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">)](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

Questions to think about (Naïve Bayes)

Can you use Naïve Bayes for a combination of discrete and real-valued Xi?

How can we easily model the assumption that just 2 of the n attributes as dependent?

What does the decision surface of a Naïve Bayes classifier look like?

How would you select a subset of Xi's?

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 $P(Y|X)$ or decision boundary 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:

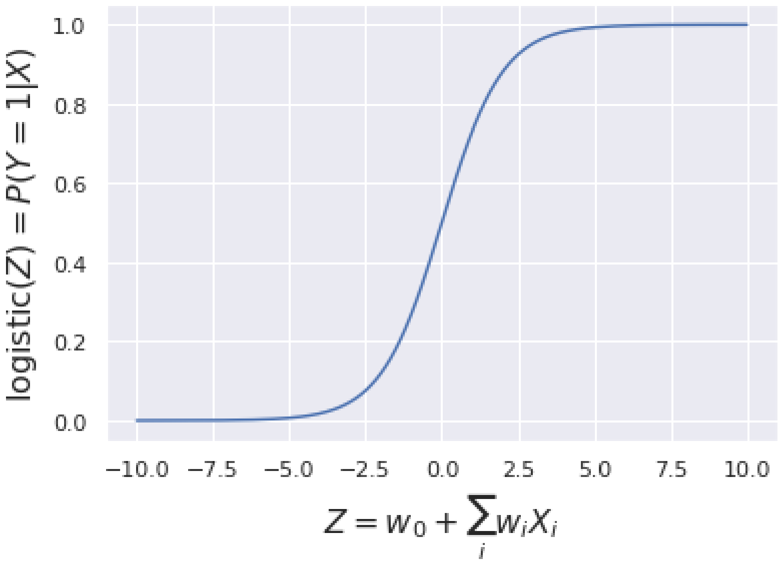
$$P(Y = 1|X) = \frac{1}{1 + \exp(-(w_0 + \sum_i w_i X_i))} = \frac{\exp(w_0 + \sum_i w_i X_i)}{\exp(w_0 + \sum_i w_i X_i) + 1}$$

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'$Z = w_0+\sum_i w_i X_i$',fontsize=16)
plt.ylabel(r'logistic$(Z) = P(Y=1|X)$',fontsize=16)
```

Out[2]:
```
Text(0, 0.5, 'logistic$(Z) = P(Y=1|X)$')
```



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

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

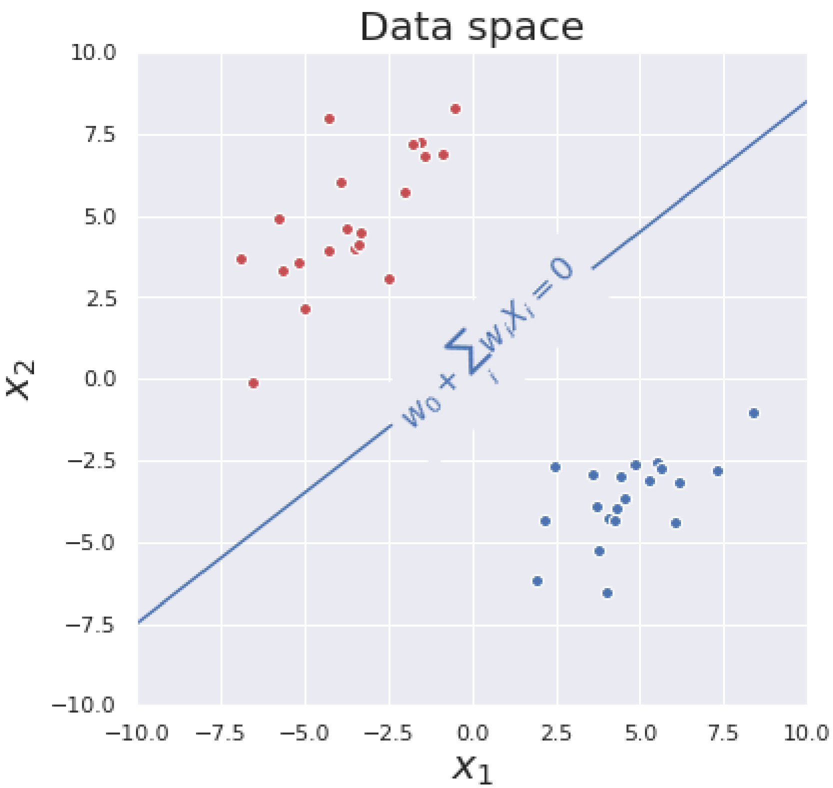
This is a linear decision boundary!

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

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

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

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.

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

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

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

Training Logistic Regression

Let's focus on binary classfication

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

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

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:

$$\hat{\mathbf{w}}_{\mathrm{MLE}} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(X^{(j)}, Y^{(j)}|\mathbf{w})$$

Problem: We don’t have a model for $P(X)$ or $P(X|Y)$ – only for $P(Y|X)$

Training Logistic Regression

Discriminative philosophy – Don't waste effort learning $P(X)$, focus on $P(Y|X)$

- that's all that matters for classification!

Maximum (Conditional) Likelihood Estimation:

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

Conditional log likelihood:

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

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

Conditional log likelihood - simpler view

$$z_i = w_0 + \sum_{i=1}^{d} w_i x_i^j$$

$$\begin{aligned}
l(\mathbf{w}) &\equiv \ln \prod_j P(y^j | \mathbf{x}^j, \mathbf{w}) \\
&= \ln \prod_{j, y^j = 1} \left(\frac{\exp(z_j)}{1 + \exp(z_j)} \right) \prod_{j, y^j = 0} \left(\frac{1}{1 + \exp(z_j)} \right) \\
&= \ln \prod_{j, y^j = 1} \left(\exp(z_j) \right) \prod_j \left(\frac{1}{1 + \exp(z_j)} \right) \\
&= \sum_j \left[y^j \left(z_j \right) - \ln\left(1 + \exp(z_j)\right) \right]
\end{aligned}$$

Maximizing Conditional Log Likelihood

$$l(\mathbf{w}) \equiv \ln \prod_j P(y^j | \mathbf{x}^j, \mathbf{w})$$

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

$$\hat{\mathbf{w}}_{\mathrm{MCLE}} = \underset{\mathbf{w}}{\operatorname{argmax}}\ l(\mathbf{w})$$

- Good news: $l(\mathbf{w})$ is concave in $\mathbf{w}$. Local optimum = global optimum
- Bad news: no closed-form solution to maximize $l(\mathbf{w})$
- Good news: concave functions easy to optimize (unique maximum)

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:

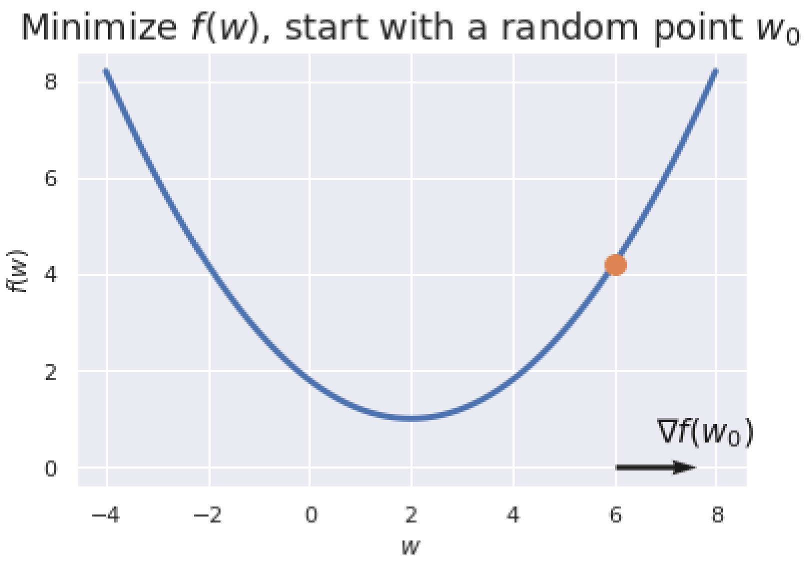
$$f(w) = 0.2(w - 2)^2 + 1$$

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
```

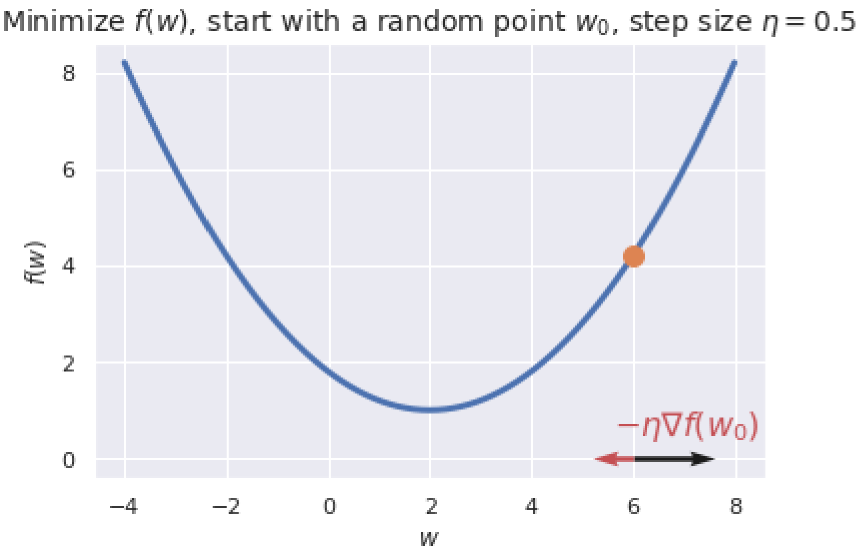
In [6]:

```
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 = 18);
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')
```



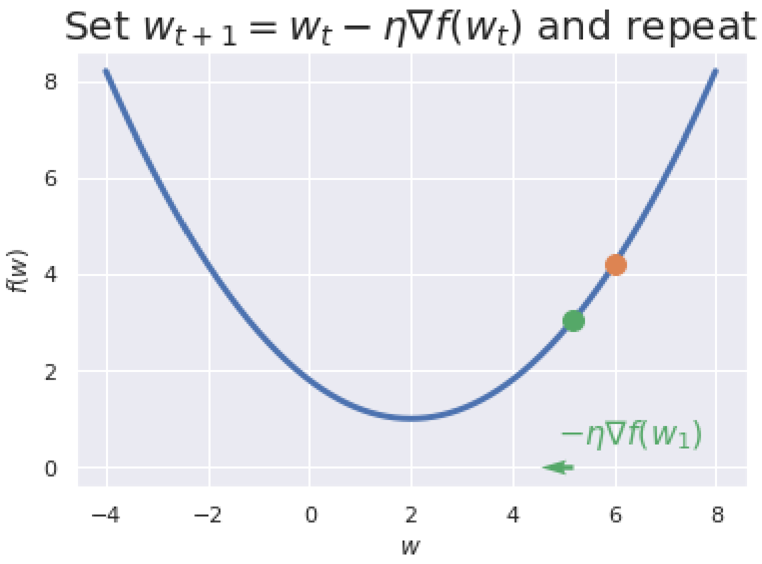
In [7]:

```
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 = 14);
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')
```



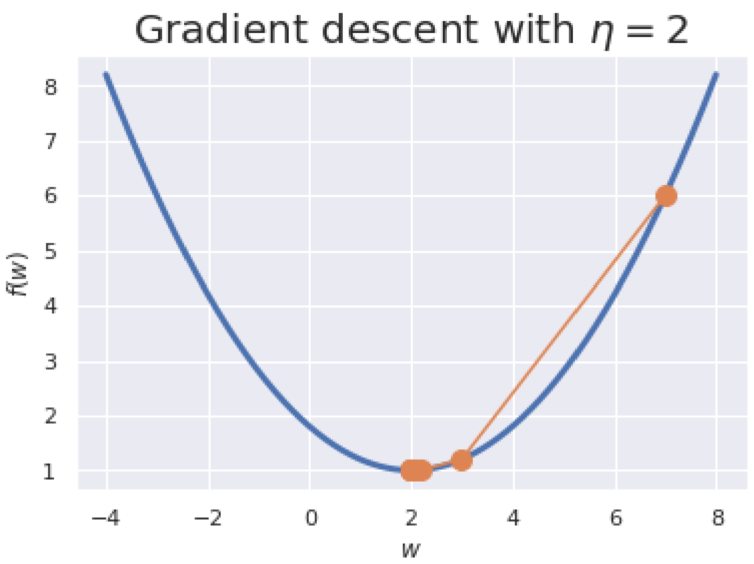
In [8]:

```
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]:
```python
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 = 2

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)
```

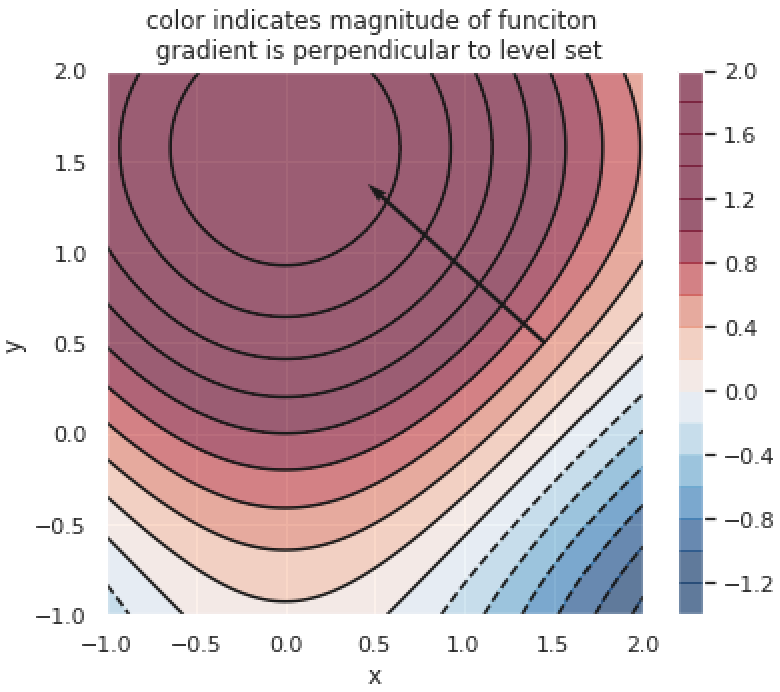
Out[9]:
```
[<matplotlib.lines.Line2D at 0x144bb4908>]
```



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

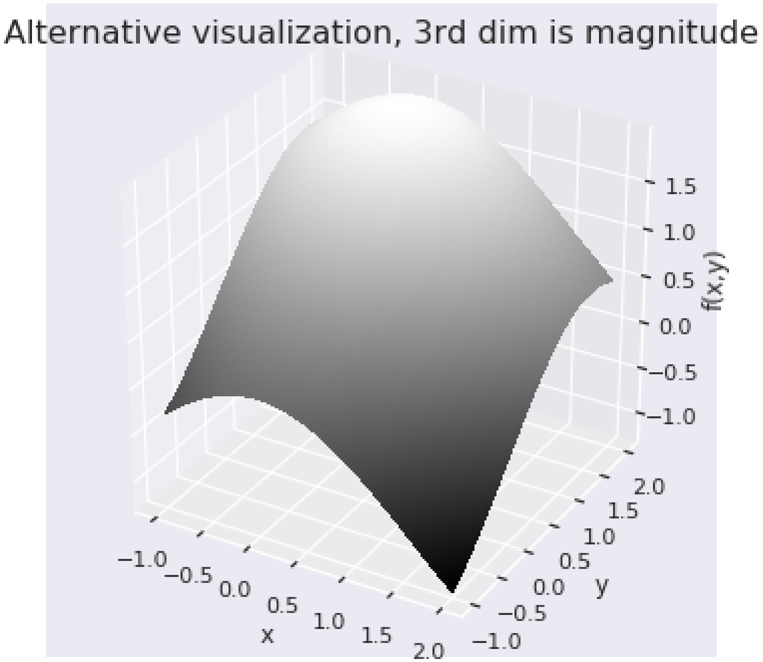
In [10]:

```
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', fontsize=16);
```



Logistic regression gradient ascent

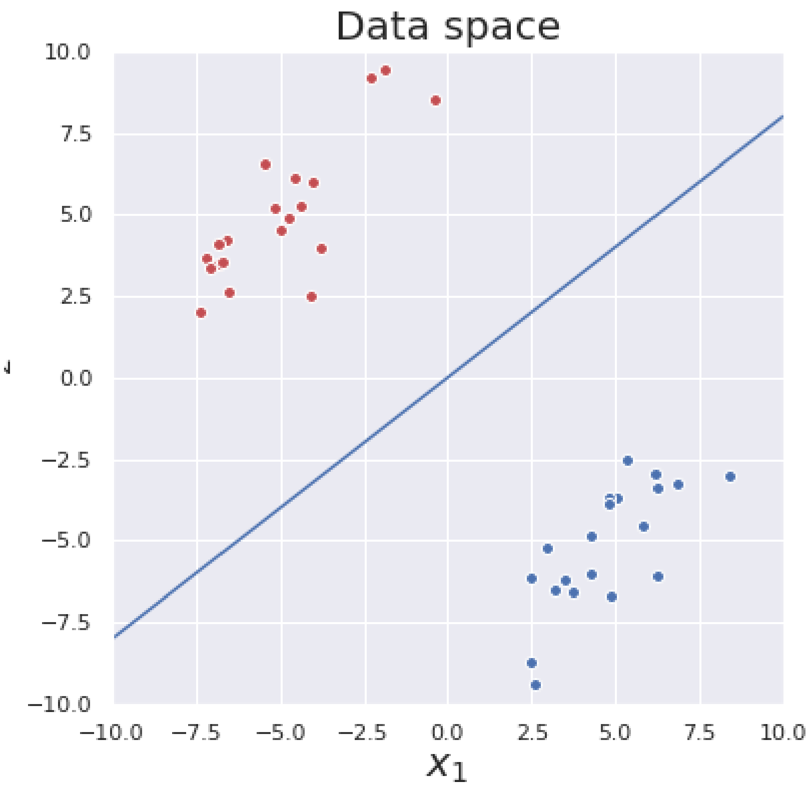
Simple simulated example

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

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

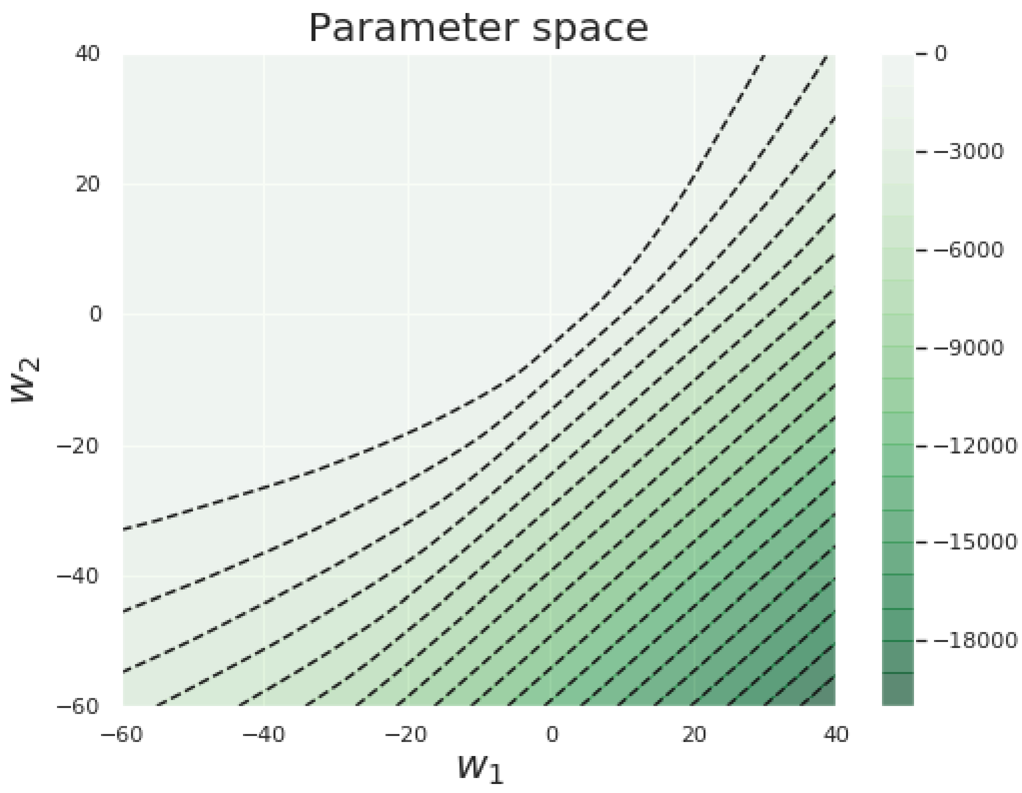
We omit w_0 in the example below for simplicity

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='Greens_r',vmin=np.min(L_w),vmax=0,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 $i = 1 \ldots d$:

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

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=(9,7))
cs = plt.contourf(W1, W2, L_w,20,cmap='Greens_r',vmin=np.min(L_w),
                  vmax=0,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'$\nabla L(w)/10$','k');
```

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 $i = 1 \ldots d$:

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

What is the $[y^j - \hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w^{(t)}})]$ term doing?

- $\hat{P}(Y^j = 1 | \mathbf{x}^j, \mathbf{w^{(t)}})$ is our current prediction of the label.
- compare this to actual label
- multiple difference by feature value

Gradient Descent (Ascent) is simplest of approaches

Compare to:

Stochastic Gradient Descent

Typically, the loss / function to minimize is a sum over the loss for each individual point: $L(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} L_i(\mathbf{w})$.

We use $\nabla L_i(\mathbf{w})$ instead of $\nabla L(\mathbf{w})$. Since we sample over the points uniformly, they all have equal proability, and the expected value of $\nabla L_i(\mathbf{w})$ is:

$$E_I \nabla L_i(\mathbf{w}) = \sum_{i=1}^{n} P(i) L_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} L_i(\mathbf{w}) = \nabla L(\mathbf{w}).$$

- $\nabla L_i(\mathbf{w})$ is faster to compute
- we make n updates for each epoch
- $\nabla L_i(\mathbf{w})$ has higher variance than $\nabla L(\mathbf{w})$ and therefore introduces noise into the trajectory. However, this still leads to a much faster convergence and the noise can be beneficial as it allows for some exploration.
- SGD converges in $O(1/\epsilon)$ and GD in $O(1/\log \epsilon)$ steps. However, in practice it is much faster

Stochastic Gradient Descent

Algorithm:

- Choose a starting point (typically random or 0)
- While not converged, repeat:
    - for each point i in a reshuffled order of the points:
        - compute gradient $\nabla L_i(\mathbf{w})$
        - choose a step size (start large and decrease)
        - $w \leftarrow \mathbf{w} - \eta \nabla L_i(\mathbf{w})$.
- Return after stopping criterion satisfied

Batch gradient descent

To reduce the noise in the gradients at individual datapoints, one approach is to:

- use a batch of B datapoints sampled from the dataset at each step.
- in each iteration, one can go over all the dataset in batches.

Algorithm:

- Choose a starting point (typically random or 0)
- While not converged, repeat:
    - for each batch B in a reshuffled order of the points:
        - compute gradient $\nabla L_B(\mathbf{w}) = \sum_{i \in B} \nabla L_i(\mathbf{w})$
        - choose a step size (start large and decrease)
        - $w \leftarrow \mathbf{w} - \eta \nabla L_B(\mathbf{w})$.
- Return after stopping criterion satisfied

Effect of step-size η:

- Large: Fast convergence but larger residual error, also possible oscillations
- Small: Slow convergence but small residual error

Extra Reading:

Learning rate decay, and other gradient descent methods

- This is Sebastian Ruder's blog post (https://ruder.io/optimizing-gradient-descent/index.html#adagrad). You can see animations by Alec Radford on this blogpost (http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html) for demos. You can also explore this interactive visualization from Roberts Dionne (http://www.robertsdionne.com/bouncingball/).
- In the examples above, we had a fixed learning rate for simplicity, but the choice of the learning rate is very important and affects the behavior and convergence time of the algorithm.
- When using SGD, we can have a large learning rate because the gradients are mostly pointing in the same direction. Later in training, we are closer to the optimum and the gradients are more noisy. We want to slow down the training to average the noise. We can use the validation dataset to perform this:
    - when the validation set loss stops decreasing, we reduce the learning rate
    - if the validation set still doesn't decrease, stop
    - compute the validation loss after multiple iterations to have a less fluctuating estimate.

