$\LaTeX$ 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");

# matplotlib objects
from matplotlib import mlab;
from matplotlib import gridspec;

# 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")
```

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
});
```

EECS 545: Machine Learning

Lecture 10: Bayesian Linear Regression & Gaussian Processes

- Instructor: **Jacob Abernethy**
- Date: February 15, 2015

Lecture Exposition Credit: Valli, Ben, and Saket

References

This lecture draws upon the following resources:

- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://www.springer.com/us/book/9780387310732). 2006.
- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[CS229]** Ng, Andrew. CS 229: Machine Learning (http://cs229.stanford.edu/). Autumn 2015.
    - Gaussian Processes (http://cs229.stanford.edu/section/cs229-gaussian_processes.pdf)
    - More on Gaussians (http://cs229.stanford.edu/section/more_on_gaussians.pdf)

Outline

- Finish SVM and Dual Optimization
- More on Multivariate Gaussians
    - Partitioned Marginals and Conditionals
    - Bayes' Theorem for Gaussians
- Bayesian Linear Regression
- Gaussian Process Regression
    - Gaussian Processes

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.

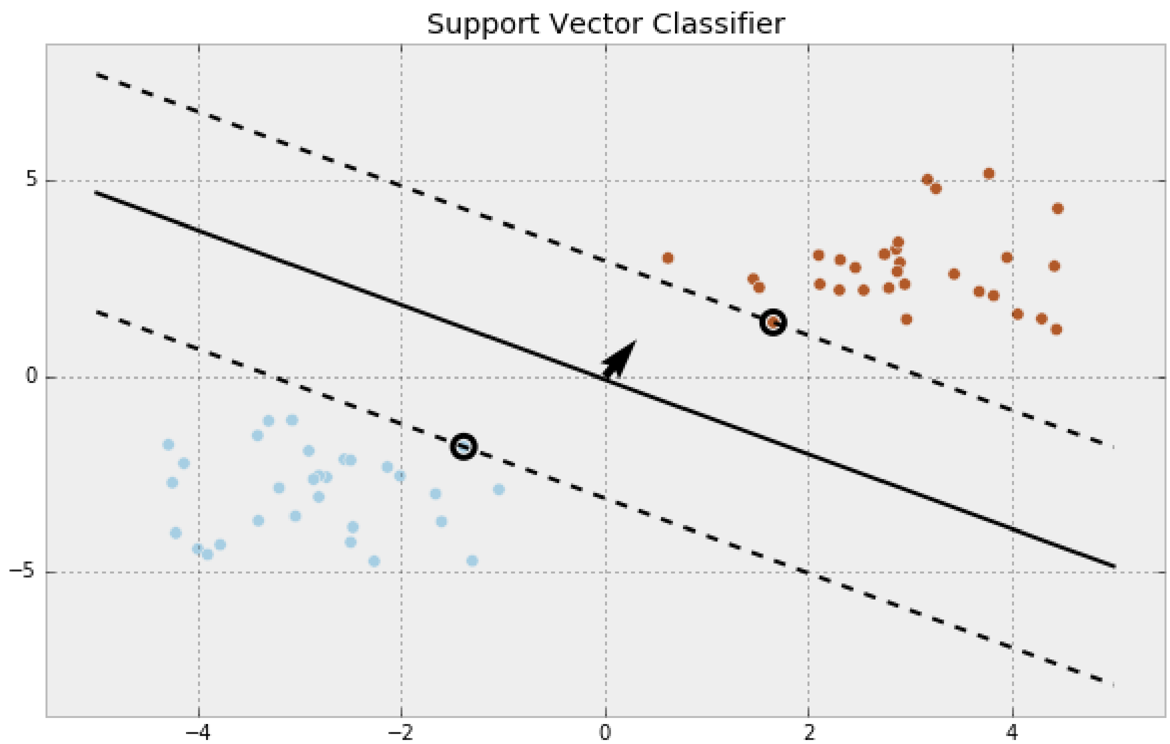
- "best" linear classifier in terms of generalization
- misclassification unlikely with a wide margin between classes.

Maximum Margin Classifier: Example Code

In [3]:
```
# 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 [4]:
```
# 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

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

- 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

$$\begin{array}{ll} \text{maximize}_{\mathbf{w},b} & \rho(\mathbf{w}, b) \\ \text{subject to} & y_i(\mathbf{w}^T\mathbf{x}_i + b) > 0 \end{array}$$

Canonical Form

- Let $m := \min_{i=1,...,n} |\mathbf{w_1}^T\mathbf{x}_i + b_1|$ (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

$$\begin{array}{ll} \text{maximize } \min\limits_{i} \ {}_{\mathbf{w},b} & \dfrac{|\mathbf{w}^T\mathbf{x}_i + b|}{||\mathbf{w}||} \\ \text{subject to} & y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \forall i \\ & y_i(\mathbf{w}^T\mathbf{x}_i + b) = 1 \text{ for some } i \end{array}$$

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

$$\begin{array}{ll} \text{minimize}_{\mathbf{w},b} & \dfrac{1}{2}||\mathbf{w}||^2 \\ \text{subject to} & y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \forall i \end{array}$$

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

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

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

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

- 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**

$$
\begin{array}{ll}
\text{minimize}_{\mathbf{x}\in \mathrm{R}^d} & f(\mathbf{x}) \\
\text{subject to} & g_i(\mathbf{x}) \leq 0, i = 1, \dots, m \\
& h_j(x) = 0, j = 1, \dots, n
\end{array}
$$

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 objective is given by $L_D(\alpha, \beta) = \ \min_{\mathbf{x}} L(\mathbf{x}, \alpha, \beta)$
- The Dual Optimization problem is given by $\max_{\alpha, \beta : \alpha_i \geq 0} \quad L_D(\alpha, \beta)$
- Note, L_D is concave, because it is a piece-wise minimimum of affine functions.
- The Lagrange Primal objective is given by $L_P(\mathbf{x}) := \max_{\alpha, \beta : \alpha_i \geq 0} \quad L(\mathbf{x}, \alpha, \beta) = \begin{cases} f(x) & \text{if } x \text{ is feasible} \\ \infty & \text{otherwise} \end{cases}$
- Notice that the Lagrange Primal Optiminization problem, $\min_{\mathbf{x}} L_P(\mathbf{x})$, is identical to the original optimization problem!

Review: Strong and Weak Duality

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

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

- 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^*, 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. $\forall\, i,\, \alpha_i^* g_i(\mathbf{x}^*) = 0$ (complimentary slackness)

Review: KKT (Proof of 1 and 5)

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

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 \begin{align} & L(\mathbf{w}, b, \mathbf{\xi}, \alpha, \beta) = \frac{1}{2}{||\mathbf{w}||}^2 + \frac{C}{n}\sum*i \xi_i \ & \quad \quad - \sum \limits*{i = 1}^n \alpha*i (y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i) - \sum \limits*{i = 1}^n \beta_i \xi_i \end{align}

OSMH: Dual Problem

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

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

- Thus, the dual problem given by the following optimization

$$
\begin{aligned}
&\text{maximize}_{\alpha, \beta} \qquad && L_D(\alpha, \beta) \\
&\text{subject to} && \alpha \geq 0, \beta \geq 0
\end{aligned}
$$

OSMH: The Unconstrained Minimization

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

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

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

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

OSMH: Dual Problem Revisited

(Note the inner product!)

