$\LaTeX$ command declarations here.

In [1]:
```
from __future__ import division

# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import matplotlib as mpl;
from mpl_toolkits.mplot3d import Axes3D
if "bmh" in plt.style.available: plt.style.use("bmh");

# scientific
import numpy as np;
import scipy as scp;
import scipy.stats;

# scikit-learn
import sklearn;
from sklearn.kernel_ridge import KernelRidge;

# python
import random;

# warnings
import warnings
warnings.filterwarnings("ignore")
```

```
Vendor:  Continuum Analytics, Inc.
Package: mkl
Message: trial mode expires in 30 days
```

In [2]:
```
# rise config
from notebook.services.config import ConfigManager
cm = ConfigManager()
cm.update('livereveal', {
              'theme': 'simple',
              'start_slideshow_at': 'selected',
              'transition':'fade',
              'scroll': False
})
```

Out[2]:
```
{'scroll': False,
 'start_slideshow_at': 'selected',
 'theme': 'simple',
 'transition': 'fade'}
```

EECS 545: Machine Learning

Lecture 09: Kernel Methods & Support Vector Machines

- Instructor: **Jacob Abernethy**
- Date: February 10, 2015

Lecture Exposition Credit: Ben, Saket, & Valli

References

This lecture draws upon the following resources:

- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://www.springer.com/us/book/9780387310732). 2006.
- **[CS229]** Ng, Andrew. CS 229: Machine Learning (http://cs229.stanford.edu/). Autumn 2015.
    - Lecture Notes 03: Support Vector Machines & Kernels (http://cs229.stanford.edu/notes/cs229-notes3.pdf)
- Eric Kim 2013, Everything You Wanted to Know about the Kernel Trick (http://www.eric-kim.net/eric-kim-net/posts/1/kernel_trick.html)

Outline

- Dual Representations
    - *Review*: Kernel Trick
    - *Example*: Linear Regression
- Kernel Regression
- Support Vector Machines

Dual Representations: Linear Regression

> Following **[PRML]** Chapter 6.1

Review: Kernel Trick

By using different definitions for inner product, we can

- compute inner products in a high dimensional space
- with computational complexity of a low dimensional space

Many algorithms can be expressed completely in terms of kernels $\kappa(x, x')$, rather than other operations on x.

- In this case, you can replace one kernel with another, and get a new algorithm that works over a different domain.

Dual Representations: Kernel Trick

- The dual representation, and its solutions, are entirely written in terms of kernels.
- The elements of the Gram matrix $K = \Phi\Phi^T$
$$K_{ij} = \kappa(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$
- These represent the pairwise similarities among all the observed feature vectors.
  - We may be able to compute the kernels more efficiently than the feature vectors.

Dual Representations: Linear Regression

Recall the **error function** for regularized linear regression,

$$\begin{aligned} J(w) &= \frac{1}{2}\sum_{n=1}^{N}(w^T \phi(x_n) - t_n)^2 + \frac{\lambda}{2} w^T w \\ &= \frac{1}{2} w^T \Phi^T \Phi w - w^T \Phi^T t + \frac{1}{2} t^T t + \frac{\lambda}{2} w^T w \end{aligned}$$

Solution: $w_{ML} = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T t$

- Recall the N x M design matrix that is central to this solution.
- We can approach the solution a different way

Review: The Design Matrix

The **design matrix** is a matrix $\Phi \in \mathbb{R}^{N \times M}$, applying

- the M basis functions (M: number of columns)
- to N data points (N: number of rows)

Each *row* is a feature vector. Our goal is $\boxed{\Phi w \approx t}$.

$$\Phi = \begin{Bmatrix} \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_{M-1}(x_1) \\ \phi_0(x_2) & \phi_1(x_2) & \cdots & \phi_{M-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_N) & \phi_1(x_N) & \ldots & \phi_{M-1}(x_N) \end{Bmatrix}$$

Review: The Gram Matrix

For regression, a key item is the "*covariance*" matrix,

$$\Phi^T \Phi \in \mathbb{R}^{M \times M}$$

(Actual cov. matrix requires mean centering normalizing)

Here, we will use the **Gram matrix** (*pairwise similarity*)

$$K = \Phi \Phi^T \in \mathbb{R}^{N \times N}$$

Note $K_{ij} = \phi(x_i)^T \phi(x_j)$ encapsulates the pairwise similarities of all training points

- Kernel methods use only K , not Φ.

Dual Representations: Linear Regression

We want to min: $J(w) = \frac{1}{2} \sum_{n=1}^{N} (w^T \phi(x_n) - t_n)^2 + \frac{\lambda}{2} w^T w$

Taking $\nabla J(w) = 0$, we obtain:

$$\begin{aligned} w &= -\frac{1}{\lambda} \sum_{n=1}^{N} (w^T \phi(x_n) - t_n) \phi(x_n) \\ &= \sum_{n=1}^{N} a_n \phi(x_n) = \Phi^T a \end{aligned}$$

Notice: w can be written as a linear combination of the $\phi(x_n)$!

Transform $J(w)$ to $J(a)$ by substituting $w = \Phi^T a$

- Where $a_n = -\frac{1}{\lambda}\left\{w^T \phi(x_n) - t_n)\right\}$
- Let $a = (a_1, \ldots, a_N)^T$ be the parameter, instead of w.

Dual Representations: Linear Regression

Dual: Substituting $w = \Phi^T a$,

$$\begin{aligned} J(a) &= \frac{1}{2} w^T \Phi^T \Phi w - w^T \Phi^T t + \frac{1}{2} t^T t + \frac{\lambda}{2} w^T w \\ &= \frac{1}{2}(a^T \Phi)\Phi^T \Phi(\Phi^T a) - (a^T \Phi)\Phi^T t + \frac{1}{2} t^T t + \frac{\lambda}{2}(a^T \Phi)(\Phi^T a) \\ &= \frac{1}{2} a^T K K a - a^T K t + \frac{1}{2} t^T t + \frac{\lambda}{2} a^T K a \end{aligned}$$

Dual Representations: Linear Regression

Dual: Substituting $w = \Phi^T a$,

$$\begin{aligned} J(a) &= \frac{1}{2} w^T \Phi^T \Phi w - w^T \Phi^T t + \frac{1}{2} t^T t + \frac{\lambda}{2} w^T w \\ &= \frac{1}{2} a^T (\Phi\Phi^T)(\Phi\Phi^T) a - a^T (\Phi\Phi^T) t + \frac{1}{2} t^T t + \frac{\lambda}{2} a^T (\Phi\Phi^T) a \\ &= \frac{1}{2} a^T K K a - a^T K t + \frac{1}{2} t^T t + \frac{\lambda}{2} a^T K a \end{aligned}$$

Dual Representations: Linear Regression

Dual: Substituting $w = \Phi^T a$,

$$J(a) = \frac{1}{2} a^T K K a - a^T K t + \frac{1}{2} t^T t + \frac{\lambda}{2} a^T K a$$

Prediction: Hypothesis becomes

$$y(x) = w^T \phi(x) = a^T \Phi \phi(x) = a^T \mathbf{k}(x)$$

where

$$\mathbf{k}(x) = \Phi \phi(x) = [k(x_1, x), \ldots, k(x_n, x)]^T$$

We still need to solve for a!