Momentum

Ravines (where the surface curves steeply in one dimension) are problematic because SGD can oscillate.

- Momentum helps accelerate SGD in the relevant direction and dampens oscillations.
- This is done using a fraction γ of the update vector of the past time step that is added to the current update:

$$\Delta w_t = \gamma \Delta w_{t-1} + \nabla L(w_t)$$
$$w_{t+1} = w_t - \Delta w_t$$

- γ is usually set to 0.9. The momentum term increases the update for dimensions for which the gradients point in the same directions, and decreases the update for dimensions that are changing. This leads to faster convergence and less oscillation.

Nesterov Accelerated gradient

- NAG is a way to incorporate some look ahead into the update. The algorithm first takes a partial step in the direction of the previous update then computes the gradient in that new location:

$$\Delta w_t = \gamma \Delta w_{t-1} + \nabla L(w_t - \gamma \Delta w_{t-1})$$
$$w_{t+1} = w_t - \Delta w_t$$

- NAG first makes a jump in the direction of the previous accumulated gradient then makes a "correction" by computing the gradient at that location.

Adagrad

- Adagrad adapts the learning rate to the dimensions of w: it makes less sparse dimensions (or ones that have a larger magnitude features) have lower learning rates than more sparse dimensions (or ones that have a smaller magnitude).
$$w_{t+1,i} = w_{t,i} - \frac{\eta}{G_{t,ii} + \epsilon} \nabla L(w)_i$$
- G_t is a diagonal matrix with the sum of the squares of the gradient of the ith element at each i, i entry.
- When using Adagrad, we don't need to tune the learning rate. However, as training goes on, the updates become smaller and smaller and the algorithm can stagnate. This is solved by the following algorithms:

Adadelta

- Adadelta resolves the slowing learning rate by reducing the dependence on the sum of the gradients so far through the introduction of a forgetting factor. Adadelta computes the weighted sum:
$$E[\nabla L(w)^2]_t = \gamma E[\nabla L(w)^2]_{t-1} + (1 - \gamma) \nabla L(w)_t^2$$
- where γ is set to values similar to the momentum rate.
$$\delta w_t = \frac{\eta}{E[\nabla L(w)^2]_t + \epsilon} \nabla L(w)_t$$

RMSprop

- RMSprop was proposed at the same time as Adadelta, and is very similar.

End of extra reading.

- You can also read about other methods such as Newton's method, Conjugate gradient ascent, IRLS (see Bishop 4.3.3)

What happens if data is linearly separable?

Decision boundary:

$$w_0 + \sum_{i=1}^{d} w_i x_i^j = 0$$

What about:

$$(10w_0) + \sum_{i=1}^{d} (10w_i) x_i^j = 0$$

or

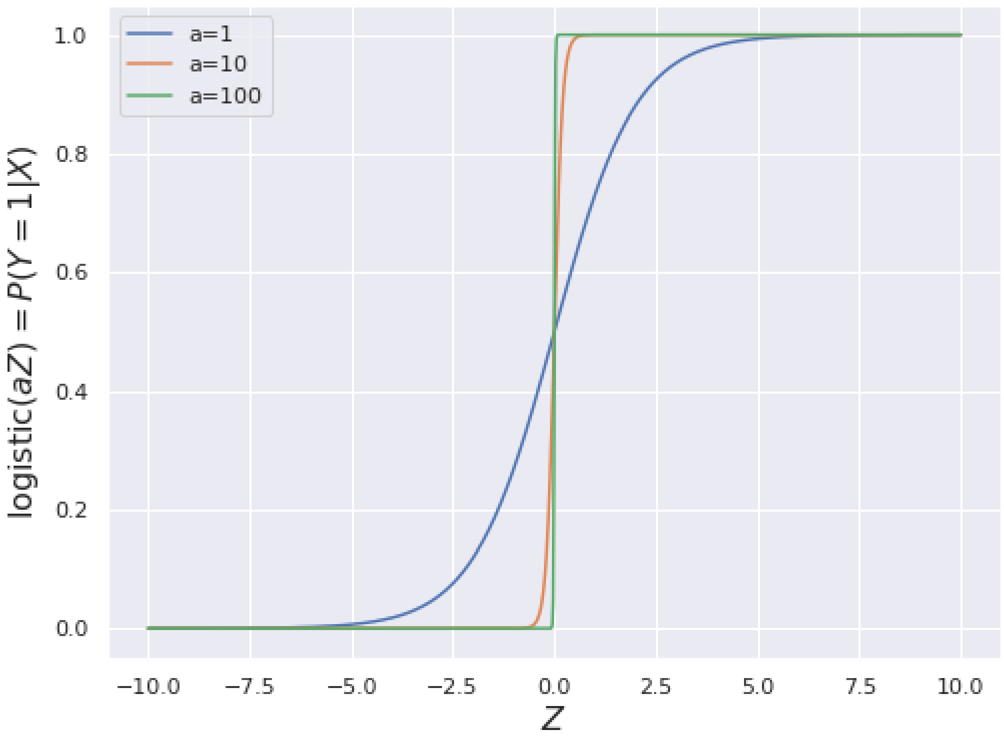
$$(10000w_0) + \sum_{i=1}^{d} (10000w_i) x_i^j = 0$$

Same boundary! Which one has higher log likelihood?

In [18]:

```
plt.figure(figsize=(8,6))
z = np.linspace(-10,10,1000)
plt.plot(z,1/(1+np.exp(-z)), label = 'a=1')
plt.plot(z,1/(1+np.exp(-10*z)), label = 'a=10')
plt.plot(z,1/(1+np.exp(-100*z)), label = 'a=100')
plt.legend(); plt.xlabel(r'$Z$',fontsize=16);
plt.ylabel(r'logistic$(a Z) = P(Y=1|X)$',fontsize=16);
```

```
/Users/lwehbe/env/py3/lib/python3.7/site-packages/ipykernel_launcher.py:5: Run
timeWarning: overflow encountered in exp
  """
```



Need to regularize the weights

- $w \rightarrow \infty$ if the data is linearly separable
- For MAP, need to define prior on W
    - given $W = (w_1, \dots w_d)$
    - 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: $W \sim \frac{1}{2\pi\sigma^2}\exp\left(-\frac{1}{2\sigma^2}\sum_i w_i^2\right)$

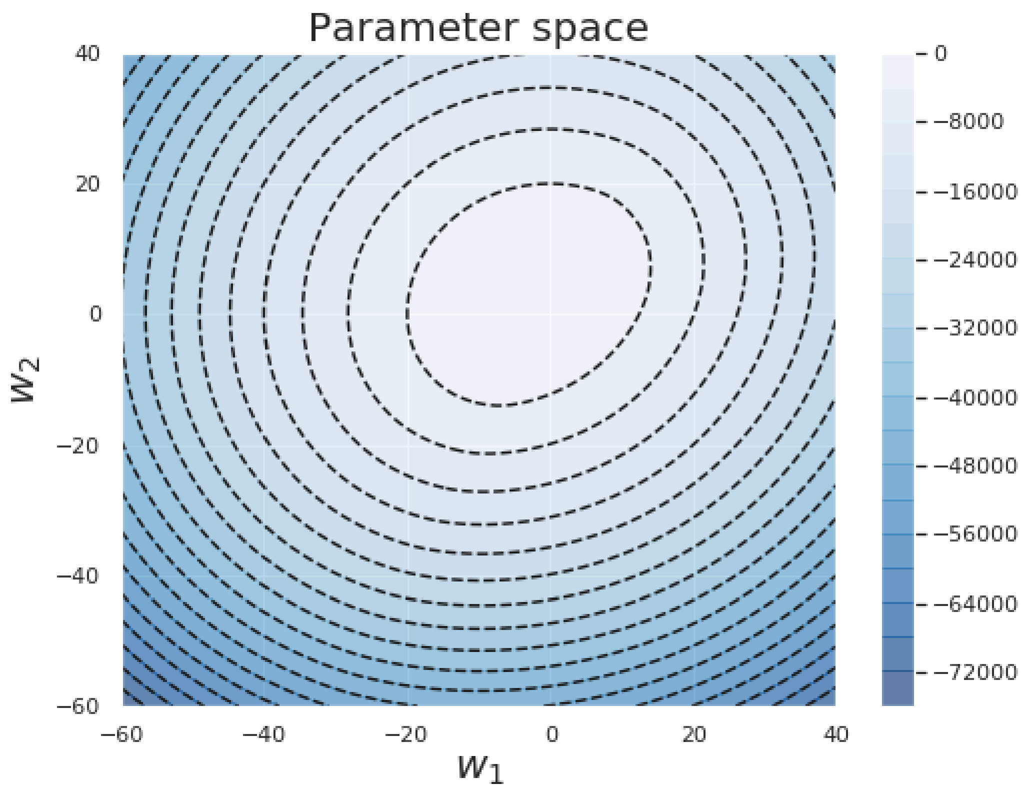
$$W^{MAP} = \underset{W}{\text{argmax}}\ \ln P(Y|W,X) - \left(\frac{1}{2\sigma^2}\sum_i w_i^2\right)$$

