NYC DATA SCIENCE ACADEMY

Python Machine Learning Class 4: Classification 2

Data Science Bootcamp

Outline

- **Support Vector Machines**
  - Separating Hyperplanes
  - The Support Vector Classifier
  - Kernels
- **Tree-Based Methods**
  - Decision Trees
  - Bagging and Random Forests

Support Vector Machines

- **Support vector machines** (SVMs) are supervised learning methods used for classification analysis.
- Unlike linear discriminant analysis or logistic regression, **SVMs** approach the two-class classification problem in a direct way: construct linear decision boundaries, by explicitly separating the data in two different classes as well as possible.
- The decision boundaries are called **hyperplanes** in the feature space.

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Hyperplanes

- A **hyperplane** of a *p-dimensional* space *V* is a subspace of dimension *p*-1, which can be described with a single linear equation of the form (in Cartesian coordinates):

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

- It is more convenient to write the equation above in matrix form:

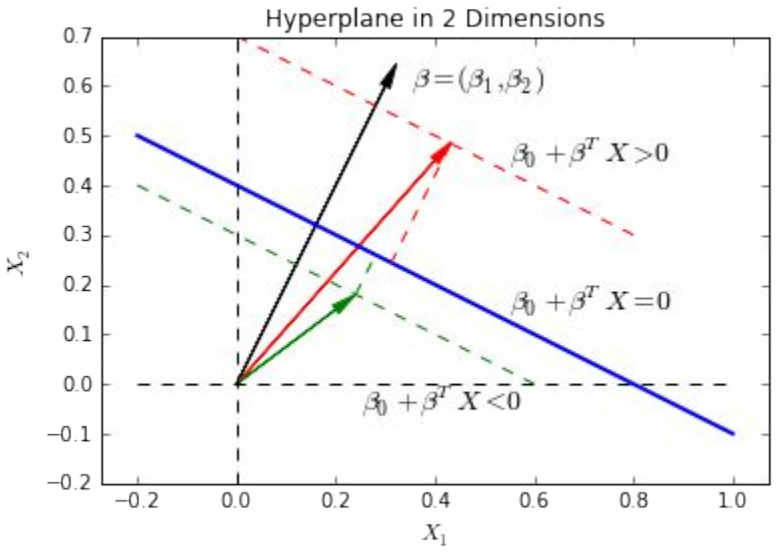
$$\beta_0 + X\beta^T$$

where $\beta = (\beta_1, \ldots \beta_p)$ and $X = (X_1, \ldots X_p)$ are *p-dimensional* vectors.

- In a 2-dimensional space, a hyperplane is a line and in a 3-dimensional space it is a plane.

Hyperplanes

- The coefficient vector β is the **normal vector** - a vector orthogonal to the surface of that hyperplane.
- In some cases we need to work with the normalized form: $\beta^* = \beta/|\beta|$ or equivalently, to require that $\sum_i^p \beta_i^2 = 1$.



Hyperplanes

- Here are some properties:
  - For any point x_0 in the hyperplane,

$$\beta^T x_0 = -\beta_0$$

  - The signed distance of any point x to the hyperplane is given by:

$$f(x) = \frac{1}{|\beta|}(\beta^T x + \beta_0)$$

Separating Hyperplanes

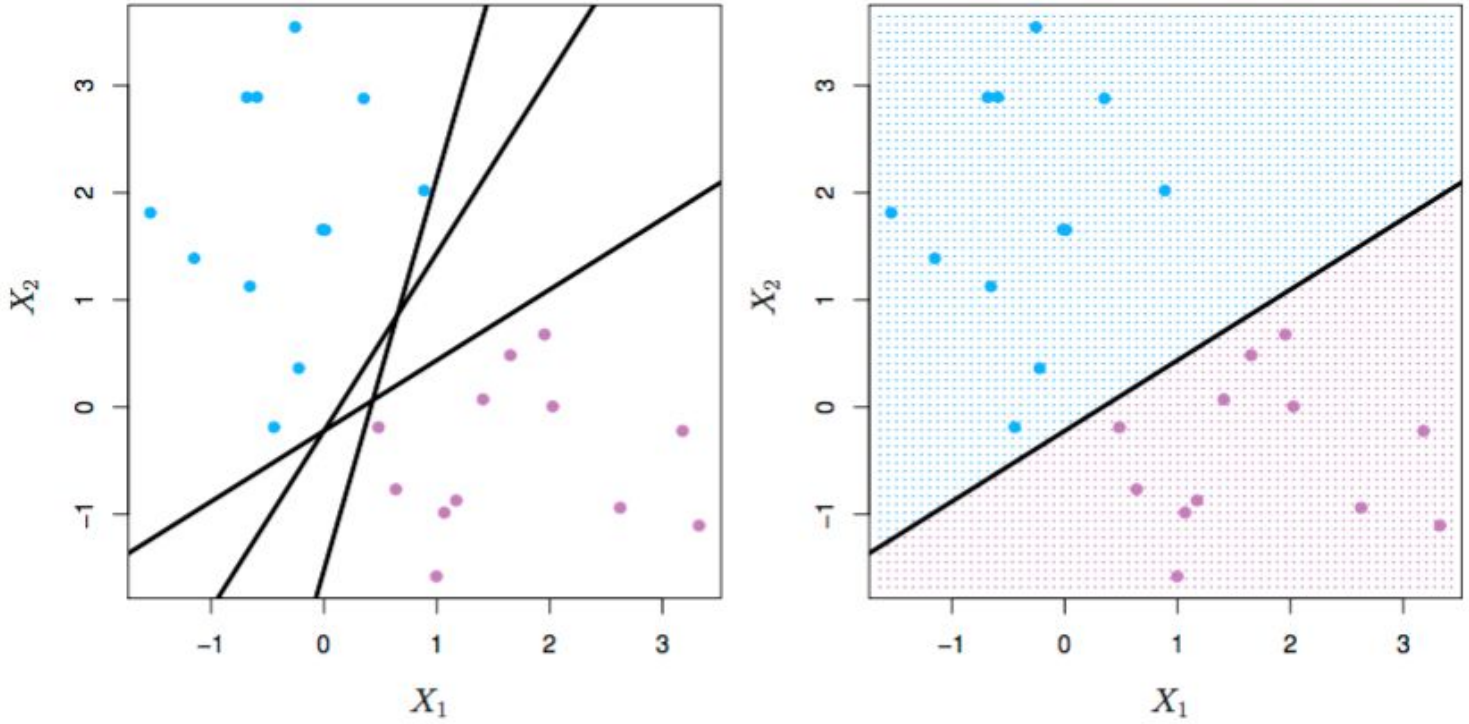
- If we assume that the data can be well *separated by a hyperplane* defined by $f(X) = \beta_0 + \beta^T X = 0$, then:
  - $f(X) > 0$, for points on one side of the hyperplane,
  - $f(X) < 0$, for points on the other side.
- If we code the two classes as:
  - $y = 1$, for $f(X) > 0$, and
  - $y = -1$, for $f(X) < 0$,

  then the distance times the class becomes positive:

$$y_i \cdot f(X_i) > 0$$

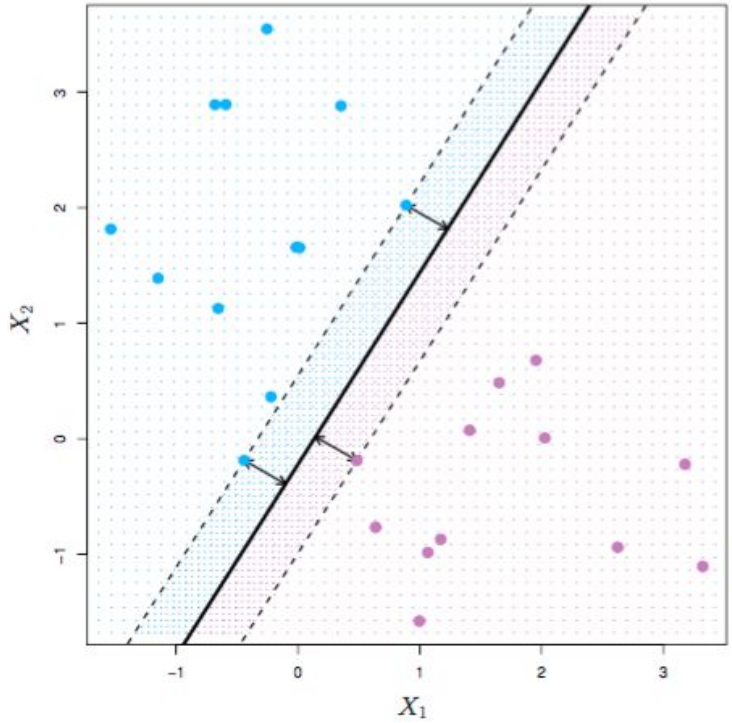
Separating Hyperplanes

- The figure on the left shows three of the infinitely many possible separating lines; the figure on the right shows the values of function $f(X)$ on the two sides of the hyperplane are of opposite signs.



