$\LaTeX$ command declarations here.

In [1]:
```
# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
if "bmh" in plt.style.available: plt.style.use("bmh");

# scientific
import numpy as np;

from scipy import linalg
import matplotlib as mpl
from matplotlib import colors

from sklearn.discriminant_analysis import LinearDiscriminantAnalysi
s
from sklearn.discriminant_analysis import QuadraticDiscriminantAnal
ysis

# rise config
from notebook.services.config import ConfigManager
cm = ConfigManager()
cm.update('livereveal', {
              'theme': 'simple',
              'start_slideshow_at': 'selected',
})
```

Out[1]:
```
{u'start_slideshow_at': 'selected', u'theme': 'simple', u'transiti
on': u'none'}
```

EECS 545: Machine Learning

Lecture 06: Probability Models and Logistic Regression

- Instructor: **Jacob Abernethy**
- Date: January 27, 2016

Lecture Exposition Credit: Benjamin Bray, Saket Dewangan

HW2 + Kaggle

- Check out http://kaggle.com (http://kaggle.com), an online platform for machine learning competitive challenges
- Homework 2 requires not one but two submissions to "in-class" Kaggle challenges
- There will be a performance requirement (i.e. need your_score > score_benchmark)
- Winners will get bragging rights and a prize in lecture

Small Aside: check out the Michigan Data Science Team

- http://mdst.eecs.umich.edu (http://mdst.eecs.umich.edu)
- Like doing Kaggle competitions for fun? We give prizes!
- We got a little mention in this morning's University Record (http://record.umich.edu/articles/program-gives-undergraduates-use-high-performance-computing)

New Location for Lecture Content on Github

- EECS 545 Lectures now Open Source!
- Henceforth, lectures will be hosted at https://github.com/thejakeyboy/umich-eecs545-lectures (https://github.com/thejakeyboy/umich-eecs545-lectures)
- Will soon be using Github, not Canvas, for lecture notes
- We have an impressive lecture development team:
  - Ben Bray
  - Saket Dewangan
  - Valli Chockalingam
  - me

Extra Credit Opportunity #1: Lecture development

- Imagine that you:
    1. Discover some bugs in the slides
    2. Find a way to make a better visualization
    3. Have some nice content that you want to contribute as additional material, etc.
- If so: clone the repository, make a contribution, and submit it as a *pull request*!
- Contributions that we deem are great receive 0-2pts extra credit on the final exam (up to a total of 10pts)

Extra Credit Opportunity #2: HW Solutions

- Starting now, **you** can help us develop the HW solutions. **IF**
    - you write up your HW in $\LaTeX$ AND
    - your solutions are really simple and beautiful AND
    - you submit your homework early (by Friday, 3 days before due date)
- Then we may contact you to contribute your .tex file
- GSIs will compile the solutions, and for each contributed answer we'll give you roughly 1pt on your final exam (up to 10pts)

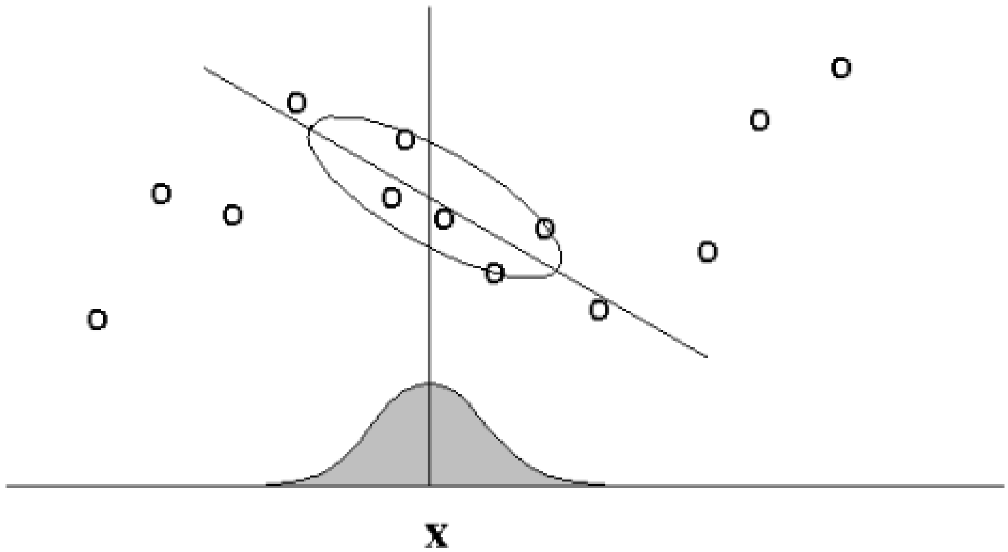
Outline

- Locally-Weighted Linear Regression
- Probabilistic Models
    - Generative Models
    - Discriminative Models
- Logistic Regression
    - Intuition, Motivation
    - Newton's Method