In [19]:

```python
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 [20]:

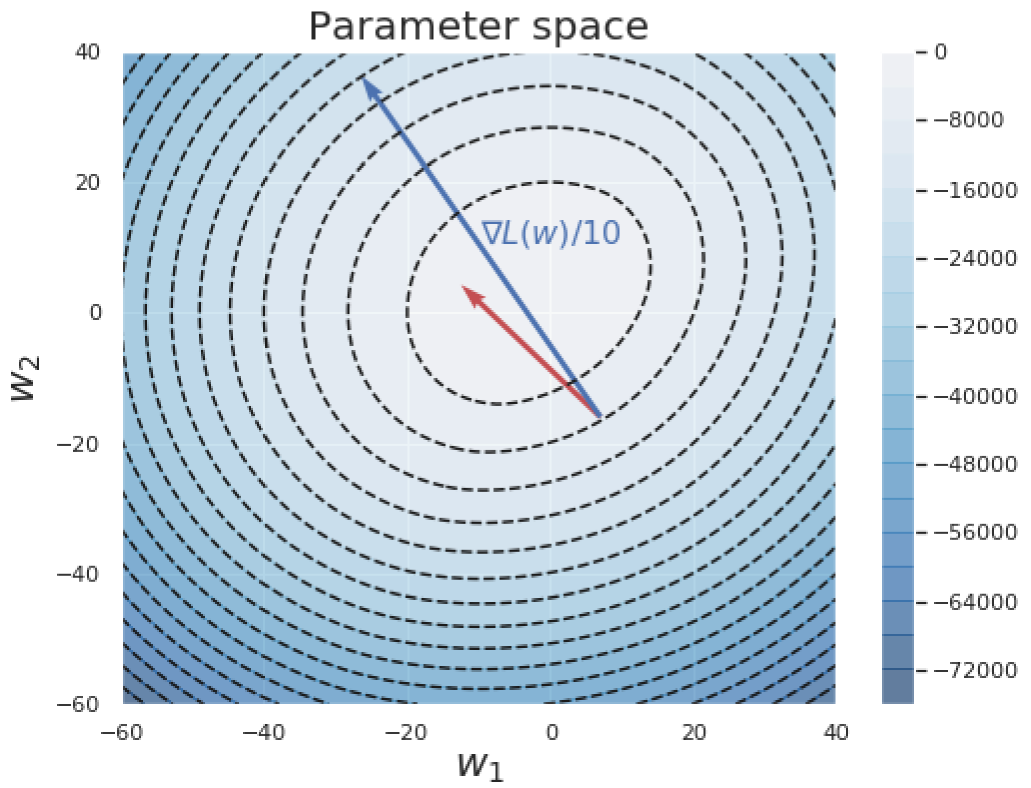
```
plt.figure(figsize=(8,6))
cs = plt.contourf(W1, W2, L_w,20,cmap='Blues_r',vmin=np.min(L_w),
                  vmax=0,alpha=0.6);
plt.colorbar()
contours = plt.contour(cs, colors='k')
plt.xlabel(r'$w_1$',fontsize=20)
plt.ylabel(r'$w_2$',fontsize=20)
plt.title('Parameter space',fontsize=20);
```



In [21]:

```
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]:
```python
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');
```



Let's compare Logistic Regression to Gaussian Naive Bayes

Consider these two assumptions:

- X_i conditionally independent of X_j given Y
- $P(Xi|Y = y_k) = \mathcal{N}(\mu_{ik}, \sigma_i)$, not $\mathcal{N}(\mu_{ik}, \sigma_{ik})$
    - i.e. shared standard deviation

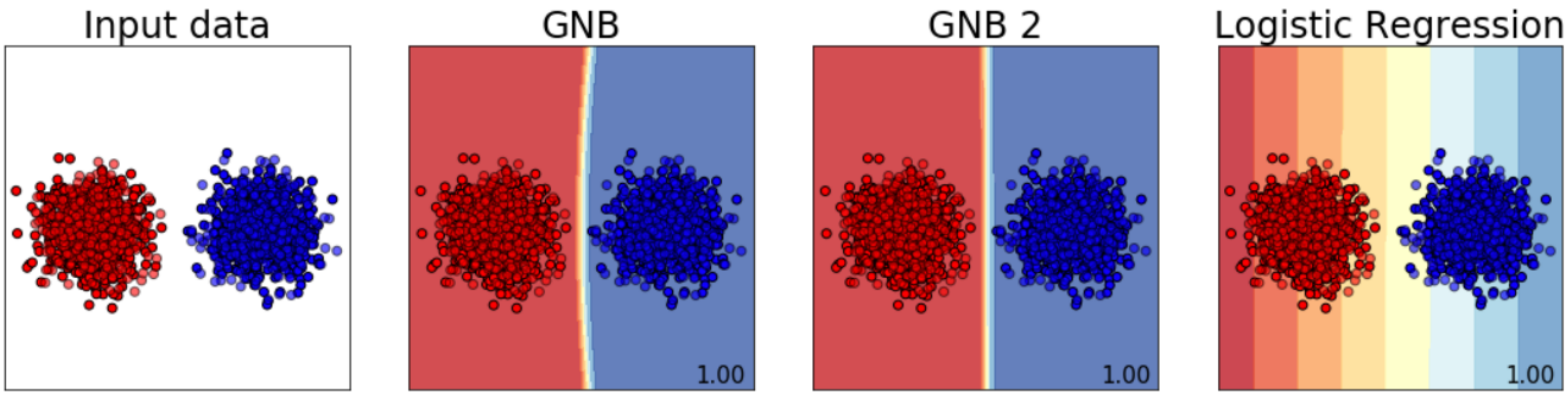
Consider three learning methods:

- GNB (assumption 1 only) --- decision surface can be non-linear
- GNB2 (assumption 1 and 2) --- decision surface linear
- LR --- decision surface linear, trained without assumption 1 or estimating $P(Xi|Y = y_k)$.

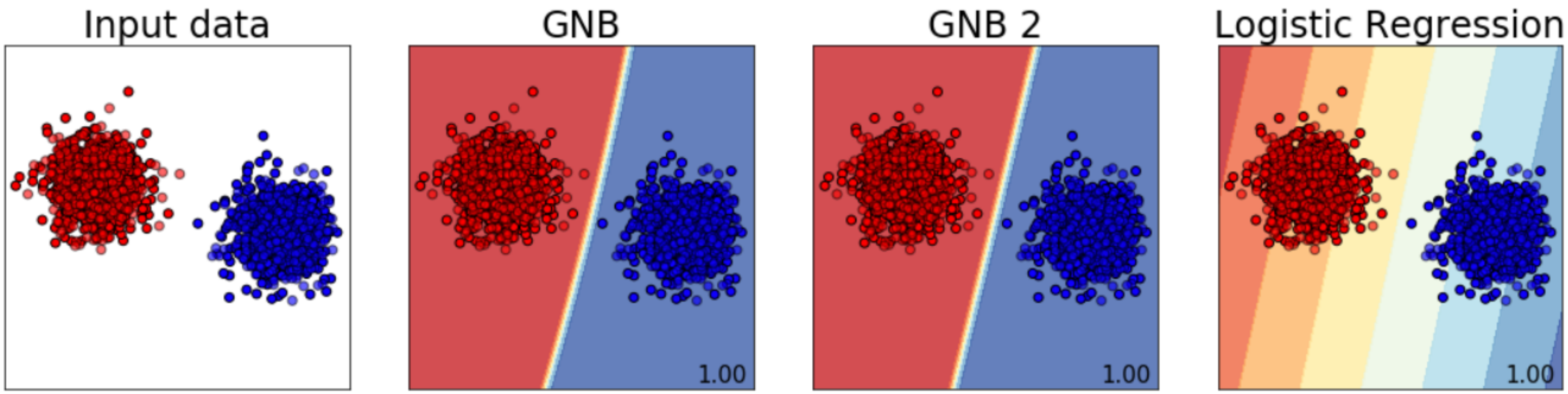
How do these methods perform if we have plenty of data and:

Both (1) and (2) are satisfied.

Assumption 1 and 2 are satisfied



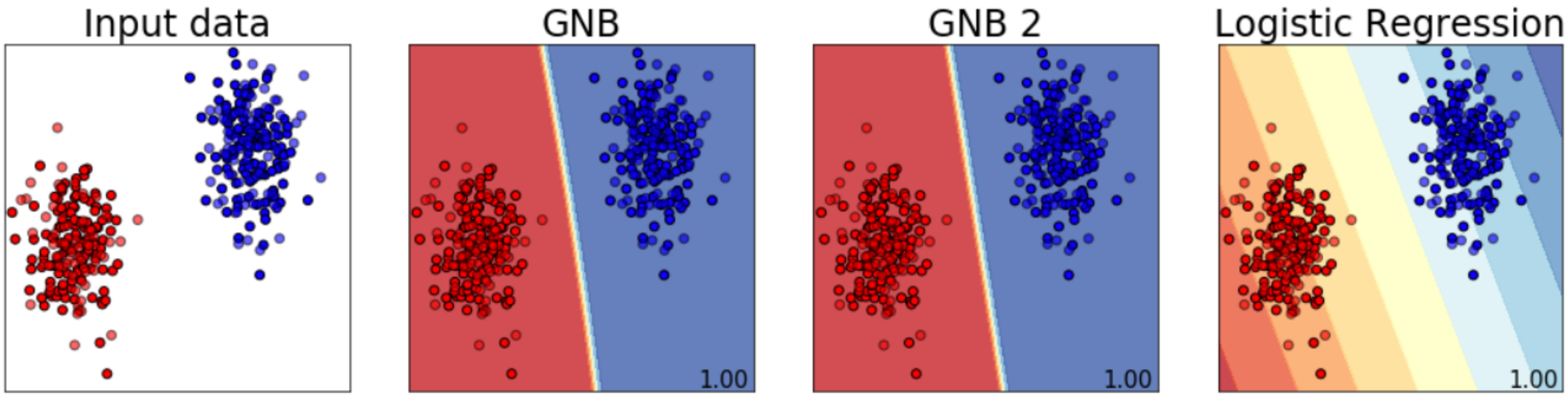
X_i's conditionally independent and variance is shared



In these cases, LR, GNB2 and GNB perform similarly

Assumption 1 and 2 are satisfied

The decision boundary of GNB and GNB2 is sensitive to the locations of the means (since the variances are the same)



Assumption 1 and 2 are satisfied

Recall the decision boundary of GNB when the variances are exactly equal:

$$\ln \frac{P(Y=1|X_1 \ldots X_d)}{P(Y=0|X_1 \ldots X_d)} = C + G(X)$$

$$G(X) = -\frac{1}{2} \sum_i \Big(x_i^2 \big(\frac{1}{\sigma_{i1}^2} - \frac{1}{\sigma_{i0}^2}\big) - 2x_i \big(\frac{\mu_{i1}}{\sigma_{i1}^2} - \frac{\mu_{i0}}{\sigma_{i0}^2}\big) + \big(\frac{\mu_{i1}^2}{\sigma_{i1}^2} - \frac{\mu_{i0}^2}{\sigma_{i0}^2}$$

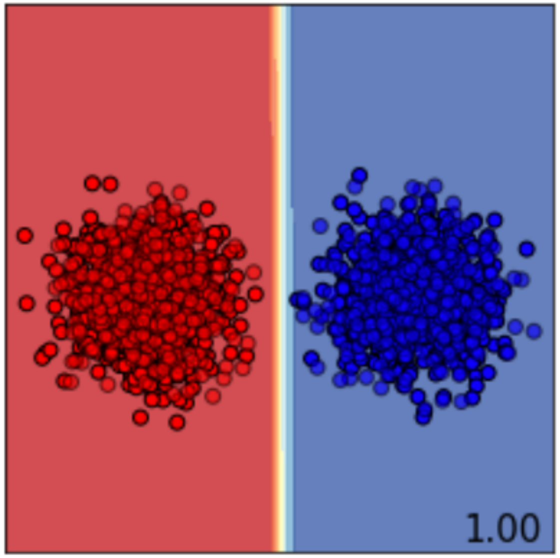
$$G(X) = \sum_i \Big(x_i \frac{\mu_{i1} - \mu_{i0}}{\sigma_i^2} \Big) - \sum_i \Big(\frac{\mu_{i1}^2 - \mu_{i0}^2}{2\sigma_i^2} \Big)$$

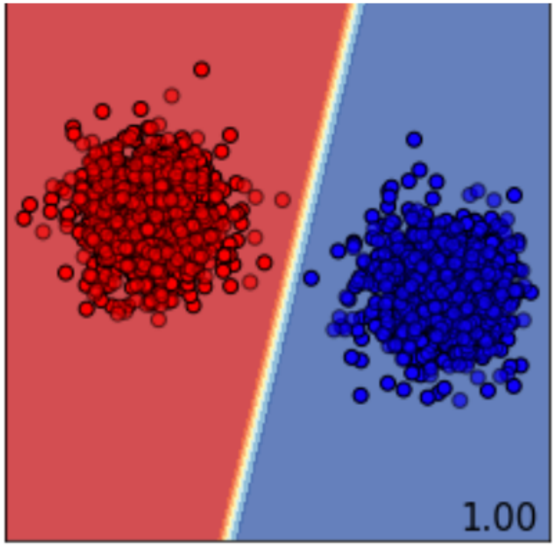
The decision boundary is linear, of the form: $\beta_0 + \sum_i \beta_i x_i = 0$.

The parameters are determined using the distance between centers, weighted by variance on each dimension.

If the variances of the Xi are the same (across classes and across i), the decision boundary of GNB2 and GNB is determined by the distance to the mean (perpendicular bisector)

Independently, if one of the coordinates of the two means are the same, then the decision boundary becomes parallel to that axis





