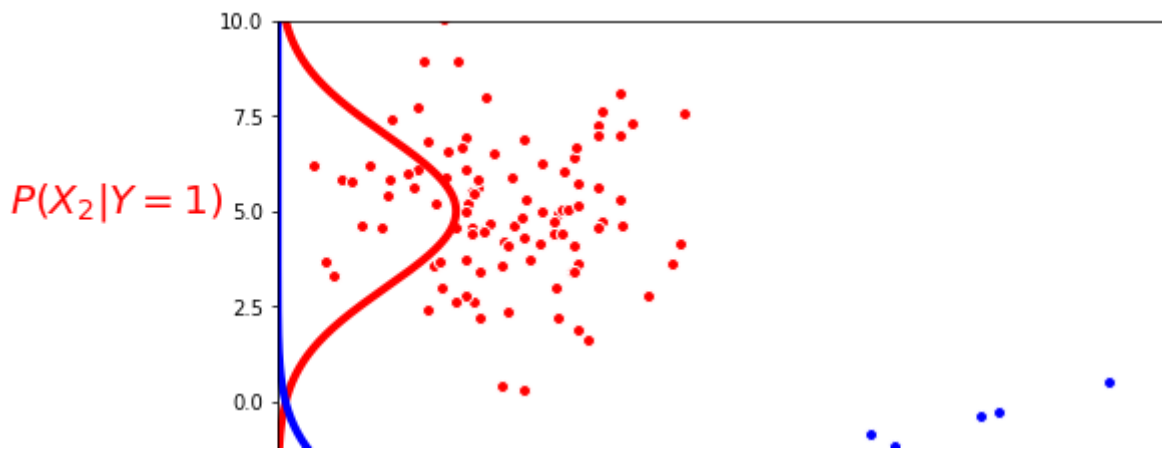
plt.plot(P_X2_1*2*lim_plot-lim_plot, x1, 'r', linewidth=4)
plt.text(-16, 5, r'$P(X_2|Y=1)$', color = 'red', fontsize=20)

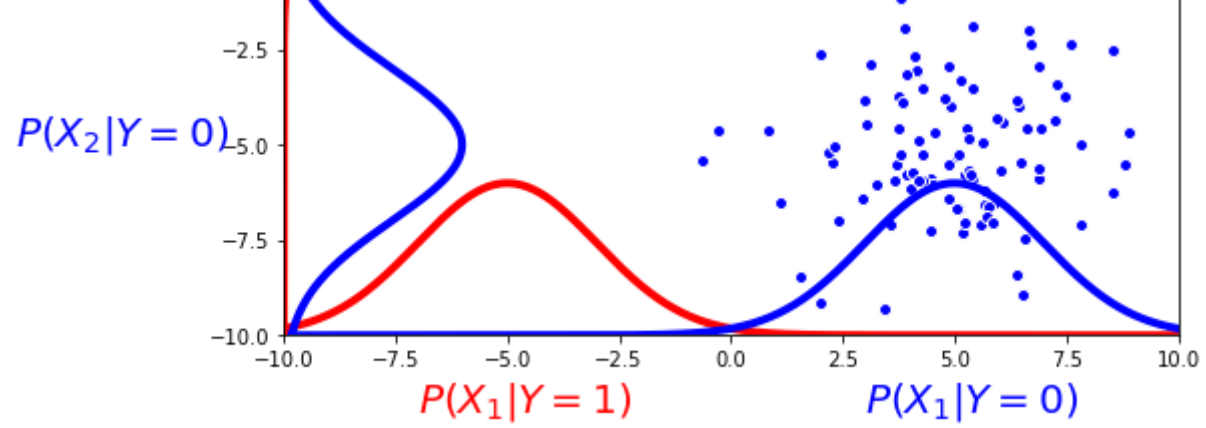
plt.plot(P_X2_0*2*lim_plot-lim_plot, x1, 'b', linewidth=4)
plt.text(-16, -5, r'$P(X_2|Y=0)$', color = 'blue', fontsize=20)

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

```

Out[3]: [-10, 10, -10, 10]





```
In [8]: # 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)
```

```

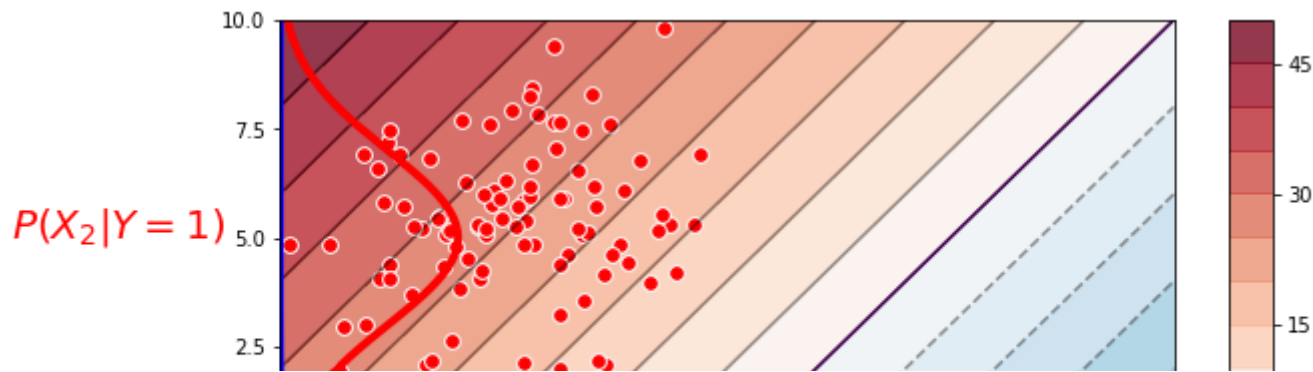
In [12]: plt.figure(figsize=(10,8))

