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

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

Lecture outcomes:

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

In [1]:

```
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)
```

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 $f : X \to Y$, 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).

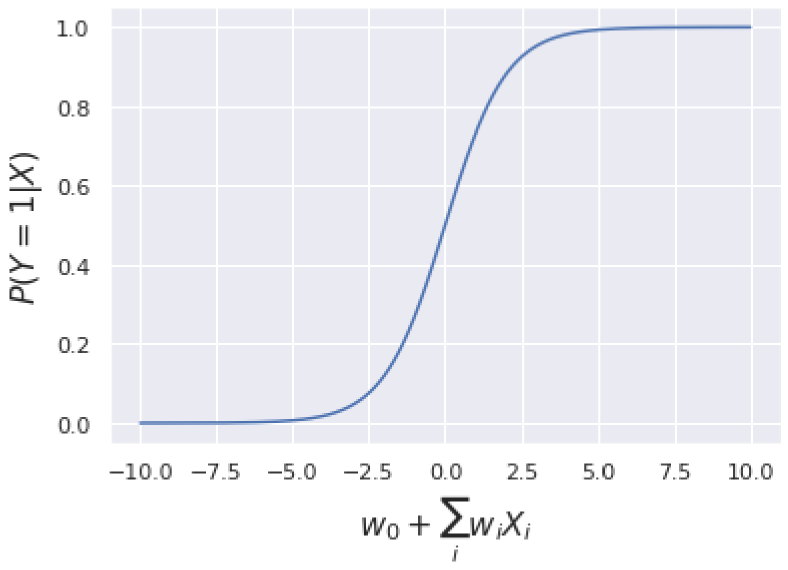
$P(Y|X)$ is modeled as:

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

It uses the logistic (or sigmoid) function:

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

```
In [2]: 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[2]: 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

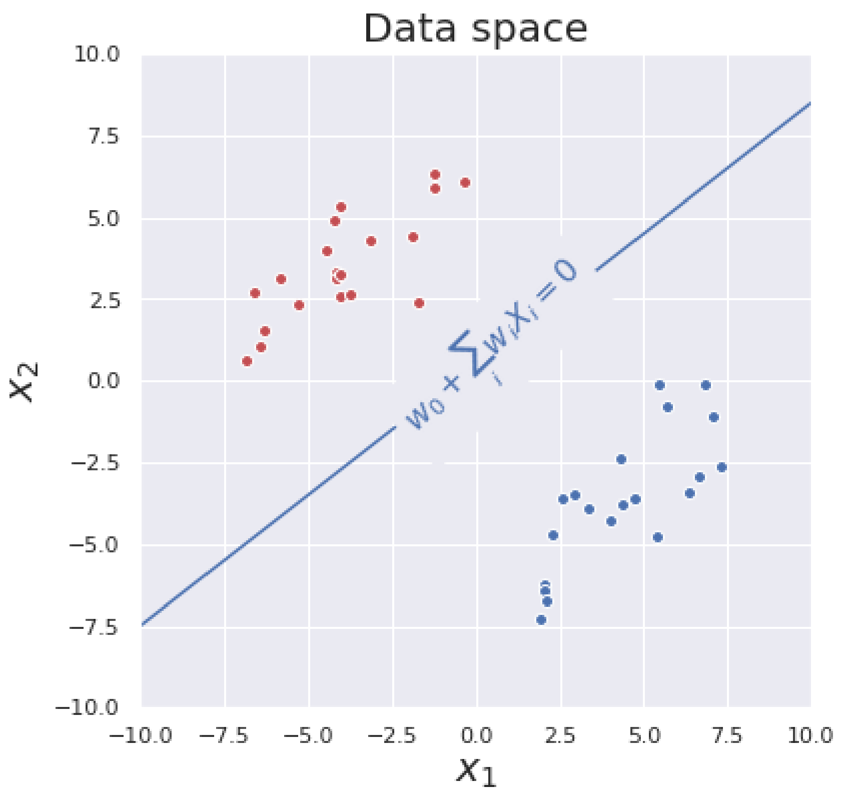
$$w_0 + \sum_i w_i X_i \quad > 0?$$

This is a linear decision boundary!

In [3]:
```
from scipy.stats import multivariate_normal
# 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 [4]:

```
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')

# 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);
```



Logistic Regression is a Linear Classifier

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

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

The weights w_i are optimized such that when $w_0 + \sum_i w_i X_i > 0$ the example is more likely to be positive and when $w_0 + \sum_i w_i X_i < 0$ it's more likely to be negative.

