10-315 Introduction to Machine Learning (SCS Majors)
Lecture 7: Logistic Regression

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

Lecture outcomes:

- Logistic Regression
- Gradient Descent Review
- Comparing LR and GNB

The Naïve Bayes Algorithm

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

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

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

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

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 $\hat{\theta}_{ijk}$
    - θ_{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^{new}

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

Method 1: Maximum (Conditional) Likelihood Estimation

Method 2: Maximum A Posteriori Probability Estimation

Gaussian Naïve Bayes Algorithm – continuous $\boldsymbol{X_i}$ (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 μ_{ik} and standard deviation σ_{ik}

- Prediction: Classify Y^{new}

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

Estimating Parameters: Y discrete, X_i continuous

Maximum (Conditional) Likelihood Estimation

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

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

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

Let's simulate the behavior of GNB!

We saw:

- What happens if the variances are the same across classes?
- What could happen if the variables are not really conditionally independent?

In [25]:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from scipy.stats import norm
import seaborn as sns
sns.set_theme()

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 = (1
00,2))
X_negative = norm.rvs(loc=[mu_1_0,mu_2_0], scale=[sigma_1_0, sigma_2_0], size = (1
00,2))


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')
```

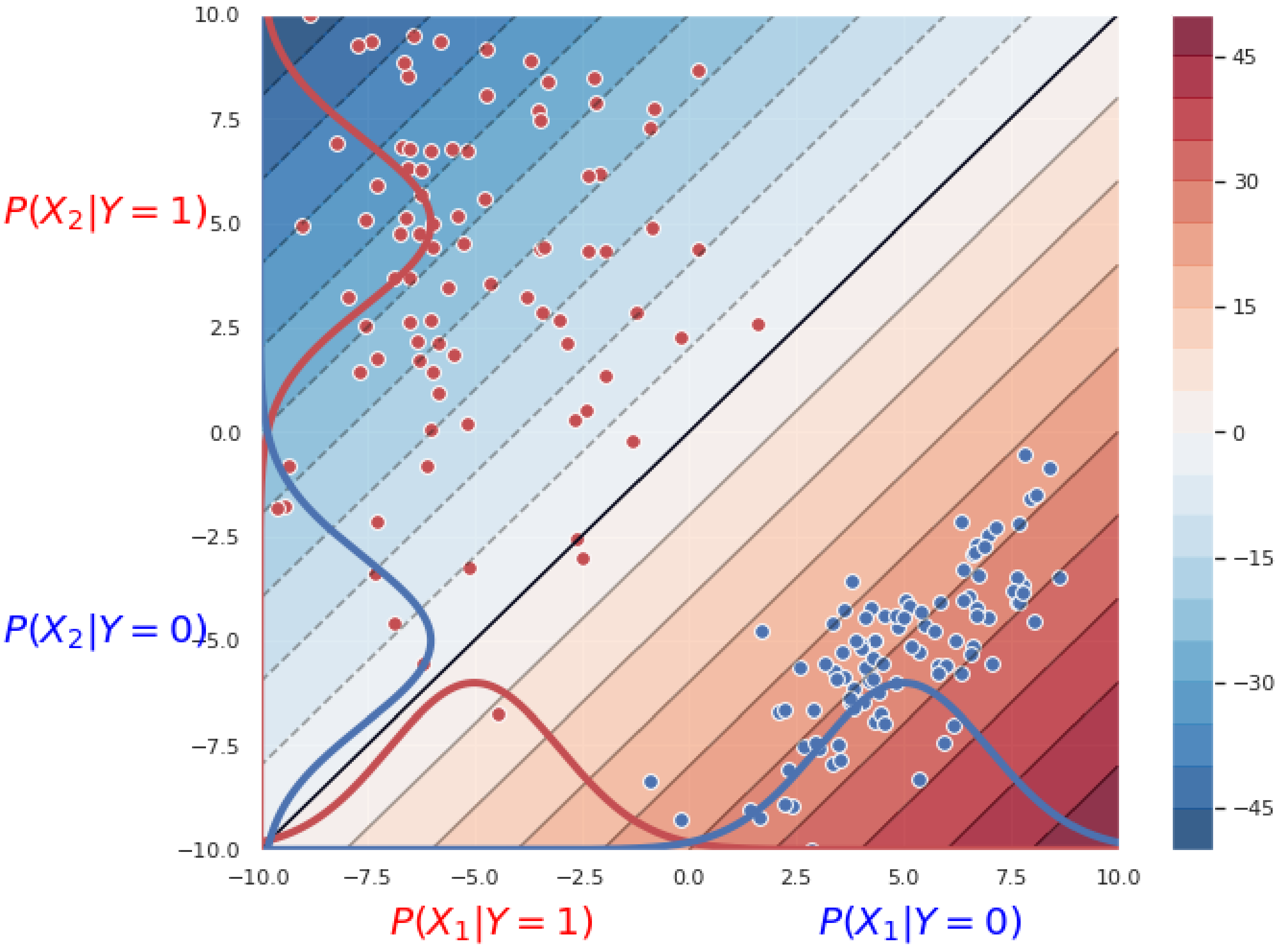
Out[25]:

```
[-10, 10, -10, 10]
```

In [48]:

```
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([1,1
000]))/
                                 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')
```

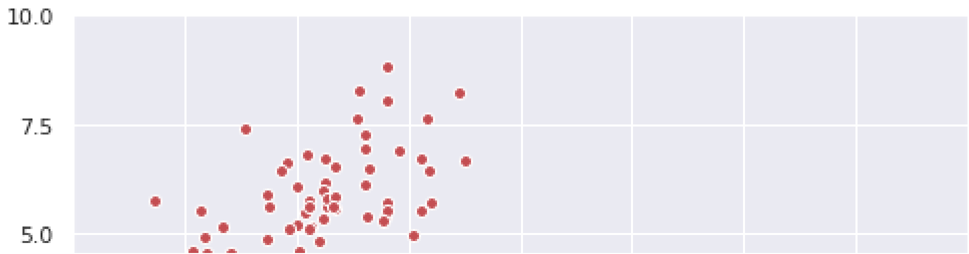
```
# Assume I perfectly estimate the parameters (not true for limited data!)
params = dict(mu_1_1 = -5, sigma_1_1 = 2,
              mu_2_1 = 5, sigma_2_1 = 2,
              mu_1_0 = 5, sigma_1_0 = 2,
              mu_2_0 = -5, sigma_2_0 = 2
)

plot_GNB(X_positive,X_negative,params)
```

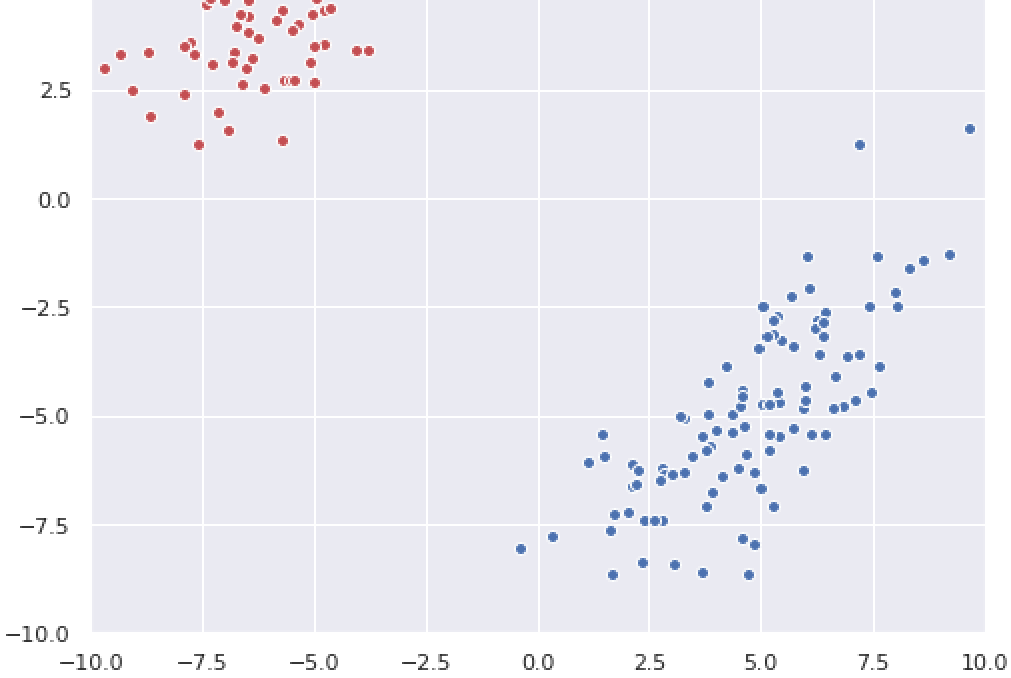


In [28]:

```python
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]]
```





2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

Is GNB a linear separator?

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

Decision rule:

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

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

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

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

$$
\begin{aligned}
&= \ln \frac{P(Y=1)}{P(Y=0)} + \sum_i \ln \frac{\sigma_{i0}}{\sigma_{i1}} - \frac{1}{2} \sum_i \Big(x_i^2 \big(\frac{1}{\sigma_{i1}^2} - \frac{1}{\sigma_{i0}^2}\big) - 2x_i \\
&\qquad + \big(\frac{\mu_{i1}^2}{\sigma_{i1}^2} - \frac{\mu_{i0}^2}{\sigma_{i0}^2}\big)\Big)
\end{aligned}
$$

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

- We get a linear decision boundary. Otherwise, it's a quadratic decision boundary (unless somehow we estimate exactly the same standard deviations).

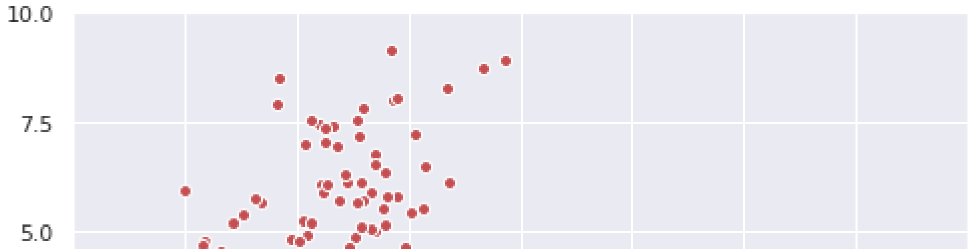
In [39]:

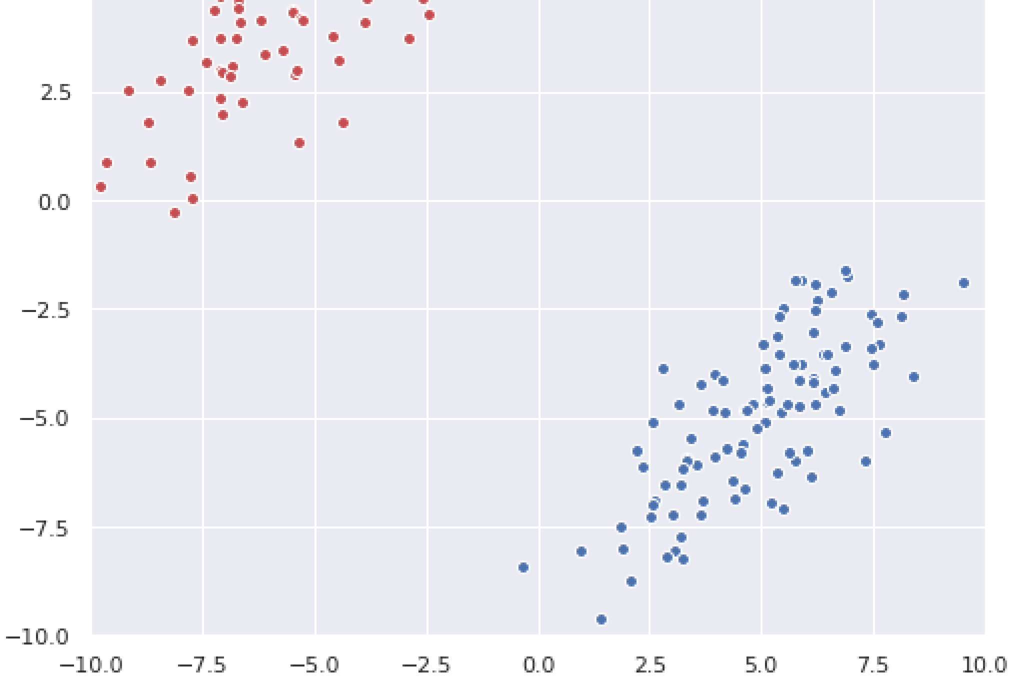
```
# Same param as before
mu_1_1 = -5; sigma_1_1 = 2
mu_2_1 = 5; sigma_2_1 = 2
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

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[39]:

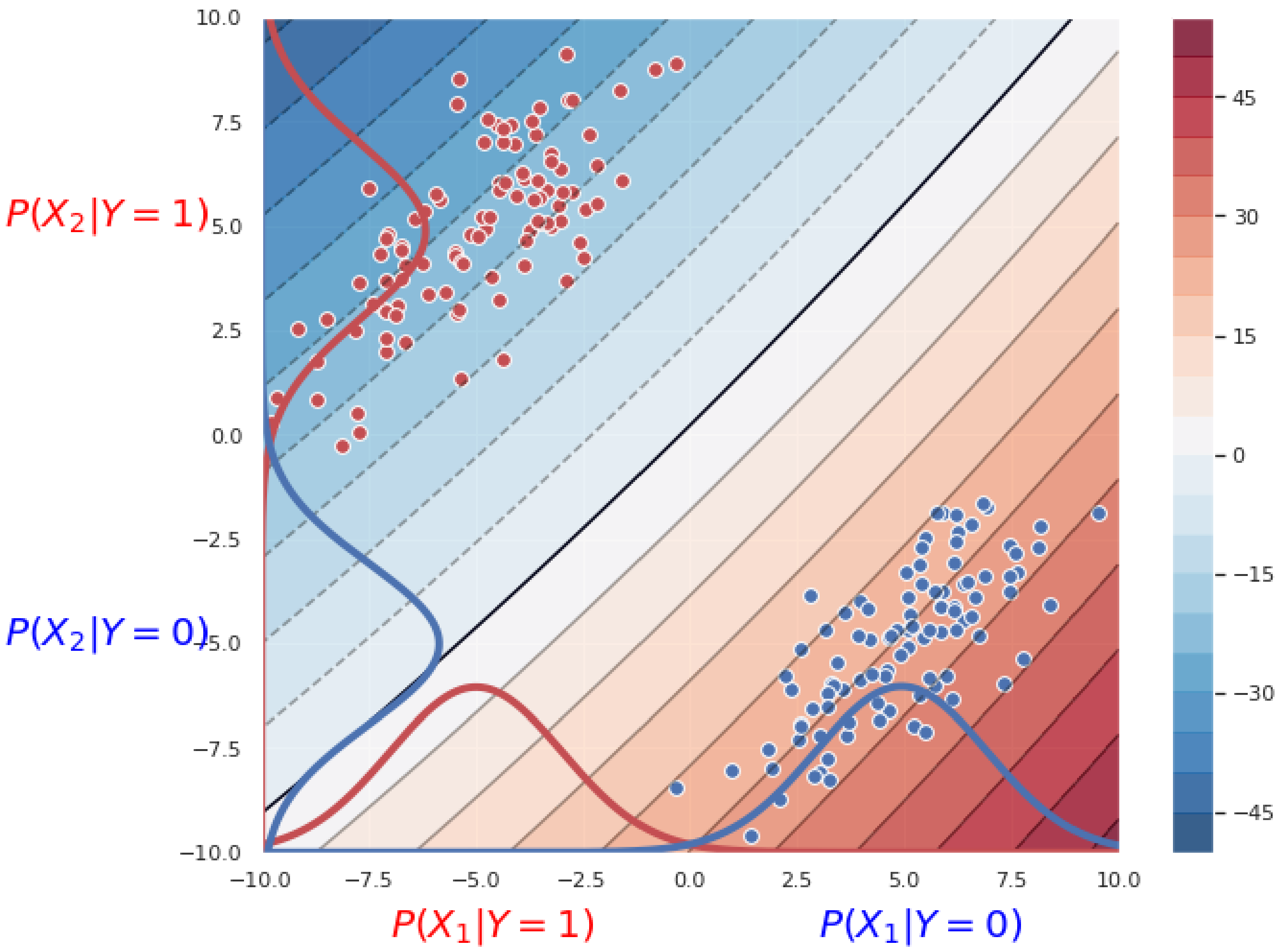
```
[-10, 10, -10, 10]
```




2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

In [40]:

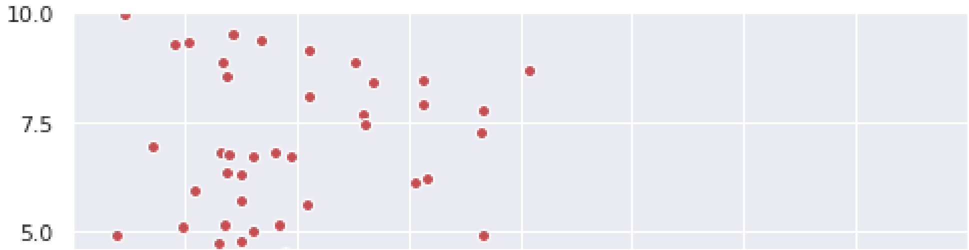
```python
params = dict()
# Estimate - Different variance
params['mu_1_1'], params['mu_2_1'] = np.mean(X_positive,axis=0)
params['sigma_1_1'], params['sigma_2_1'] = np.std(X_positive,axis=0)
params['mu_1_0'], params['mu_2_0'] = np.mean(X_negative,axis=0)
params['sigma_1_0'], params['sigma_2_0'] = np.std(X_negative,axis=0)

plot_GNB(X_positive,X_negative,params)
```

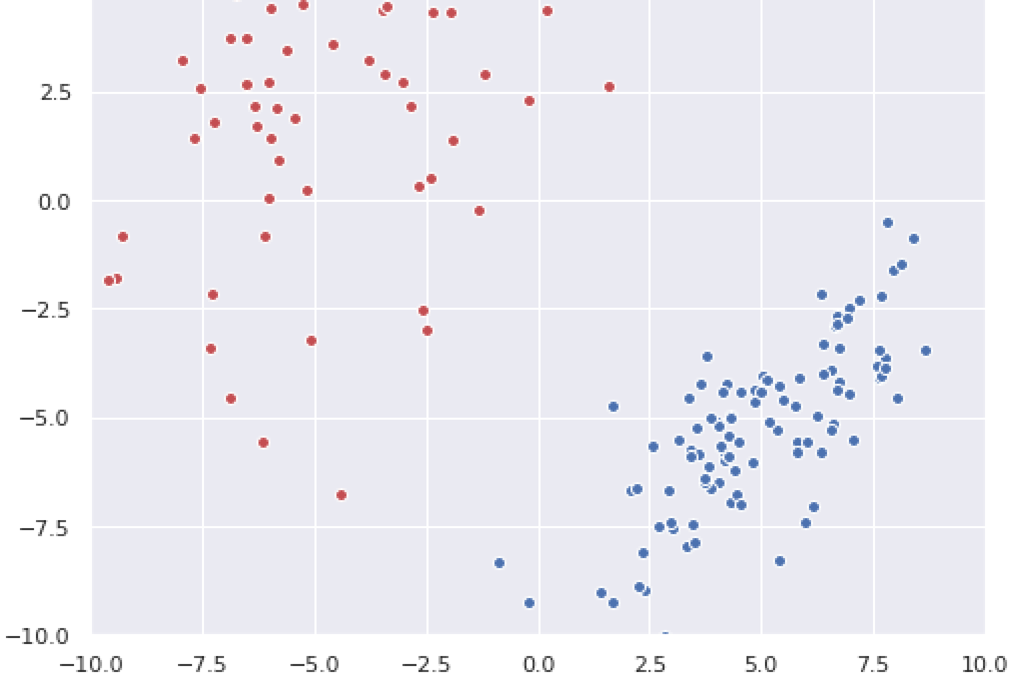


In [41]:
```
# Let's set up another example in which the variances are actually different
mu_1_1 = -5; sigma_1_1 = 3
mu_2_1 = 5; sigma_2_1 = 4
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

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]]
```

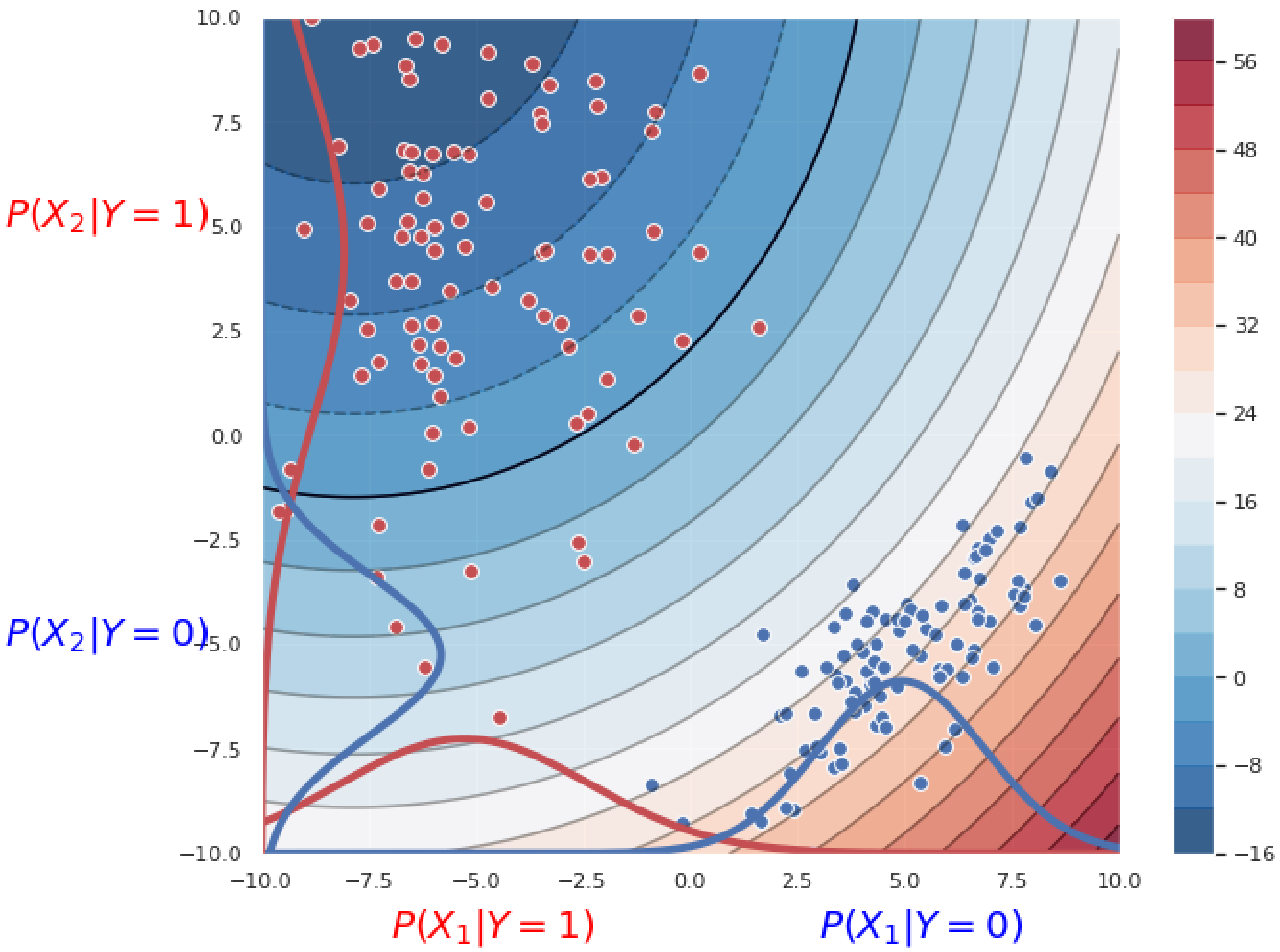
Out[41]: [-10, 10, -10, 10]