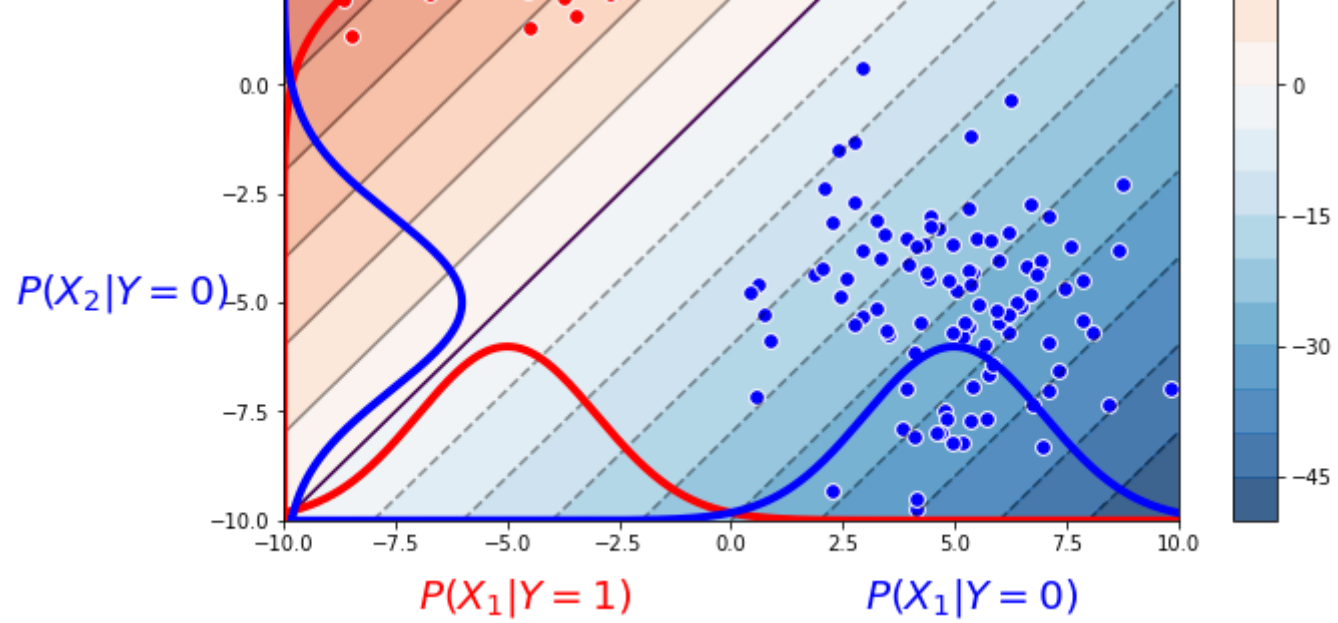
# plot contour plot
cs = plt.contourf(X1, X2, fX,20,cmap='RdBu_r',alpha=0.8);
plt.colorbar()
contours = plt.contour(cs, colors='k',alpha=0.4)
plt.contour(contours,levels=[0],linewidth=5)

# 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
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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')

```

Out[12]: [-10, 10, -10, 10]





```
In [24]: def ratio_log_compute(X1,X2,params):  
    pY0 =0.5; pY1 = 1- pY0  
    pY1pXY1 = pY1*norm.pdf(X1,params['mu_1_1'],params['sigma_1_1'])*norm.pdf(X2,pa  
    rams['mu_2_1'],params['sigma_2_1'])  
    pY0pXY0 = pY0*norm.pdf(X1,params['mu_1_0'],params['sigma_1_0'])*norm.pdf(X2,pa  
    rams['mu_2_0'],params['sigma_2_0'])  
    return np.log(pY1pXY1/pY0pXY0)
```

```

In [14]: 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_compute(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)

    # 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')

```



## 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 save variance

```
In [15]: 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)

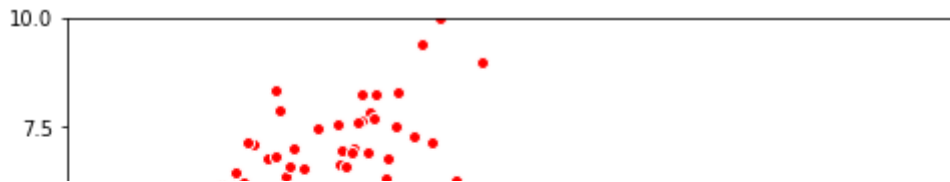
# Sample data from these distributions
X_positive = multivariate_normal.rvs(mean=[mu_1_1,mu_2_1], cov=cov_positive, size
= (100))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0], cov=cov_negative, size
= (100))