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

OSMH: Eliminating Constraints

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

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

OSMH: Observations

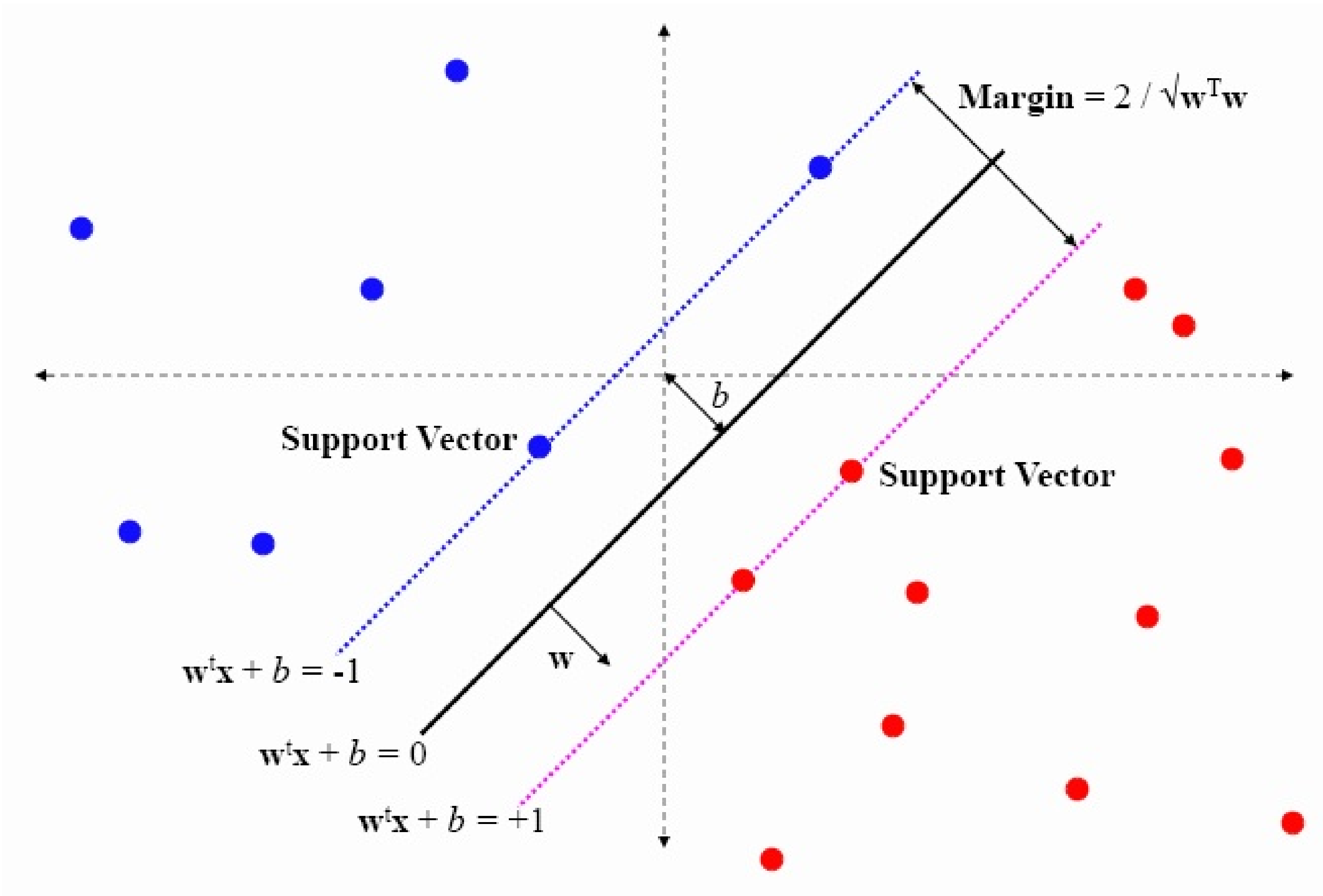
- Let $\mathbf{w}^*, b^*$ and ξ^* be the primal optimal solutions and α^* and β^* be the dual optimal solutions.
- From the KKT conditions, we have $\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* y_i \mathbf{x}_i$. So, the optimal normal vector to the hyperplane is a linear combination of datapoints!

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 $0 \le y_i(\mathbf{w}^{*T}\mathbf{x}_i + b^*) < 1$, 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

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

OSMH: Support Vector Machines

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

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

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

In [5]:

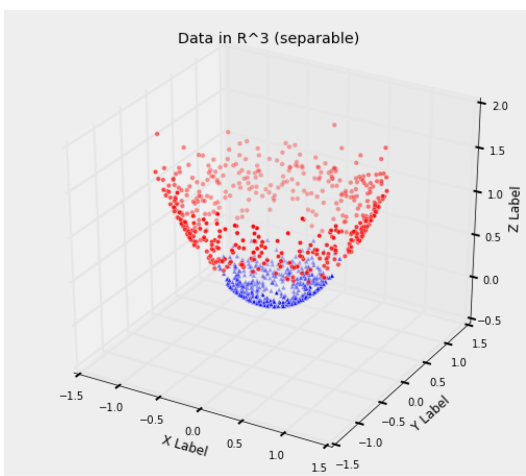
```
%matplotlib inline

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]
```

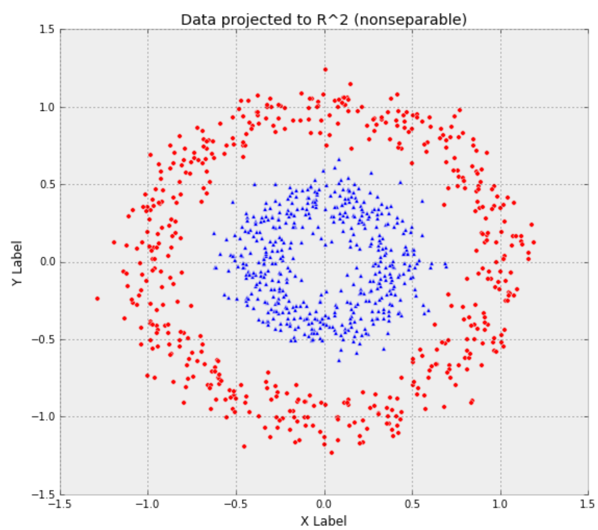
```python
A = np.array([fn_kernel(x,y) for x,y in zip(np.ravel(X1_orig), np.r
avel(Y1_orig))])
X1 = A[:, 0]
Y1 = A[:, 1]
Z1 = A[:, 2]

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

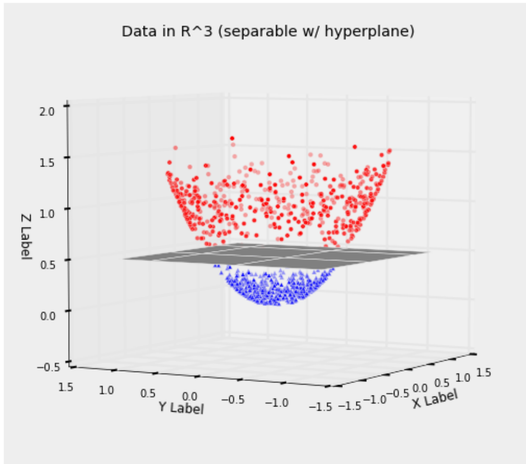
In [6]:
```
# Polynomial Kernel Example
plot_no_decision_boundary()
```

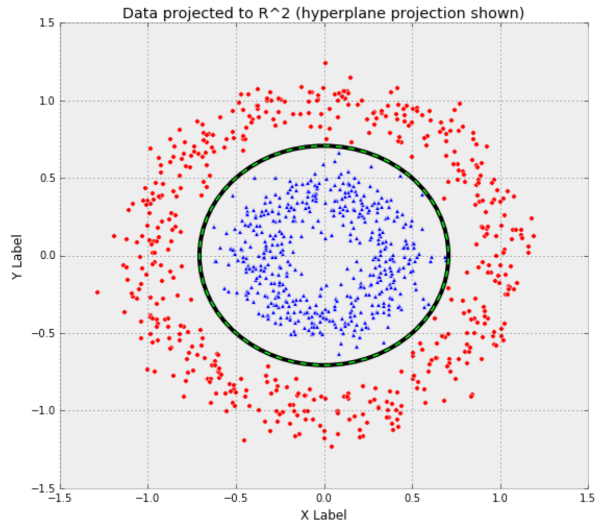




SVM: Decision Boundary

In [7]:
```
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 tolerance).

See Platt (1998) for details.

Break Time!

More on Multivariate Gaussians

> Taken from **[PRML]** §2.3, **[MLAPP]** §4.3, 4.4, and **[CS229]**

Review: Multivariate Gaussians

Recall the **Multivariate Normal / Gaussian** distribution with

- mean $\mu \in \mathrm{R}^D$
- covariance matrix $\Sigma \in \mathrm{R}^{D \times D}$

$$\mathrm{N}(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu) \right]$$

Partitioned Gaussian Distributions

Partition $x \sim \mathrm{N}(\mu, \Sigma)$ as $x = [x_a, x_b]^T$, and

- Mean and covariance

$$\mu = \begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix} \quad \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}$$

- Precision Matrix

$$\Lambda = \Sigma^{-1} = \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}$$

Partitioned Marginals

Exercise: Marginals are obtained by taking a subset of rows and columns:

$$\begin{aligned} P(x_a) &= \int P(x_a, x_b)\, dx_b \\ &= \mathrm{N}(x_a \mid \mu_a, \Sigma_{aa}) \end{aligned}$$

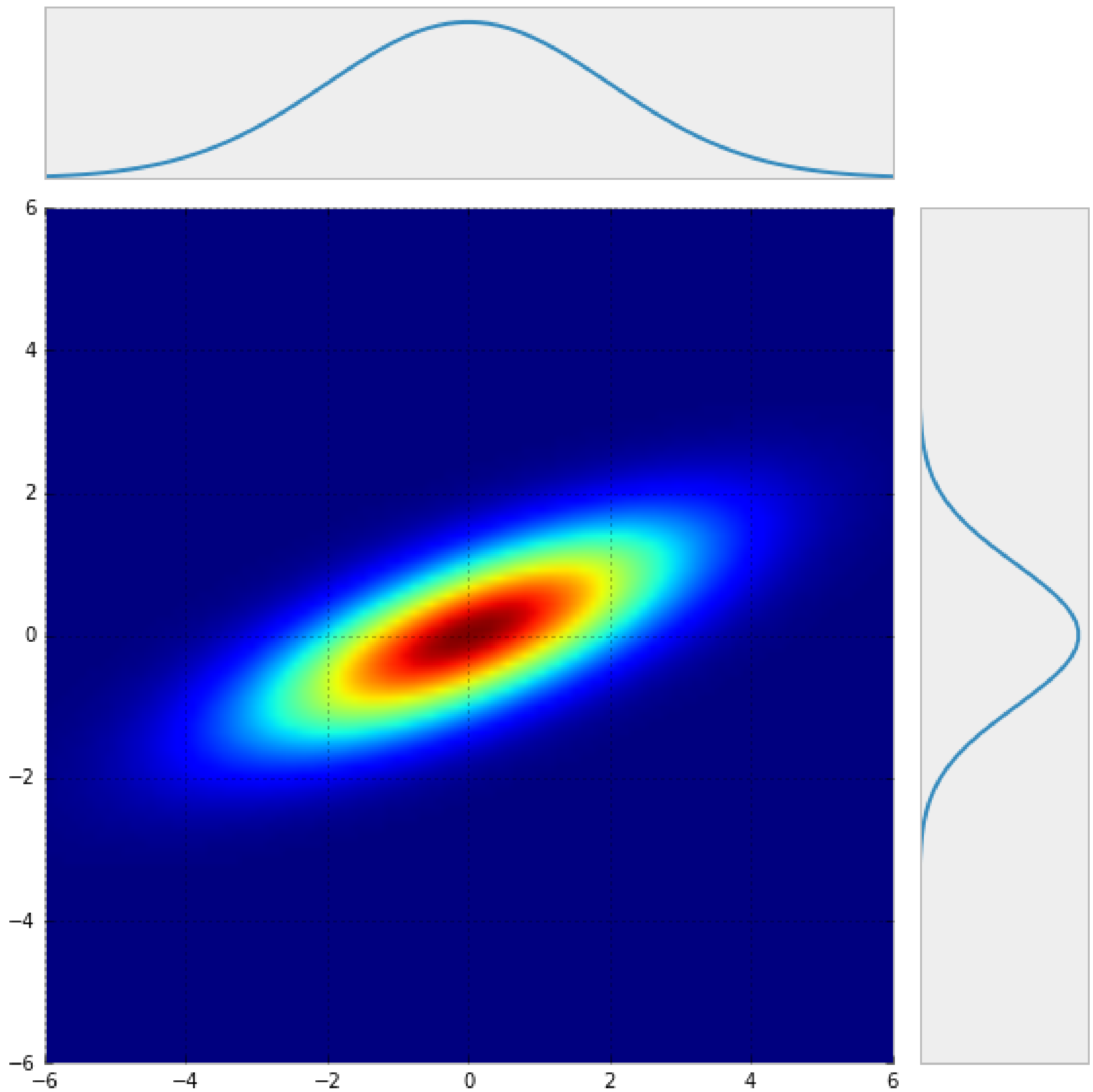
> Marginals are Gaussian!

Partitioned Marginals: Example Code

In [8]:
```
def plot_mvn(sigmax, sigmay, mux, muy, corr):
    # dimensions
    radius = 3 * max(sigmax, sigmay);
    # create grid
    x = np.linspace(mux-radius, mux+radius, 100);
    y = np.linspace(muy-radius, muy+radius, 100);
    X, Y = np.meshgrid(x, y);

    # data limits
    xlim = (x.min(), x.max());
    ylim = (y.min(), y.max());

    # bivariate and univariate normals
    sigmaxy = corr * np.sqrt(sigmax * sigmay);
    Z = mlab.bivariate_normal(X, Y, sigmax, sigmay, mux, muy, sigma
xy);
    zx = np.sum(Z, axis=0); #mlab.normpdf(x, mux, sigmax);
    zy = np.sum(Z, axis=1); #mlab.normpdf(y, muy, sigmay);

    # figure
    fig = plt.figure(figsize=(8,8));

    # subplots
    gs = gridspec.GridSpec(2, 2, width_ratios=[5,1], height_ratios=
[1,5]);
    ax_xy = fig.add_subplot(gs[1,0]);
    ax_x  = fig.add_subplot(gs[0,0], sharex=ax_xy);
    ax_y  = fig.add_subplot(gs[1,1], sharey=ax_xy);

    # plot
    ax_xy.imshow(Z, origin='lower', extent=xlim+ylim, aspect='aut
o');
    ax_x.plot(x, zx);
    ax_y.plot(zy, y);

    # hide labels
    ax_x.xaxis.set_visible(False);
    ax_x.yaxis.set_visible(False);
    ax_y.xaxis.set_visible(False);
    ax_y.yaxis.set_visible(False);

    # layout & title
    plt.tight_layout();
```

