10-701 INTRODUCTION TO MACHINE LEARNING (PHD)
LECTURE 5: LOGISTIC REGRESSION

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Reading: (http://www.cs.cmu.edu/~tom/mlbook/NBayesLogReg.pdf">) Generative and Disciminative 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 X_i?
- 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 X_i's?

In [100]:
```
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? I.E. 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

CONSIDER THE FOLLOWING NAIVE BAYES SETUP

Learns $f : \mathcal{X} \to \{0, 1\}$, where

- $\mathbf{x}$ 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).
- assume all X_j are conditionally independent given Y
- model $P(X_j | Y = y_k)$ as Gaussian $\mathcal{N}(\mu_{jk}, \sigma_j)$
- model $P(Y)$ as Bernoulli(θ)

$$P(Y = 1|X) = \frac{P(Y = 1)P(X|Y = 1)}{P(Y = 1)P(X|Y = 1) + P(Y = 0)P(X|Y = 0)} = \frac{1}{1 + \frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}}$$

$$= \frac{1}{1 + \exp\left(\ln\left(\frac{P(Y=0)P(X|Y=0)}{P(Y=1)P(X|Y=1)}\right)\right)} = \frac{1}{1 + \exp\left(\ln\frac{1-\theta}{\theta} + \sum_j \frac{\mu_{j0}-\mu_{j1}}{\sigma_j^2} x_j + \frac{\mu_{j0}^2-\mu_{j1}^2}{\sigma_j^2}\right)}$$

$$= \frac{1}{1 + \exp\left(-(w_0 + \sum_{j=1}^{d} w_j x_j)\right)}$$

LOGISTIC REGRESSION IS A DISCRIMINATIVE CLASSIFIER

Learns $f : \mathcal{X} \to \{0, 1\}$, where

- $\mathbf{x}$ 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).

$P(Y = 1|X = \mathbf{x})$ is modeled as:

$$P(Y = 1|X = \mathbf{x}) = \frac{1}{1 + \exp\left(-(w_0 + \sum_{j=1}^{d} w_j x_j)\right)} = \frac{\exp(w_0 + \sum_{j=1}^{d} w_j x_j)}{\exp(w_0 + \sum_{j=1}^{d} w_j x_j) + 1}$$

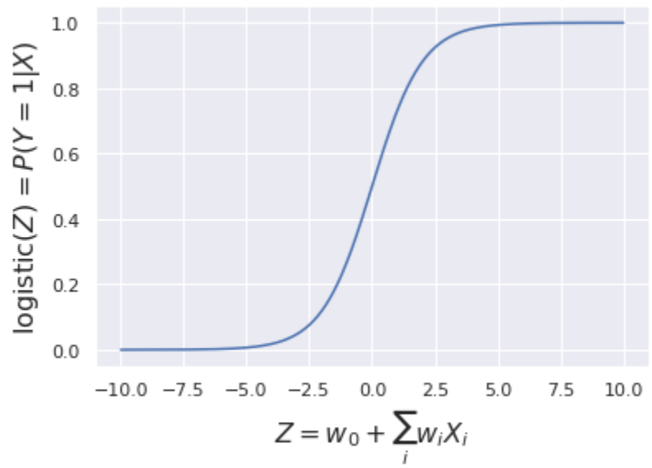
It uses the logistic (or sigmoid) function:

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

(Note: the parameters are not tied to correspond to the naive bayes parameters on the previous slide. See comparisons at end of lecture)

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?

$$\frac{P(Y=1|X)}{P(Y=0|X)} = \frac{\frac{\exp(w_0+\sum_{j=1}^{d} w_j x_j)}{\exp(w_0+\sum_{j=1}^{d} w_j x_j)+1}}{\frac{1}{\exp(w_0+\sum_{j=1}^{d} w_j x_j)+1}} = \exp(w_0 + \sum_{j=1}^{d} w_j x_j)$$

- Asking: is $P(Y=1|X) > P(Y=0|X)$ is the same as asking:

$$\ln \frac{P(Y=1|X)}{P(Y=0|X)} > 0?$$

- i.e. is

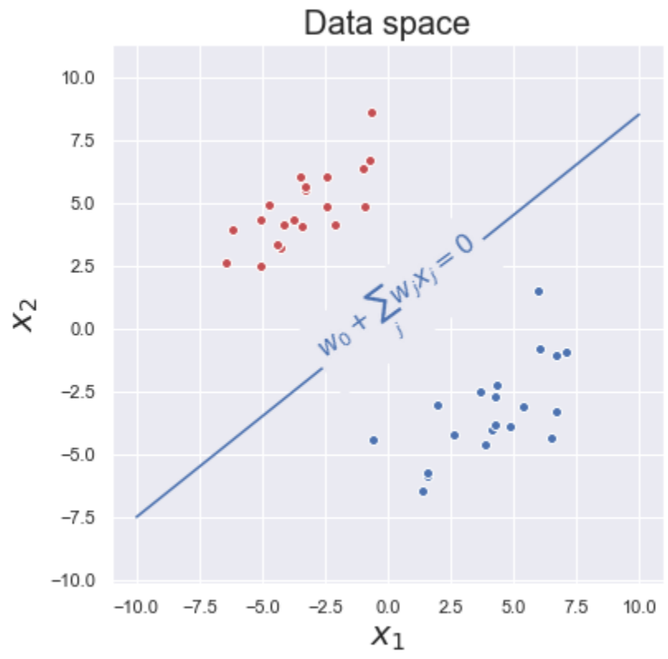
$$w_0 + \sum_{j=1}^{d} w_j x_j \quad > 0?$$

- This is a linear decision boundary!

In [2]:

```
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 [6]:
```
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'$w_0+\sum_j w_j x_j = 0$',fontsize=16)

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

- Repeat what we did in Lecture 1: redefine $\mathbf{x}$ to have an additional dimension that is always 1, and now use the vector $\mathbf{w} = [w_0, w_1, \ldots, w_d]$

$$P(Y = 1|X) = \frac{\exp(\mathbf{w}^\top \mathbf{x})}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$
$$P(Y = 0|X) = \frac{1}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$

- The weights w_j are optimized such that when $\mathbf{w}^\top \mathbf{x} > 0$ the example is more likely to be positive and when $\mathbf{w}^\top \mathbf{x} < 0$ it's more likely to be negative.

$\mathbf{w}^\top \mathbf{x} = 0, \qquad P(Y = 1|X) = \frac{1}{2}$

$\mathbf{w}^\top \mathbf{x} \to \infty, \qquad P(Y = 1|X) \to 1$

$\mathbf{w}^\top \mathbf{x} \to -\infty, \qquad P(Y = 1|X) \to 0$

TRAINING LOGISTIC REGRESSION

- Let's focus on binary classfication

$$P(Y = 1|X) = \frac{\exp(\mathbf{w}^\top \mathbf{x})}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$
$$P(Y = 0|X) = \frac{1}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$

- **How to learn $\mathbf{w} = [w_0, w_1 \ldots w_d]$?**
- Training data: $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^n$, with $\mathbf{x}^{(i)} = \left(x_1^{(i)}, x_2^{(i)}, \ldots, x_d^{(i)}\right)$
- Maximum Likelihood Estimation:

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

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:

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

CONDITIONAL LOG LIKELIHOOD:

$$P(Y=1|X) = \frac{\exp(\mathbf{w}^\top \mathbf{x})}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$

$$P(Y=0|X) = \frac{1}{\exp(\mathbf{w}^\top \mathbf{x}) + 1}$$

$$\begin{aligned} l(\mathbf{w}) &\equiv \ln \prod_{i=1}^{n} P(Y = y^{(i)} | X = \mathbf{x}^{(i)}, \mathbf{w}) \\ &= \ln \prod_{i, y^{(i)}=1} \left(\frac{\exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)}{1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)} \right) \prod_{i, y^{i}=0} \left(\frac{1}{1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)} \right) \\ &= \ln \prod_{i, y^{(i)}=1} \left(\exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right) \right) \prod_{i} \left(\frac{1}{1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)} \right) \\ &= \sum_{i} \left[y^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)}\right) - \ln\left(1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right) \right] \end{aligned}$$

MAXIMIZING CONDITIONAL LOG LIKELIHOOD

$$l(\mathbf{w}) \equiv \ln \prod_{i=1}^{n} P(Y = y^{(i)} | X = \mathbf{x}^{(i)}, \mathbf{w})$$

$$= \sum_{i} \left[y^{i} \left(\mathbf{w}^{\top} \mathbf{x}^{(i)} \right) - \ln\left(1 + \exp\left(\mathbf{w}^{\top} \mathbf{x}^{(i)}\right)\right) \right]$$

$$\hat{\mathbf{w}}_{\text{MCLE}} = \underset{\mathbf{w}}{\text{argmax}}\, l(\mathbf{w})$$

- 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 $\eta > 0$**

$$\Delta \mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$
$$w_j^{(t+1)} = w_j^{(t)} + \eta \frac{\partial l(\mathbf{w})}{\partial w_j}|_{w^{(t)}}$$

OPTIMIZING CONCAVE/CONVEX FUNCTION

- It's more common to encounter gradient descent which is used 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

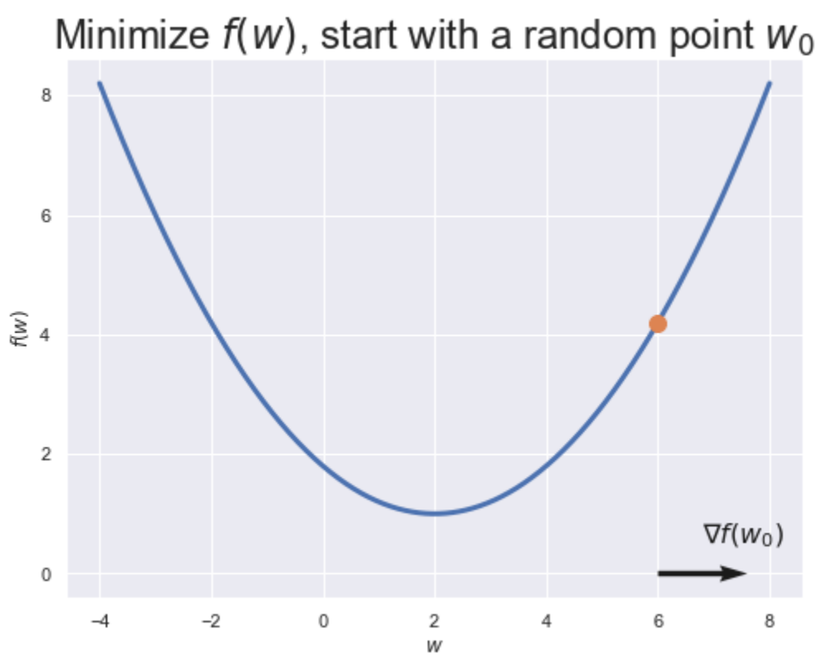
Review, let's start with a simple function:

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

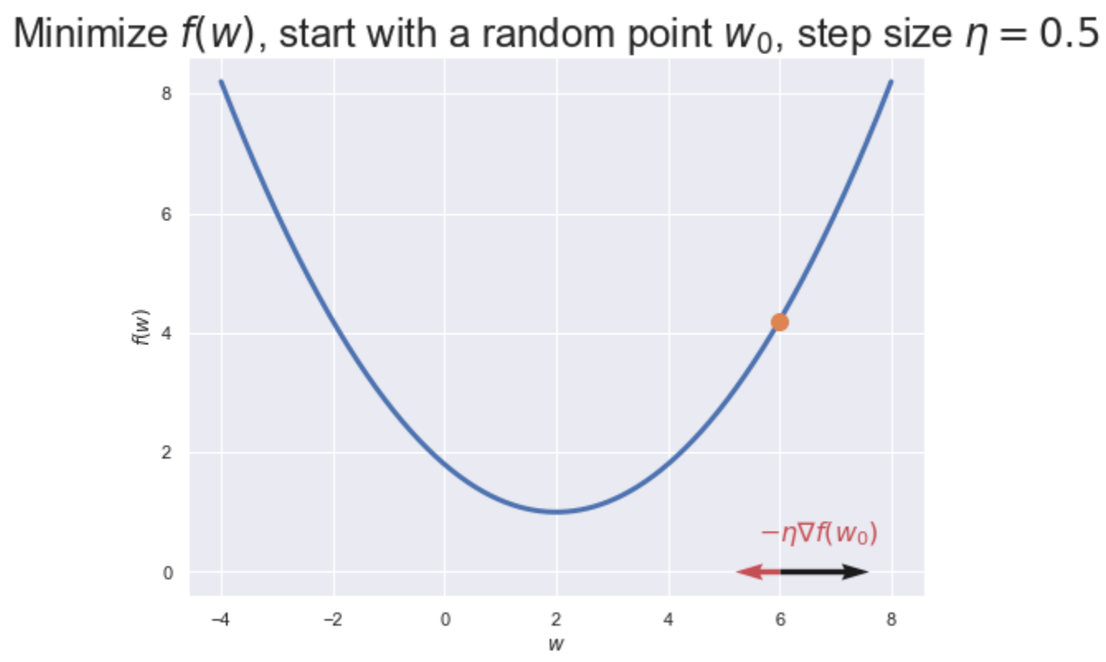
We know that this function is convex (2nd derivative exists and is positive).

In [7]:
```
f = lambda w: 0.2*(w-2)**2+1
dfdw = lambda w: 0.4*w - 0.8
```

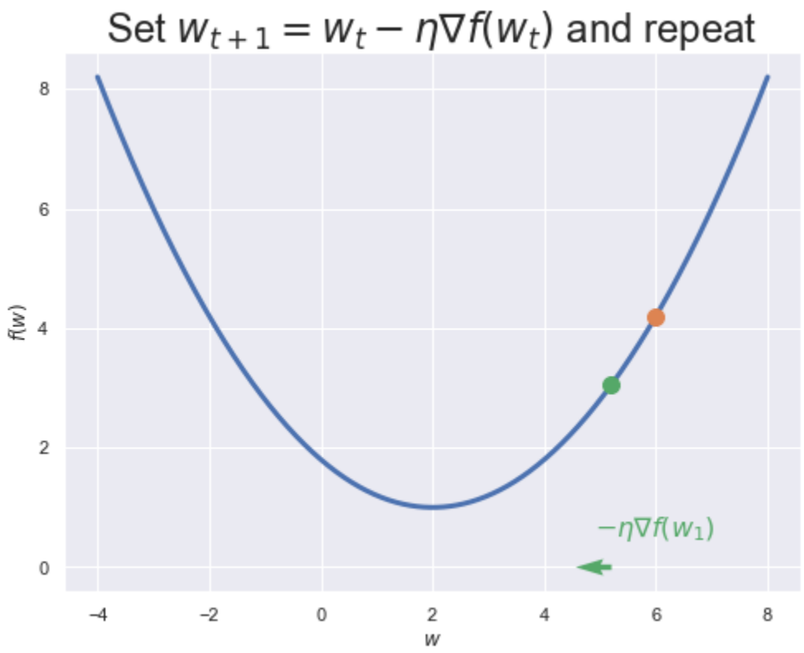
In [22]:
```
plt.figure(figsize=(8,6))
w = np.linspace(-4,8,1000)
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')
plt.title(r'Minimize $f(w)$, start with a random point $w_0$',fontsize = 24);
w_0 = 6
plt.plot(w_0, f(w_0), "o",markersize=10)

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 [28]:
```
plt.figure(figsize=(8,6))
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 = 24);
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')
```

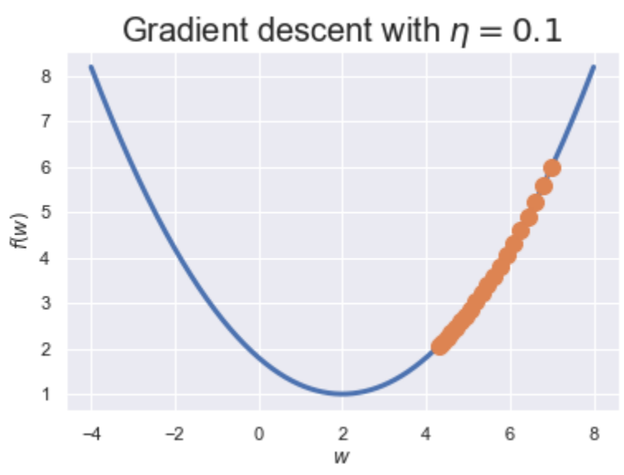


In [23]:
```
plt.figure(figsize=(8,6))
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

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 = 24);

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')
```



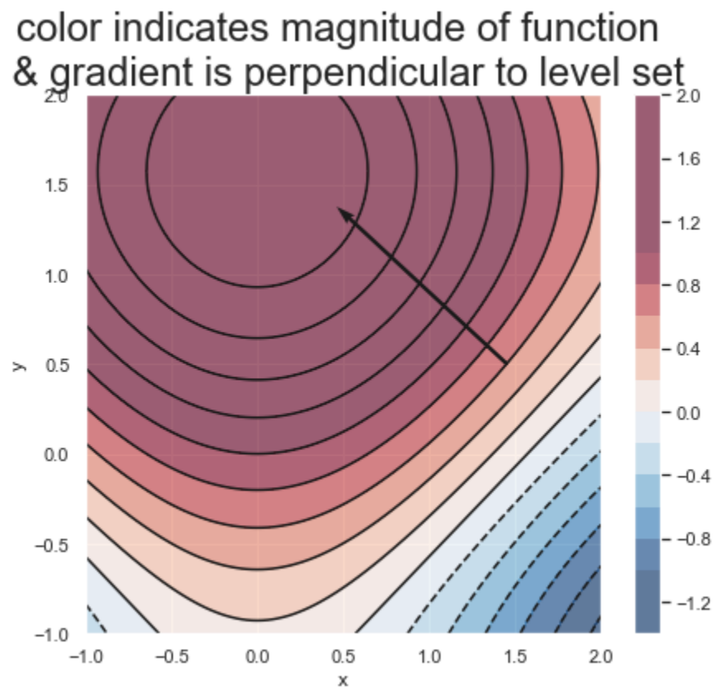
In [108]:
```
plt.plot(w, f(w), linewidth=3 )
plt.xlabel(r'$w$')
plt.ylabel(r'$f(w)$')

# w_1 = w_0 - dfdw(w_0)*eta
w_t = np.zeros(20)
w_t[0] = 7  # w_0

eta = 0.1

for i in range(1,20):
    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[108]:
```
[<matplotlib.lines.Line2D at 0x1373cd2b0>]
```



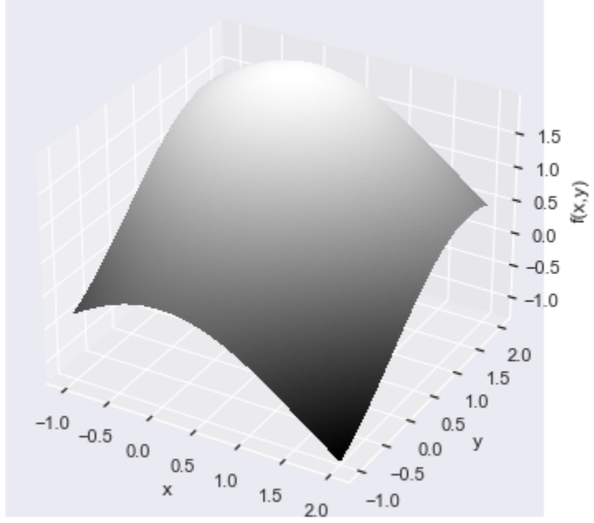
LET'S PLOT A FUNCTION WITH TWO VARIABLES AND LOOK AT THE GRADIENT

In [18]:
```
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=(7,6))
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')
plt.title('color indicates magnitude of function \n & gradient is perpendicular to level set', fontsize=24
)

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



In [29]:
```
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);
```

```
/Users/lwehbe/env/py3/lib/python3.7/site-packages/ipykernel_launcher.py:5: MatplotlibDeprecationWarnin
g: Calling gca() with keyword arguments was deprecated in Matplotlib 3.4. Starting two minor releases l
ater, gca() will take no keyword arguments. The gca() function should only be used to get the current a
xes, or if no axes exist, create new axes with default keyword arguments. To create a new axes with non
-default arguments, use plt.axes() or plt.subplot().
  """
```