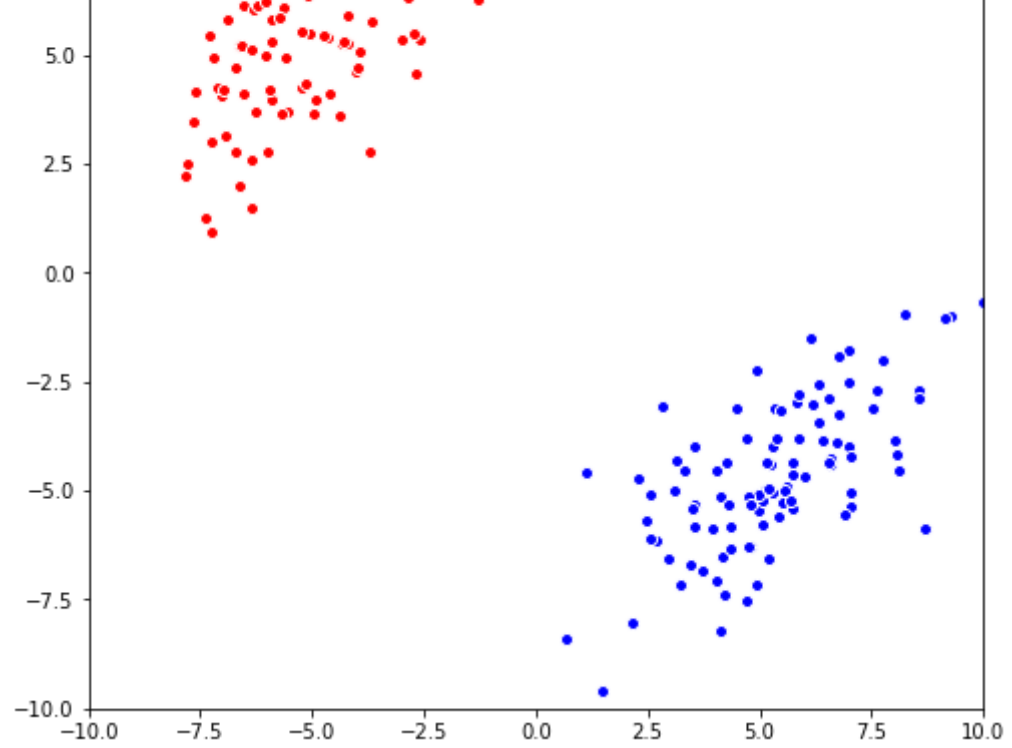
plt.figure(figsize=(8,8))

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]]
```

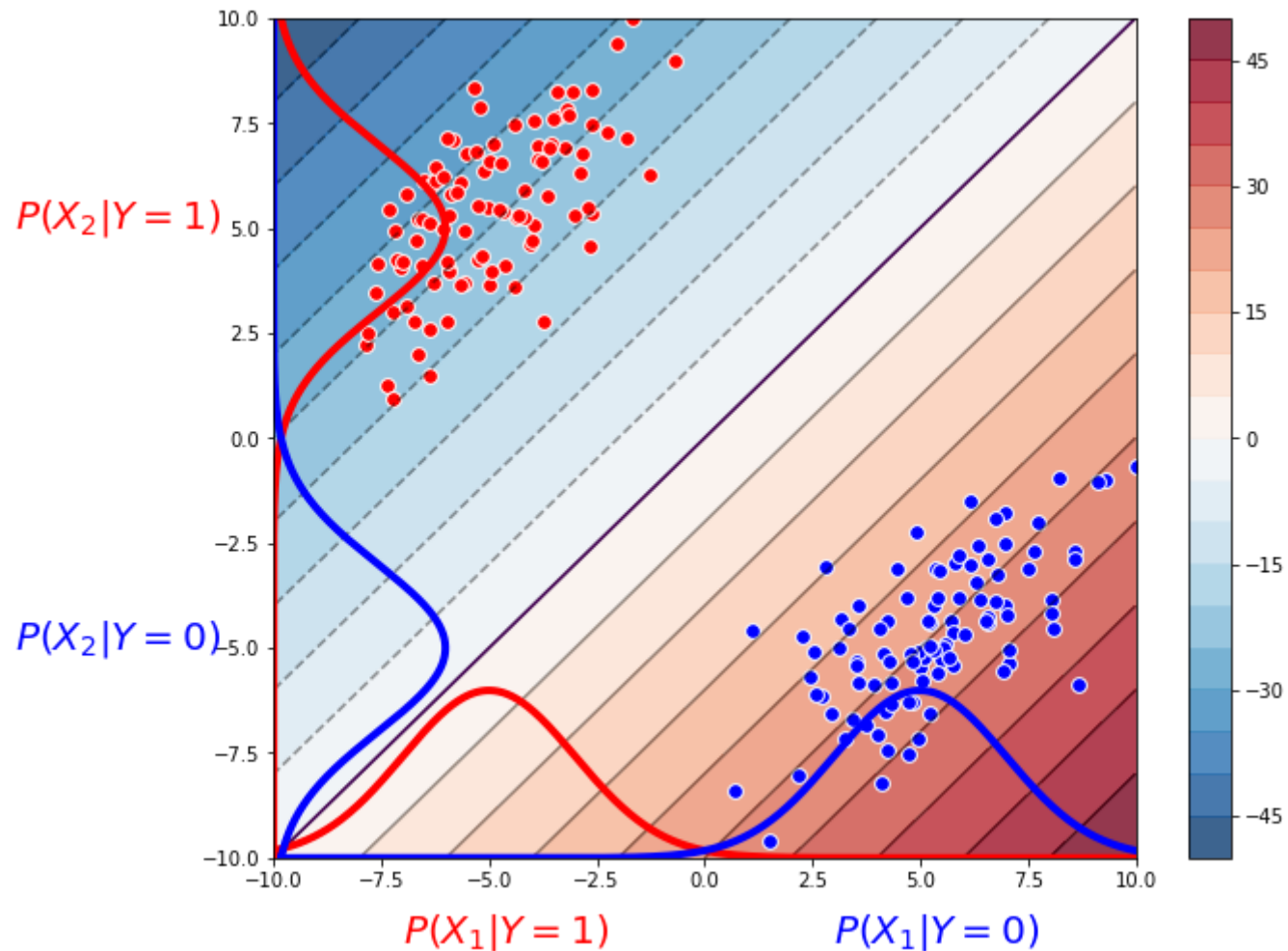
Out[15]: [-10, 10, -10, 10]





```
In [16]: # 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 [17]: *# 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)
```