$w_0 + \sum_i w_i X_i = 0, P(Y = 1|X) = \frac{1}{2}$

$w_0 + \sum_i w_i X_i \to \infty, P(Y = 1|X) \to 1$

$w_0 + \sum_i w_i X_i \to -\infty, P(Y = 1|X) \to 0$

Training Logistic Regression

Let's focus on binary classfication

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

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

How to learn $w_0, w_1 ... w_d$?

Training data: $\{(X^{(j)}, Y^{(j)})\}_{j=1}^{n}$, with $X^{(j)} = \left(X_1^{(j)}, X_2^{(j)}, \ldots X_d^{(j)}\right)$

Maximum Likelihood Estimation:

$$\hat{\mathbf{w}}_{\text{MLE}} = \underset{\mathbf{w}}{\text{argmax}} \prod_{j=1}^{n} P(X^{(j)}, Y^{(j)}|\mathbf{w})$$

Optimizing concave/convex function

- $l(\mathbf{w})$ concave, we can maximize it via gradient ascent

Gradient:

$$\nabla_{\mathbf{w}} l(\mathbf{w}) = \left[\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_d} \right]$$

Update rule for gradient ascent, with **learning rate** $\boldsymbol{\eta > 0}$

$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

$$w_i^{(t+1)} = w_i^{(t)} + \eta \frac{\partial l(\mathbf{w})}{\partial w_i} |_{w_t}$$

Optimizing concave/convex function

- It's more common to use gradient descent to minimize a convex fuction

Update rule for gradient **descent**, with learning rate $\eta > 0$

$$\Delta \mathbf{w} = -\eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

$$w_i^{(t+1)} = w_i^{(t)} - \eta \frac{\partial l(\mathbf{w})}{\partial w_i} |_{w_t}$$

(maximizing $l(\mathbf{w})$ is the same as minimizing $l'(\mathbf{w}) = -l(\mathbf{w})$)

Gradient Descent

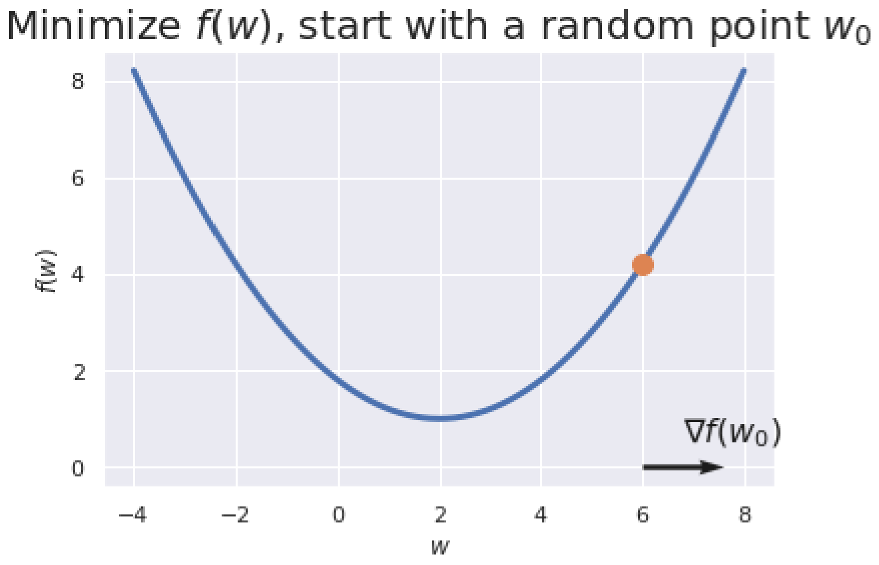
Review, let's start with a simple function:

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

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

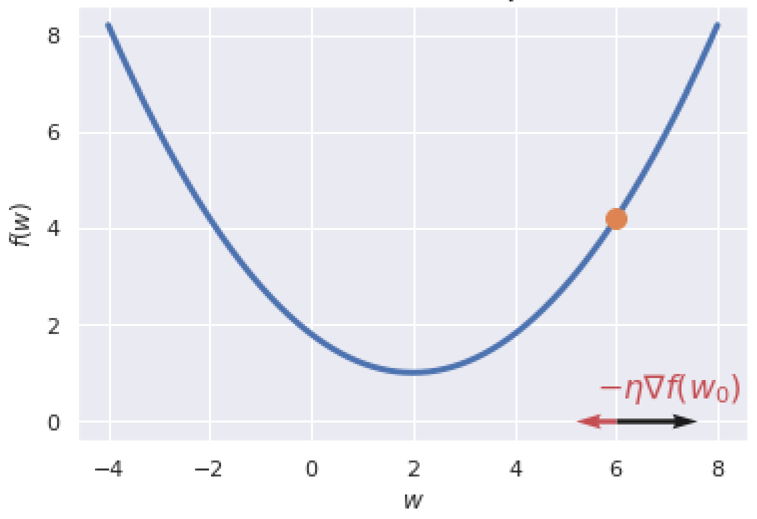
In [5]:
```
f = lambda w: 0.2*(w-2)**2+1
dfdw = lambda w: 0.4*w - 0.8
```