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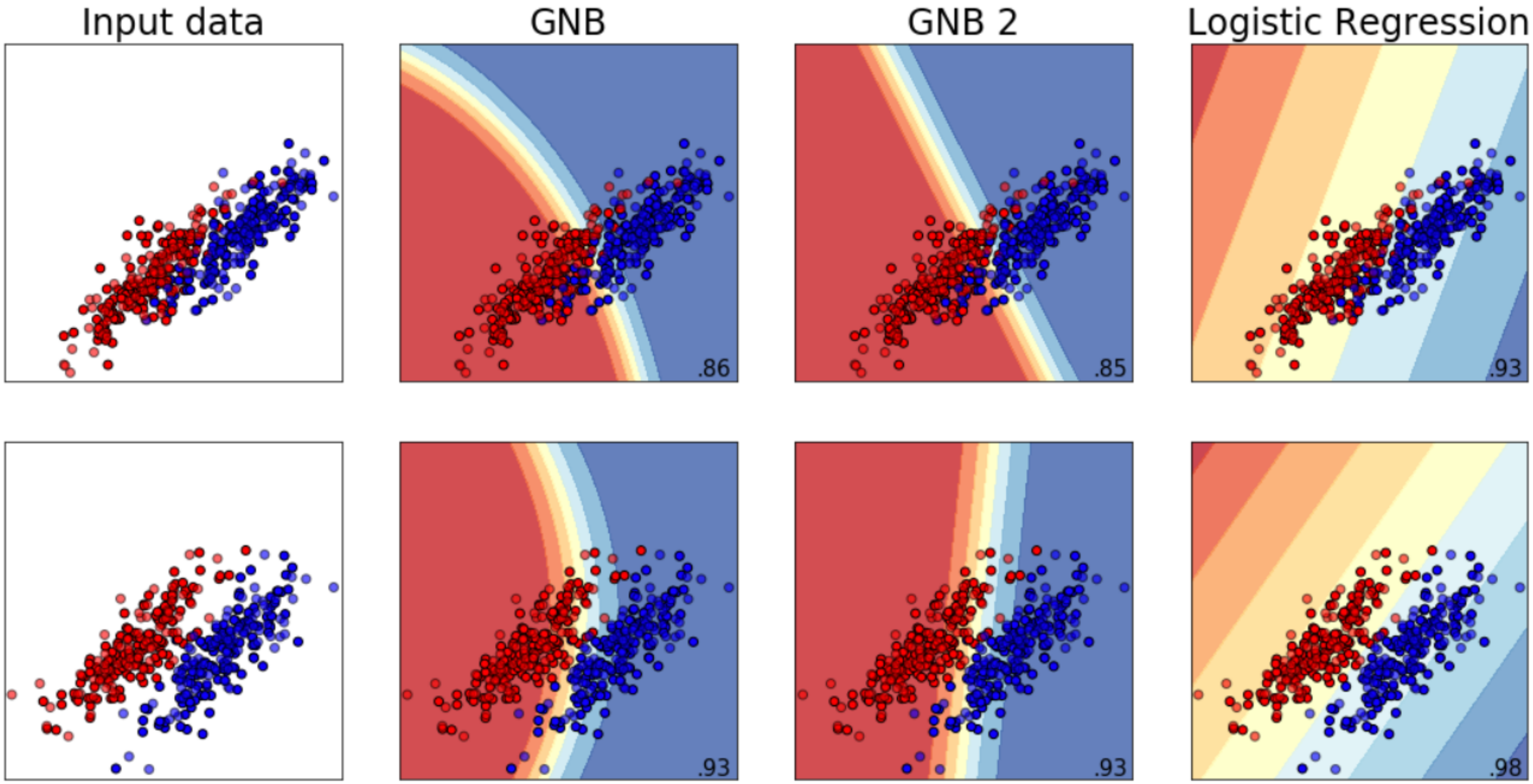
How do these methods perform if we have plenty of data and:

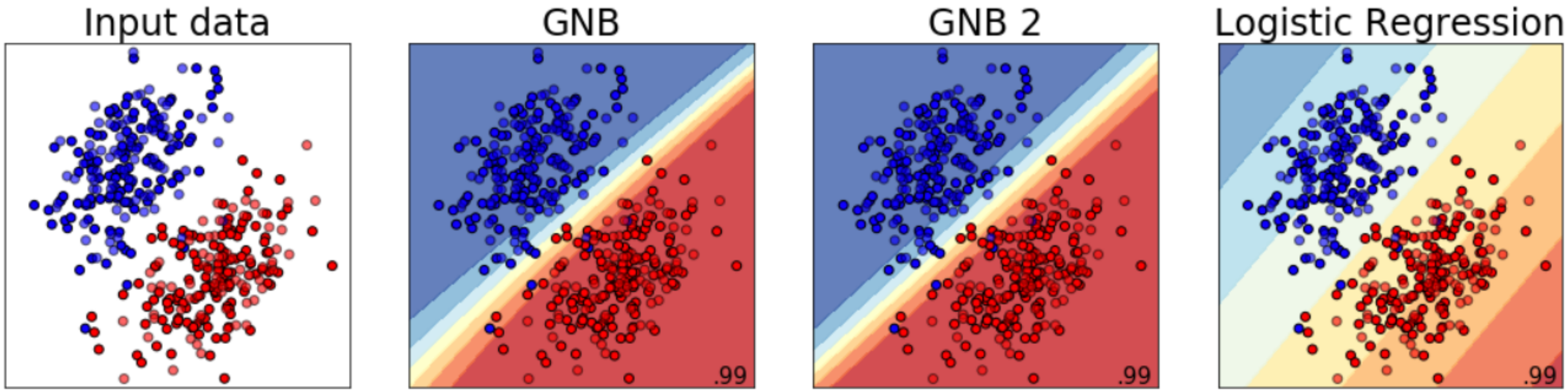
(2) is satisfied, but not (1).

Assumption 2 satisfied and not 1



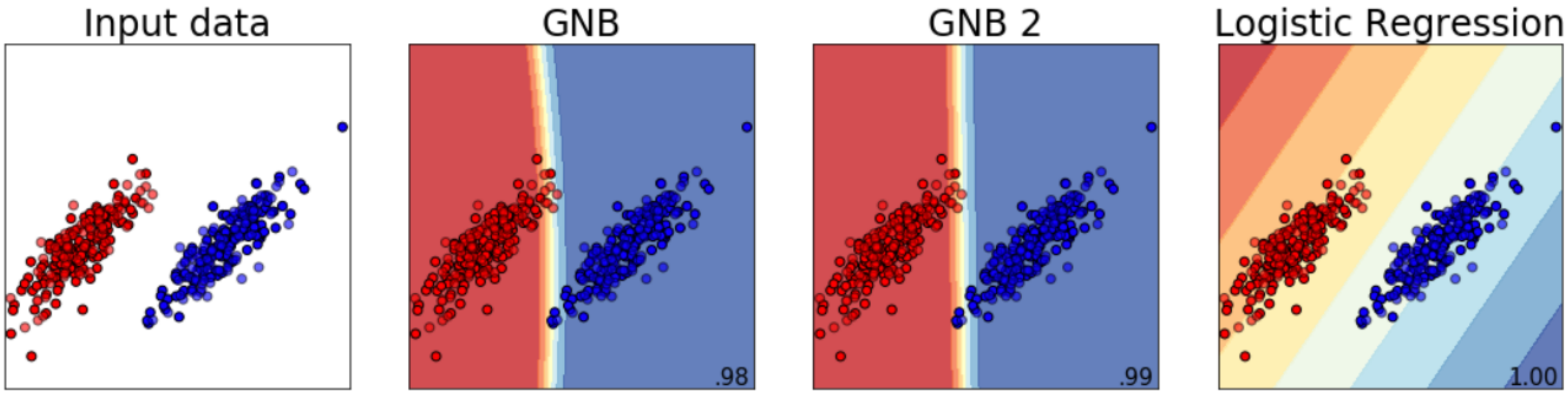
GNB2 can break (also GNB) in these examples

Assumption 2 satisfied and not 1



GNB2 and GNB can also work well

Assumption 2 satisfied and not 1



Why doesn't GNB2 learn the same boundary as LR?

The decision boundary for GNB 2 is linear, of the form: $\beta_0 + \sum_i \beta_i x_i = 0.$

But each parameters is linked to the individual means and standard deviation of each dimension x_i, e.g.:

$$\beta_i = \frac{\mu_{i1} - \mu_{i0}}{\sigma_i^2}$$

GNB 2 is therefore less flexible than LR.

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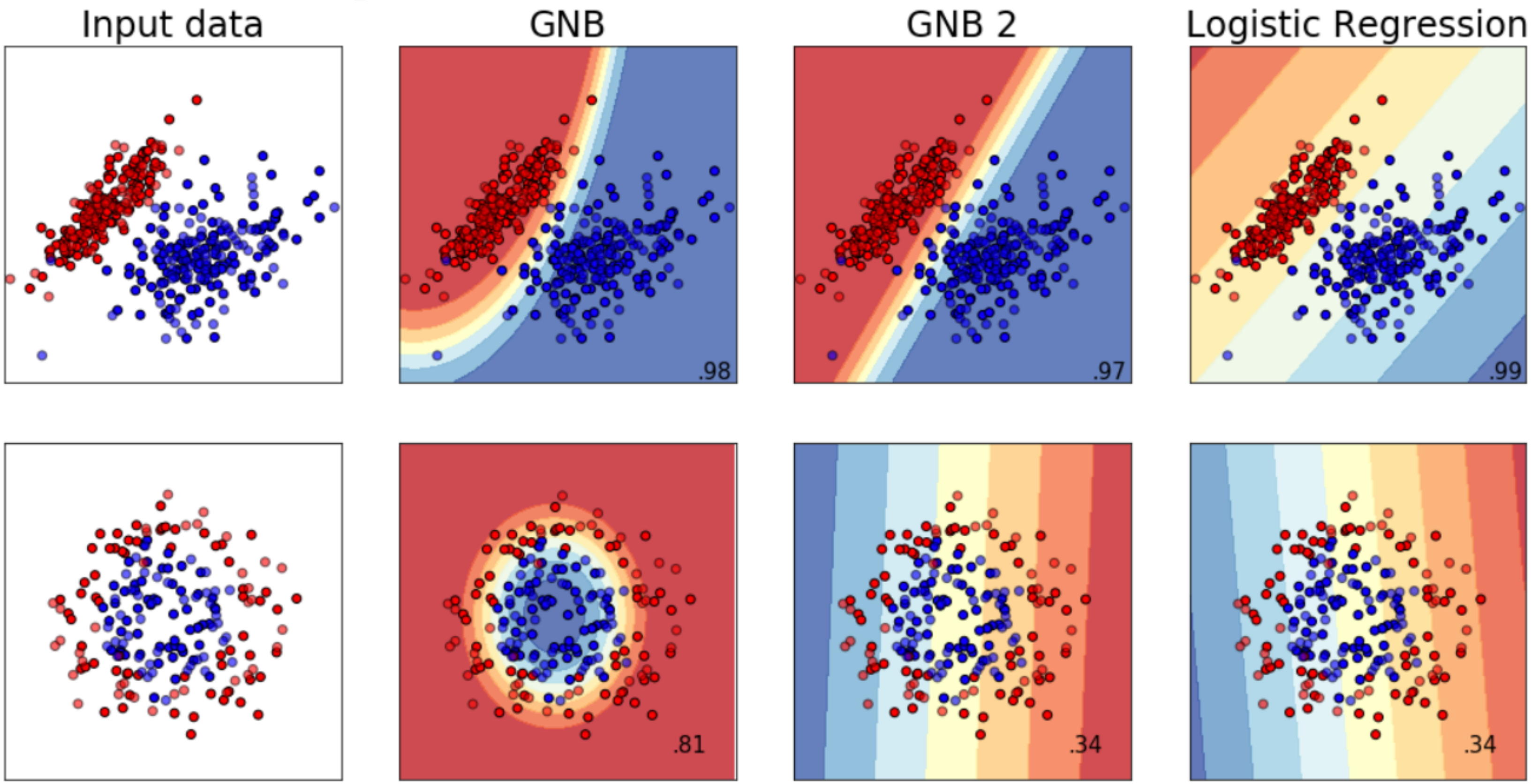
How do these methods perform if we have plenty of data and:

Neither (1) nor (2) is satisfied.

Assumptions 1 and 2 are not satisfied



Depending on the dataset, GNB and LR have different performances.
Even though LR and GNB2 can be expressed in the same way, LR has more flexibly to learn parameters that fit the data, and they are don't have to be tied to the marginal means and variance

Let's compare Logistic Regression to Gaussian Naive Bayes

Which method works better if we have **infinite** training data, and...

- Both (1) and (2) are satisfied: LR = GNB2 = GNB
- (1) is satisfied, but not (2) : GNB > GNB2, GNB ? LR, LR > GNB2
- Neither (1) nor (2) is satisfied: GNB>GNB2, LR > GNB2, LR??GNB

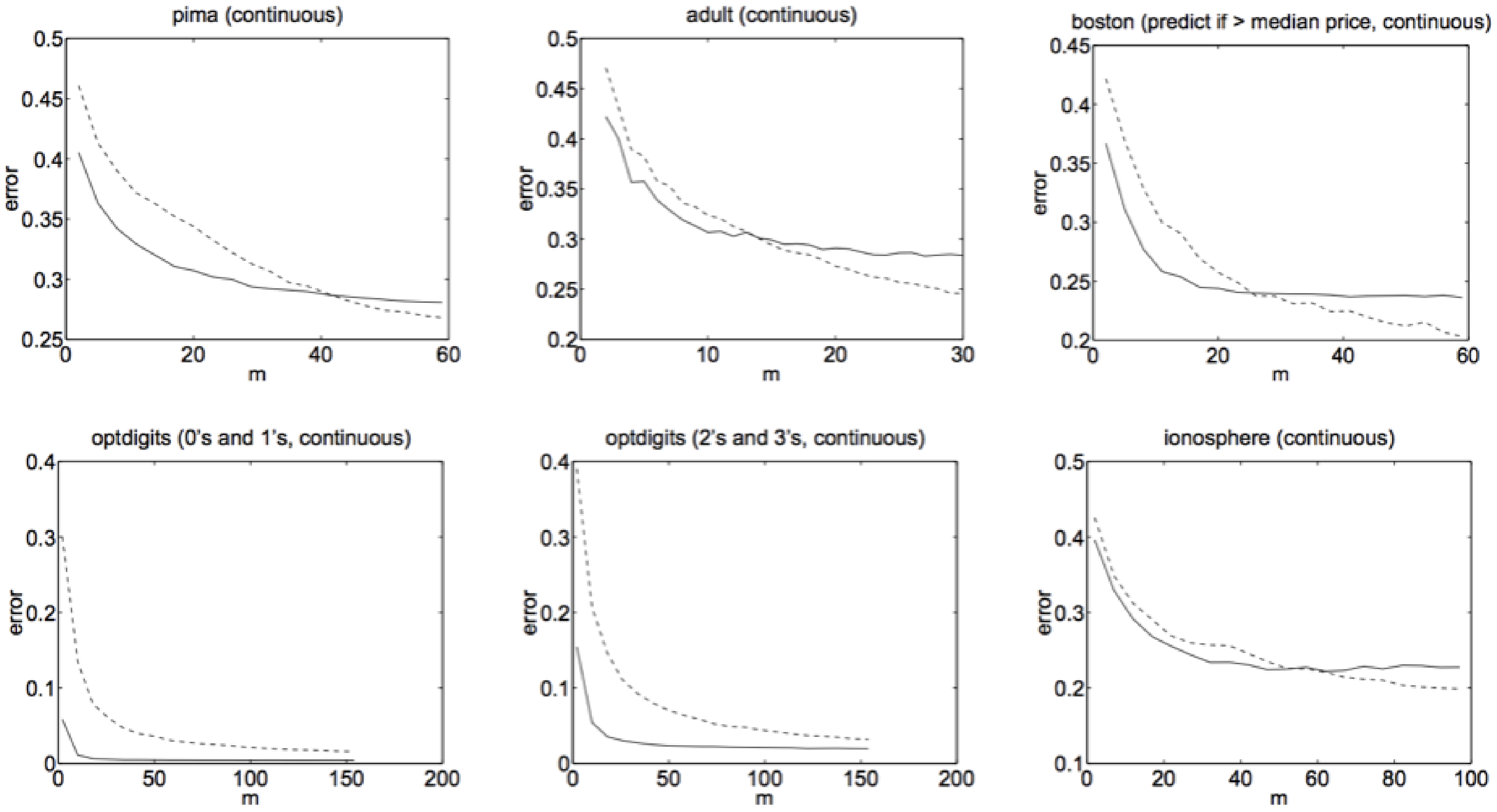
Naïve Bayes vs. Logistic Regression

The bottom line:

- GNB2 and LR both use linear decision surfaces, GNB need not
- Given infinite data, LR is better or equal to GNB2 because training procedure does not make assumptions 1 or 2 (though our derivation of the form of P(Y|X) did).

What happens if we have finite training data?

[Ng & Jordan, 2002] ==> GNB converges more quickly



- GNB2 converges more quickly to its perhaps-less-accurate asymptotic error. (more bias than LR)
- And GNB is both more biased (assumption 1) and less (no linearity assumption) than LR, so either might outperform the other.

What you should know

- Generative vs. Discriminative classifiers

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