```
1.7522444858114437 1.966082854951404
1.8771045185177992 1.8285375175548788
```

## 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  $\mathcal{N}(\mu_{ik}, \sigma_{ik})$ :

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

# 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  $\mathcal{N}(\mu_{ik}, \sigma_{ik})$ :

$$\begin{aligned} p(X_i = x|Y = y_k) &= \frac{1}{\sqrt{2\pi\sigma_{ik}^2}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{ik})^2}{\sigma_{ik}^2}\right) \\ \ln \frac{P(Y = 1|X_1 \dots X_d)}{P(Y = 0|X_1 \dots X_d)} &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{P(X_i|Y = 1)}{P(X_i|Y = 0)} \\ &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\frac{1}{\sigma_{i1}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{i1})^2}{\sigma_{i1}^2}\right)}{\frac{1}{\sigma_{i0}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{i0})^2}{\sigma_{i0}^2}\right)} \end{aligned}$$

# 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  $\mathcal{N}(\mu_{ik}, \sigma_{ik})$ :

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



$$\begin{aligned}
\ln \frac{P(Y = 1|X_1 \dots X_d)}{P(Y = 0|X_1 \dots X_d)} &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{P(X_i|Y = 1)}{P(X_i|Y = 0)} \\
&= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\frac{1}{\sigma_{i1}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{i1})^2}{\sigma_{i1}^2}\right)}{\frac{1}{\sigma_{i0}}} \\
&= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\sigma_{i0}}{\sigma_{i1}} - \frac{1}{2} \sum_i \left( x_i^2 \left( \frac{1}{\sigma_{i1}^2} - \frac{1}{\sigma_{i0}^2} \right) - 2x_i \left( \frac{\mu_{i1}}{\sigma_{i1}^2} - \frac{\mu_{i0}}{\sigma_{i0}^2} \right) \right)
\end{aligned}$$

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

# 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  $\mathcal{N}(\mu_{ik}, \sigma_{ik})$ :

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

$$\begin{aligned}
\ln \frac{P(Y = 1|X_1 \dots X_d)}{P(Y = 0|X_1 \dots X_d)} &= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{P(X_i|Y = 1)}{P(X_i|Y = 0)} \\
&= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\frac{1}{\sigma_{i1}} \exp\left(-\frac{1}{2} \frac{(x_i - \mu_{i1})^2}{\sigma_{i1}^2}\right)}{\frac{1}{\sigma_{i0}}} \\
&= \ln \frac{P(Y = 1)}{P(Y = 0)} + \sum_i \ln \frac{\sigma_{i0}}{\sigma_{i1}} - \frac{1}{2} \sum_i \left( x_i^2 \left( \frac{1}{\sigma_{i1}^2} - \frac{1}{\sigma_{i0}^2} \right) - 2x_i \left( \frac{\mu_{i1}}{\sigma_{i1}^2} - \frac{\mu_{i0}}{\sigma_{i0}^2} \right) \right)
\end{aligned}$$

What happens if we force  $\hat{\sigma}_{i0} = \hat{\sigma}_{i1}$ ?

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

```

In [18]: # 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))

plt.figure(figsize=(8,8))

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')

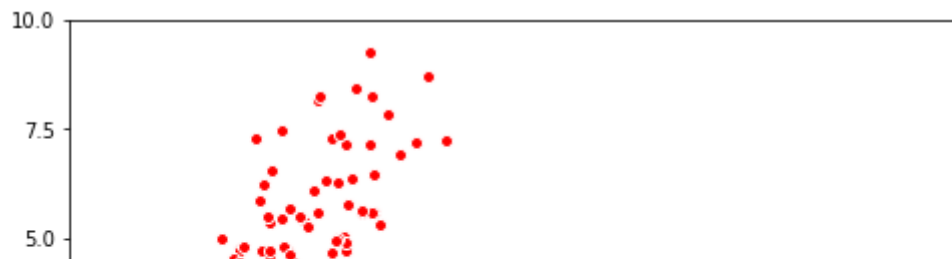
```

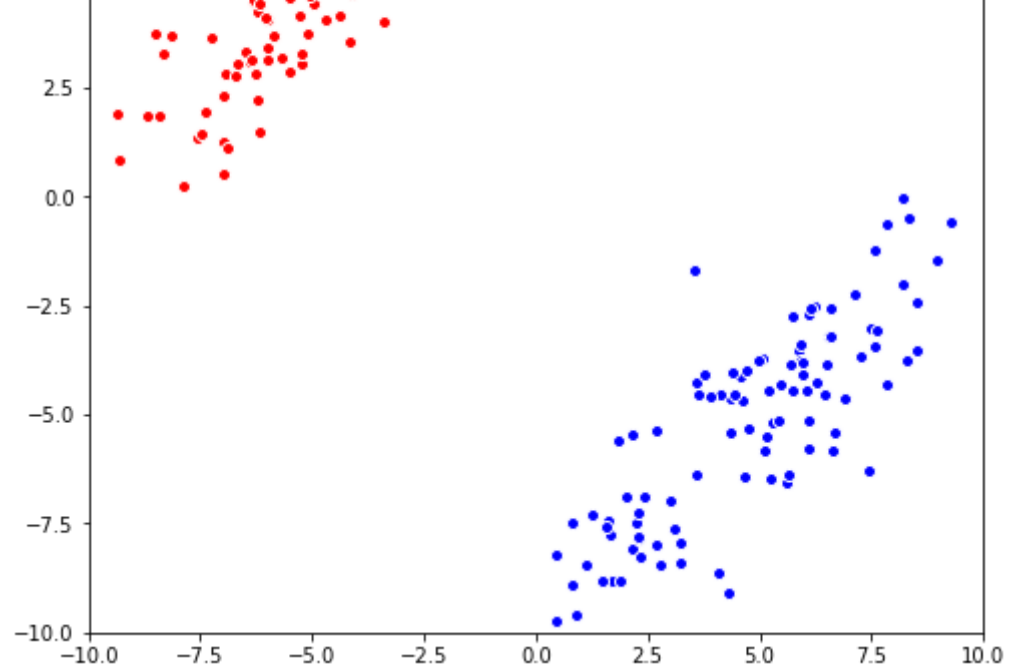
```