In [6]:
```
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')
```

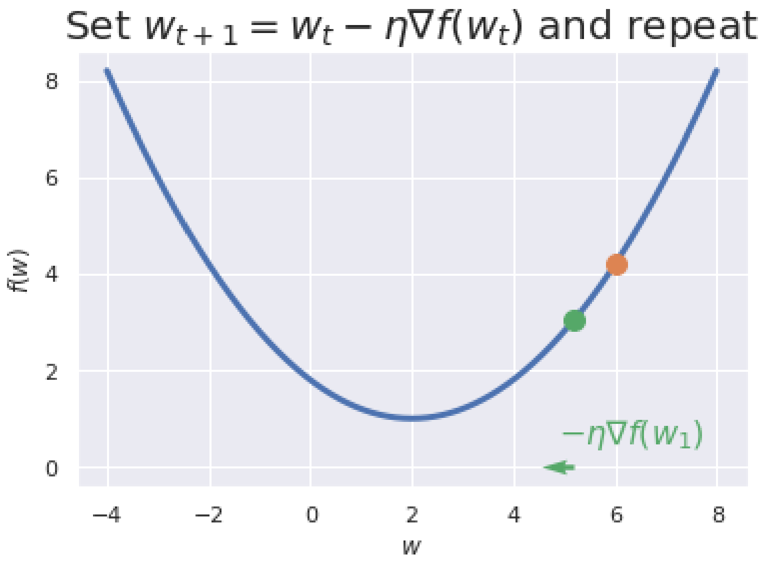


```
In [7]: plt.plot(w, f(w), linewidth=3 )
        plt.xlabel(r'$w$')
        plt.ylabel(r'$f(w)$')

        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)

        draw_vector_2D(plt, w_0, 0, dfdw(w_0),0, r' ','k')

        eta=0.5

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

Minimize $f(w)$, start with a random point w_0, step size $\eta = 0.5$

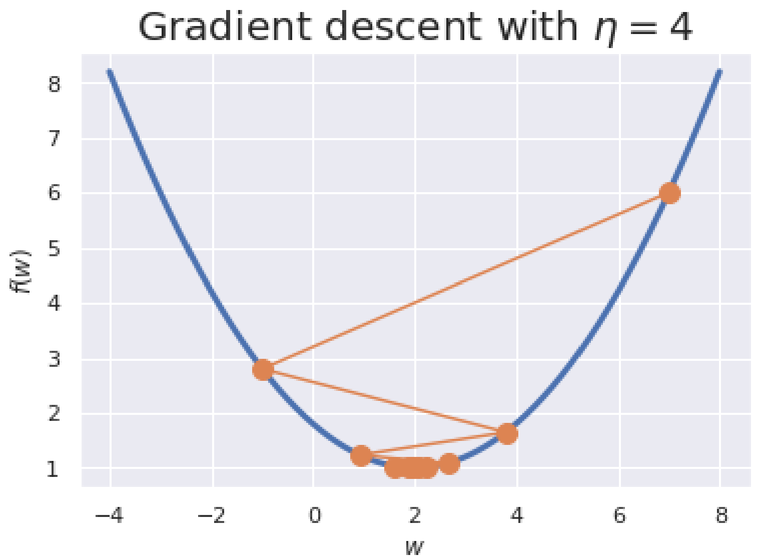


In [8]:
```
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

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_0, f(w_0), "o",markersize=10)
plt.plot(w_1, f(w_1), "o",markersize=10)

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



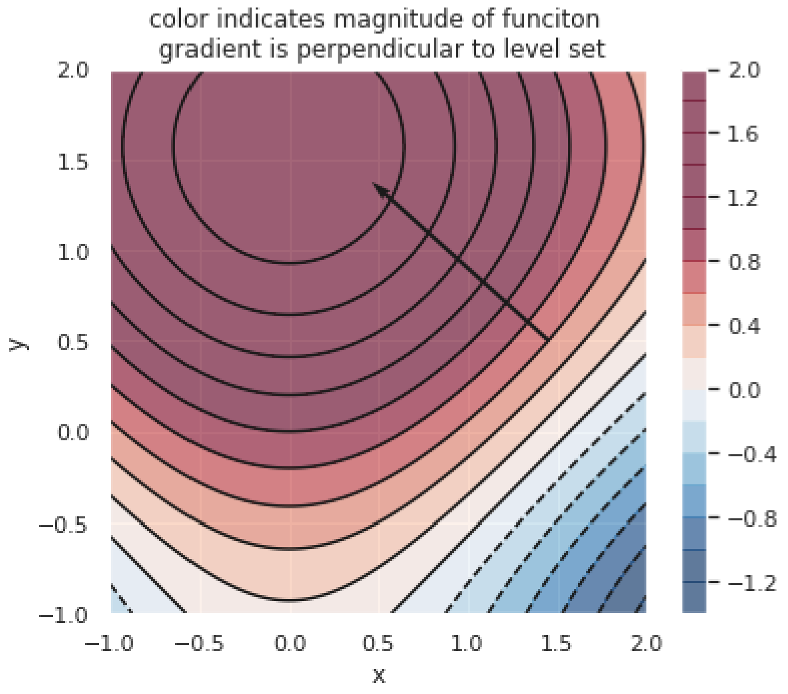
```
In [9]: plt.plot(w, f(w), linewidth=3 )
        plt.xlabel(r'$w$')
        plt.ylabel(r'$f(w)$')

        # 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[9]: [<matplotlib.lines.Line2D at 0x142f191d0>]
```

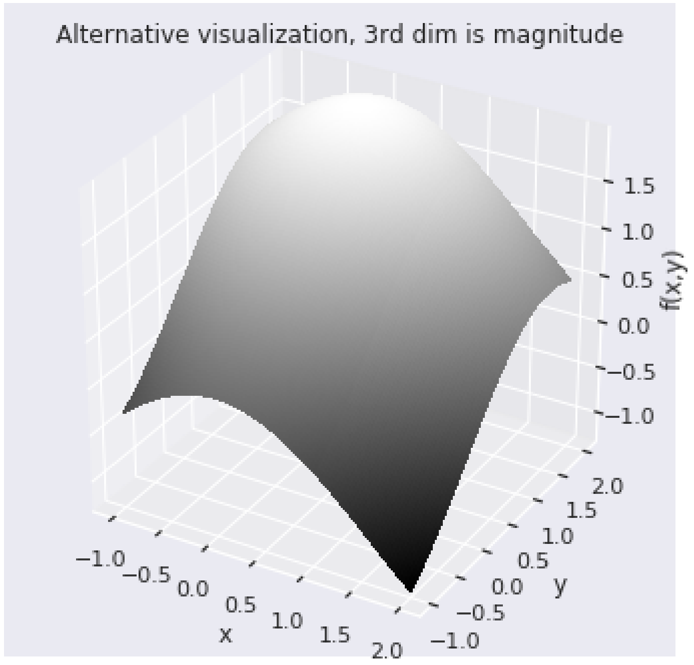


Let’s plot a function with two variables and look at the gradient

In [10]:
```
x = np.linspace(-1,2,100);y = np.linspace(-1,2,100); X,Y = np.meshgrid(x, y)

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

plt.figure(figsize=(6,5))
cs = plt.contourf(X, Y, f_XY,20,cmap='RdBu_r',vmin=-1,vmax=1,alpha=0.6);plt.colorb
ar()
contours = plt.contour(cs, colors='k')
plt.xlabel('x');plt.ylabel('y')
plt.title('color indicates magnitude of funciton \n gradient is perpendicular to l
evel set')

draw_vector_2D(plt, 1.45,0.5,-np.sin(1.45),np.cos(0.5),'','k')
```



```
In [11]: from mpl_toolkits.mplot3d import Axes3D
         %matplotlib inline
         %config InlineBackend.print_figure_kwargs = {'bbox_inches':None}
         fig = plt.figure(figsize=(6,6))
         ax = fig.gca(projection='3d')
         Z = np.cos(X)+np.sin(Y)
         # Plot the surface.
         surf = ax.plot_surface(X, Y, Z, cmap='gray',
                                linewidth=0, antialiased=False, rcount=200, ccount=200)
         ax.set_xlabel('x');ax.set_ylabel('y');ax.set_zlabel('f(x,y)');
         ax.set_title('Alternative visualization, 3rd dim is magnitude');
```

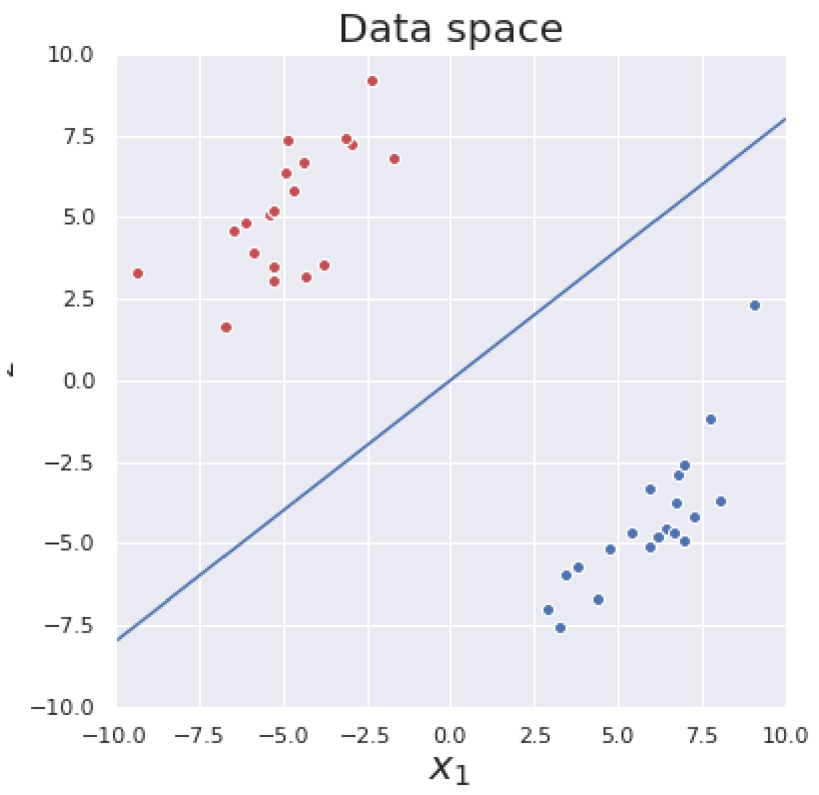


Logistic regression gradient ascent

Simple simulated example

In [12]:
```
# 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]] )
# 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
))])
```

```
In [13]: 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.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);
```



Log likelihood plot

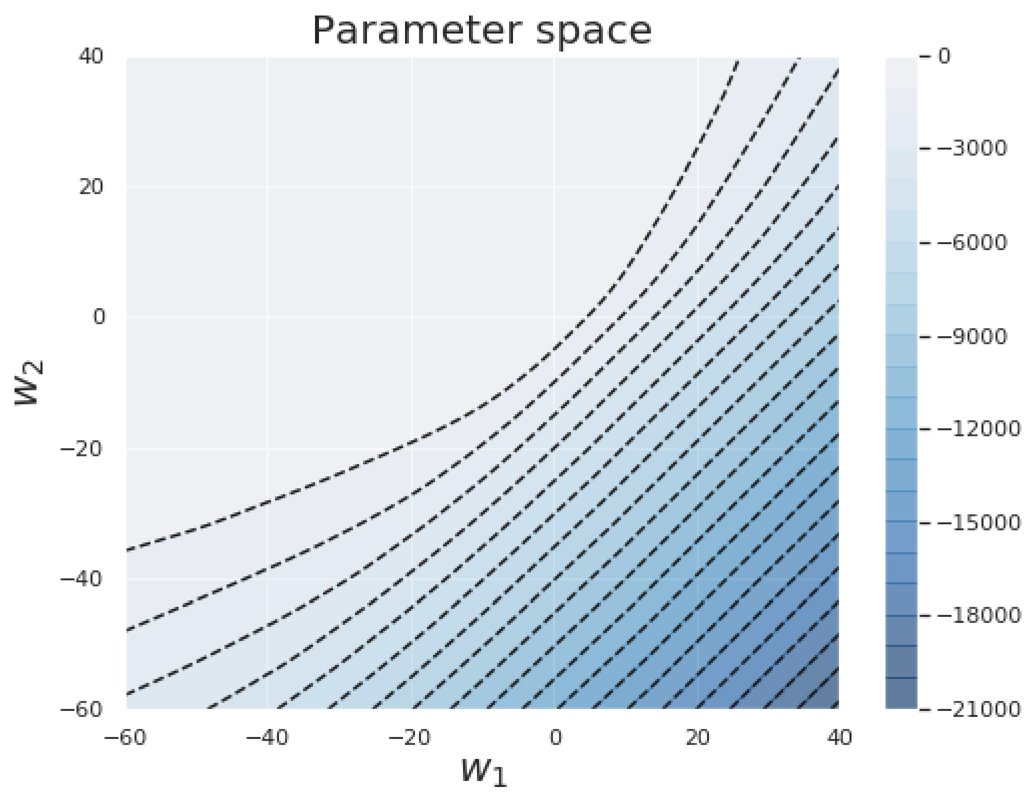
$$l(\mathbf{w}) = \sum_j \left[y^j \left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) - \ln\left(1 + \exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right)\right)\right]$$

We omit w_0 in the example below for simplicity

In [14]:

```
w1x = np.linspace(-60,40,100)
w2x = np.linspace(-60,40,100)
W1,W2 = np.meshgrid(w1x, w2x)

## ommiting w_0 just for illustration
def loglikelihood(w1,w2):
    w = np.array([[w1],[w2]]) # make w_vec
    loglihood = np.sum(Y*X.dot(w) - np.log(1+ np.exp(X.dot(w))))
    return loglihood

L_w = np.vectorize(loglikelihood)(*np.meshgrid(w1x, w2x))
```

In [15]:
```
plt.figure(figsize=(8,6))

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);
```



Gradient computation

$$l(\mathbf{w}) = \sum_j \left[y^j \left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) - \ln\left(1 + \exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right)\right)\right]$$

$$\frac{\partial l(\mathbf{w})}{\partial w_0} = \sum_j \left[y^j - \frac{\exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j\right)}{\left(1 + \exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j\right)\right)} \right]$$

$$= \sum_j \left[y^j - \hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w}^{(\mathbf{t})}) \right]$$

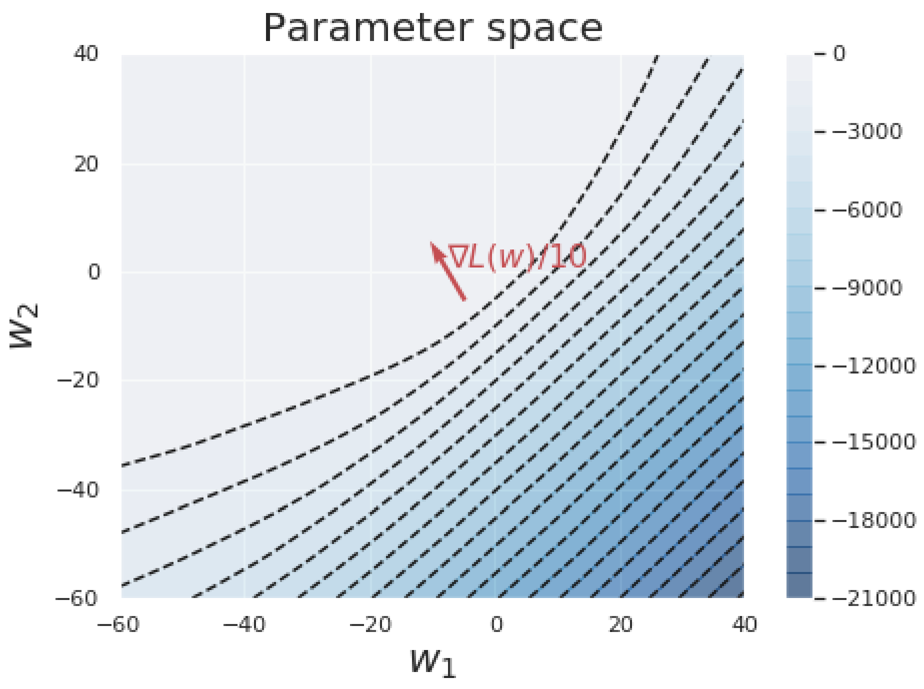
for $i = 1 \ldots d$:

$$\frac{\partial l(\mathbf{w})}{\partial w_0} = \sum_j x_i^j \left[y^j - \hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w}^{(\mathbf{t})}) \right]$$