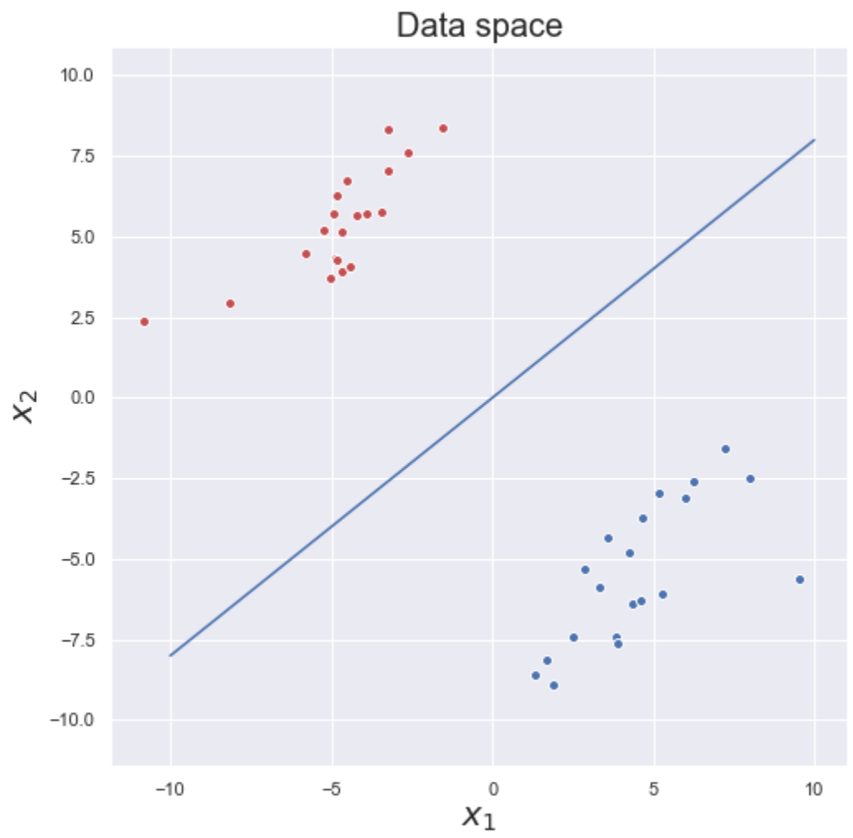


LOGISTIC REGRESSION GRADIENT ASCENT

Simple simulated example

In [30]:
```
# 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 [46]:
```
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]),plt.axis('equal')
plt.xlabel(r'$x_1$',fontsize=20)
plt.ylabel(r'$x_2$',fontsize=20)
plt.title('Data space',fontsize=20);
```



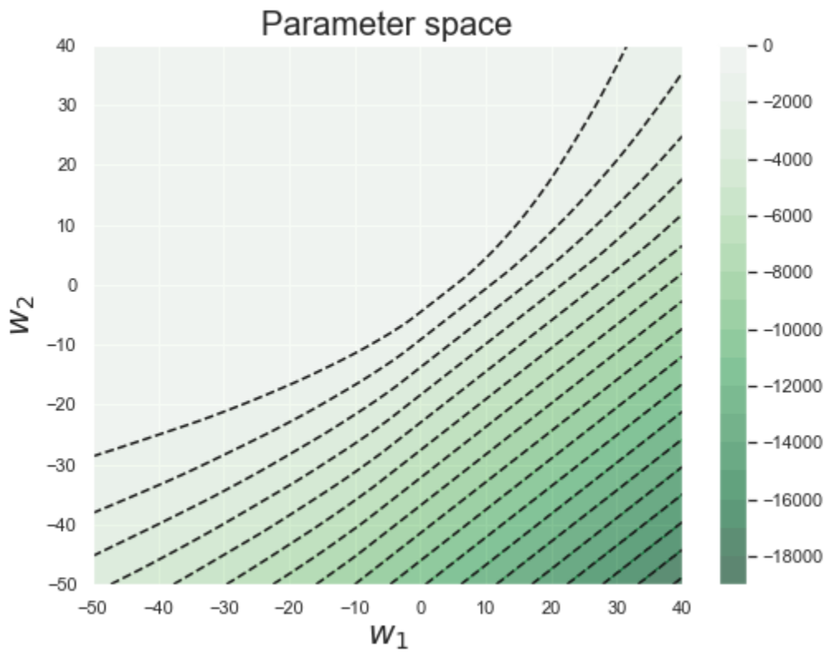
LOG LIKELIHOOD PLOT

$$l(\mathbf{w}) = \sum_i \left[y^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)} \right) - \ln\left(1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)} \right)\right)\right]$$

WE OMIT w_0 IN THE EXAMPLE BELOW FOR SIMPLICITY

In [58]:
```
w1x = np.linspace(-50,40,100)
w2x = np.linspace(-50,40,100)
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 [60]:
```
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

$$l(\mathbf{w}) = \sum_i \left[y^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)} \right) - \ln\left(1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right)\right]$$

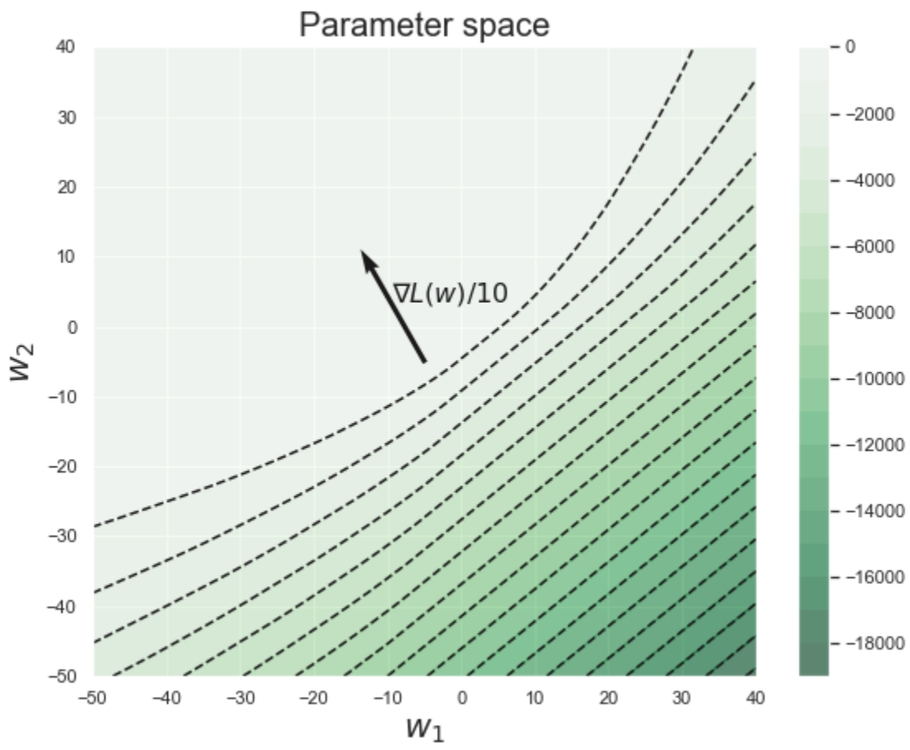
$$\mathbf{w}^\top \mathbf{x}^{(i)} = \sum_{j=1}^{d} w_j x_j^{(i)}$$

$$\frac{\partial l(\mathbf{w})}{\partial w_j} = \sum_i \left[y^{(i)} x_j^{(i)} - x_j^{(i)} \frac{\exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)}{\left(1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right)} \right]$$

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

In [63]:
```
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 [67]:
```
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 $< \epsilon$)

for $j = 0...d$:

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

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

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

GRADIENT DESCENT (ASCENT) IS SIMPLEST OF APPROACHES

COMPARE TO: STOCHASTIC GRADIENT DESCENT

- Typically, the loss / function to minimize is a mean 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:
    - $E\nabla L_i(\mathbf{w}) = \sum_{i=1}^{n} P(i) L_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} L_i(\mathbf{w}) = \nabla L(\mathbf{w})$.
- $\nabla L_i(\mathbf{w})$ 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.

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)
        - $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla L_i(\mathbf{w})$.
- 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)
        - $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla L_B(\mathbf{w})$.
- 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 algorithms on the next slide.

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:

$$w_0 + \sum_{j=1}^{d} w_j x_j^{(i)} = 0$$

What about:

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

or

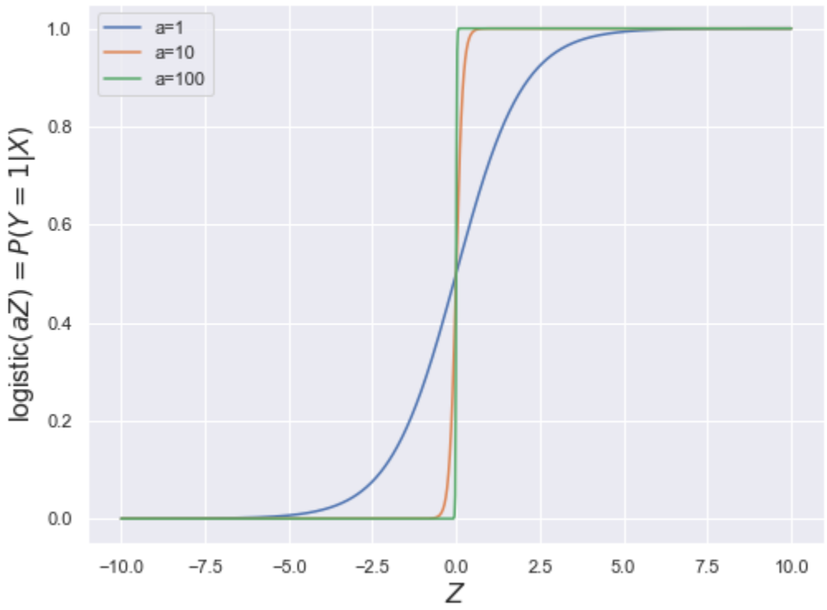
$$10000w_0 + \sum_{j=1}^{d} 10000w_j x_j^{(i)} = 0$$

Same boundary! Which one has higher log likelihood?

$$l(\mathbf{w}) \equiv \ln \prod_i P(Y = y^{(i)} | X = \mathbf{x}^{(i)}, \mathbf{w}) = \sum_i \left[y^{(i)} \left(\mathbf{w}^\top \mathbf{x}^{(i)} \right) - \ln\left(1 + \exp\left(\mathbf{w}^\top \mathbf{x}^{(i)}\right)\right)\right]$$

In [68]:
```
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: RuntimeWarning: overflow enc
ountered in exp
  """
```



NEED TO REGULARIZE THE WEIGHTS

- $\mathbf{w} \rightarrow \infty$ 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:

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

ADDING A PRIOR ON W

Zero Mean Gaussian prior on W:

$$P(W_j = w_j) = \frac{1}{2\pi\sigma^2}\exp\left(-\frac{w_j^2}{2\sigma^2}\right)$$

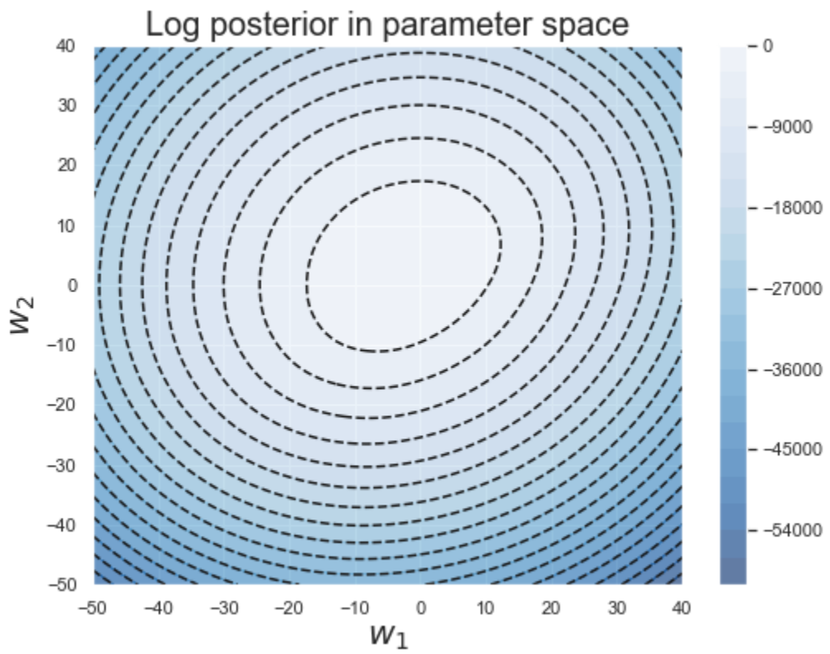
$$\mathbf{w}^{MAP} = \underset{\mathbf{w}}{\operatorname{argmax}} \ln P(Y|W, X) - \frac{\sum_{j=0}^{d} w_j^2}{2\sigma^2}$$

This “pushes” parameters towards zero and corresponds to Regularization

- Helps avoid very large weights and overfitting
- More on this later in the semester

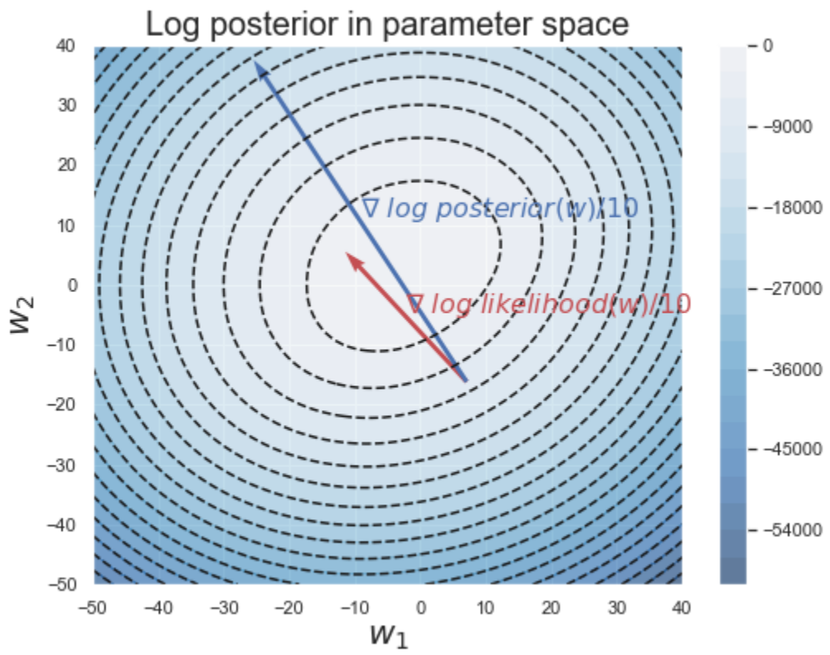
In [69]:
```
lmbda = 10 # this is 1/(2*sigma**2)

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 [77]:
```
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('Log posterior in parameter space',fontsize=20);
```



In [90]:
```
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 [98]:
```
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('Log posterior in 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'$\nabla ~ log~ likelihood(w)/10$','r');
gw1, gw2 = gradient_posterior(w1,w2,X, Y)
draw_vector_2D(plt, w1,w2,gw1/10,gw2/10, r'$\nabla ~ log~ posterior(w)/10$','b');
```



LET'S COMPARE LOGISTIC REGRESSION TO GAUSSIAN NAIVE BAYES

Consider these two assumptions:

- X_1 conditionally independent of X_2 given Y
- $P(X_j|Y = y_k) = \mathcal{N}(\mu_{jk}, \sigma_j)$, not $\mathcal{N}(\mu_{jk}, \sigma_{jk})$
    - i.e. shared standard deviation

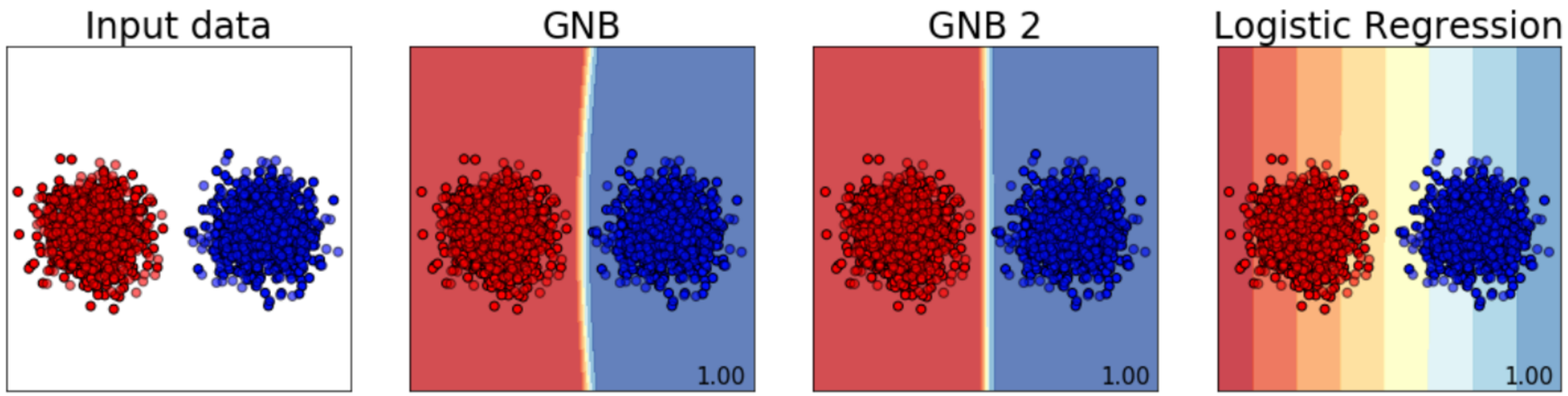
Consider three learning methods:

- 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 $P(X_j|Y = y_k)$.

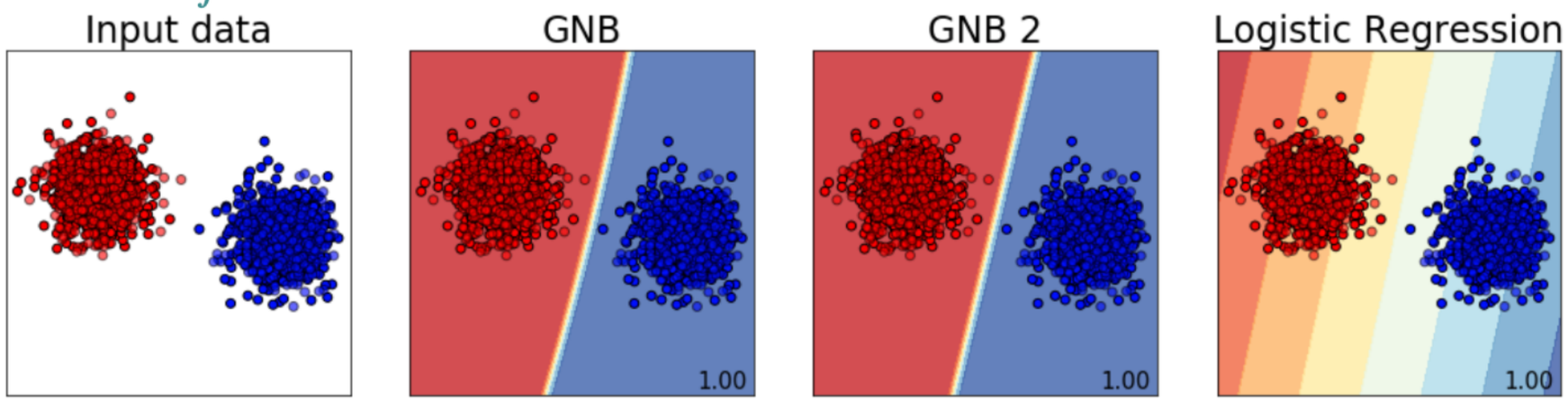
How do these methods perform if we have plenty of data and:

Both (1) and (2) are satisfied.

ASSUMPTION 1 AND 2 ARE SATISFIED



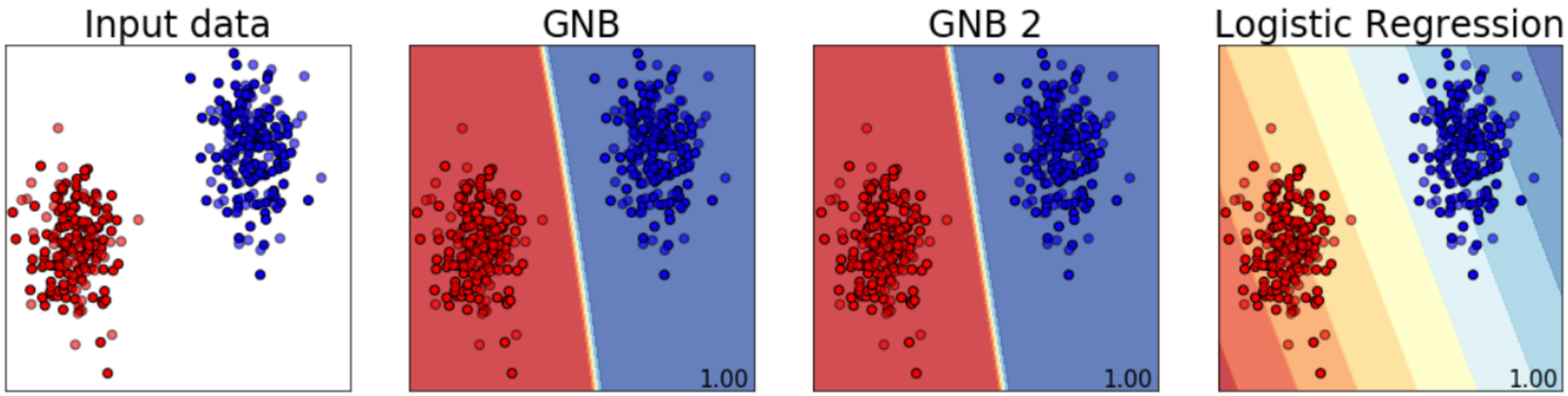
X_j's conditionally independent and variance is shared



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:

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

$$G(X) = -\frac{1}{2} \sum_i \left(x_j^2 (\frac{1}{\sigma_{j1}^2} - \frac{1}{\sigma_{j0}^2}) - 2x_j (\frac{\mu_{j1}}{\sigma_{j1}^2} - \frac{\mu_{j0}}{\sigma_{j0}^2}) + (\frac{\mu_{j1}^2}{\sigma_{j1}^2} - \frac{\mu_{j0}^2}{\sigma_{j0}^2}) \right)$$

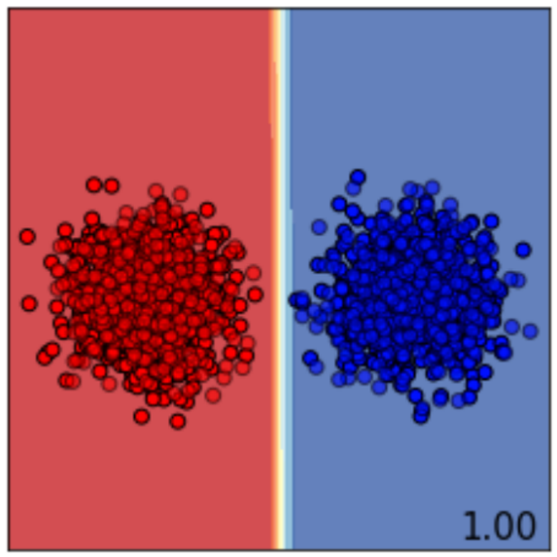
$$G(X) = \sum_j \left(x_j \frac{\mu_{j1} - \mu_{j0}}{\sigma_j^2} \right) - \sum_j \left(\frac{\mu_{j1}^2 - \mu_{j0}^2}{2\sigma_j^2} \right)$$

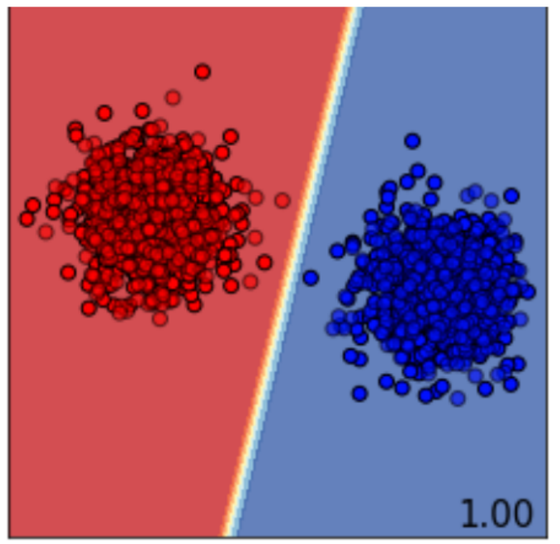
The decision boundary is linear, of the form: $\beta_0 + \sum_j \beta_j x_j = 0$.

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

If the variances of the X_js 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





LET'S COMPARE LOGISTIC REGRESSION TO GAUSSIAN NAIVE BAYES

Consider these two assumptions:

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- $P(X_j|Y = y_k) = \mathcal{N}(\mu_{jk}, \sigma_j)$, not $\mathcal{N}(\mu_{jk}, \sigma_{jk})$
    - i.e. shared standard deviation

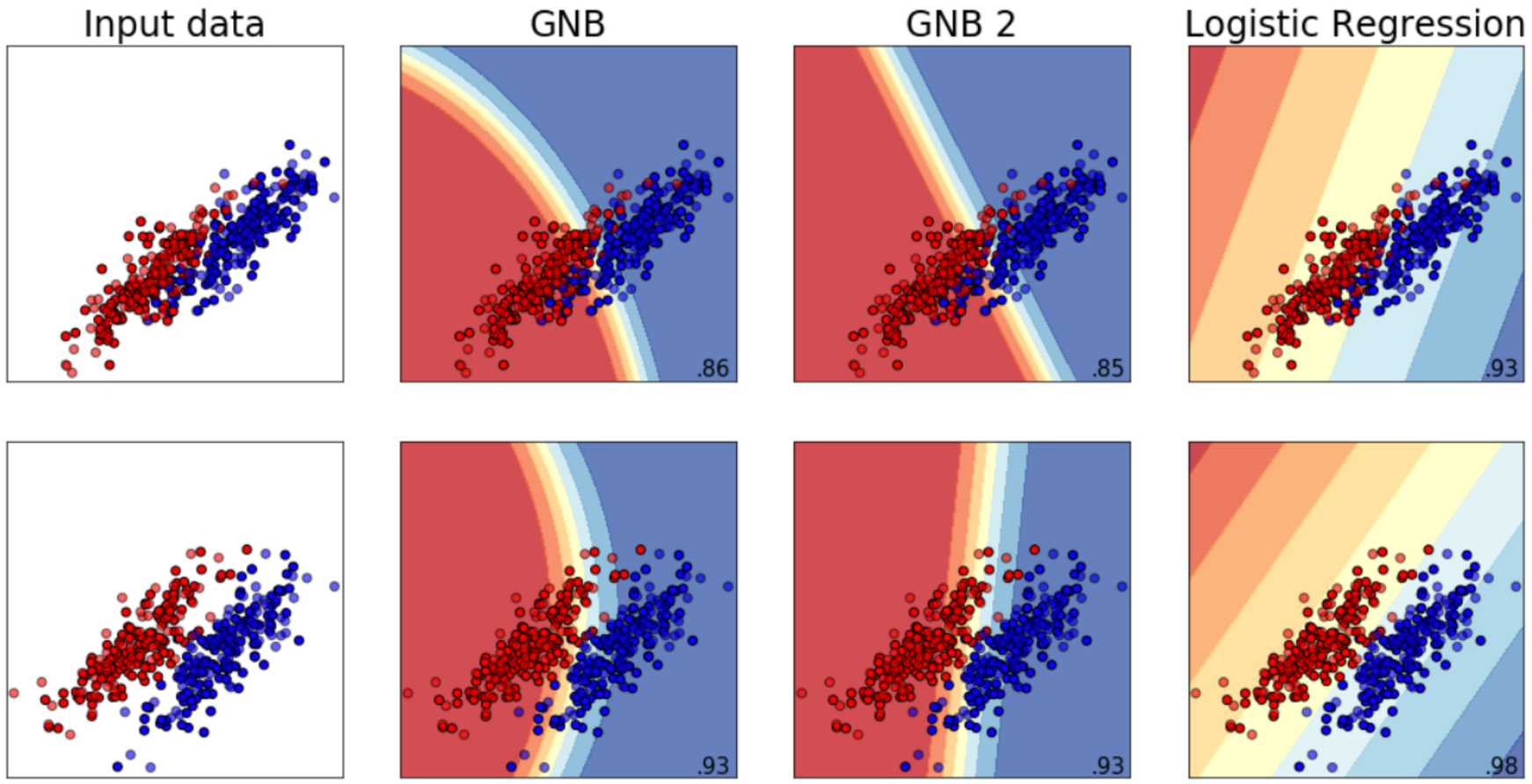
Consider three learning methods:

- 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 $P(X_j|Y = y_k)$.

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

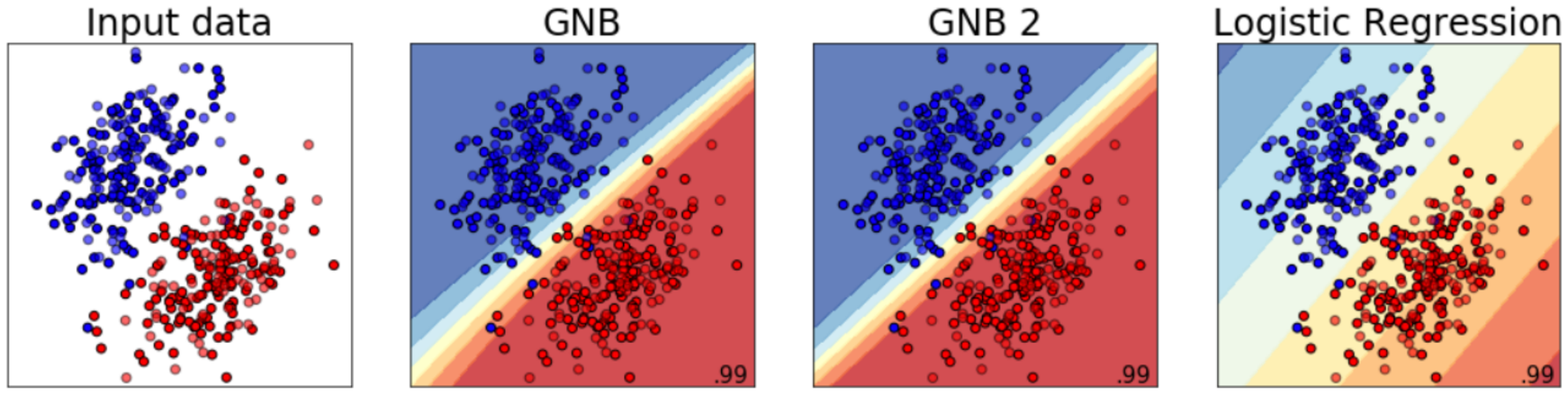
(2) is satisfied, but not (1).

ASSUMPTION 2 SATISFIED AND NOT 1



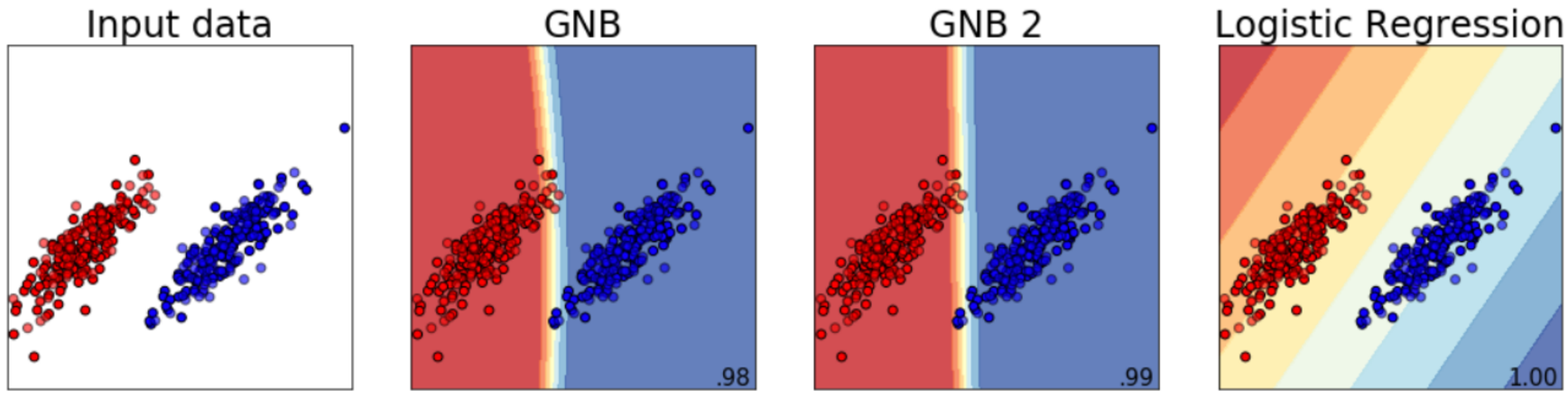
GNB2 can break (also GNB) in these examples

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: $\beta_0 + \sum_j \beta_j x_j = 0$.

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

$$\beta_j = \frac{\mu_{j1} - \mu_{j0}}{\sigma_j^2}$$

GNB 2 is therefore less flexible than LR.

LET'S COMPARE LOGISTIC REGRESSION TO GAUSSIAN NAIVE BAYES

Consider these two assumptions:

- X_1 conditionally independent of X_2 given Y
- $P(X_j|Y = y_k) = \mathcal{N}(\mu_{jk}, \sigma_j)$, not $\mathcal{N}(\mu_{jk}, \sigma_{jk})$
    - i.e. shared standard deviation

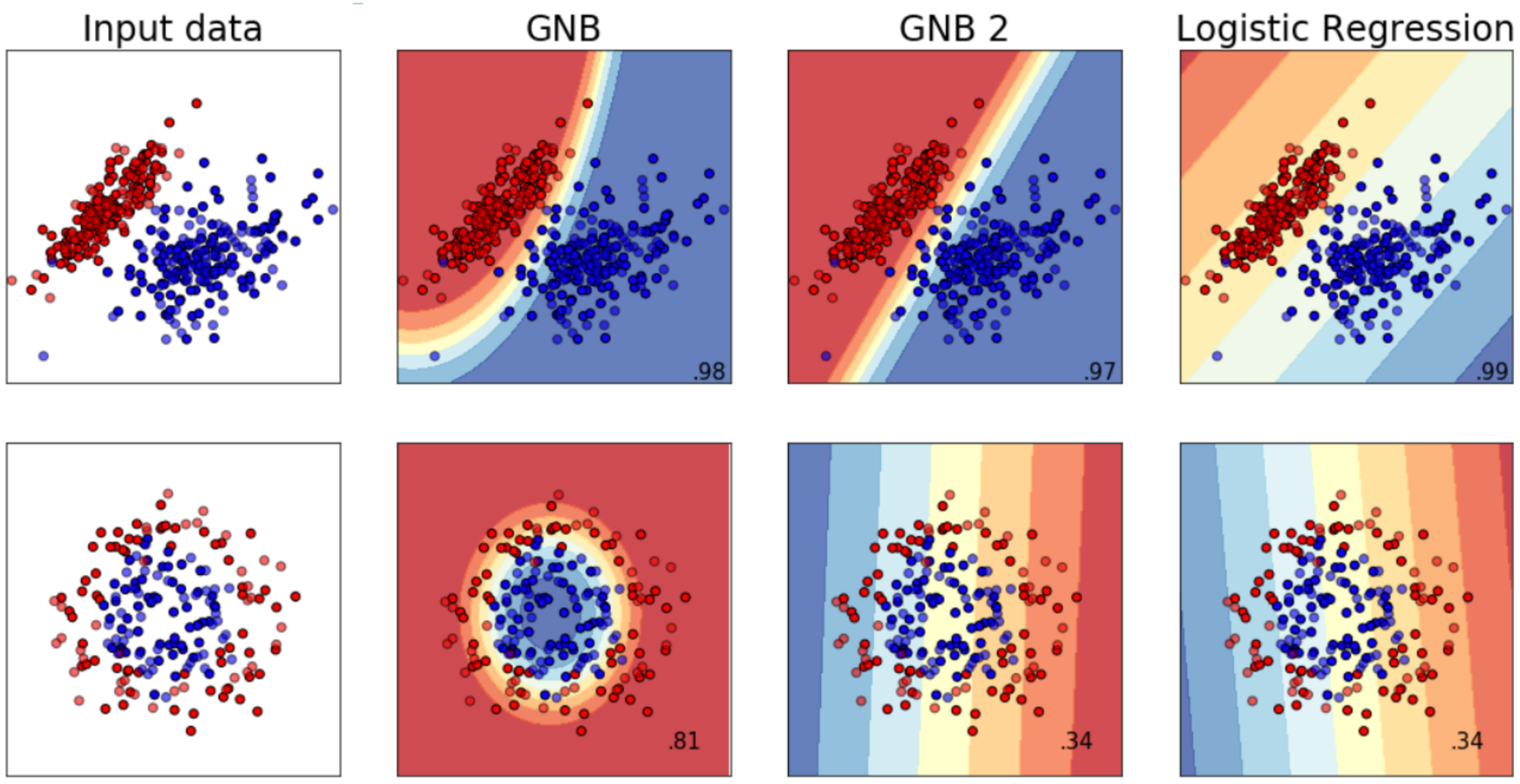
Consider three learning methods:

- 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 $P(X_j|Y = y_k)$.

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

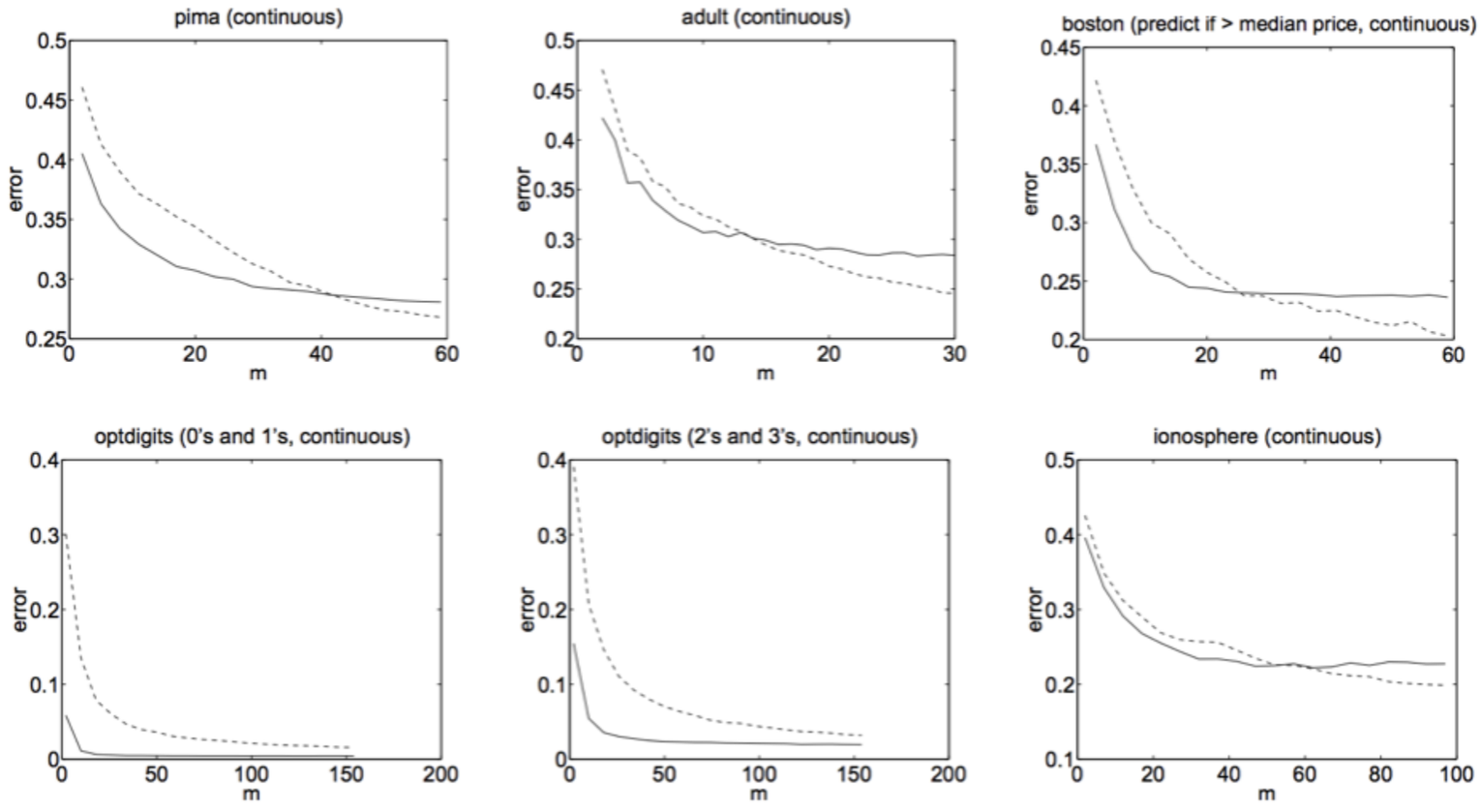
NAÏVE BAYES VS. LOGISTIC REGRESSION

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 ⇒ global optimum with gradient ascent
    - Maximum conditional a posteriori corresponds to regularization