[[4 3]
 [3 4]]

```

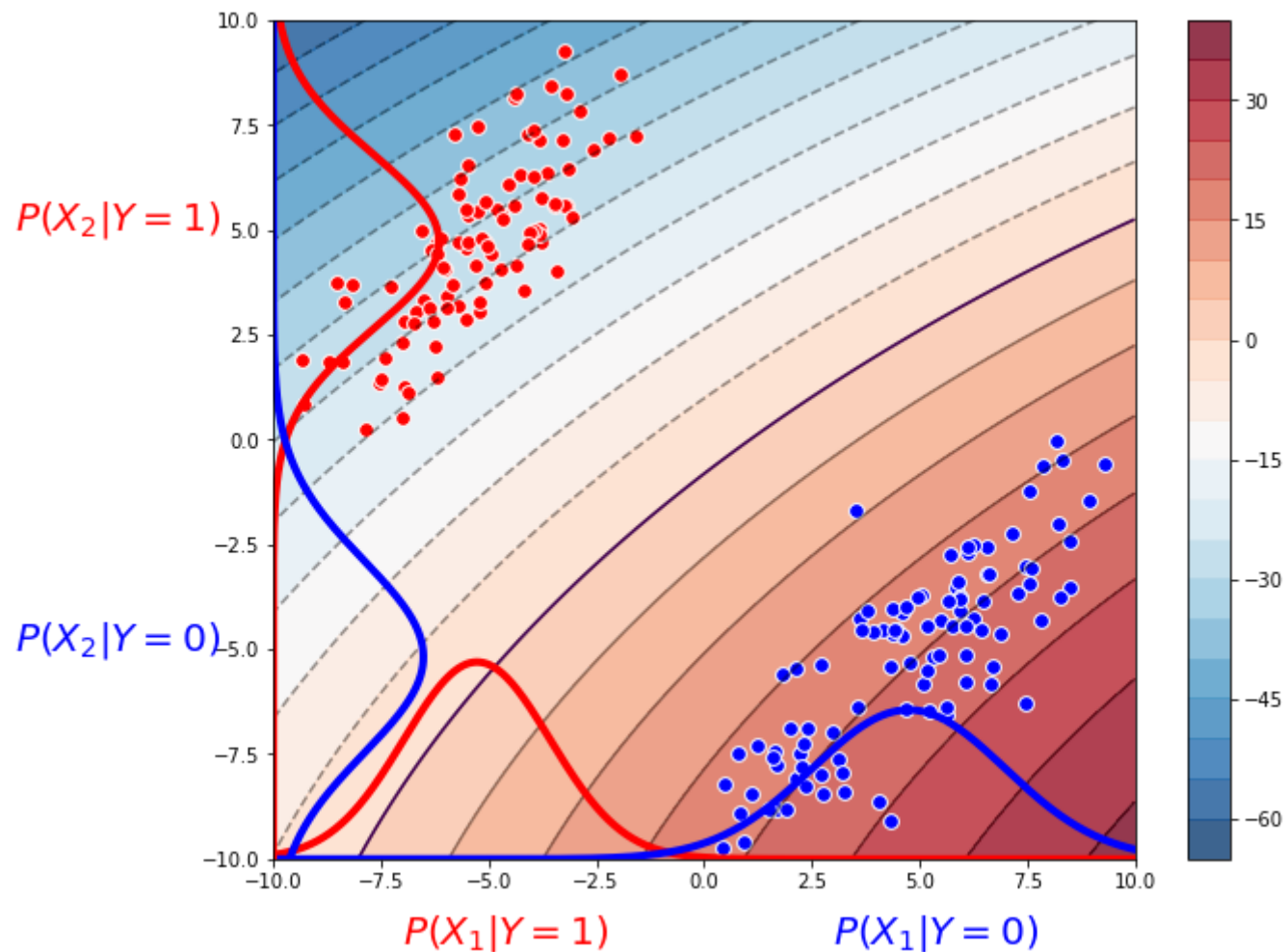
Out[18]: [-10, 10, -10, 10]





```
In [19]: 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)

plot_GNB(X_positive,X_negative,params)
```





```

In [20]: # 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]] )

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))

plt.figure(figsize=(8,8))

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')