In [16]:

```
def gradient_likelihood(w1,w2,X,Y):
    w = np.array([[w1],[w2]])
    P_Y_1 = np.exp(X.dot(w))/(1+ np.exp(X.dot(w)))
    gw1 = X[:,0:1].T.dot(Y-P_Y_1)
    gw2 = X[:,1:2].T.dot(Y-P_Y_1)
    return gw1, gw2
```

In [17]:
```
plt.figure(figsize=(7,5))
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);

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



Gradient ascent for logistic regression

Iterate until convergence (until change $< \epsilon$)

$$w_0^{(t+1)} = w_0^{(t)} + \eta \sum_j \left[y^j - \hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w^{(t)}}) \right]$$

for $i = 1 ... d$:

$$w_i^{(t+1)} = w_i^{(t)} + \eta \sum_j x_i^j \left[y^j - \hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w^{(t)}}) \right]$$

$\hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w^{(t)}})$ is our current prediction of the label.

- compare this to actual label
- multiple difference by feature value

Gradient Ascent (Descent) is simplest of approaches

Compare to:

- Stochastic Gradient Descent
- Batch Gradient Descent
- Newton

...

- Convergence?

Effect of step-size ⍰ Large □ ⇒ Fast convergence but larger residual error Also possible oscillations Small □ ⇒ Slow convergence but small residual error

Need to regularize the weights

- $w \to \infty$ if the data is linearly separable
- For MAP, need to define prior on W
    - given $W = (w_1, \dots w_d)$
    - 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:

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

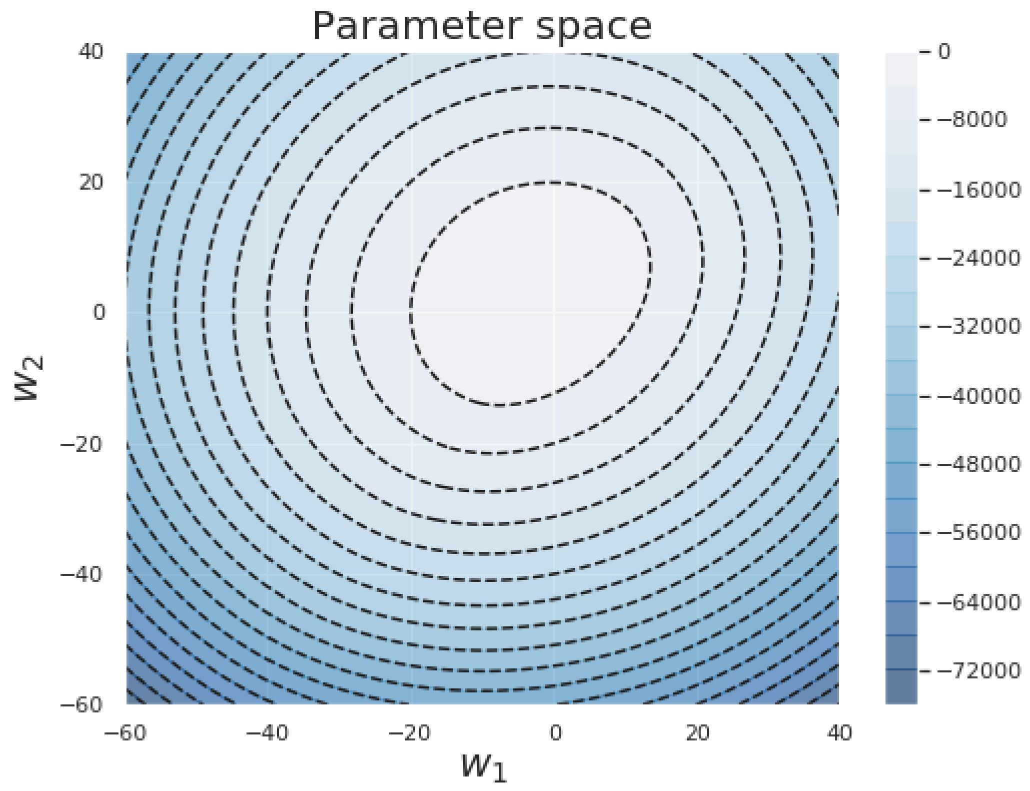
Zero Mean Gaussian prior on W: $W \sim \frac{1}{2\pi\sigma^2}\exp\left(-\frac{1}{2\sigma^2}\sum_i w_i^2\right)$

$$W^{MAP} = \underset{W}{\text{argmax}}\ \ln P(Y|W,X) - \left(\frac{1}{2\sigma^2}\sum_i w_i^2\right)$$

In [18]:

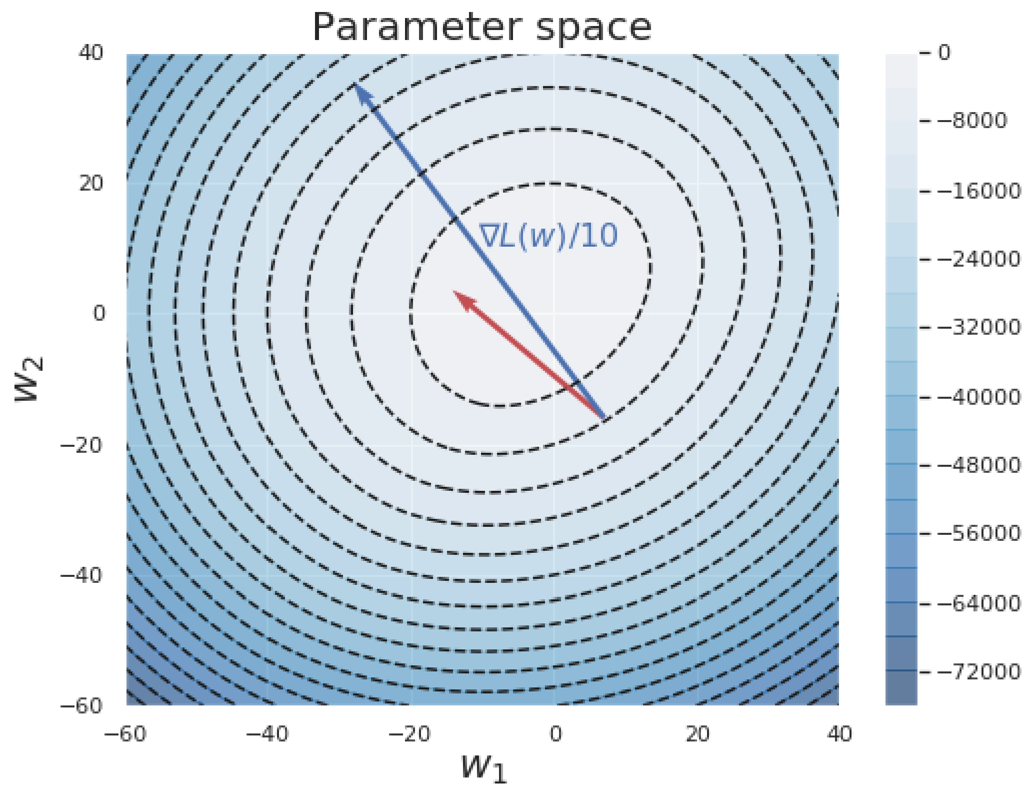
```
lmbda = 10 # this is 1/(2*sigma**2)