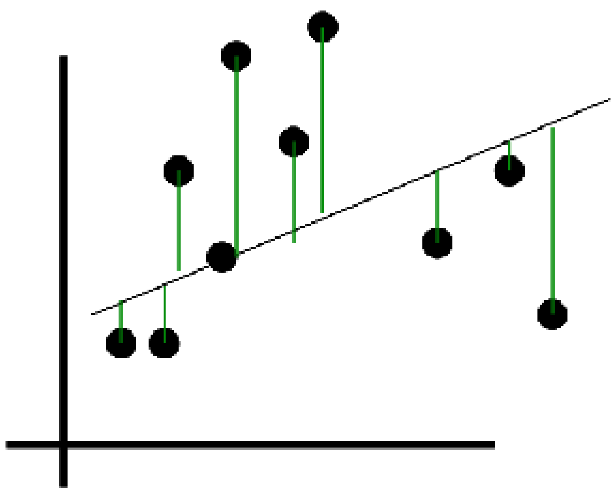
Locally-Weighted Linear Regression

Locally-Weighted Linear Regression

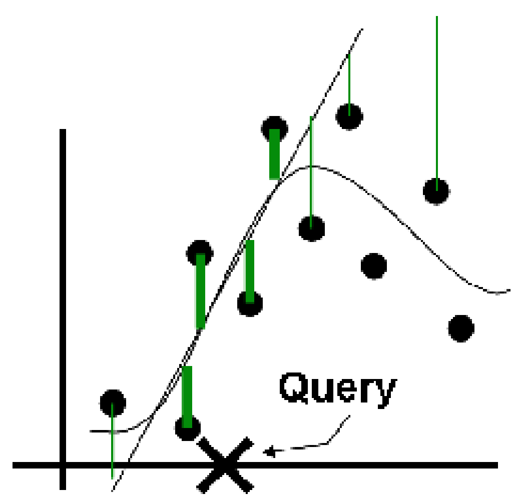
Main Idea: When predicting $f(x)$, give high weights for *neighbors* of x.



Regular vs. Locally-Weighted Linear Regression



Regular linear regression



Locally weighted linear regression

Regular vs. Locally-Weighted Linear Regression

Linear Regression

1. Fit w to minimize $\sum_k (t_k - w^T \phi(x_k))^2$
2. Output $w^T \phi(x_k)$

Locally-weighted Linear Regression

1. Fit w to minimize $\sum_k r_k(t_k - w^T \phi(x_k))^2$ for some weights r_k
2. Output $w^T \phi(x_k)$

Locally-Weighted Linear Regression

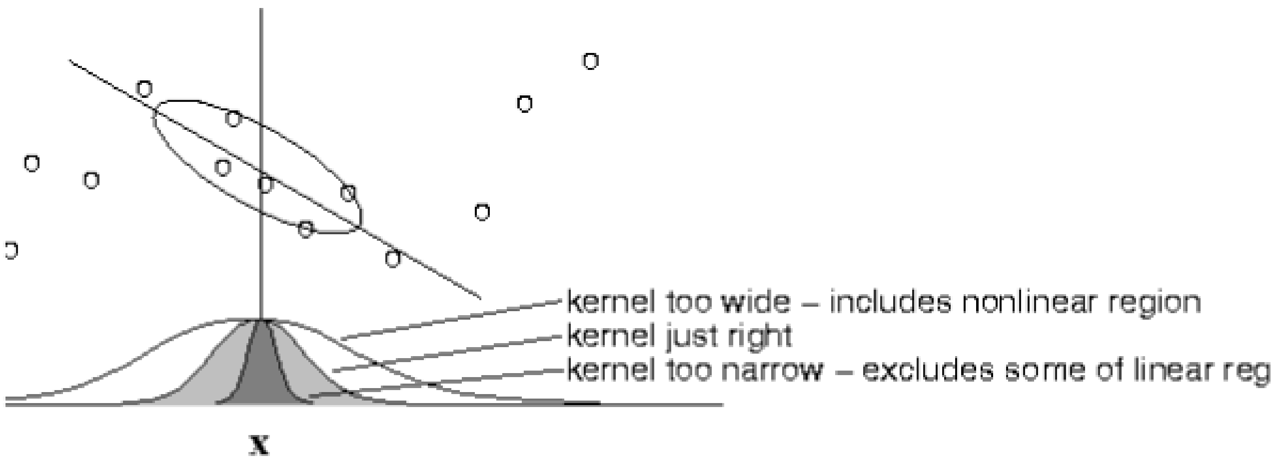
- The standard choice for weights r uses the **Gaussian Kernel**, with **kernel width** τ

$$r_k = \exp\left(-\frac{||x_k - x||^2}{2\tau^2}\right)$$

- Note r_k depends on both x (query point); must solve linear regression for each query point x.
- Can be reformulated as a modified version of least squares problem.

Locally-Weighted Linear Regression

- Choice of kernel width matters.
  - (requires hyperparameter tuning!)



> The estimator is minimized when kernel includes as many training points as can be accomodated by the model. Too large a kernel includes points that degrade the fit; too small a kernel neglects points that increase confidence in the fit.

Let's back up a little...

Probabilistic Models & Bayesian Statistics

> *Disclaimer:* These slides were written by a Bayesian :)

Probabilistic Models & Bayesian Statistics

Last time, there were several questions about **priors**.

- Represent prior beliefs about acceptable values for model parameters.
- *Example:* In linear regression, L_2 regularization can be interpreted as placing a **Gaussian Prior** on the regression coefficients.

Probabilistic Models & Bayesian Statistics

All statistical models and machine learning algorithms make assumptions.

- All reasoning is based on implicit assumptions.
- A **Bayesian** will tell you that his prior is a way of explicitly stating those assumptions.

Probabilistic Models & Bayesian Statistics

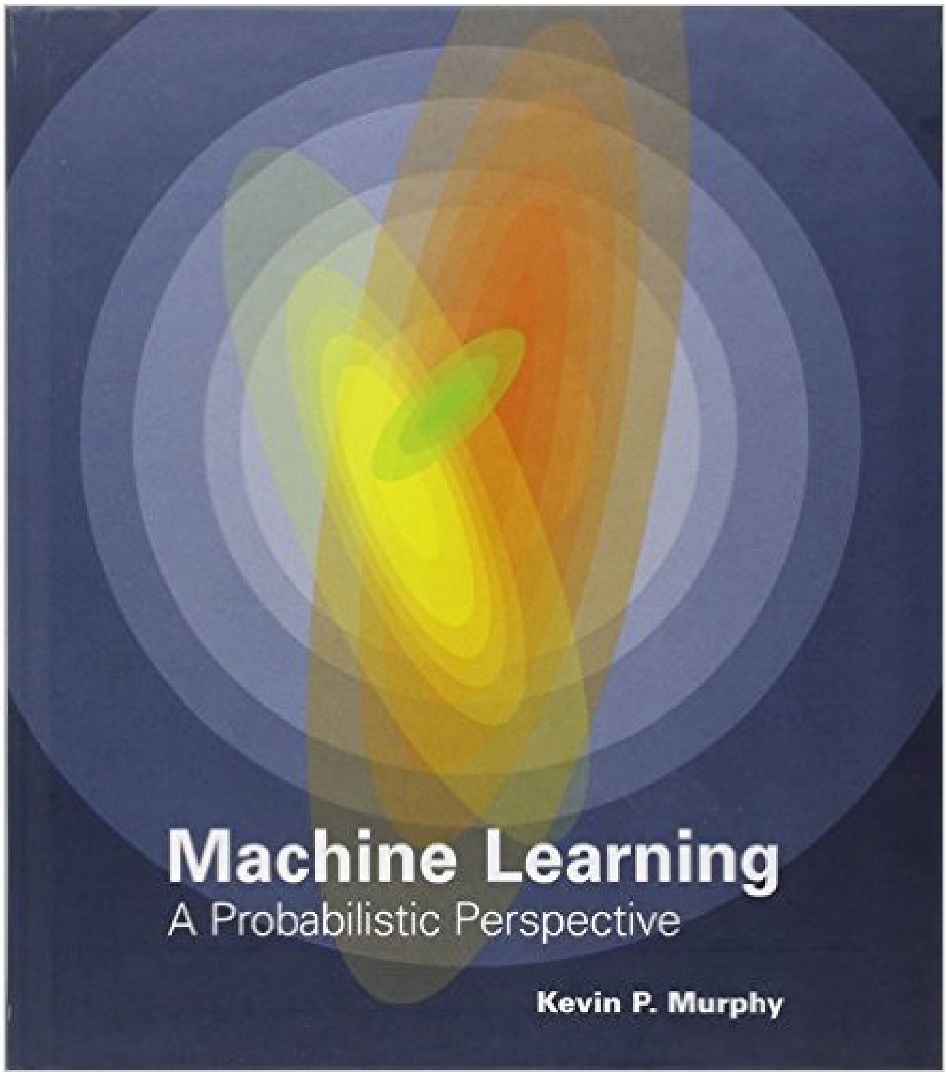
This can all get very philosophical, but...

- Bayesian reasoning is best seen as a useful tool.
- Many concepts in machine learning have Bayesian interpretations.
  - Choice of loss / error function, regularization, etc.

We'll mention these things as they come up.

Probabilistic Models & Bayesian Statistics

For a fully Bayesian take on machine learning, check out the **Murphy** textbook:



Review: Classification

- **Goal:** Assign each feature vector x to one of K distinct classes C_k, where $k = 1, \dots, K$.
  - Data X
  - Labels Y
- The case $K = 2$ is **Binary Classification**
  - $t = 1$ means $x \in C_1$
  - $t = 0$ means $x \in C_2$ (or sometimes $t = -1$
- For the case $K > 2$, use **one-hot encoding**,
$$t = (0, 1, 0, \dots, 0, 0)^T \implies x \in C_2$$

Generative Models

A **generative model** learns a joint model $P(Y, X) = P(X \mid Y)P(Y)$.

- Perform inference using the **posterior**, via Bayes' Rule:
$$P(Y \mid X) = \frac{P(X \mid Y)P(Y)}{P(X)}$$
- Specifies how to generate observed features X if labels Y are known
- By comparing the synthetic data and real data, we get a sense of how good the generative model is.

Generative Models: Examples

Simple examples:

- Naive Bayes (Later)
- Gaussian Discriminant Analysis (Later)

More abstract examples:

- Linear Regression
- Most Bayesian models

Discriminative Models

Conversely, a **discriminative model** fits $P(Y \mid X)$ directly from data.

- Goal: select a hypothesis to *discriminates* between class labels
- Does not (necessarily) provide the ability to *generate* new random examples
- allows us to focus purely on the classification task

We will discuss the pros and cons of each method later.

Discriminative Models

The discriminative approach will typically

- have fewer parameters to estimate
- make fewer assumptions about data distribution
    - Linear (logistic regression) vs quadratic (GDA) in the input dimension
- make fewer generative assumptions about the data
    - However, reconstruction features from labels may require prior knowledge

Break Time!

> Thanks to Bryan for the GIF!

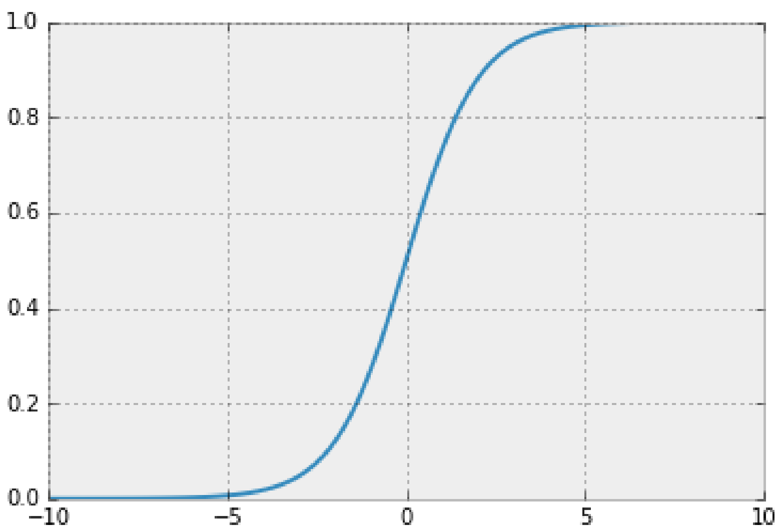
Logistic Regression

Sigmoid and Logit Functions

The **logistic sigmoid function** is

$$\sigma(a) = \frac{1}{1 + \exp(-a)} = \frac{\exp(a)}{1 + \exp(a)}$$

In [2]:
```
def sigmoid(a):
    return 1 / (1 + np.exp(-a));

xvals = np.linspace(-10,10,100);
plt.plot(xvals, sigmoid(xvals));
```

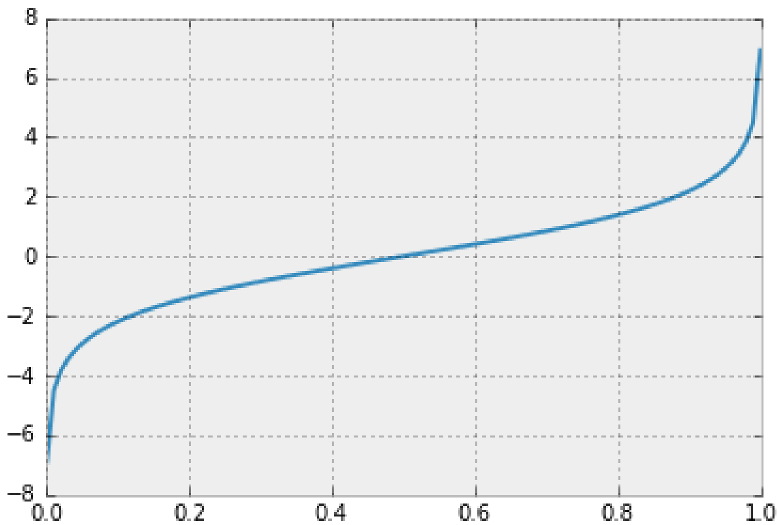


Sigmoid and Logit Functions

Its inverse is the **logit function** or the log-odds ratio,

$$a = \ln\left(\frac{\sigma}{1 - \sigma}\right)$$

In [3]:
```
def logit(sigma):
    return np.log(sigma / (1-sigma));

xvals = np.linspace(0.001, 0.999, 100);
plt.plot(xvals, logit(xvals));
```



Sigmoid and Logit Functions

The sigmoid function generalizes to the **normalized exponential** or **softmax** function

Given any real numbers $q_1, \ldots, q_n$, we can generate a distribution on n objects using:

$$p_k = \frac{\exp(q_k)}{\sum_j \exp(q_j)}$$

Logistic Regression

- Simpest discriminative model that is **linear** in the parameters.
- Models the **class posterior** using a sigmoid applied to a linear function of the feature vector:

$$y \sim \text{Bernoulli}[\sigma(w^T \phi(x))]$$
$$P(y|\phi(x)) = y(\phi(x)) = \sigma(w^T \phi(x))$$

- We can solve the paramter w by maximizing the likelihood of the training data.

Logistic Regression: Why Sigmoid?

- For two classes, **Bayes' theorem** says:

$$p(C_1|x) = \frac{p(x|C_1) \cdot p(C_1)}{p(x|C_1) \cdot p(C_1) + p(x|C_2) \cdot p(C_2)}$$

- The **log odds** is defined to be:

$$a = \ln \frac{p(C_1|x)}{p(C_2|x)} = \ln \frac{p(x|C_1) \cdot p(C_1)}{p(x|C_2) \cdot p(C_2)}$$

- In terms of the log odds, the posterior is defined as:

$$p(C_1|x) = \frac{1}{1 + \exp(-a)} = \sigma(a)$$

Logistic Regression: Intuition

- Given data x and learned weights w, pick the label with the largest **posterior probability**

$$P(t = 1|x, w) = \sigma(w^T \phi(x))$$
$$P(t = 0|x, w) = 1 - \sigma(w^T \phi(x))$$

- This is equivalent to setting a threshold at $p = 0.5$.
    - Classify x as positive $(y = 1)$ if $\sigma(w^T \phi(x)) > 0.5$
    - This creates a **linear decision boundary** in the feature space! (for $\phi(x) \in \mathbb{R}^d$)

Logistic Regression: Intuition

- Classify x as positive if $\sigma(w^T \phi(x)) > 0.5$.

$$\sigma(w^T \phi(x)) = \frac{\exp(w^T \phi(x))}{1 + \exp(w^T \phi(x))} > 0.5$$
$$\implies \boxed{w^T \phi(x) > 0}$$

- This is the equation for a half-plane in $\mathbb{R}^d$, with **normal vector** w!

Logistic Regression: Linear Decision

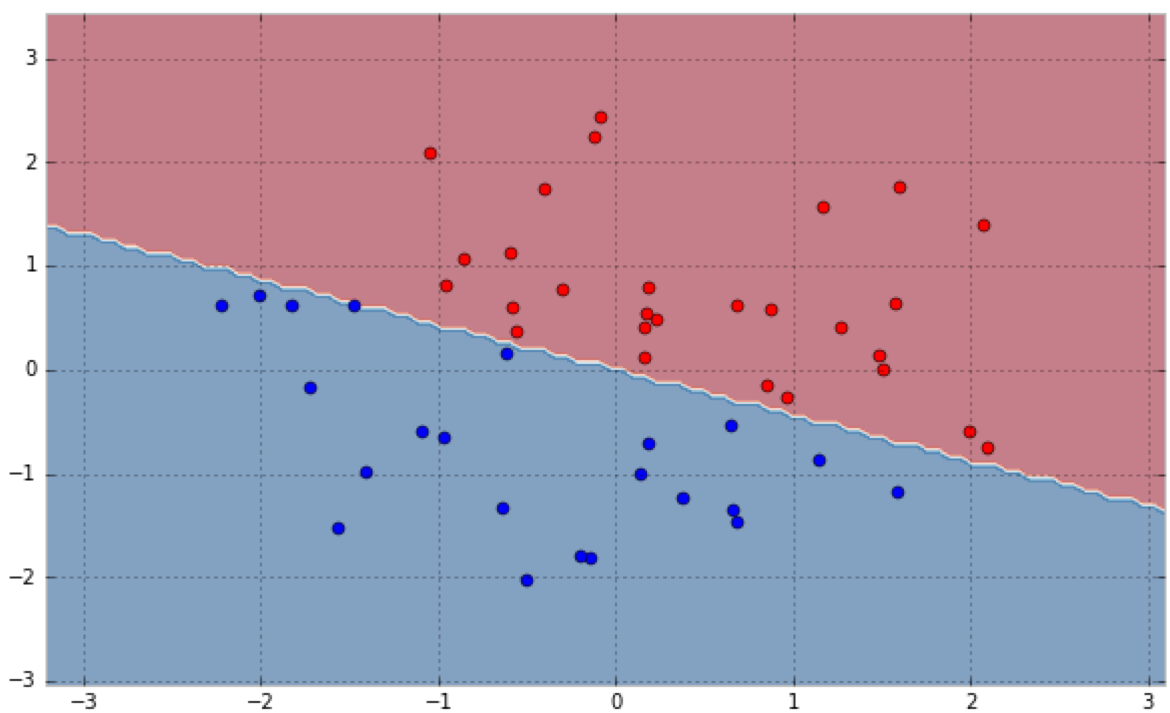
In [4]:

```python
# source code for plot on NEXT SLIDE!
def plot_linear_boundary():
    # random data + normal
    x = np.random.randn(2,50);
    w = np.random.randn(2);
    # classify based on w
    labels = np.dot(w.T, x) > 0;
    blue, red = x[:,labels==0], x[:,labels==1];

    # grid over plot window
    xx = np.linspace( min(x[0])-1, max(x[0])+1, 100);
    yy = np.linspace( min(x[1])-1, max(x[1])+1, 100);
    X,Y = np.meshgrid(xx, yy);

    # compute w.T*x for each point on grid
    Z = np.array([X.ravel(), Y.ravel()]);
    Z = np.dot(w.T, Z).reshape(X.shape) < 0;

    plt.contourf(X, Y, Z, cmap="RdBu", alpha=0.5);
    plt.plot(blue[0], blue[1], 'ob', red[0], red[1], 'or');
```

Logistic Regression: Linear Decision

In [5]:

```python
plt.figure(figsize=(10,6))
plot_linear_boundary();
```



Logistic Regression: Likelihood

- We saw before that the **likelihood** for each binary label is:

$$P(t=1|x,w)=\sigma(w^T\phi(x))$$
$$P(t=0|x,w)=1-\sigma(w^T\phi(x))$$

- With a clever trick, this

$$P(t|x,w)=\sigma(w^T\phi(x))^t\cdot(1-\sigma(w^T\phi(x)))^{1-t}$$

Logistic Regression

- For a data set $\{(\phi(x_n),t_n)\}$ where $t_n\in\{0,1\}$, the **likelihood function** is

$$P(t|w)=\prod_{n=1}^{N}y_n^{t_n}(1-y_n)^{1-t_n}$$

  - where $y_n=P(C_1|\phi(x_n))=\sigma(w^T\phi(x_n))$
- Minimize the **loss** or **negative log-likelihood**, $E(w)=-\ln P(t|w)$
  - maximizes the likelihood

Derivation: $\nabla_w \ln P(t|w)$

$$=\sum_{n=1}\nabla_w\left[t_n\ln\sigma(w^T\phi(x_n))+(1-t_n)\ln(1-\sigma(w^T\phi(x_n))\right]$$

$$=\sum_{n=1}^{N}\left(t_n\frac{y_n(1-y_n)}{y_n}-(1-t_n)\frac{y_n(1-y_n)}{1-y_n}\right)\nabla_w\left[w^T\phi(x_n)\right]$$

$$=\sum_{n=1}^{N}(t_n(1-y_n)-(1-t_n)y_n)\nabla_w\left[w^T\phi(x_n)\right]$$

$$=\sum_{n=1}^{N}(t_n-y_n)\phi(x_n)=\sum_{n=1}^{N}\left[t_n-\sigma(w^T\phi(x_n))\right]\phi(x_n)$$

Logistic Regression: Gradient Descent

We have just shown that the gradient of the loss is

$$\nabla_w E(w) = \sum_{n=1}^{N} (y_n - t_n)\phi(x_n)$$

$$y_n = P(C_1|\phi(x_n)) = \sigma(w^T\phi(x_n))$$

- This resembles the gradient expression from linear regression with least squares!

$$\begin{array}{rl} \text{Logistic} & y_n - t_n = \sigma(w^T\phi(x_n)) - t_n \\ \text{Linear} & y_n - t_n = w^T\phi(x_n) - t_n \end{array}$$

Newton's Method: Overview

- **Goal:** Minimize a general function $F(w)$ in one dimension by solving for

$$f(w) = \frac{\partial F}{\partial w} = 0$$

- **Newton's Method:** To find roots of f, Repeat until convergence:

$$w \leftarrow w - \frac{f(w)}{f'(w)}$$

Newton's Method: Geometric Intuition

- Find the roots of $f(w)$ by following its **tangent lines**. The tangent line to f at w_{k-1} has equation

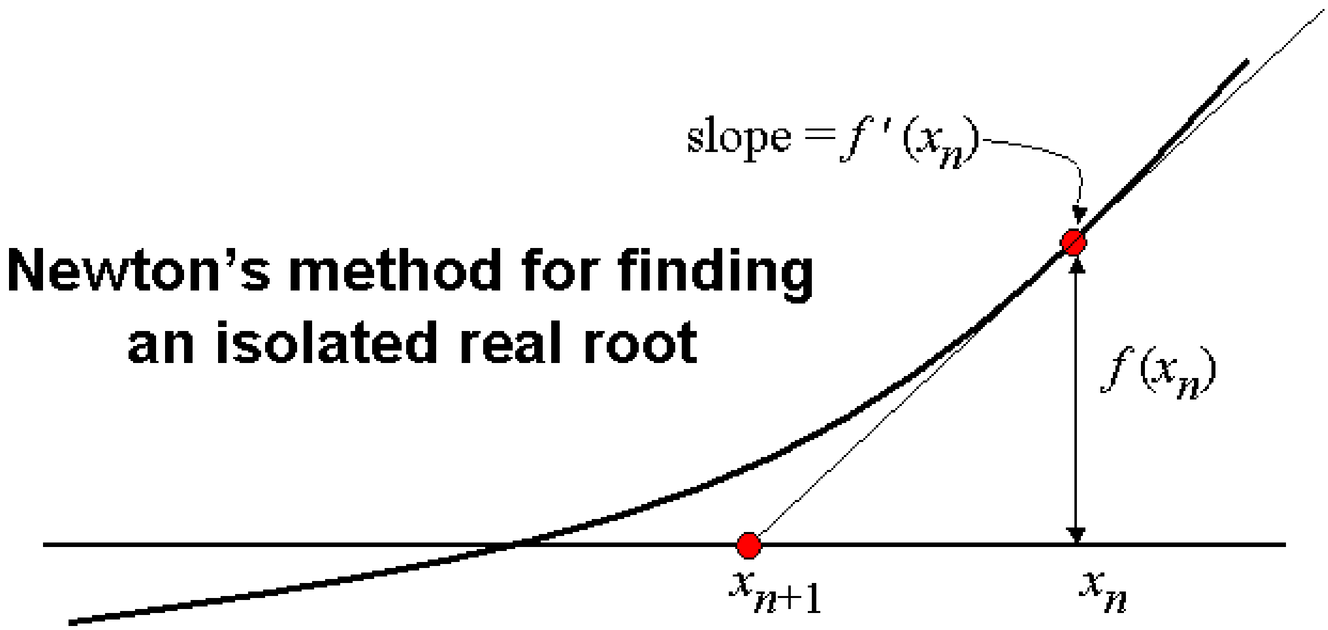
$$\ell(w) = f(w_{k-1}) + (w - w_{k-1})f'(w_{k-1})$$

- Set next iterate w_{k+1} to be **root** of tangent line:

$$f(w_{k-1}) + (w - w_{k-1})f'(w_{k-1}) = 0$$

$$\implies \boxed{w = w_{k-1} - \frac{f(w_{k-1})}{f'(w_{k-1})}}$$

Newton's Method: Geometric Intuition

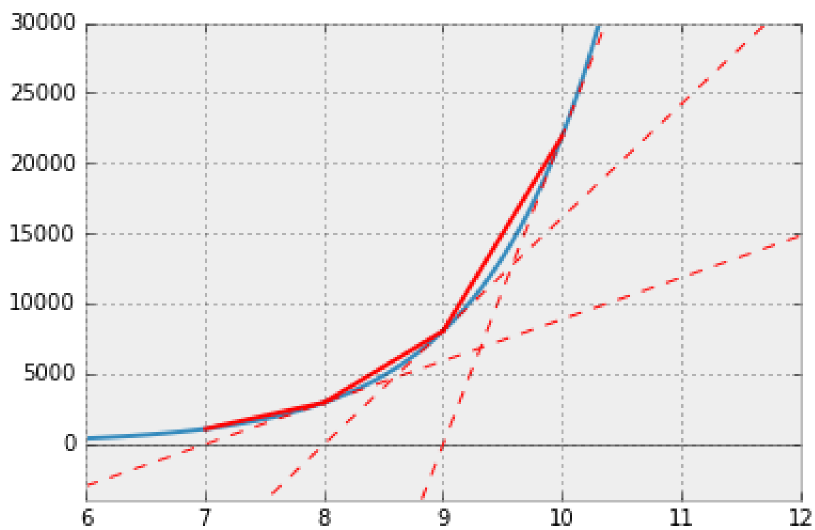


$$x_{n+1} = x_n - \frac{f'(x_n)}{f(x_n)}$$

In [6]:

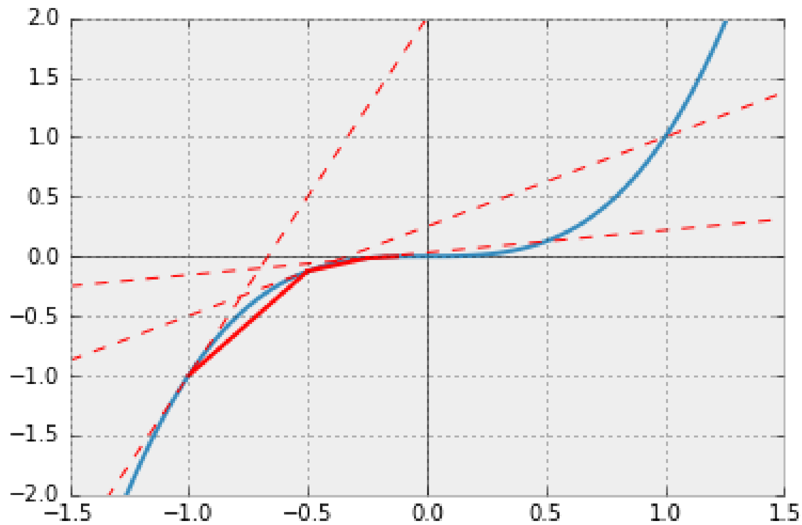
```
# custom newton's method -- see Canvas
from newton_plot import *;

def fn(x): return np.exp(x) - x**2;
def d1(x): return np.exp(x) - 2*x;
def d2(x): return np.exp(x) - 2;

lst = [];
print("Newton's Method:", newton_exact(d1, d2, 10, lst=lst, max
n=4));
plot_optimization(plt.gca(), fn, d1, lst, xlim=(6,12), ylim=(-4000,
30000), tangents=True);
```

```
Newton's Method did not converge.
("Newton's Method:", 6.018373602193873)
```



In [7]:
```
# custom newton's method -- see Canvas
from newton_plot import *;

def fn(x): return x**3;
def d1(x): return 3 * x**2;
def d2(x): return 6 * x;

lst = [];
print("Newton's Method:", newton_exact(d1, d2, -1, lst=lst, max
n=4));
plot_optimization(plt.gca(), fn, d1, lst, xlim=(-1.5,1.5), ylim=
(-2,2), tangents=True);
```

```
Newton's Method did not converge.
("Newton's Method:", -0.0625)
```



Newton's Method: Recap

To minimize $F(w)$, find roots of $F'(w)$ via Newton's Method.

Repeat until convergence:

$$\boxed{w \leftarrow w - \frac{F'(w)}{F''(w)}}$$

Newton's Method: Multivariate Case

Replace second derivative with the **Hessian Matrix**,

$$H_{ij}(w) = \frac{\partial^2 F}{\partial w_i \partial w_j}$$

Newton update becomes:

$$\boxed{w \leftarrow w - H^{-1}\nabla_w F}$$

Recall: Linear Regression

- For linear regression, least squares has a **closed-form solution**:
$$w_{ML} = (\Phi^T\Phi)^{-1}\Phi^T t$$
- This generalizes to weighted least squares, with diagonal weight matrix R,
$$w_{WLS} = (\Phi^T R\Phi)^{-1}\Phi^T Rt$$

Logistic Regression: Newton's Method

- For logistic regression, however, $\nabla_w E(w) = 0$ is **nonlinear**, and no closed-form solution exists.

We must iterate!

- Newton's method is a good choice in many cases.

Iterative Solution

- Apply Newton's method to solve $\nabla_w E(w) = 0$
- This involves least squares with weights $R_{nn} = y_n(1 - y_n)$
- Since R depends on w, and vice-versa, we get...

Iteratively-Reweighted Least Squares (IRLS)

Repeat Until Convergence:
1. $w^{(new)} = w_{WLS} = (\Phi^T R \Phi)^{-1} \Phi^T R z$
2. $z = \Phi w^{(old)} - R^{-1}(y - t)$

Merging the two steps, a more computationally efficient version is obtained:
$w^{(new)} = w^{(old)} + (\Phi^T R \Phi)^{-1} \Phi^T (t - y)$