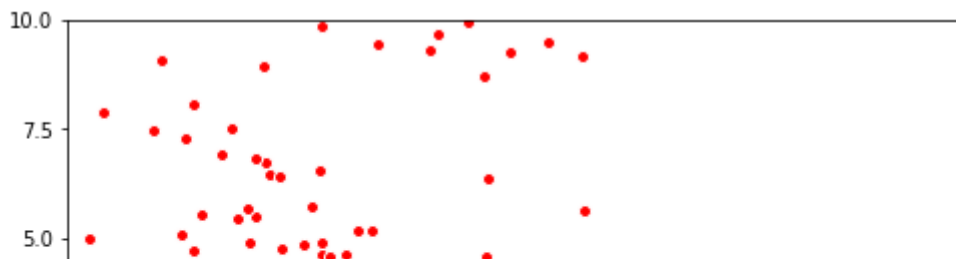
```

```

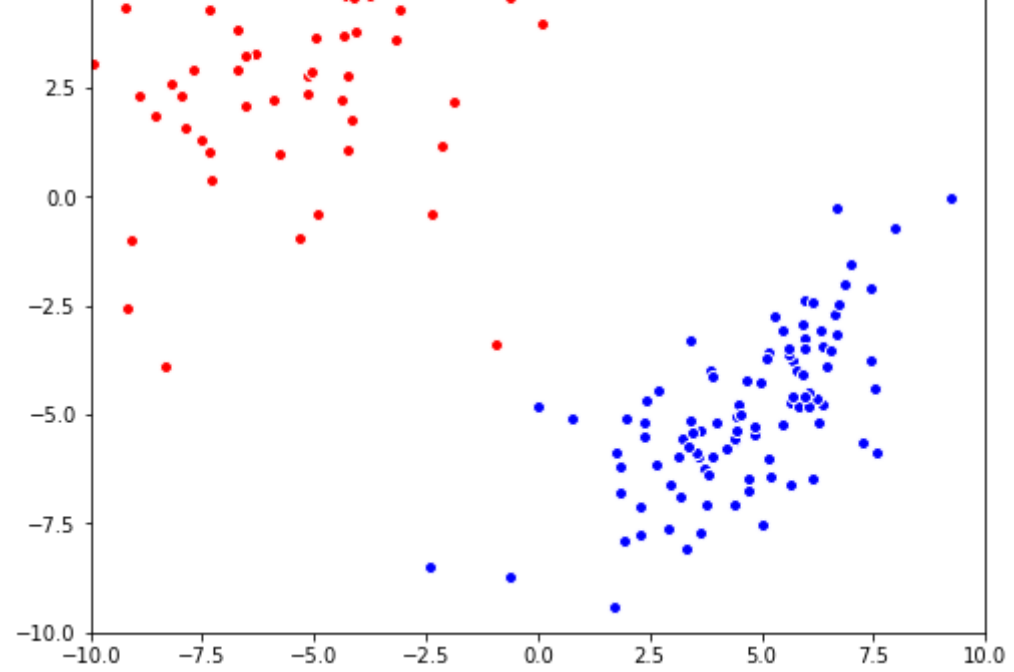
[[ 9  3]
 [ 3 16]]

```

Out[20]: [-10, 10, -10, 10]

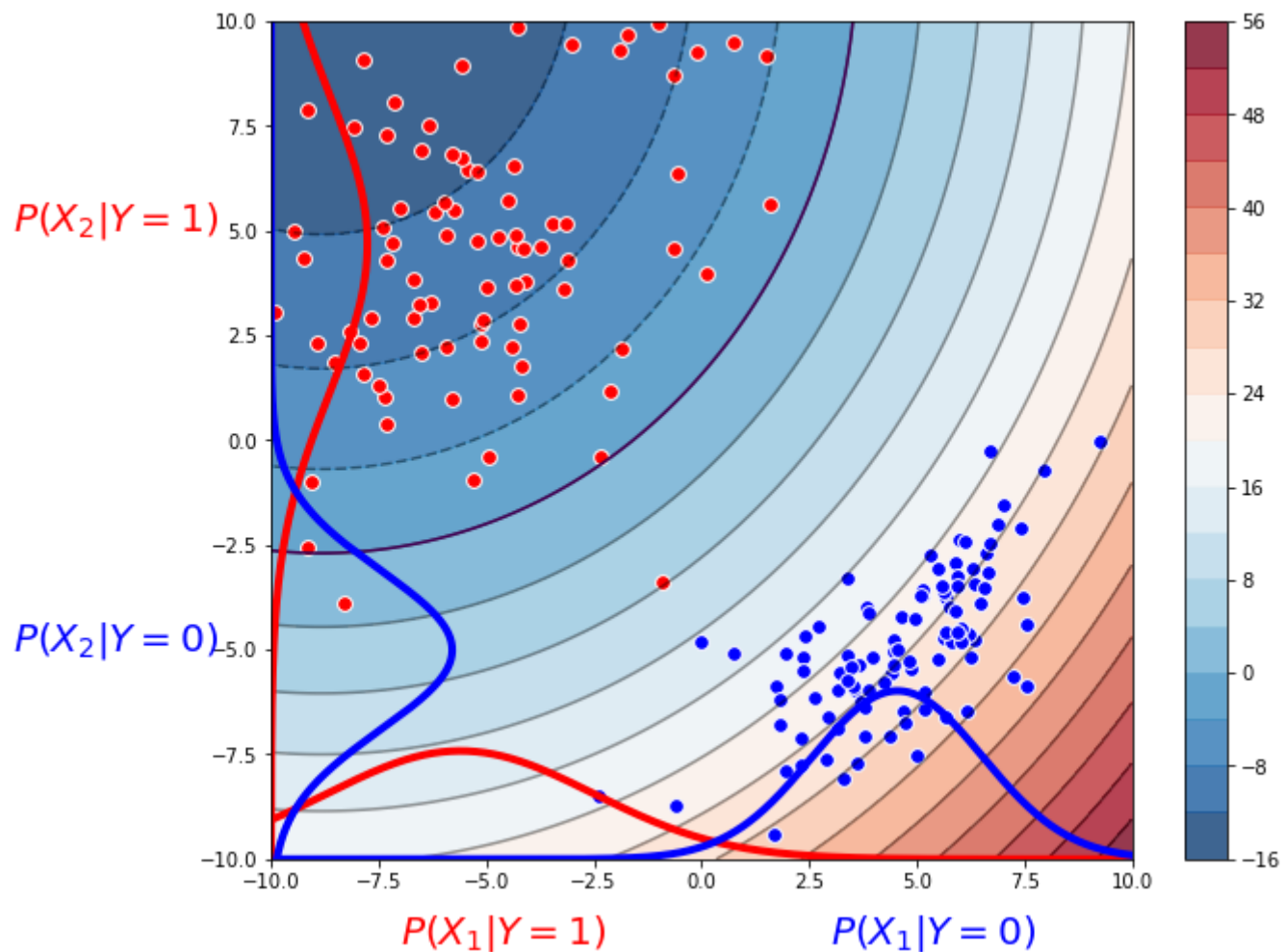