2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

In [42]:

```
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)
```

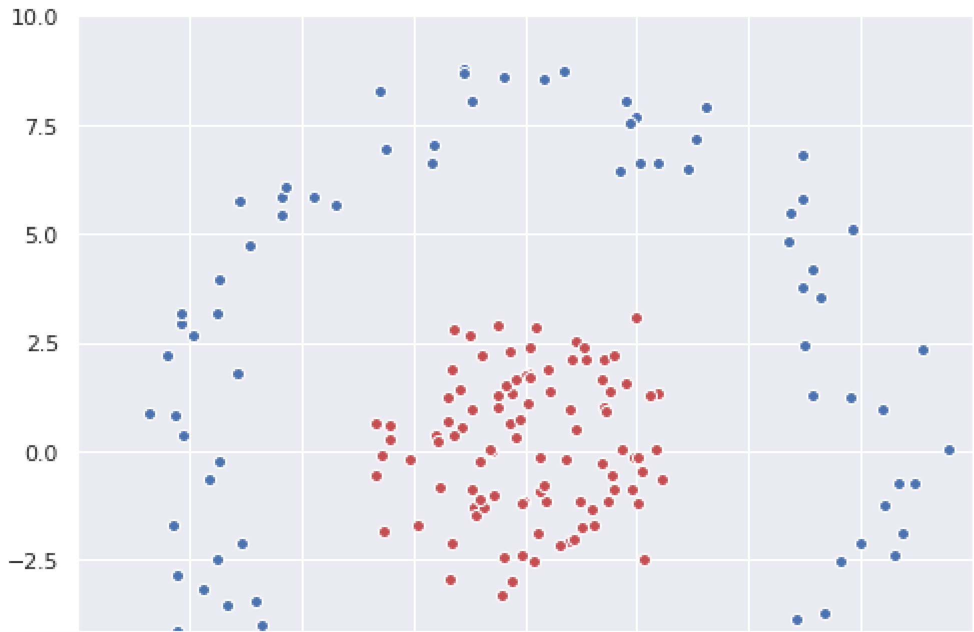


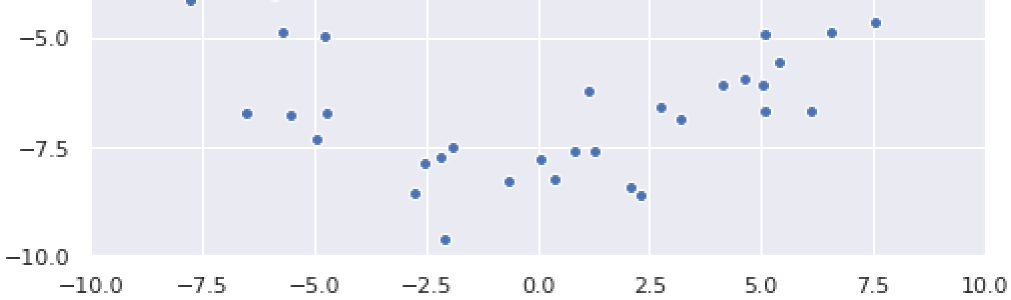
In [36]:

```
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[36]:

```
[-10, 10, -10, 10]

<Figure size 360x360 with 0 Axes>
```



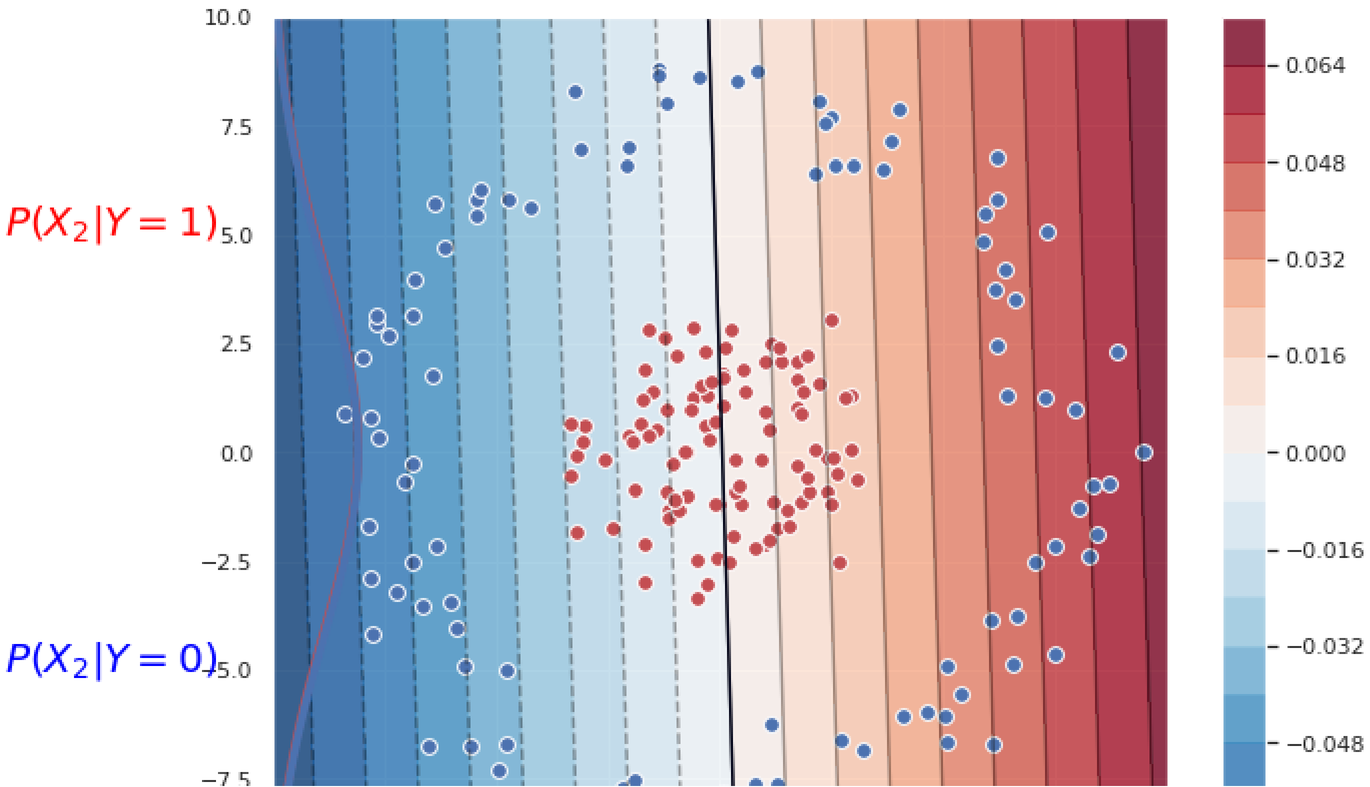


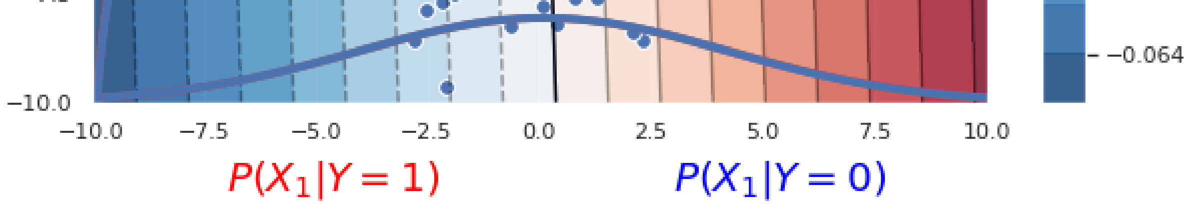
−5.0
−7.5
−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

In [37]:

```python
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)
```

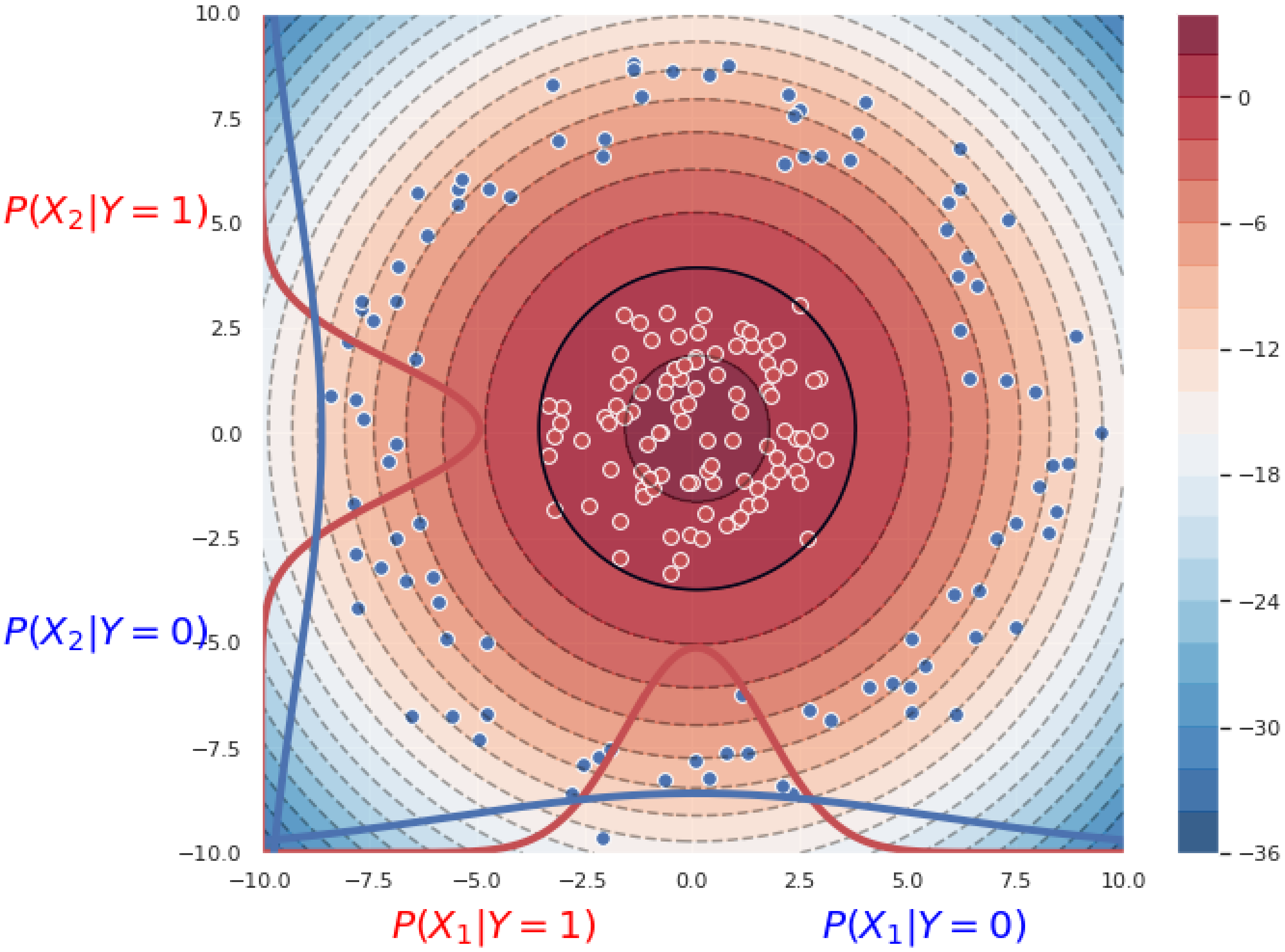
```
/Users/lwehbe/env/py3/lib/python3.7/site-packages/matplotlib/contour.py:1000:
UserWarning: The following kwargs were not used by contour: 'linewidth'
  s)
```





−10.0
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
−0.064
$P(X_1|Y=1)$
$P(X_1|Y=0)$

In [38]:
```python
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)
```



The last example is a case where the conditional independence assumption is incorrect

- but GNB does very well

Naïve Bayes is a *Generative* classifier

Generative classifiers:

- Assume a functional form for $P(X, Y)$ (or $P(X|Y)$ and $P(Y)$)
- we can view $P(X|Y)$ as describing how to sample random instances X given Y.

Instead of learning P(X|Y), can we learn P(Y|X) directly or learn the decision boundary directly?

Discriminative classifiers

- Assume some functional form for $P(Y|X)$ or for the decision boundary
- Estimate parameters of $P(Y|X)$ directly from training data

Logistic Regression is a discriminative classifier

Learns $f : X \rightarrow Y$, where

- X is a vector of real-valued or discrete features, $(X_1, \ldots, X_d)$
- Y is boolean (can also be extended for K discrete classes).

$P(Y|X)$ is modeled as:

$$P(Y = 1|X) = \frac{1}{1 + \exp(-(w_0 + \sum_i w_i X_i))} = \frac{\exp(w_0 + \sum_i w_i X_i)}{\exp(w_0 + \sum_i w_i X_i) + 1}$$

It uses the logistic (or sigmoid) function:

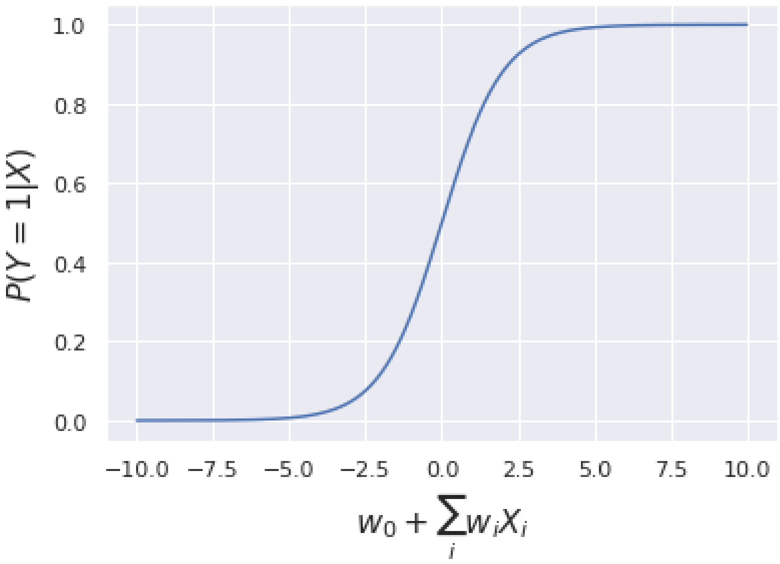
$$\frac{1}{1 + \exp -z}$$

In [478]:

```
z = np.linspace(-10,10,1000)
plt.plot(z,1/(1+np.exp(-z)))
plt.xlabel(r'$w_0+\sum_i w_i X_i$',fontsize=16)
plt.ylabel(r'$P(Y=1|X)$',fontsize=16)
```

Out[478]:

```
Text(0, 0.5, '$P(Y=1|X)$')
```



What is the form of the decision boundary?

$$\frac{P(Y=1|X)}{P(Y=0|X)} = \frac{\frac{\exp(w_0+\sum_i w_i X_i)}{\exp(w_0+\sum_i w_i X_i)+1}}{\frac{1}{\exp(w_0+\sum_i w_i X_i)+1}} = \exp(w_0 + \sum_i w_i X_i)$$

Asking $P(Y=1|X) > P(Y=0|X)$ is the same as asking if $\ln \frac{P(Y=1|X)}{P(Y=0|X)} > 0.$

i.e. is

$$w_0 + \sum_i w_i X_i \quad > 0?$$

This is a linear decision boundary!

In [ ]:
```
# similar to previous example
mu_1_1 = -4; sigma_1_1 = 2;mu_2_1 = 4; sigma_2_1 = 2
mu_1_0 = 4; sigma_1_0 = 2;mu_2_0 = -4; 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
= (20))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0], cov=cov_negative, size
= (20))
```

In [500]:

```
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')

# hand picked line
plt.plot(x1, x1*0.8+0.5)
from labellines import labelLine
labelLine(plt.gca().get_lines()[-1],0.6,label=r'$w_0+\sum_i w_i X_i = 0$',fontsize
=16)

plt.axis([-10,10,-10,10],'equal')
plt.xlabel(r'$x_1$',fontsize=20); plt.ylabel(r'$x_2$',fontsize=20)
plt.title('Data space',fontsize=20);
```

Gradient Descent

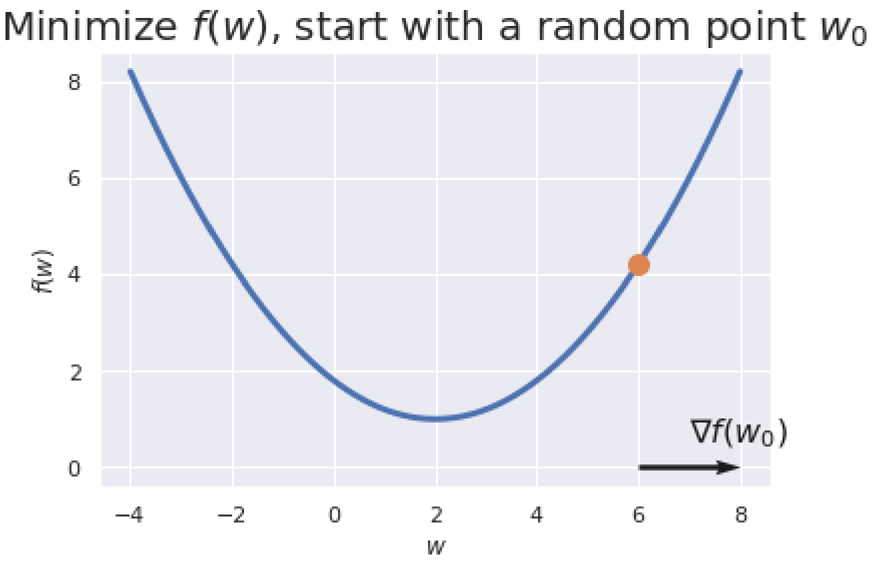
Review, let's start with a simple function:

$$f(w) = 0.2(w - 2)^2 + 1$$

We know that this function is convex (2nd derivative exists and is positive).

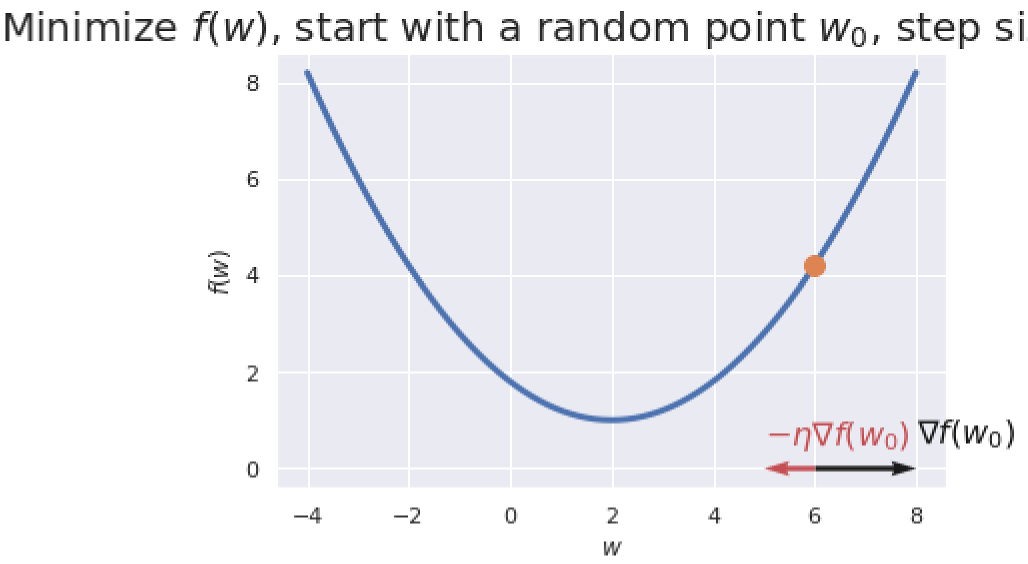
In [450]:

```
f = lambda w: 0.2*(w-2)**2+1
dfdw = lambda w: 0.4*w - 0.4

w = np.linspace(-4,8,1000)
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

plt.title(r'Minimize $f(w)$, start with a random point $w_0$',fontsize = 20);
w_0 = 6
plt.plot(w_0, f(w_0), "o",markersize=10)

def draw_vector_2D(ax, x, y, lenx, leny,name,color='k'):
#     grad = np.array([-np.sin(x),np.cos(y)])
    ax.quiver(x,y,lenx, leny, color=color,angles='xy', scale_units='xy', scale=1)
    ax.text(x+lenx/2, y+leny/2+0.5,name,fontsize = 16,color=color)

draw_vector_2D(plt, w_0, 0, dfdw(w_0),0, r'$\nabla f(w_0)$','k')
```



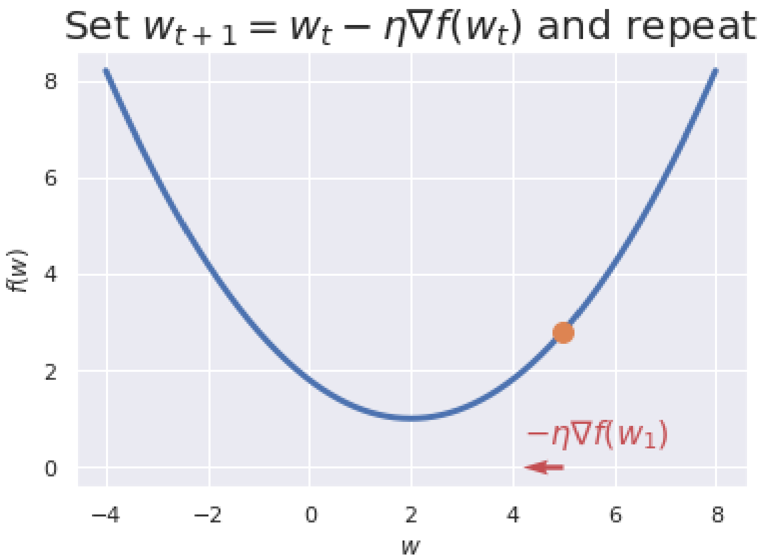
In [440]:

```
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

plt.title(r'Minimize $f(w)$, start with a random point $w_0$, step size $\eta=0.5
$',fontsize = 20);
w_0 = 6
plt.plot(w_0, f(w_0), "o",markersize=10)

def draw_vector_2D(ax, x, y, lenx, leny,name,color='k'):
    ax.quiver(x,y,lenx, leny, color=color,angles='xy', scale_units='xy', scale=1)
    ax.text(x+lenx, y+0.5,name,fontsize = 16,color=color)

draw_vector_2D(plt, w_0, 0, dfdw(w_0),0, r'$\nabla f(w_0)$','k')

eta=0.5

draw_vector_2D(plt, w_0, 0, - dfdw(w_0)*eta,0, r'$-\eta\nabla f(w_0)$','r')
```



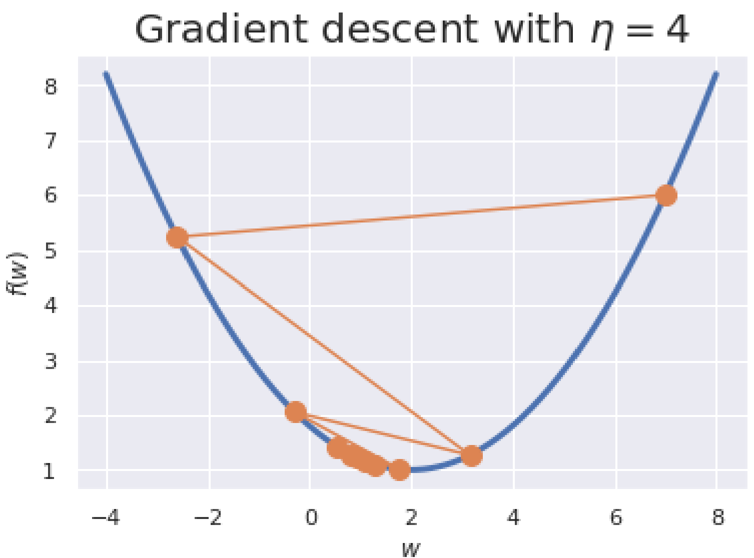
In [441]:

```
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

w_1 = w_0 - dfdw(w_0)*eta

plt.title(r'Set $w_{t+1} = w_{t}  - \eta \nabla f(w_t)$ and repeat', fontsize = 20
);

plt.plot(w_1, f(w_1), "o",markersize=10)

draw_vector_2D(plt, w_1, 0, - dfdw(w_1)*eta,0, r'$-\eta\nabla f(w_1)$','r')
```



In [442]:
```
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

# w_1 = w_0 - dfdw(w_0)*eta
w_t = np.zeros(10)
w_t[0] = 7  # w_0

eta = 4

for i in range(1,10):
    w_t[i] =  w_t[i-1] - eta * dfdw(w_t[i-1] )

plt.title(r'Gradient descent with $\eta={}$'.format(eta), fontsize = 20);

plt.plot(w_t, f(w_t), "o-",markersize=10)

# draw_vector_2D(plt, w_1, 0, - dfdw(w_1)*eta,0, r'$-\eta\nabla f(w_1)$','r')
```

Out[442]:
```
[<matplotlib.lines.Line2D at 0x14528e9b0>]
```



Multiple variables

Now let's assume the following logistic model does

In [451]:

```
x = np.linspace(-1,2,100)
y = np.linspace(-1,2,100)
X,Y = np.meshgrid(x, y)
sigma = 1

f_XY = np.cos(X)+np.sin(Y)


plt.figure(figsize=(11,9))

cs = plt.contourf(X, Y, f_XY,20,cmap='RdBu_r',vmin=-1,vmax=1,alpha=0.6);
plt.colorbar()
contours = plt.contour(cs, colors='k')
plt.xlabel('x')
plt.ylabel('y')



draw_vector_2D(plt, 1.45, 0.5, -np.sin(1.45),np.cos(0.5), 'gradient \n(perpendicular to \nlevel set of function)','k')
```

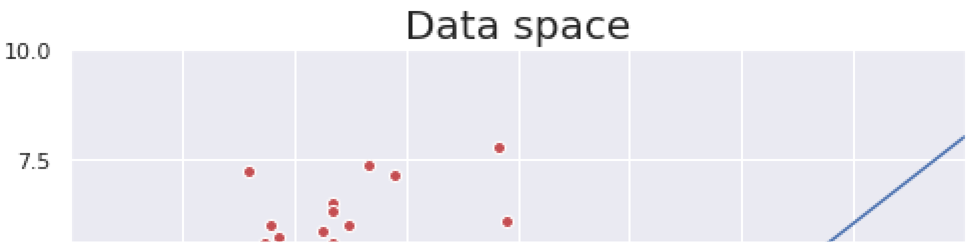
In [472]:

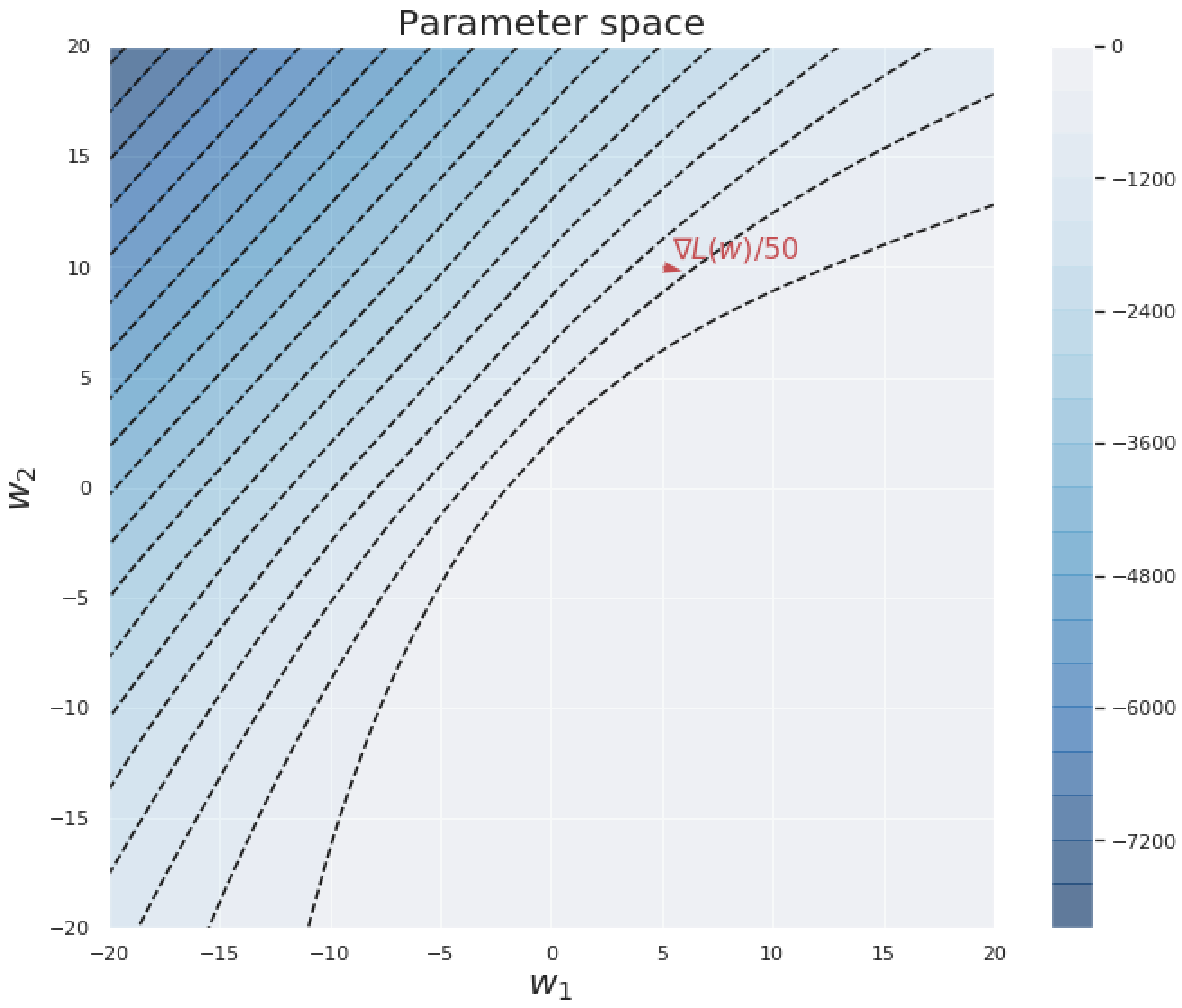
```python
# Previous example
mu_1_1 = -5; sigma_1_1 = 2
mu_2_1 = 5; sigma_2_1 = 2
mu_1_0 = 5; sigma_1_0 = 2
mu_2_0 = -5; sigma_2_0 = 2

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
= (20))
X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0], cov=cov_negative, size
= (20))

X = np.vstack([X_positive, X_negative])
Y = np.vstack([np.ones((X_positive.shape[0],1)),np.zeros((X_negative.shape[0],1
))])

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.plot(x1, x1*0.8)

plt.axis([-10,10,-10,10],'equal')
plt.xlabel(r'$x_1$',fontsize=20)
plt.ylabel(r'$x_2$',fontsize=20)
plt.title('Data space',fontsize=20)


w1x = np.linspace(-20,20,100)
w2x = np.linspace(-20,20,100)
W1,W2 = np.meshgrid(w1x, w2x)
```

```
## ommiting w_0 just for illustration
def loss_compute(w1,w2,X,Y):
    w = np.array([[w1],[w2]]) # make w_vec
    loss = np.sum(Y*X.dot(w) - np.log(1+ np.exp(X.dot(w))))
#     loss /= (X_positive.shape[0]+ X_negative.shape[0])
    #     loss += - (w1**2 + w2**2)*10
    return loss

plt.figure(figsize=(11,9))

L_w = np.zeros((len(w1x),len(w2x)))

for i1,w1 in enumerate(w1x):
    for i2,w2 in enumerate(w2x):
        L_w[i1,i2] = loss_compute(w1,w2,X,Y)


cs = plt.contourf(W1, W2, L_w,20,cmap='RdBu_r',vmin=-np.max(np.abs(L_w)),
                                                            vmax=np.max(np.abs(L_w
)),
                                                            alpha=0.6);
plt.colorbar()
contours = plt.contour(cs, colors='k')
plt.xlabel(r'$w_1$',fontsize=20)
plt.ylabel(r'$w_2$',fontsize=20)
plt.title('Parameter space',fontsize=20)


## ommiting w_0 just for illustration
def gradient_compute(w1,w2,X,Y):
    # positive samples
#     X = np.vstack([X_positive,X_negative])
#     Y = np.vstack([np.ones((X_positive.shape[0],1)),np.zeros((X_negative.shape
[0],1))])
#     print(Y.shape)
    w = np.array([[w1],[w2]])
```

```python
    P_Y_1 = np.exp(X.dot(w))/(1+ np.exp(X.dot(w)))
    print(P_Y_1.shape)
    gw1 = - X[:,0:1].T.dot((Y-P_Y_1))
    gw2 = - X[:,1:2].T.dot((Y-P_Y_1))
    print(gw1, gw2)
    return gw1, gw2

w1 = 5; w2 = 10
gw1, gw2 = gradient_compute(w1,w2,X, Y)
draw_vector_2D(plt, w1,w2,gw1/50,gw2/50, r'$\nabla L(w)/50$','r');
```

```
[[4 3]
 [3 4]]
(40, 1)
[[42.5819951]] [[-8.84456482]]
```


Data space
10.0
7.5



Parameter space
$\nabla L(w)/50$
w_1
w_2

Function with training data and parameters… loss vs hypothetical function

Need to regularize the weights

- $w \rightarrow \infty$ if the data is linearly separable
- For MAP, need to define prior on W
    - given $W = (w_1, \ldots w_d)$
    - let's assume prior $P(w_i) = \mathcal{N}(0, \sigma)$
- A kind of Occam's razor (simplest is best) prior
- Helps avoid very large weights and overfitting

Adding a prior on W

MAP estimation picks the parameter W that has maximum posterior probability $P(W|Y,X)$ given the conditional likelihood $P(Y|W,X)$ and the prior $P(W)$.

Using Bayes rule again:

$$
\begin{aligned}
W^{MAP} &= \underset{W}{\operatorname{argmax}}\ P(W|Y,W) \\
&= \underset{W}{\operatorname{argmax}}\ \frac{P(Y|W,X)P(W,X)}{P(Y,X)} \\
&= \underset{W}{\operatorname{argmax}}\ P(Y|W,X)P(W,X) \\
&= \underset{W}{\operatorname{argmax}}\ P(Y|W,X)P(W)P(X) \qquad \text{let's assume} P(W,X) = P(W)P(X) \\
&= \underset{W}{\operatorname{argmax}}\ P(Y|W,X)P(W) \\
&= \underset{W}{\operatorname{argmax}}\ \ln P(Y|W,X) + \ln P(W)
\end{aligned}
$$

Zero Mean Gaussian prior on W: $W \sim \frac{1}{2\pi\sigma^2} \exp\left(-\frac{1}{2\sigma^2}\sum_i w_i^2\right)$

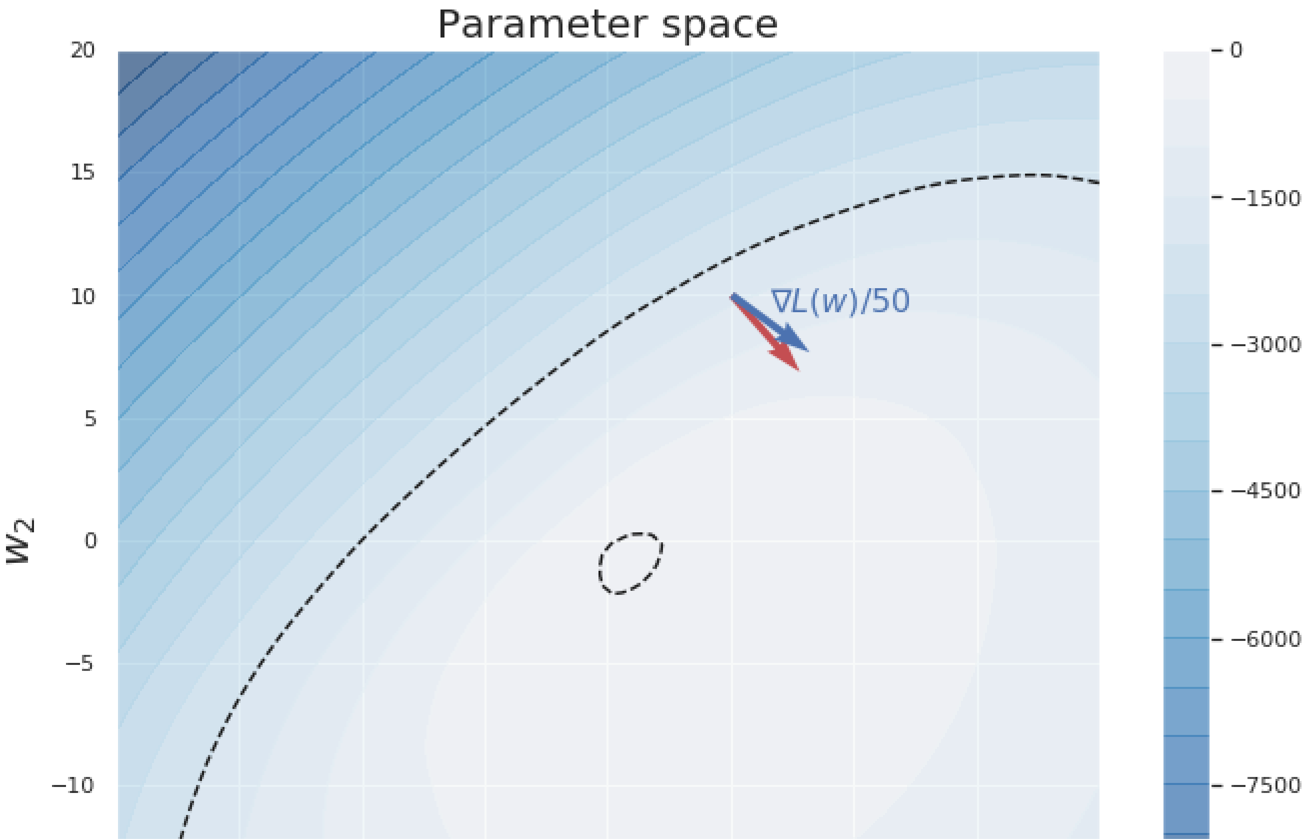
In [471]:

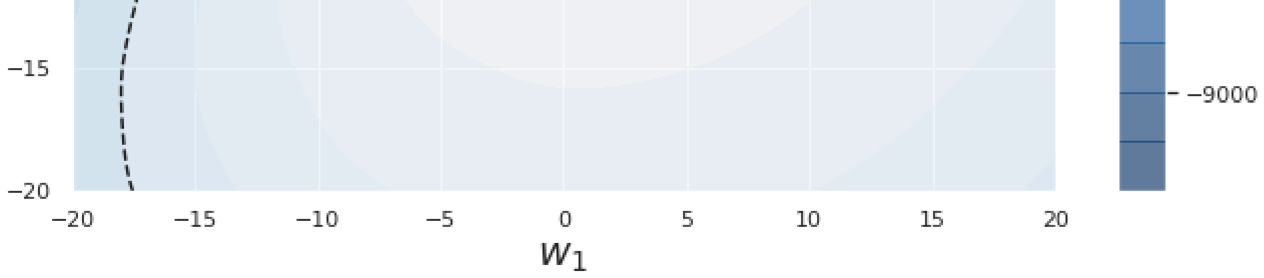
```
# # Previous example
# mu_1_1 = -5; sigma_1_1 = 4
# mu_2_1 = 5; sigma_2_1 = 3
# mu_1_0 = 5; sigma_1_0 = 2
# mu_2_0 = -5; sigma_2_0 = 2

# 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, siz
e = (20))
# X_negative = multivariate_normal.rvs(mean=[mu_1_0,mu_2_0], cov=cov_negative, siz
e = (20))


# 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.plot(x1, x1*0.8)

# plt.axis([-10,10,-10,10],'equal')
# plt.xlabel(r'$x_1$',fontsize=20)
# plt.ylabel(r'$x_2$',fontsize=20)
# plt.title('Data space',fontsize=20)


# w1x = np.linspace(-20,20,100)
# w2x = np.linspace(-20,20,100)
# W1,W2 = np.meshgrid(w1x, w2x)


## ommiting w_0 just for illustration
```

```
lmbda = 2
def loss_compute(w1,w2,X,Y):
    w = np.array([[w1],[w2]]) # make w_vec
    loss = np.sum(Y*X.dot(w) - np.log(1+ np.exp(X.dot(w))))
#     loss /= (X_positive.shape[0]+ X_negative.shape[0])
    #     loss += - (w1**2 + w2**2)*10
    loss += - (w1**2 + w2**2)*lmbda
    return loss

plt.figure(figsize=(11,9))

L_w = np.zeros((len(w1x),len(w2x)))

for i1,w1 in enumerate(w1x):
    for i2,w2 in enumerate(w2x):
        L_w[i1,i2] = loss_compute(w1,w2,X,Y)


cs = plt.contourf(W1, W2, L_w,20,cmap='RdBu_r',vmin=-np.max(np.abs(L_w)),
                                                            vmax=np.max(np.abs(L_w
)),
                                                            alpha=0.6);
plt.colorbar()
contours = plt.contour(cs,levels=[-10,-2000], colors='k')
plt.xlabel(r'$w_1$',fontsize=20)
plt.ylabel(r'$w_2$',fontsize=20)
plt.title('Parameter space',fontsize=20)


## ommiting w_0 just for illustration
def gradient_compute(w1,w2,X,Y):
    # positive samples
#     X = np.vstack([X_positive,X_negative])
#     Y = np.vstack([np.ones((X_positive.shape[0],1)),np.zeros((X_negative.shape
[0],1))])
#     print(Y.shape)
    w = np.array([[w1],[w2]])
    P_Y_1 = 1/(1+ np.exp(X.dot(w)))
```

```
    print(P_Y_1.shape)
    gw1 = - X[:,0:1].T.dot((Y-P_Y_1))
    gw2 = - X[:,1:2].T.dot((Y-P_Y_1))
    print(gw1, gw2)
    return gw1, gw2

w1 = 5; w2 = 10
gw1, gw2 = gradient_compute(w1,w2,X, Y)
draw_vector_2D(plt, w1,w2,gw1/50,gw2/50, r' ','r');
draw_vector_2D(plt, w1,w2,(gw1+lmbda*w1*2)/50,(gw2+lmbda*w2*2)/50, r'$\nabla L(w)/
50$','b');
```

```
(40, 1)
[[138.18196438]] [[-156.60707659]]
```





In [335]:
```
lmbda*w1*2
```
Out[335]:
```
10
```