def logposterior(w1,w2):
    w = np.array([[w1],[w2]]) # make w_vec
    loglihood = np.sum(Y*X.dot(w) - np.log(1+ np.exp(X.dot(w))))
    loglihood += - (w1**2 + w2**2)*lmbda
    return loglihood

L_w = np.vectorize(logposterior)(*np.meshgrid(w1x, w2x))
```

In [19]:
```
plt.figure(figsize=(8,6))
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);
```



In [20]:
```
def gradient_posterior(w1,w2,X,Y):
    w = np.array([[w1],[w2]])
    P_Y_1 = np.exp(X.dot(w))/(1+ np.exp(X.dot(w)))
    gw1 = X[:,0:1].T.dot(Y-P_Y_1)- 2*lmbda*w1#

    gw2 =X[:,1:2].T.dot(Y-P_Y_1) - 2*lmbda*w2 #

    return gw1, gw2
```

```
In [22]: plt.figure(figsize=(8,6))
         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);

         w1 = 7; w2 = -16
         gw1, gw2 = gradient_likelihood(w1,w2,X, Y)
         draw_vector_2D(plt, w1,w2,gw1/10,gw2/10, r' ','r');
         gw1, gw2 = gradient_posterior(w1,w2,X, Y)
         draw_vector_2D(plt, w1,w2,gw1/10,gw2/10, r'$\nabla L(w)/10$','b');
```



What you should know

LR is a linear classifier: decision rule is a hyperplane

- LR optimized by conditional likelihood
    - no closed-form solution
    - concave $\Rightarrow$ global optimum with gradient ascent
    - Maximum conditional a posteriori corresponds to regularization

```
In [ ]:
```