```
In [21]: params = dict()
# Estimate - Different variance
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)

plot_GNB(X_positive,X_negative,params)
```





```
In [22]: from sklearn import datasets

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

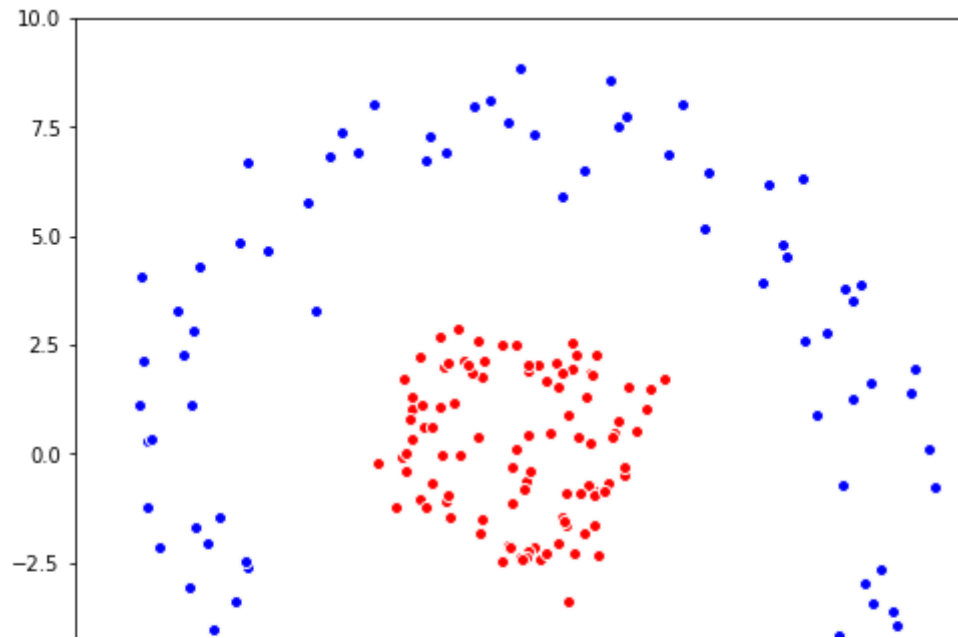
# scale
X_positive = X[y==1]*8
X_negative = X[y==0]*8

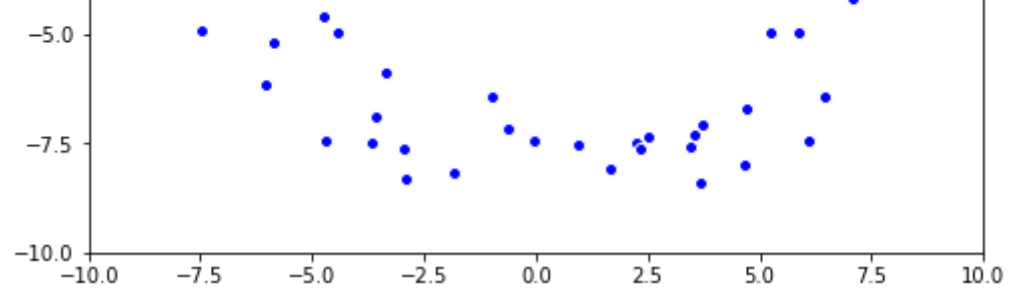
plt.figure(figsize=(8,8))

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[22]: [-10, 10, -10, 10]

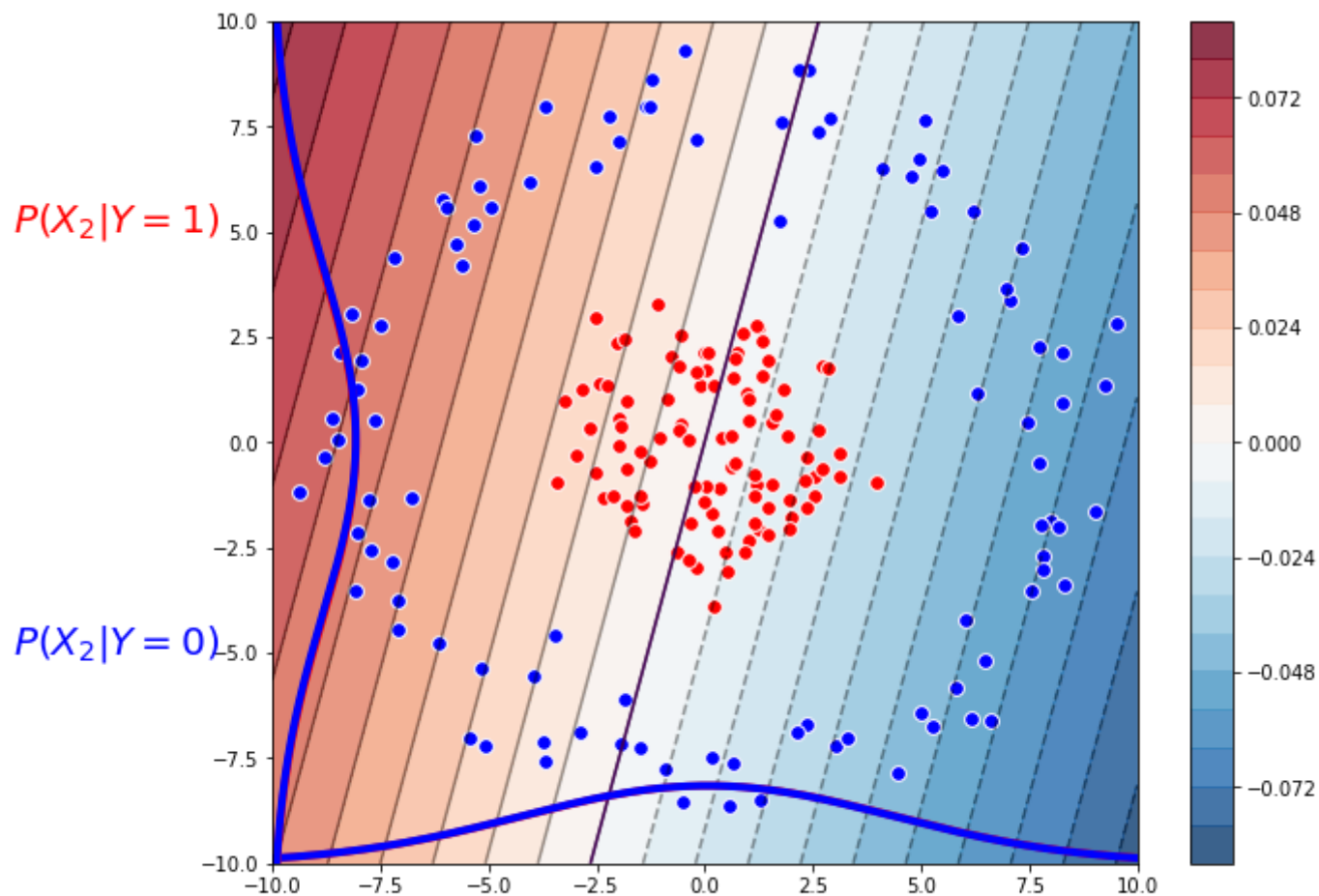
<Figure size 360x360 with 0 Axes>





```
In [49]: 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)

plot_GNB(X_positive,X_negative,params)
```