Dual Representations: Summary

1. Transform $J(w)$ to $J(a)$ by using $w = \Phi^T a$ and the Gram matrix $K = \Phi\Phi^T$
2. Find a to minimize $J(a)$

$$\boxed{a = (K + \lambda I_N)^{-1} t}$$

3. For predictions (for query point/test example x)

$$y(x) = w^T \phi(x) = a^T \Phi\phi(x) = \mathbf{k}(x)^T (K + \lambda I_N)^{-1} t$$

   - where $\mathbf{k}(x)$ has elements $\kappa(x_1, x), \ldots, \kappa(x_n, x)$

Dual Representations: Primal vs. Dual

Primal: $w = (\Phi^T \Phi + \lambda I_M)^{-1} \Phi^T t$

- invert $\Phi^T \Phi \in \mathbb{R}^{M \times M}$
- cheaper since usually $N >> M$
- must explicitly construct features

Dual: $a = (K + \lambda I_N)^{-1} t$

- invert Gram matrix $K \in \mathbb{R}^{N \times N}$
- use kernel trick to avoid feature construction
- use kernels $\kappa(x, x')$ to represent similarity over vectors, images, sequences, graphs, text, etc..

Kernel Regression

> For more details, see **[PRML]** Chapter 6.3

Kernel Regression

Recall the **Gaussian Kernel**:

$$\kappa(x, z) = \exp\left\{-\frac{\|x - z\|^2}{2\sigma^2}\right\} = \exp\{-\gamma\|x - z\|^2\}$$

From training data $\{(x_1, t_1), \ldots, (x_N, t_N)\}$, **Kernel Regression** outputs:

$$y(x) = \frac{1}{\sum_{n=1}^{N} \kappa(x, x_n)} \sum_{n=1}^{N} \kappa(x, x_n) t_n$$

- approximates $y(x)$ with a weighted sum of nearby points
- any distance metric or kernel can be used

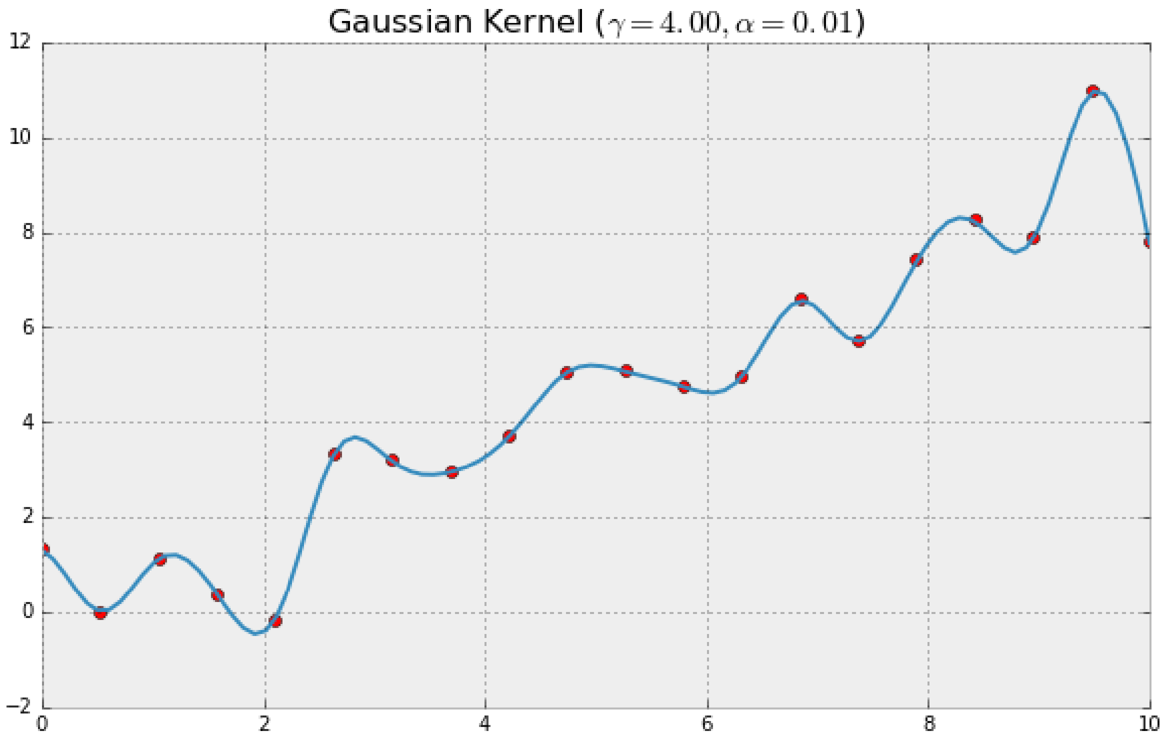
Kernel Regression: Example Code

In [3]:

```
def plot_kernel_ridge(X, y, gamma=0.5, alpha=0.1):
    # kernel (ridge) regression
    krr = KernelRidge(kernel="rbf", gamma=gamma, alpha=alpha);
    krr.fit(X,y);

    # predict
    x_plot = np.linspace(min(X), max(X), 100)[:,np.newaxis];
    y_plot = krr.predict(x_plot);

    # plot
    plt.figure(figsize=(10,6));
    plt.plot(X, y, 'or');
    plt.plot(x_plot, y_plot)
    plt.title(r"Gaussian Kernel ($\gamma=%0.2f, \alpha=%0.2f$)" %
(gamma,alpha), fontsize=16)
```

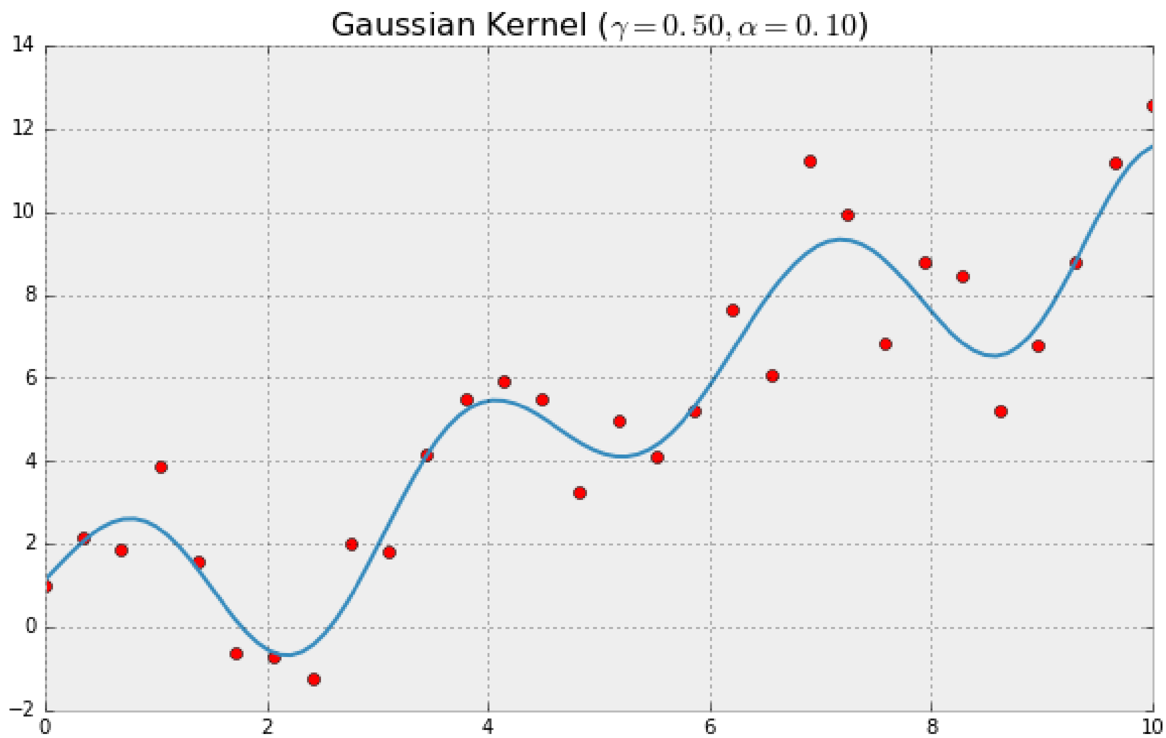
Kernel Regression: Linear + Noise

In [4]:
```
n = 20;
# linear + noise
X = np.linspace(0,10,n)[:,np.newaxis];
y = (X + np.random.randn(n,1)).ravel();
# plot
plot_kernel_ridge(X, y,gamma=4,alpha=0.01);
```



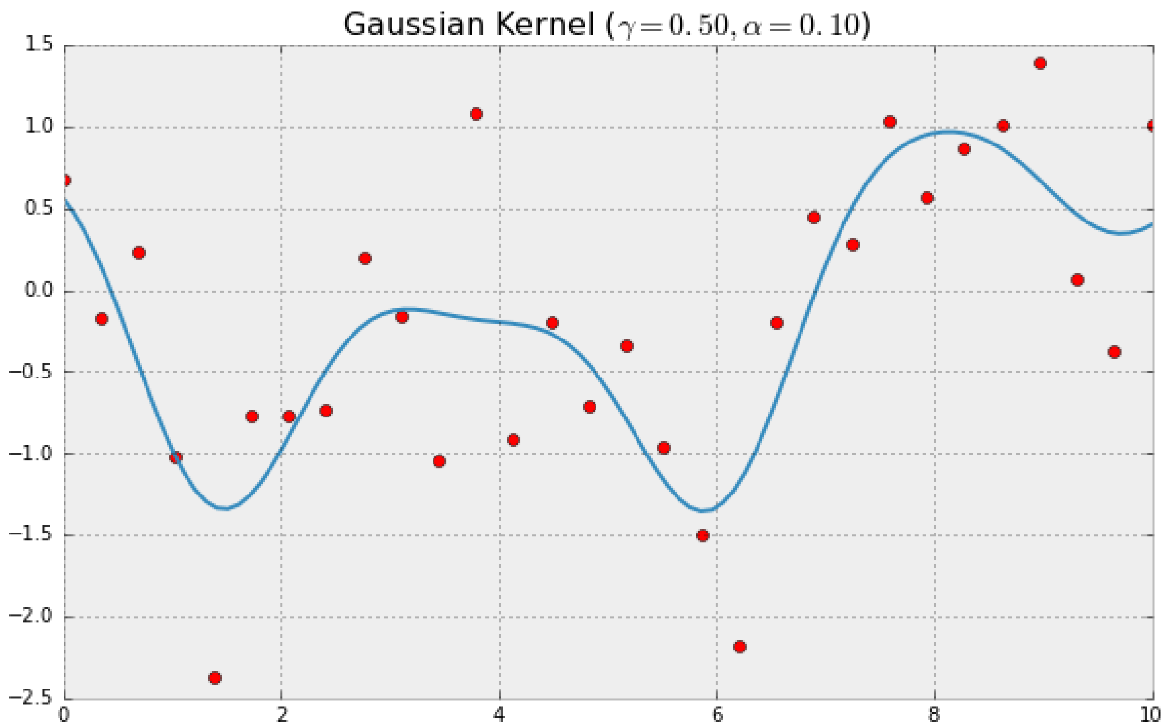
Kernel Regression: Sine + Linear + Noise

In [5]:
```
n = 30;
# sine + linear + noise
X = np.linspace(0,10,n)[:,np.newaxis];
y = (2*np.sin(X*2) + X + np.random.randn(n,1)).ravel();
# plot
plot_kernel_ridge(X, y);
```



Kernel Regression: Completely Random

In [6]:
```
n = 30;
# completely random
X = np.linspace(0,10,n)[:,np.newaxis];
y = (np.random.randn(n)).ravel();
# plot
plot_kernel_ridge(X, y);
```



Kernel Regression: Classification

It is very easy to adapt kernel regression to **classification**!

- Data $\mathcal{D} = \{(x_1, t_1), \dots, (x_N, t_N)\}$, Kernel $\kappa(x, x')$

Regression: if $t \in \mathbb{R}$, return weighted average:

$$y(x) = \frac{1}{\sum_{n=1}^N \kappa(x, x_n)} \sum_{n=1}^N \kappa(x, x_n) t_n$$

Classification if $t \in \pm 1$, return weighted majority:

$$h(x) = \text{sign}\left(\sum_{n=1}^N \kappa(x, x_n) t_n \right)$$

Comparison to Locally-Weighted Linear Regression

Locally-weighted Linear Regression

1. Fit w to minimize $\sum_{n=1}^{N} r_n(t_n - w^T\phi(x_n))^2$ for weights r_n
2. Output $w^T\phi(x)$

Use Gaussian Kernel, $r_n = \exp\left\{-\frac{\|x-x_n\|^2}{2\sigma^2}\right\}$

Comparison to Locally-Weighted Linear Regression

Similarities: Both methods are "instance-based learning".

- Only observations (training set) close to the query point are considered (highly weighted) for regression computation.
- Kernel determines how to assign weights to training examples (similarity to the query point x)
- Free to choose types of kernels
- Both can suffer when the input dimension is high.

Comparison to Locally-Weighted Linear Regression

Differences:

- *LWLR:* Weighted regression; slow, but more accurate
- *KR:* Weighted mean; faster, but less accurate

Break Time!

Support Vector Machines

Review: Linear Classifiers

Linear classifiers make decisions based on a linear (or more generally affine) combination of features.

- *Generative*: Fisher's LDA, GDA, Naive Bayes
- *Discriminative*: Logistic Regression, Perceptron

> What is the "best" linear classifier?

Vapnik's Principle:

> "When solving a problem of interest, do not solve a more general problem as an intermediate step."
>
> "Don't solve a harder problem than you have to"

Discriminative vs. Generative?

- Generative models require estimation of (conditional) densities or mass functions.
- Often much easier to just determine the "decision boundary."

Hyperplanes

An affine subspace one dimension fewer than its ambient space.

- The hyperplanes of a 2-D space are 1-D lines.
- The hyperplanes of a 3-D space are 2-D planes.

Mathematically, a **hyperplane** is of the form

$$\mathbb{H} = \{\mathbf{x} : \mathbf{w}^T\mathbf{x} + b = 0\}$$

where $\mathbf{w} \in \mathbb{R}^d$, $b \in \mathbb{R}$ and d is the number of features.

Point-Plane Distance

Given a hyperplane $\mathbb{H} = \{\mathbf{x} : \mathbf{w}^T\mathbf{x} + b = 0\}$ and a point $\mathbf{z} \notin \mathbb{H}$, we can write z as:

$$\mathbf{z} = \mathbf{z}_0 + r \cdot \frac{\mathbf{w}}{||\mathbf{w}||}$$

- for a unique $\mathbf{z}_0 \in \mathbb{H}$ and $r \neq 0$
- The distance is then given by $|r|$

> Note to slide devs: this is a great place for a picture!

Calculating $|r|$

$$\begin{aligned} \mathbf{w}^T \mathbf{z} + b &= \mathbf{w}^T \mathbf{z}_0 + b + \mathbf{w}^T \left(r \cdot \frac{\mathbf{w}}{||\mathbf{w}||} \right) \\ &= r \frac{\mathbf{w}^T \mathbf{w}}{||\mathbf{w}||} = r||\mathbf{w}|| \end{aligned}$$

Therefore, we have $\boxed{|r| = \frac{|\mathbf{w}^T \mathbf{z} + b|}{||\mathbf{w}||}}$

Separating Hyperplanes

Provide a way of solving 2-class classification problems.

Idea: divide the vector space $\mathbb{R}^d$ where d is the number of features into 2 "decision regions" with a $\mathbb{R}^{d-1}$ subspace (a hyperplane).

Maximum Margin Classifier

(Functional) Margin: The distance from a separating hyperplane to the closest datapoint of any class.

Max. Margin Classifiers: separate data by looking for the hyperplane that maximizes the margin.

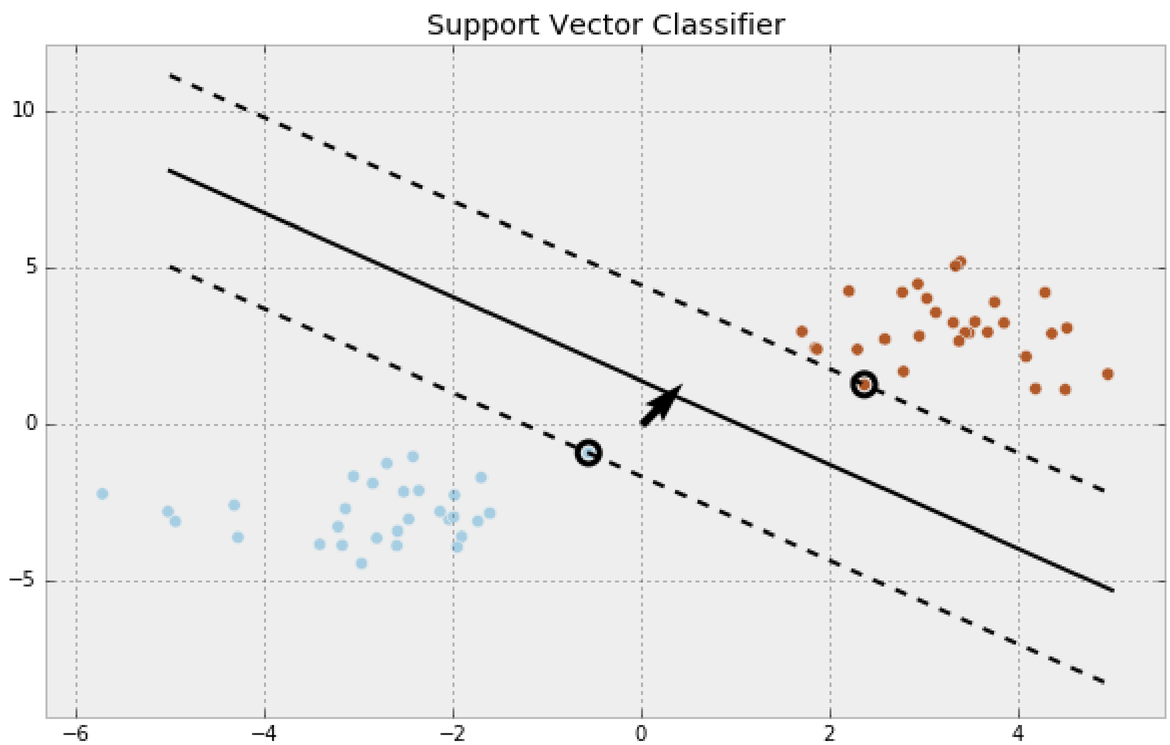
- "best" linear classifier in terms of generalization
- misclassification unlikely with a wide margin between classes.

Maximum Margin Classifier: Example Code

In [7]:
```
# ADAPTED FROM SCIKIT-LEARN EXAMPLE
# (http://scikit-learn.org/stable/modules/svm.html)

def max_margin_classifier(ax, X, Y):
    clf = sklearn.svm.SVC(kernel='linear')
    clf.fit(X, Y)

    # get the separating hyperplane
    w = clf.coef_[0]
    m = -w[0] / w[1]
    xx = np.linspace(-5, 5)
    yy = m * xx - (clf.intercept_[0]) / w[1]

    # plot the parallel lines to the separating hyperplane that pas
s through the
    # support vectors
    t = clf.support_vectors_[0]
    yy_down = m * xx + (t[1] - m * t[0])
    t = clf.support_vectors_[-1]
    yy_up = m * xx + (t[1] - m * t[0])

    ax.plot(xx, yy, 'k-')
    ax.plot(xx, yy_down, 'k--')
    ax.plot(xx, yy_up, 'k--')

    ax.scatter(clf.support_vectors_[:, 0], clf.support_vectors_[:,
1],
            s=120, facecolors='none', edgecolors='k', linewidth=3);
    ax.scatter(X[:, 0], X[:, 1], c=Y, cmap=plt.cm.Paired, s=40)

    ax.axis('tight')

    return w

def plot_svc():
    # Create 30 random points
    np.random.seed()
    X = np.r_[np.random.randn(30, 2) - [3, 3], np.random.randn(30,
2) + [3, 3]]
    Y = [0] * 30 + [1] * 30

    fig = plt.figure(figsize=(10,6))
    ax = fig.add_subplot(111)
    w = max_margin_classifier(ax, X, Y)
    plt.quiver(0, 0, 2 * w[0], 2 * w[0]/w[1],
               angles='xy', scale_units='xy', scale=2)

    plt.title("Support Vector Classifier");
```

Maximum Margin Classifier: Example

In [8]:
```
# Note: The separating hyperplane is the line between the two dotte
d lines.
# The two dotted lines specify the margin and points on the margin
are circled.
plot_svc();
```



Margin Equation

The margin ρ of a hyperplane is given by

$$\rho = \rho(w, b) = \min_{i=1,\ldots,n} \frac{|\mathbf{w}^T \mathbf{x}_i + b|}{||\mathbf{w}||}$$

- where $\mathbf{x}_i$ is the i^{th} datapoint from the training set.

Finding the Max-Margin Hyperplane

As with other linear classifiers, let the classifier be given by

$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

The maximum margin separating hyperplane is then given by the following optimization problem

$$\begin{aligned} \underset{\mathbf{w},b}{\text{maximize}} \quad & \rho(\mathbf{w}, b) \\ \text{subject to} \quad & y_i(\mathbf{w}^T x_i + b) > 0 \end{aligned}$$

Canonical Form

- Let $m := \min_{i=1,\ldots,n} |\mathbf{w_1}^T\mathbf{x}_i + b_1|$ (Simply renaming $\mathbf{w}$ as $\mathbf{w}_1$ and b as b_1 .
- Then, scaling $\mathbf{w}_1$ and b_1 by $\frac{1}{m}$ keeps the hyperplane unaffected.
- $\mathbf{w_2} = \frac{\mathbf{w_1}}{m}$ and $b_2 = \frac{b_1}{m}$ express the hyperplane in canonical form.

Restatement of Optimization Problem

Using the canonical form, we can rewrite the optimization problem as

$$\begin{aligned} \underset{\mathbf{w},b}{\text{maximize}} \min_i \quad & \frac{|\mathbf{w}^T\mathbf{x}_i + b|}{||\mathbf{w}||} \\ \text{subject to} \quad & y_i(\mathbf{w}^T x_i + b) \geq 1, \forall i \\ & y_i(\mathbf{w}^T x_i + b) = 1 \text{ for some } i \end{aligned}$$

Simplifying further (**Exercise:** try to verify this!), we have

$$\begin{aligned} \underset{\mathbf{w},b}{\text{minimize}} \quad & \frac{1}{2}||\mathbf{w}||^2 \\ \text{subject to} \quad & y_i(\mathbf{w}^T x_i + b) \geq 1, \forall i \end{aligned}$$

Linear Separability

- Two classes of data are said to be **linearly separable** if there exists a hyperplane that separates them without any errors.
- So far, we have looked at primarily linearly separable data where a single hyperplane will do for classification.
- We can extend on this notion to a multiclass scenario by considering data to be linearly separable if there exists a set of hyperplanes that can classify each class of examples from the rest (again without errors).

Ideas for dealing with data that aren't linearly separable

- Use "slack" variables that allow for misclassification and penalize misclassification.
- Extend linear classifiers with kernels.

Optimal Soft-Margin Hyperplane (OSMH)

Learn a linear classifier which solves

$$\begin{aligned} \underset{\mathbf{w},b,\xi}{\text{minimize}} \quad & \frac{1}{2}||\mathbf{w}||^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} \quad & y_i(\mathbf{w}^T x_i + b) \geq 1 - \xi_i, i = 1, \ldots, n \\ & \xi_i \geq 0, i = 1, \ldots, n \end{aligned}$$

where we now have a new term that penalizes errors and accounts for the influence of outliers through a constant $C \geq 0$ (0 would lead us back to the hard margin case) and $\xi = [\xi_1, \ldots, \xi_n]$ are the slack variables.

OSMH: Motivation

$$\begin{aligned} \underset{\mathbf{w},b,\xi}{\text{maximize}} \quad & \frac{1}{2}||\mathbf{w}||^2 + \frac{C}{n}\sum_{i=1}^{n}\xi_i \\ \text{subject to} \quad & y_i(\mathbf{w}^T x_i + b) \geq 1 - \xi_i, i = 1, \ldots, n \\ & \xi_i \geq 0, i = 1, \ldots, n \end{aligned}$$

- The **objective function** ensures margin is large *and* the margin violations are small
- The **first set of constraints** ensures classifier is doing well
  - similar to the prev. max-margin constraint, except we now allow for slack
- The second set of constraints ensure slack vars non-neg.
  - keeps the optimization problem from "*diverging*"

The OSMH optimization problem

The OSMH optimization is a convex optimization problem

- objective function is quadratic
- inequality constraints are affine (and hence convex).

Note that strong duality holds.

Review: Lagrangian

Consider a **constrained optimization problem**

$$\begin{aligned} \underset{\mathbf{x}\in\mathbb{R}^d}{\text{minimize}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, i = 1, \ldots, m \\ & h_j(x) = 0, j = 1, \ldots, n \end{aligned}$$

The Lagrangian is then given by

$$L(\mathbf{x}, \alpha, \beta) = f(\mathbf{x}) + \sum_{i=1}^{m} \alpha_i g_i(\mathbf{x}) + \sum_{j=1}^{n} \beta_j h_j(\mathbf{x})$$

Here, α and β are the **Lagrange Multipliers / Dual Variables** associated with the inequality constraints and equality constraints repsectively.

Review: Lagrangian Dual

- The Lagrangian Dual problem is given by $L_D(\alpha, \beta) = \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta)$
- And, the Dual Optimization problem is given by $\max\limits_{\alpha,\beta:\alpha_i\geq 0} L_D(\alpha, \beta)$
- Note, L_D is concave, because it is a piece-wise minimimum of affine functions.
- The Lagrange Primal Optiminization problem is given by $\min_{\mathbf{x}} \max\limits_{\alpha,\beta:\alpha_i\geq 0} L(\mathbf{x}, \alpha, \beta)$.

  $$L_p(\mathbf{x}) = \begin{cases} f(x) & \text{if } x \text{ is feasible} \\ \infty & \text{otherwise} \end{cases}$$
- Thus, primal and original problems have the same solution!

Review: Strong and Weak Duality

$$p^* = \min_{\mathbf{x}} L_p(\mathbf{x}) = \min_{\mathbf{x}} \max_{\alpha,\beta:\alpha_i \geq 0} L(\mathbf{x}, \alpha, \beta)$$
$$d^* = \max_{\alpha,\beta:\alpha_i \geq 0} L_D(\alpha, \beta) = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta)$$

- Weak duality: $d^* \leq p^*$
- Strong duality: $p^* = d^*$
- The original problem is said to be **convex (cvx)** is $f, g_1, \ldots, g_m$ are convex and $h_1, \ldots, h_n$ are affine.
- If the original problem is cvx. and a constraint qualification holds, then $p^* = d^*$.
- Example of constraint qualification: All g_i are affine and Strict Feasibility, $\exists \mathbf{x} \text{ s.t. } \forall j, h_j(\mathbf{x}) = 0 \wedge \forall i, g_i(\mathbf{x}) < 0$

Review: Karesh-Kuhn-Tucker Conditions

Thm. If $p^* = d^*$, $\mathbf{x}^*$ is primal optimal and (α^8, β^*) are dual optimal, then the KKT conditions hold:

1. $\nabla f(\mathbf{x}^* + \sum_i \alpha_i^* \nabla g_i(\mathbf{x}^*) + \sum_j \beta_j^* \nabla h_j(x^*) = 0$
2. $\forall\, i$, $g_i(\mathbf{x}^*) \leq 0$ (by feasibility of $\mathbf{x}^*$)
3. $\forall\, j$, $h_j(\mathbf{x}^*) = 0$ (by feasibility of $\mathbf{x}^*$)
4. $\forall\, i$, $\alpha_i^* \geq 0$ (by defn. of the dual problem)
5. $\forall\, i$, $\lambda_i^* g_i(\mathbf{x}^*) = 0$ (complimentary slackness)

Review: KKT (Proof of 1 and 5)

$$\begin{aligned} f(x^*) &= L_D(\alpha^*, \beta^*) \text{ [by Strong duality]} \\ &= \min_{\mathbf{x}}(f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) + \sum_j \beta_j h_j(\mathbf{x}) \\ &\leq f(\mathbf{x}^*) + \sum_i \lambda_i^* g_i(\mathbf{x}^*) + \sum_j \beta_j h_j(\mathbf{x}^*) \\ &\leq f(x^*) \text{ [by 2 - 4]} \end{aligned}$$

Noting the inequalities are really then equalities:

- The equality of the last two lines, we get that $\forall i, \alpha_i^* g_i(\mathbf{x}^*) = 0$.
- The equality of the second and third lines imply $\mathbf{x}^*$ is a minimizer of $L(\mathbf{x}, \alpha^*, \beta^*)$ w.r.t. $\mathbf{x}$. Therefore, $\nabla_x L(\mathbf{x}^*, \alpha^*, \beta^*) = 0$.

OSMH: Lagrangian

The Lagrangian is given by

$$L(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{1}{2}||\mathbf{w}||^2 + \frac{C}{n}\sum_i \xi_i - \sum_{i=1}^{n} \alpha_i(y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 + \xi_i) - \sum_{i=1}^{n} \beta_i \xi_i$$

OSMH: Dual Problem

- So, the Lagrangian Dual is given by the following unconstrained optimization problem

$$\underset{\mathbf{w}, b, \xi}{\text{minimize}} \qquad L(\mathbf{w}, b, \xi, \alpha, \beta)$$

- Thus, the dual problem given by the following optimization

$$\begin{aligned} &\underset{\mathbf{w}, b, \xi}{\text{maximize}} && L_D(\alpha, \beta) \\ &\text{subject to} && \alpha \geq 0, \beta \geq 0 \end{aligned}$$

OSMH: The Unconstrained Minimization

For a fixed α, β, we can minimize the primal variables as follows:

- $\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i = 0, \forall i$
- $\frac{\partial L}{\partial b} = \sum_i \alpha_i y_i = 0, \forall i$
- $\frac{\partial L}{\partial \xi_i} = \frac{C}{n} - \alpha_i - \beta_i = 0, \forall i$

$||w||^2 = ||\sum_i \alpha_i y_i \mathbf{x}_i||^2 = \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$

Thus, $\boxed{L_D(\alpha, \beta) = \frac{-1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_i \alpha_i}$

OSMH: Dual Problem Revisited

(Note the inner product!)

$$\begin{aligned}
\underset{\alpha,\beta}{\text{maximize}} \quad & -\frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j < \mathbf{x}_i, \mathbf{x}_j > + \sum_i \alpha_i \\
\text{subject to} \quad & \sum_i \alpha_i y_i = 0 \\
& \forall i, \alpha_i + \beta_i = \frac{C}{n} \\
& \forall i, \alpha_i \geq 0, \beta_i \geq 0
\end{aligned}$$

OSMH: Eliminating Constraints

By eliminating β, we can write the dual optimization as the following QP

$$\begin{aligned}
\underset{\alpha}{\text{maximize}} \quad & \frac{-1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j < \mathbf{x}_i, \mathbf{x}_j > + \sum_i \alpha_i \\
\text{subject to} \quad & \sum_i \alpha_i y_i = 0 \\
& \forall i, 0 \leq \alpha_i \leq \frac{C}{n}
\end{aligned}$$

OSMH: Observations

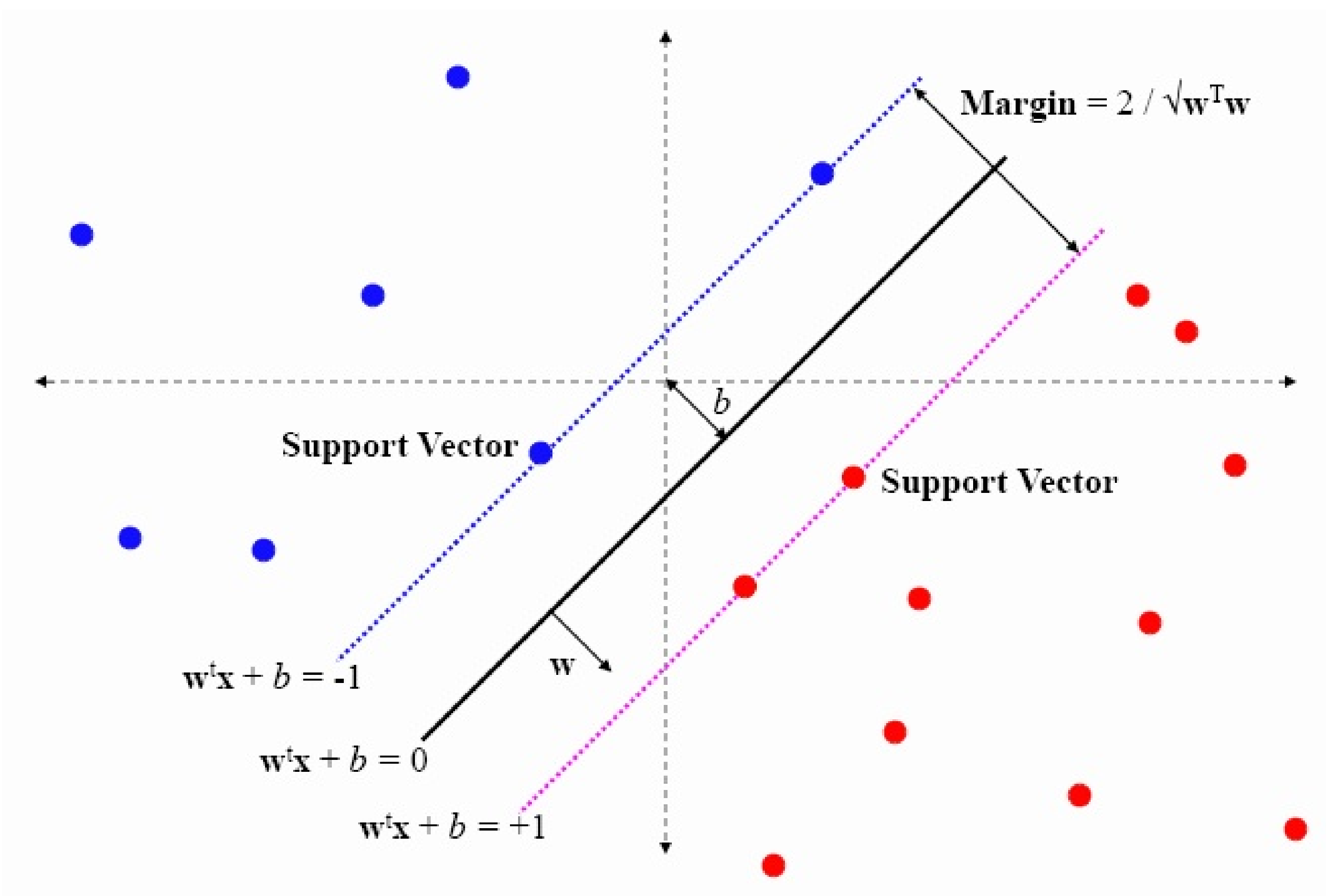
- Let $\mathbf{w}^*, b^*$ and ξ^* be the primal optimal solutions and α^* and β^* be the dual optimal solutions.
- From the KKT conditions, we have $\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i$. So, the optimal normal vector to the hyperplane is a linear combination of datapoints!