Partitioned Marginals: Bivariate Example

In [9]:
```
# sigmax, sigmay, mux, muy, corr
plot_mvn(2, 1, 0, 0, 1);
```



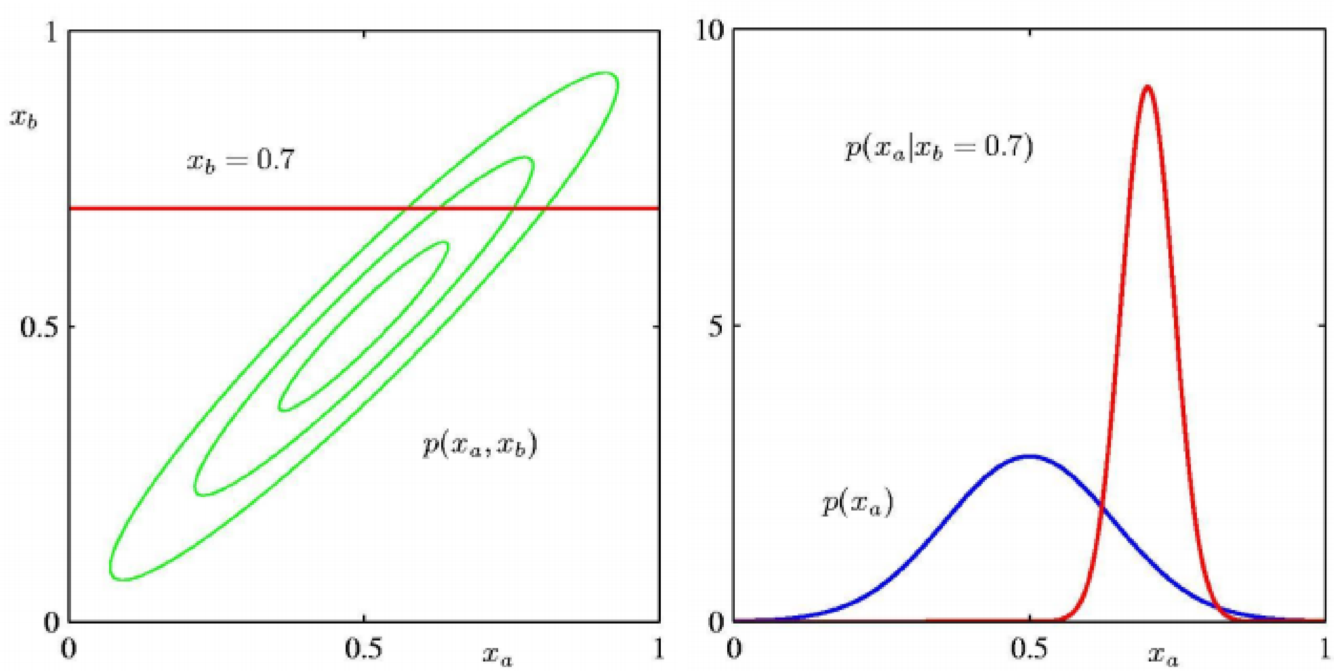
Partitioned Conditionals

Exercise: Conditionals are given by

$$
\begin{aligned}
P(x_a|x_b) &= \mathrm{N}(x_a|\mu_{a|b}, \Sigma_{a|b}) \\
\Sigma_{a|b} &= \Lambda_{aa}^{-1} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \\
\mu_{a|b} &= \Sigma_{a|b}\left[\Lambda_{aa}\mu_a - \Lambda_{ab}(x_b - \mu_b)\right] \\
&= \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b - \mu_b) \\
&= \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b)
\end{aligned}
$$

Partitioned Conditionals

> Obtained by "slicing" the joint pdf



Linear Gaussian Systems: Model

Suppose $x \in \mathrm{R}^{D_x}$ and $y \in \mathrm{R}^{D_y}$, and

$$x \sim \mathrm{N}(\mu_x, \Sigma_x)$$
$$y\,|\,x \sim \mathrm{N}(Ax + b, \Sigma_y)$$

for fixed $A \in \mathrm{R}^{D_y \times D_x}$ and $b \in \mathrm{R}^{D_y}$.

Linear Gaussian Systems: Bayes' Theorem

Exercise: Show that

$$P(y) = \mathrm{N}(y\,|\,A\mu_x + b, \Sigma_y + A\Sigma_x A^T)$$

Linear Gaussian Systems: Bayes' Theorem

Exercise: Show that

$$P(x\,|\,y) = \mathrm{N}(x\,|\,\mu_{x|y}, \Sigma_{x|y})$$

where

$$\Sigma_{x|y}^{-1} = \Sigma_x^{-1} + A^T\Sigma_y^{-1}A$$

$$\mu_{x|y} = \Sigma_{x|y}\left[A^T\Sigma_y^{-1}(y-b) + \Sigma_x^{-1}\mu_x\right]$$