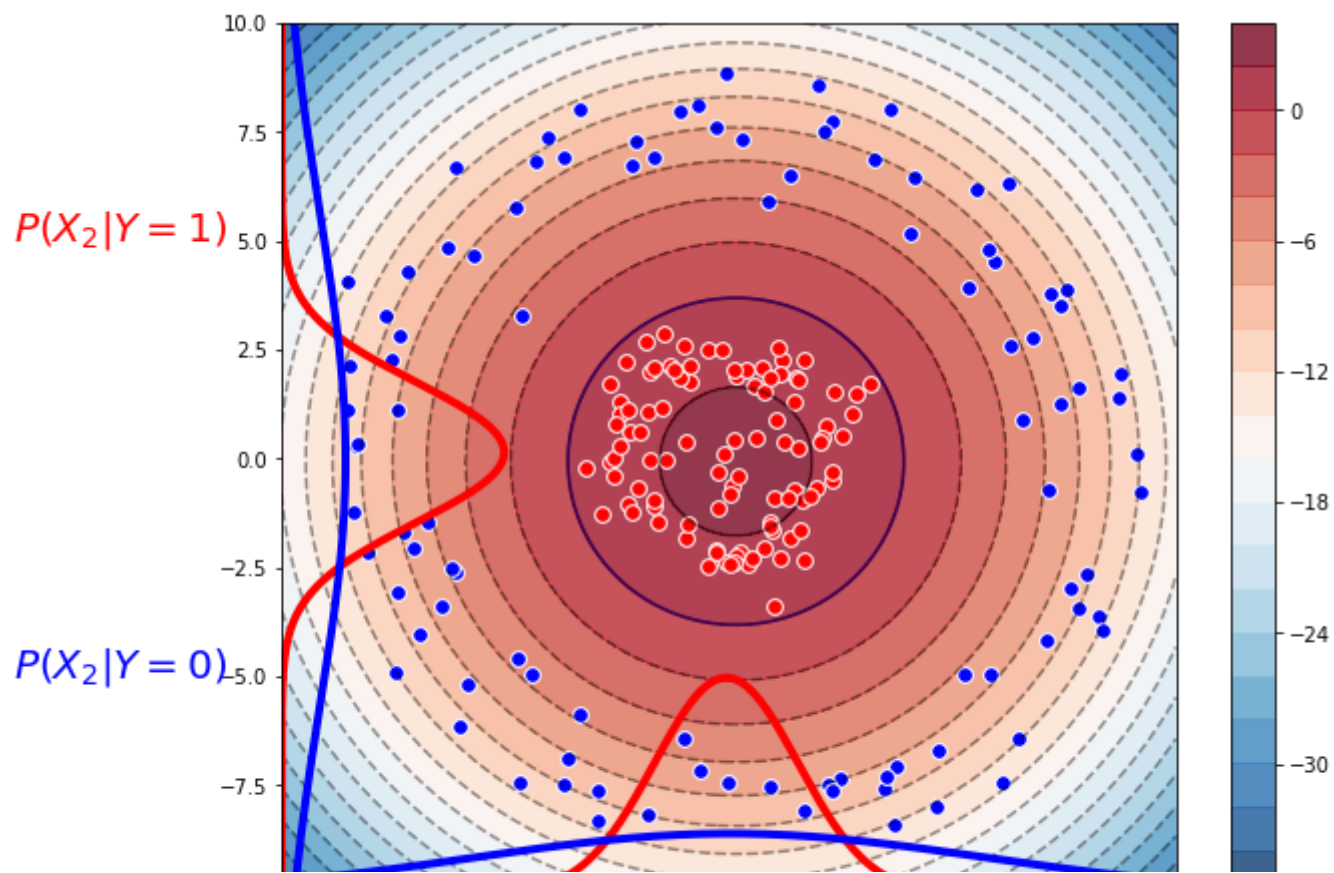
$$P(X_1|Y = 1)$$

$$P(X_1|Y = 0)$$

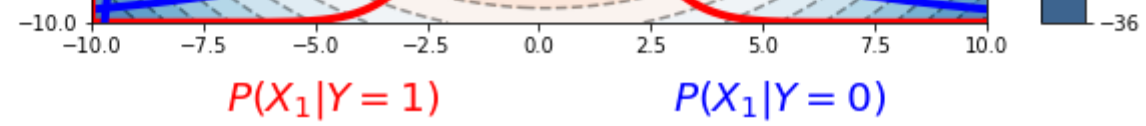
```
In [23]: params = dict()
# Estimate - Different variance
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)

plot_GNB(X_positive,X_negative,params)
```

/Users/lwehbe/env/py3/lib/python3.7/site-packages/matplotlib/contour.py:1000:  
UserWarning: The following kwargs were not used by contour: 'linewidth'  
s)







**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

In [ ]: