Class 8 – Support Vector Machines (SVM)

Classification

Pedram Jahangiry



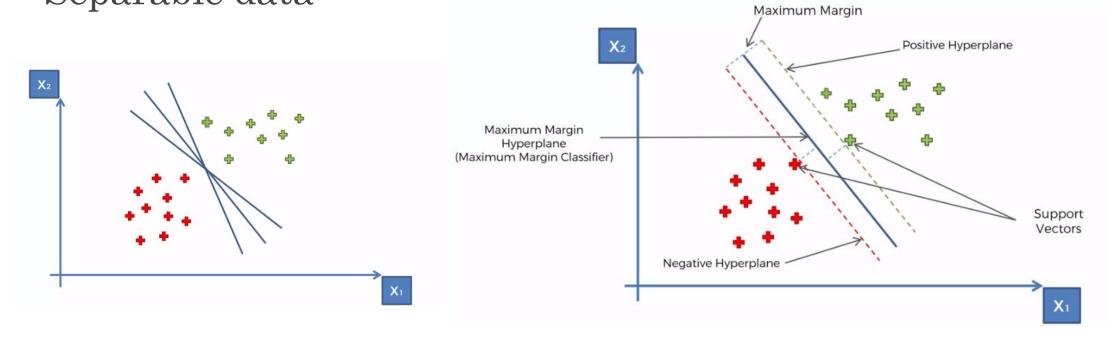
Support Vector Machines

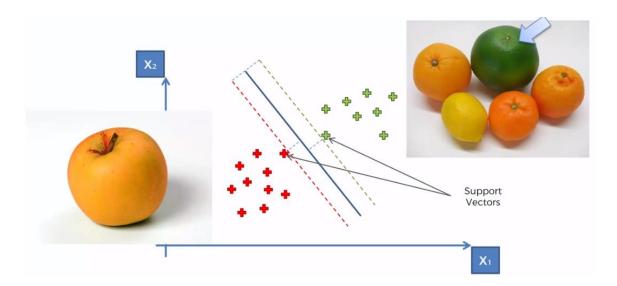
Here we approach the two-class classification problem in a direct way:

We try to find a plane that separates the classes in feature space.

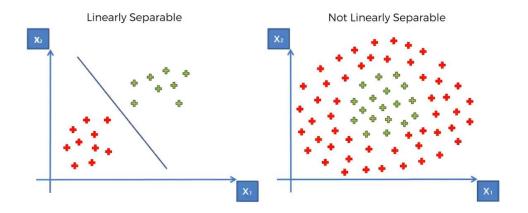
- If we cannot, we get creative in two ways:
 - 1. We soften what we mean by "separates", and
 - 2. We enrich and enlarge the feature space so that separation is possible.

Separable data

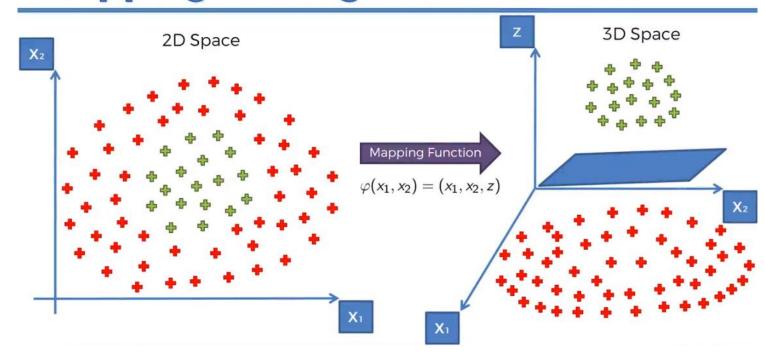




Non-Linearly Separable data

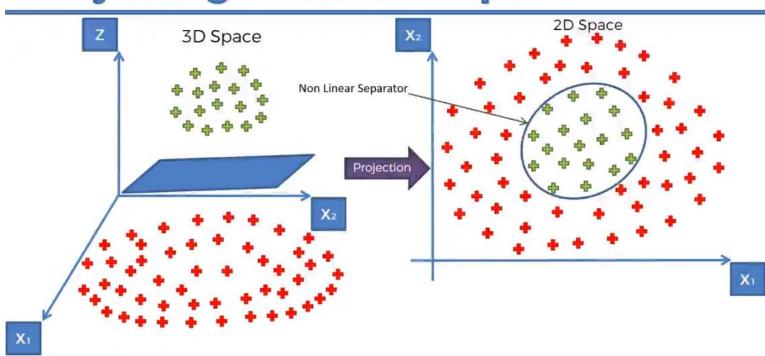


Mapping to a Higher Dimension



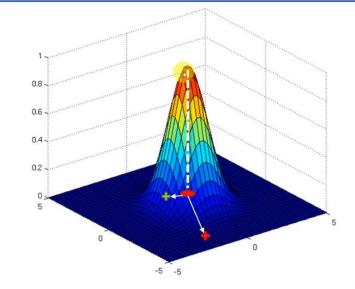
Non-Linearly Separable data (cont'd)

Projecting back to 2D Space

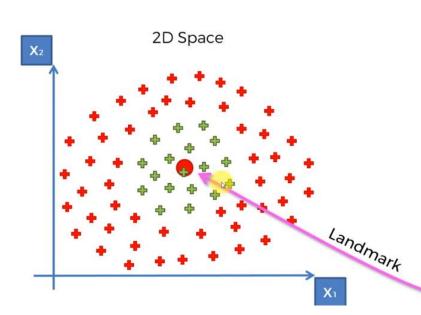


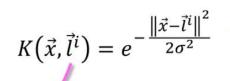
The Gaussian RBF Kernel

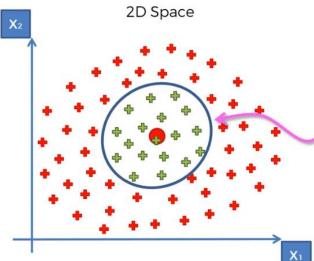
The Kernel trick!

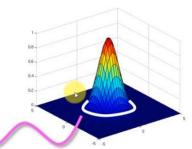


$$K(\vec{x}, \vec{l}^i) = e^{-\frac{\|\vec{x} - \vec{l}^i\|^2}{2\sigma^2}}$$



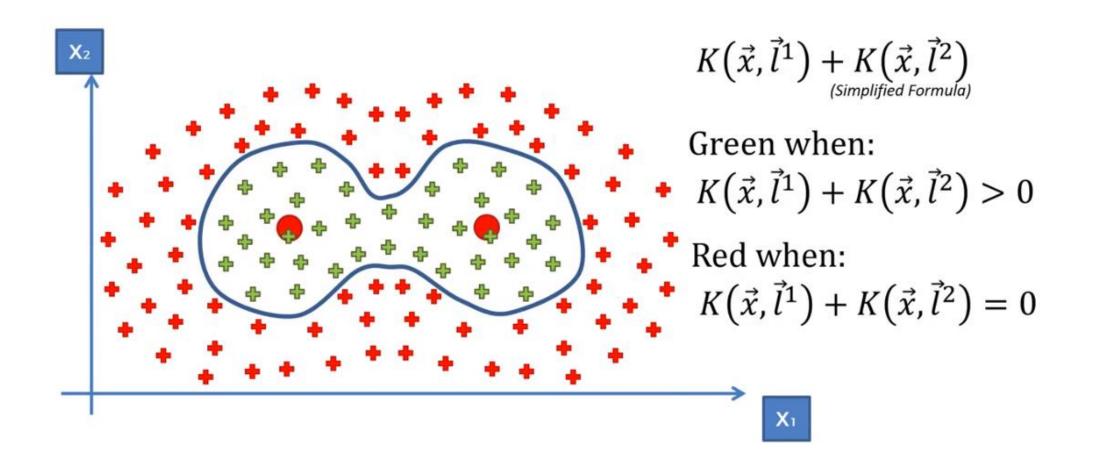




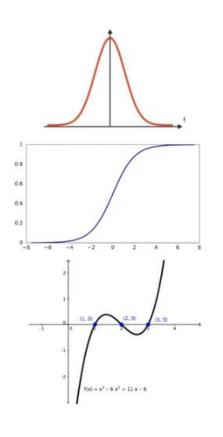


$$K(\vec{x}, \vec{l}^i) = e^{-\frac{\|\vec{x} - \vec{l}^i\|^2}{2\sigma^2}}$$

A more complex Kernel function.



Types of Kernel Functions



Gaussian RBF Kernel

$$K(\vec{x}, \vec{l}^i) = e^{-\frac{\|\vec{x} - \vec{l}^i\|^2}{2\sigma^2}}$$

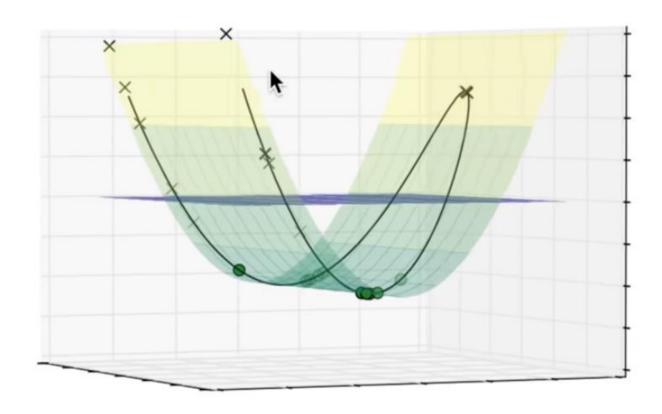
Sigmoid Kernel

$$K(X,Y) = \tanh(\gamma \cdot X^T Y + r)$$

Polynomial Kernel

$$K(X,Y) = (\gamma \cdot X^T Y + r)^d, \gamma > 0$$

Visualization of SVM



What is a Hyperplane?

- A hyperplane in p dimensions is a flat affine subspace of dimension p-1.
- In general the equation for a hyperplane has the form

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = 0$$

• In p = 2 dimensions a hyperplane is a line.

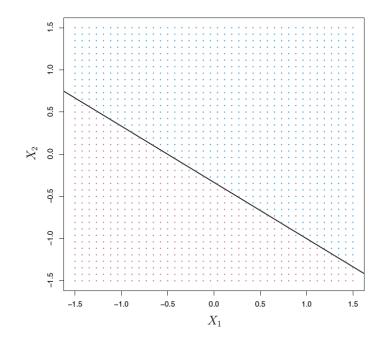
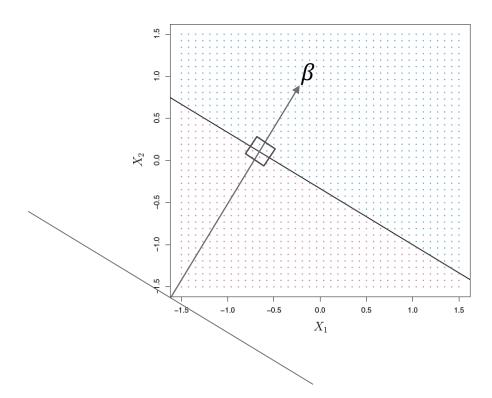


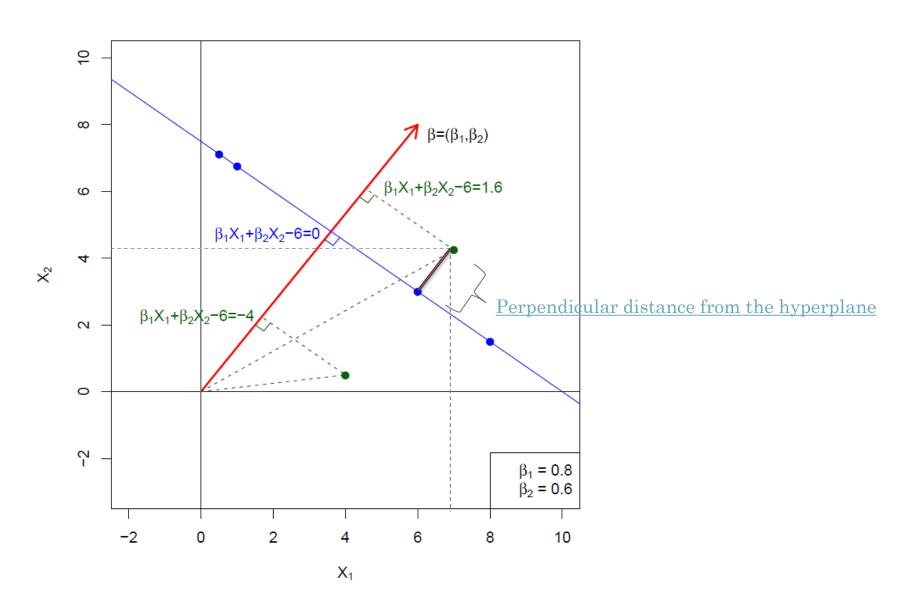
FIGURE 9.1. The hyperplane $1 + 2X_1 + 3X_2 = 0$ is shown. The blue region is the set of points for which $1 + 2X_1 + 3X_2 > 0$, and the purple region is the set of points for which $1 + 2X_1 + 3X_2 < 0$.

What is a Hyperplane?

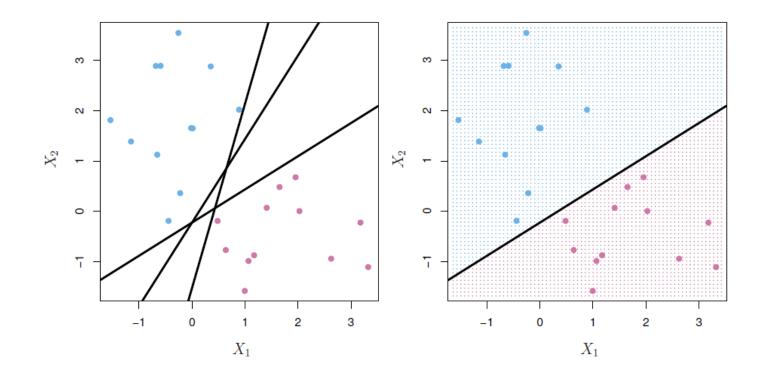
- If $\beta_0 = 0$, the hyperplane goes through the origin, otherwise not.
- The vector $\beta = (\beta_1, \beta_2, \dots, \beta_p)$ is called the normal vector it points in a direction orthogonal to the surface of a hyperplane.



Hyperplane in 2 Dimensions



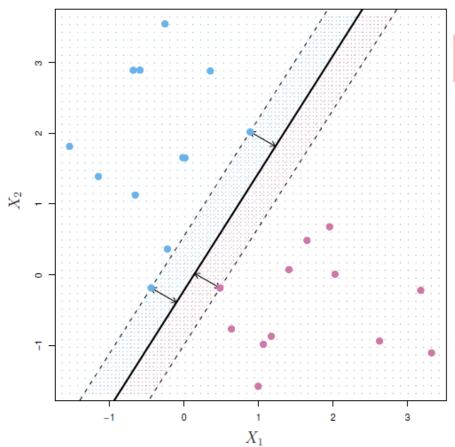
Separating Hyperplanes



- If $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$, then f(X) > 0 for points on one side of the hyperplane, and f(X) < 0 for points on the other.
- If we code the colored points as $Y_i = +1$ for blue, say, and $Y_i = -1$ for mauve, then if $Y_i \cdot f(X_i) > 0$ for all i, f(X) = 0 defines a separating hyperplane.

Maximal Margin Classifier

Among all separating hyperplanes, find the one that makes the biggest gap or margin between the two classes.



Constrained optimization problem

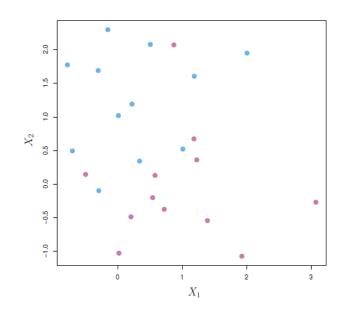
maximize
$$M$$

subject to $\sum_{j=1}^{p} \beta_j^2 = 1$,
 $y_i(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}) \geq M$
for all $i = 1, \ldots, N$.

Common problems

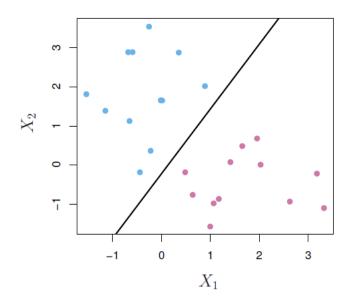
■ Non-Separable data

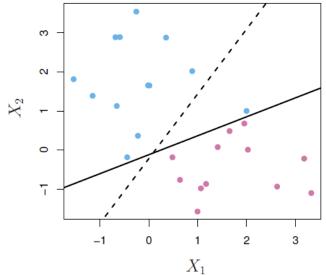
Maximal margin classifier cannot be found



■ Noisy data

Maximal margin classifier is very sensitive to outliers





Non-Separable Data

- The data in fig 9.4 are not separable by a linear boundary.
- This is often the case since N > p
- we can extend the concept of a separating hyperplane in order to develop a hyperplane that *almost* separates the classes, using a so-called *soft margin*.
- The generalization of the maximal margin classifier to the non-separable case is known as the *support vector classifier*.

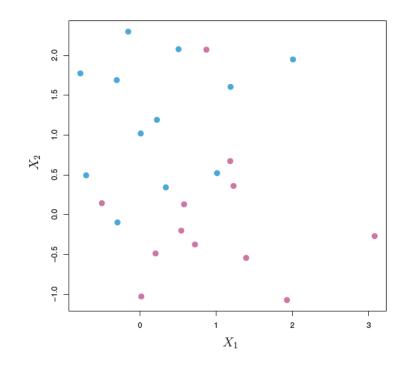


FIGURE 9.4. There are two classes of observations, shown in blue and in purple. In this case, the two classes are not separable by a hyperplane, and so the maximal margin classifier cannot be used.

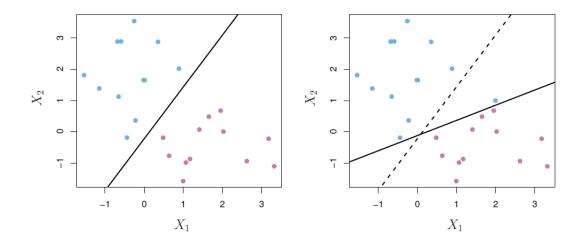
Noisy Data

In the case of noisy data, we might be willing to consider a classifier based on a hyperplane that does *not* perfectly separate the two classes, in the interest of:

- 1. Greater robustness to individual observations, and
- 2. Better classification of *most* of the training observations

That is, it could be worthwhile to misclassify a few training observations in order to do a better job in classifying the remaining observations.

The support vector classifier, sometimes called a soft margin classifier does exactly this.



Support Vector Classifier

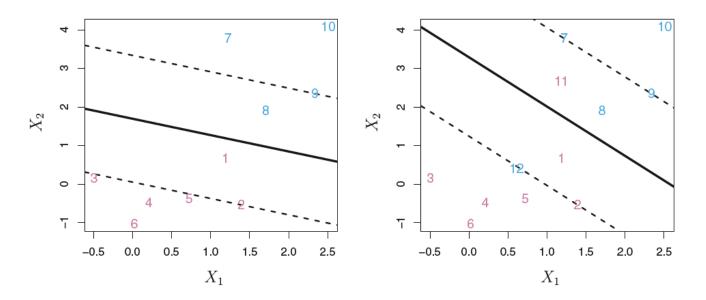


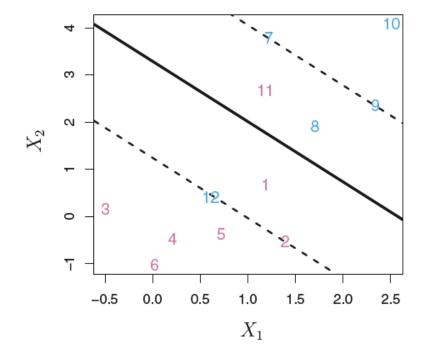
FIGURE 9.6. Left: A support vector classifier was fit to a small data set. The hyperplane is shown as a solid line and the margins are shown as dashed lines. Purple observations: Observations 3,4,5, and 6 are on the correct side of the margin, observation 2 is on the margin, and observation 1 is on the wrong side of the margin. Blue observations: Observations 7 and 10 are on the correct side of the margin, observation 9 is on the margin, and observation 8 is on the wrong side of the margin. No observations are on the wrong side of the hyperplane. Right: Same as left panel with two additional points, 11 and 12. These two observations are on the wrong side of the hyperplane and the wrong side of the margin.

Support Vector Classifier

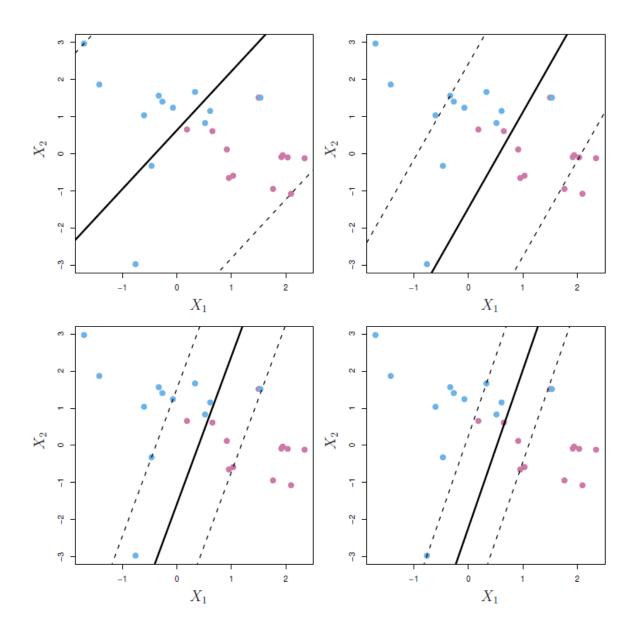
$$\max_{\beta_0, \beta_1, \dots, \beta_p, \epsilon_1, \dots, \epsilon_n, M} \text{subject to } \sum_{j=1}^p \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) \ge M(1 - \epsilon_i)$$

$$\epsilon_i \ge 0, \sum_{i=1}^n \epsilon_i \le C,$$



C is a tuning / regularization parameter

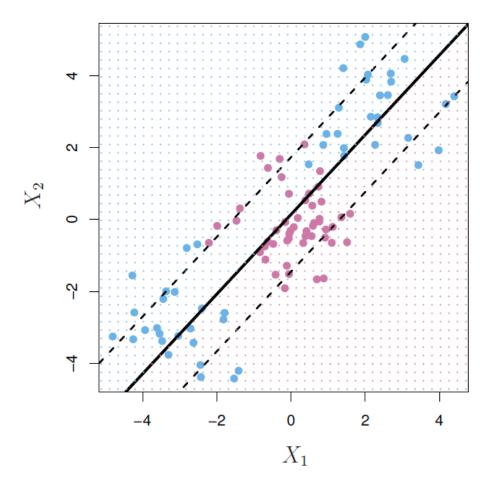


Failure of linear boundary

 Sometime a linear boundary simply won't work, no matter what value of C.

What to do?

Feature expansion (Bend the margin!)



Feature Expansion

- Enlarge the space of features by including transformations; e.g. X_1^2 , X_1^3 , X_1X_2 , $X_1X_2^2$,.... Hence go from a p-dimensional space to a M > p dimensional space.
- Fit a support-vector classifier in the enlarged space.
- This results in non-linear decision boundaries in the original space.

Example: Suppose we use $(X_1, X_2, X_1^2, X_2^2, X_1X_2)$ instead of just (X_1, X_2) . Then the decision boundary would be of the form

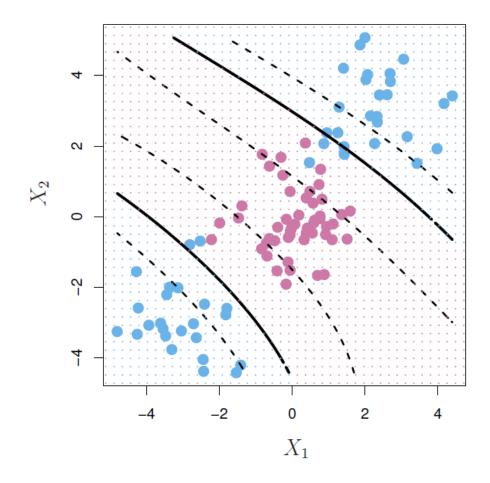
$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 = 0$$

This leads to nonlinear decision boundaries in the original space

Heading

 we use a basis expansion of cubic polynomials from 2 variables to 9.

- The support-vector classifier in the enlarged space solves the problem in the lowerdimensional space
- In a 9 dimension space, the decision boundary is a single linear boundary.
- The projections in the 2 dimensional space are multiple non-linear boundaries



$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 + \beta_6 X_1^3 + \beta_7 X_2^3 + \beta_8 X_1 X_2^2 + \beta_9 X_1^2 X_2 = 0$$

Nonlinearities and Kernels

- Polynomials (especially high-dimensional ones) get wild rather fast.
- There is a more elegant and controlled way to introduce nonlinearities in support-vector classifiers through the use of *kernels*.
- Before we discuss these, we must understand the role of inner products in support-vector classifiers.

<u>Inner products</u> and support vectors

$$\langle x_i, x_{i'} \rangle = \sum_{j=1}^p x_{ij} x_{i'j}$$
 — inner product between vectors

• The linear support vector classifier can be represented as

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$
 — n parameters

• To estimate the parameters $\alpha_1, \ldots, \alpha_n$ and β_0 , all we need are the $\binom{n}{2}$ inner products $\langle x_i, x_{i'} \rangle$ between all pairs of training observations.

It turns out that most of the $\hat{\alpha}_i$ can be zero:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i \langle x, x_i \rangle$$

 \mathcal{S} is the support set of indices i such that $\hat{\alpha}_i > 0$. See slide 14

Kernels and Support Vector Machines

- If we can compute inner-products between observations, we can fit a SV classifier. Can be quite abstract!
- Some special kernel functions can do this for us. E.g.

$$K(x_i, x_{i'}) = \left(1 + \sum_{j=1}^{p} x_{ij} x_{i'j}\right)^d$$

computes the inner-products needed for d dimensional polynomials — $\binom{p+d}{d}$ basis functions!

Try it for p = 2 and d = 2.

• The solution has the form

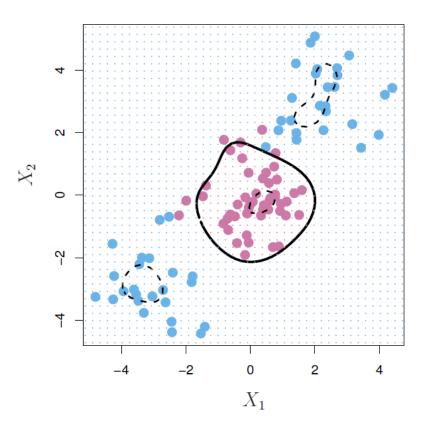
$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(x, x_i).$$

Radial Kernel

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(x, x_i)$$

$$K(x_i, x_{i'}) = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2)$$

 Radial Kernel, controls variance by squashing down most dimensions severely



SVM for more than 2 classes!

The SVM as defined works for K = 2 classes. What do we do if we have K > 2 classes?

- OVA One versus All. Fit K different 2-class SVM classifiers $\hat{f}_k(x)$, k = 1, ..., K; each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x^*)$ is largest.
- OVO One versus One. Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{k\ell}(x)$. Classify x^* to the class that wins the most pairwise competitions.

Which to choose? If K is not too large, use OVO.

Which to use: SVM or Logistic Regression

- When classes are (nearly) separable, SVM does better than LR.
- When not, Logistic Regression (LR) and SVM very similar.
- If you wish to estimate probabilities, LR is the choice.
- For nonlinear boundaries, kernel SVMs are popular. Can use kernels with Logistic Regression too, but computations are more expensive.

SVM in Python

- Find the SVM Sklearn documentation here
- Blackbox version of SVM in python:

```
from sklearn import svm
X = [[0, 0], [1, 1]]
y = [0, 1]
clf = svm.SVC(gamma='scale')
clf.fit(X, y)
```

```
>>> from sklearn import svm
>>> X = [[0, 0], [1, 1]]
>>> y = [0, 1]
>>> clf = svm.SVC(gamma='scale')
>>> clf.fit(X, y)
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='scale', kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```