OSMH: Observations

- From the complimentary slackness KKT condition, $\alpha_i^*(1 - \xi_i^* - y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*)) = 0$.
- If $\mathbf{x}_i$ satisfies $y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) = 1 - \xi_i^*$, we call $\mathbf{x}_i$ a support vector. In other words, if $\mathbf{x}_i$ is not a support vector, $\alpha_i^* = 0$.
- The above means that $\mathbf{w}^*$ depends only on the support vectors!

OSMH: Geometric Interpretation

- If $y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) > 1$, then $\xi_i^* = 0$, $\mathbf{x}_i$ is outside the margin and is not a SV.
- If $y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) = 1$, then $\xi_i^* = 0$, $\mathbf{x}_i$ is on the margin and is a SV.
- If $0 \leq y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) < 1$, then $\xi_i^* > 0$, $\mathbf{x}_i$ is within the margin and is a SV.
- If $y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) < 0$, then $\xi_i^* > 0$, $\mathbf{x}_i$ is misclassified and is a SV.



OSMH: Optimal offset

- If $\alpha_i^* < \frac{C}{n}$, then $\xi_i^* = 0$ (applying KKT Complementary Slackness to the constraint $\beta_i^* \xi_i^* = 0$).
- If $\alpha_i^* < \frac{C}{n}$ then $\beta_i^* > 0$ and so $\xi_i = 0$.
- Using the above, consider any i such that $0 < \alpha_i^* < \frac{C}{n}$. Then, $y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) = 1 - \xi_i^* = 1$.
- Solving for b^* using $y_i = \pm 1 \implies y_i^2 = 1$, we get $b^* = y_i - \mathbf{w}^{*T}\mathbf{x}_i$.

OSMH: Support Vector Machines

The dual problem and final classifier only involve the data via inner products.

- We can apply the **kernel trick** and kernelize the OSMH problem.
- The resulting classifier is known as a *Support Vector Machine*.

Let k be an inner product kernel. The SVM Classifier is given by

$$\boxed{f(\mathbf{x}) = sign(\sum_{i=1}^{n} \alpha_i^* y_i k(x, x_i) + b^*)}$$

OSMH: Support Vector Machines

Here, $\alpha^* = [\alpha_1^*, \ldots, \alpha_n^*]^T$ is the solution of

$$\boxed{\begin{array}{ll} \underset{\alpha}{\text{maximize}} & \frac{-1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j) + \sum_i \alpha_i \\ \text{subject to} & \sum_i \alpha_i y_i = 0 \\ & \forall i, 0 \le \alpha_i \le \frac{C}{n} \end{array}}$$

and $\boxed{b^* = y_i - \sum_{j=1}^{n} \alpha_j^* y_j k(x_j, x_i)}$ for some i such that $0 < \alpha_i^* < \frac{C}{n}$

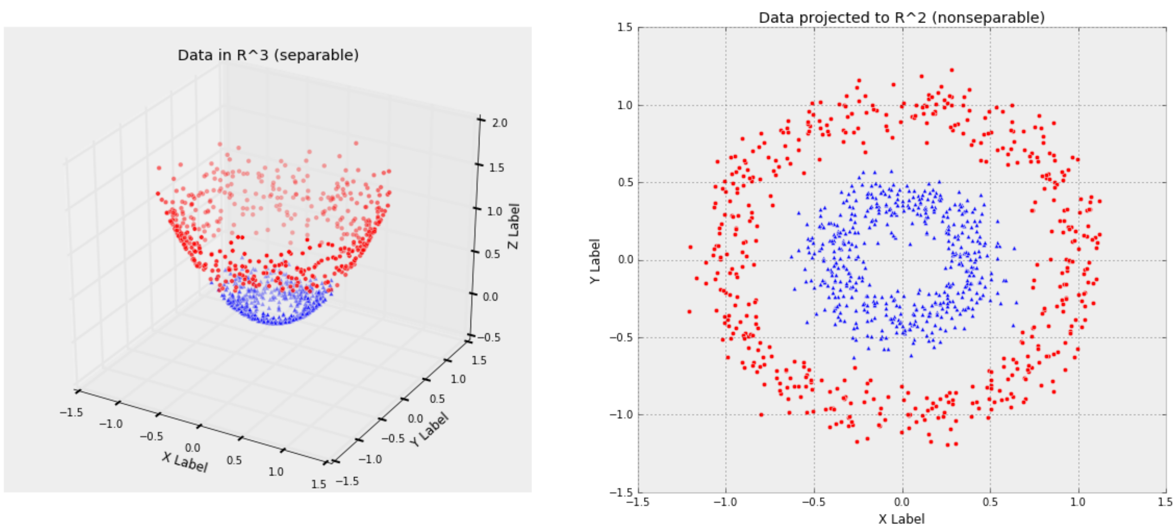
In [9]:
```
%matplotlib inline

import numpy as np
from math import sqrt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.datasets import make_circles
import matplotlib.pyplot as plt
import pylab as pl

"""
Demonstrates how a linearly nonseparable dataset in R^2 can be
linearly separable in R^3 after a transformation via an appropriate
kernel function.

Generates a 2D non-separable dataset, and projects it to R^3 using
a polynomial kernel [x1, x2] -> [x1, x2, x1^2.0 + x2^2.0], where
it is now linearly separable in R^3.

Usage:
    $ python demo_data_transform.py
"""

def randrange(n, vmin, vmax):
    return (vmax-vmin)*np.random.rand(n) + vmin

def fn_kernel(x1, x2):
    """ Implements a polynomial kernel phi(x1,y1) = [x1, y1, x1^2 +
y1^2] """
    return np.array([x1, x2, x1**2.0 + x2**2.0])

""" Generate linearly nonseparable dataset (in R^2) """

n = 1000

X, Y = make_circles(n_samples=n, noise=0.1, factor=0.4)

A = X[np.where(Y == 0)]
B = X[np.where(Y == 1)]

X0_orig = A[:, 0]
Y0_orig = A[:, 1]

X1_orig = B[:, 0]
Y1_orig = B[:, 1]

frac0 = len(np.where(Y == 0)[0]) / float(len(Y))
frac1 = len(np.where(Y == 1)[0]) / float(len(Y))

A = np.array([fn_kernel(x,y) for x,y in zip(np.ravel(X0_orig), np.r
avel(Y0_orig))])
X0 = A[:, 0]
Y0 = A[:, 1]
Z0 = A[:, 2]
```

```
A = np.array([fn_kernel(x,y) for x,y in zip(np.ravel(X1_orig), np.r
avel(Y1_orig))])
X1 = A[:, 0]
Y1 = A[:, 1]
Z1 = A[:, 2]

def plot_no_decision_boundary():
    fig = plt.figure(figsize=(20,8))
    ax = fig.add_subplot(121, projection='3d')

    ax.scatter(X0, Y0, Z0, c='r', marker='o')
    ax.scatter(X1, Y1, Z1, c='b', marker='^')

    ax.set_xlabel('X Label')
    ax.set_ylabel('Y Label')
    ax.set_zlabel('Z Label')
    ax.set_title("Data in R^3 (separable)")

    # Project data to X/Y plane
    ax2d = fig.add_subplot(122)
    ax2d.scatter(X0, Y0, c='r', marker='o')
    ax2d.scatter(X1, Y1, c='b', marker='^')

    ax2d.set_xlabel('X Label')
    ax2d.set_ylabel('Y Label')
    ax2d.set_title("Data projected to R^2 (nonseparable)")

    plt.show()

def plot_decision_boundary():
    fig = plt.figure(figsize=(20,8))
    ax = fig.add_subplot(121, projection='3d')

    ax.scatter(X0, Y0, Z0, c='r', marker='o')
    ax.scatter(X1, Y1, Z1, c='b', marker='^')

    ax.set_xlabel('X Label')
    ax.set_ylabel('Y Label')
    ax.set_zlabel('Z Label')
    ax.set_title("Data in R^3 (separable w/ hyperplane)")

    x = np.arange(-1.25, 1.25, 0.1)
    y = np.arange(-1.25, 1.25, 0.1)
    X, Y = np.meshgrid(x, y)

    Z = np.zeros(X.shape)
    Z[:,:] = 0.5

    ax.plot_surface(X, Y, Z, color='#FFFFFF')

    # Project data to X/Y plane
    ax2d = fig.add_subplot(122)
    ax2d.scatter(X0, Y0, c='r', marker='o')
```

```
    ax2d.scatter(X1, Y1, c='b', marker='^')

    ax2d.add_patch(pl.Circle((0,0), radius=sqrt(0.5),
                   fill=False, linestyle='solid', linewidth=4.0,
                   color='black'))
    ax2d.add_patch(pl.Circle((0,0), radius=sqrt(0.5),
                   fill=False, linestyle='dashed', linewidth=1.5,
                   color='#09F911'))

    ax2d.set_xlabel('X Label')
    ax2d.set_ylabel('Y Label')
    ax2d.set_title("Data projected to R^2 (hyperplane projection sh
own)")

    plt.ion()

    ax.view_init(azim = 210,elev = 5)
    plt.draw()
```

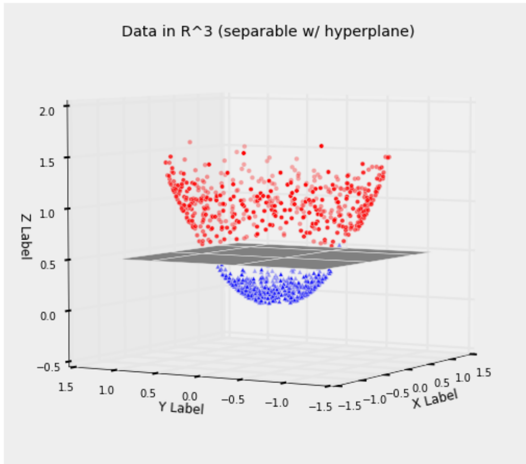
SVM: Example

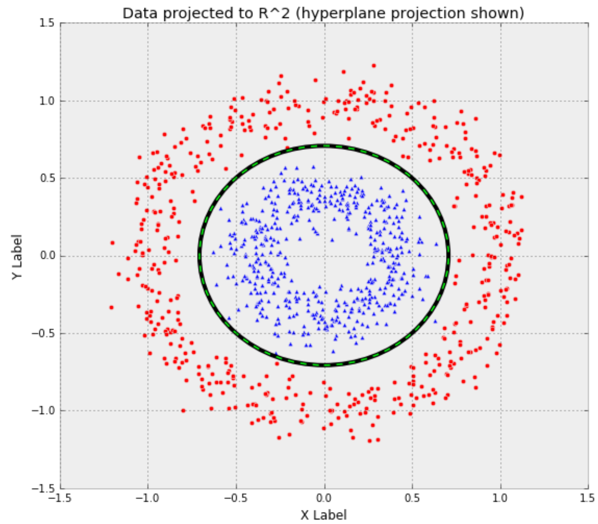
In [10]:
```
# Polynomial Kernel Example
plot_no_decision_boundary()
```



SVM: Decision Boundary

```
In [11]: plot_decision_boundary()
```





SVM: Kernels

Choice of kernels

- Gaussian or polynomial kernels are used quite often
- If simple kernels are ineffective, more elaborate kernels can be used (Radial Basis Functions provide an infinite dimensional mapping!)

SVM: Kernels

Choice of Kernel Parameters

- Ex: Gaussian Kernel; $K(x, z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$. As a heuristic, the Bandwidth (σ) can be chosen to be the distance between neighboring points whose labels will likely affect the prediction of the query point.

How to solve for the SVM dual?

- "Chunking Algorithm"
  - Start with a random subset of the data and keep iteratively adding examples which violate the optimality conditions.
  - Problem: QP problem scales with the number of SVs.
  - Most SVM problems were solved with such algorithms in expensive QP solver softwares prior to SMO (see below).

Sequential Minimal Optimization

- Divide the Dual problem into smaller sub-problems each of which consists of 2 of the linear equality constraint Lagrange multipliers (α's).
- Find a lagrange multiplier α_1 that violates the KKT conditions.
- Pick a second multiplier α_2 and optimize the pair (α_1, α_2) using **coordinate ascent**.
- Repeat the previous 2 steps until convergence (the KKT conditions are satisifed within a user-defined tolernace).

See Platt (1998) for details.