Optimal Separating Hyperplanes

- Goal: to maximize the **margin**, defined by the distance from the data point to a hyperplane, between the two classes on the training data.



- The data points that are used to determine the margins are called *support vectors*.

Maximal Margin Classifier

- The optimal separating hyperplane leads to a constrained optimization problem on margin *M*:

$$\max_{\beta_0, |\beta|=1} M$$

$$\text{subject to } y_i(x_i^T\beta + \beta_0) \geq M, i = 1, ..., N$$

- The conditions ensure that the distances from all the points to the decision boundary defined by β and β_0 are at least *M*, and we seek the largest *M* by varying the parameters.
- We can get rid of the constraint $|\beta| = 1$ by replacing the condition with:

$$y_i(x_i^T\beta + \beta_0) \geq M|\beta|$$

Maximal Margin Classifier

- For any β and β_0 satisfying the inequalities, any positively scaled multiple satisfies them too.
- If we set $|\beta| = 1/M$, we can rephrase the problem to a more convenient form by dropping the norm constraint on β:

$$\min_{\beta_0,\beta} \frac{1}{2}|\beta|^2$$

$$\text{subject to } y_i(x_i^T\beta + \beta_0) \geq 1$$

- This is a convex quadratic problem, and can be solved efficiently.

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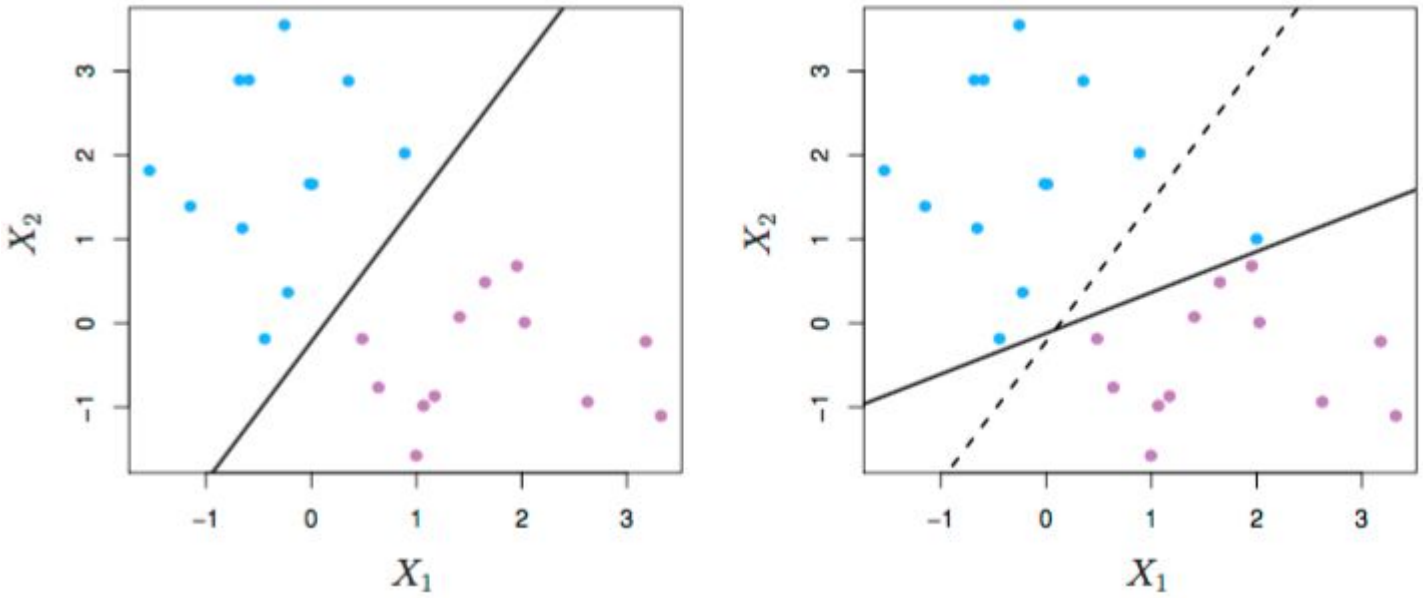
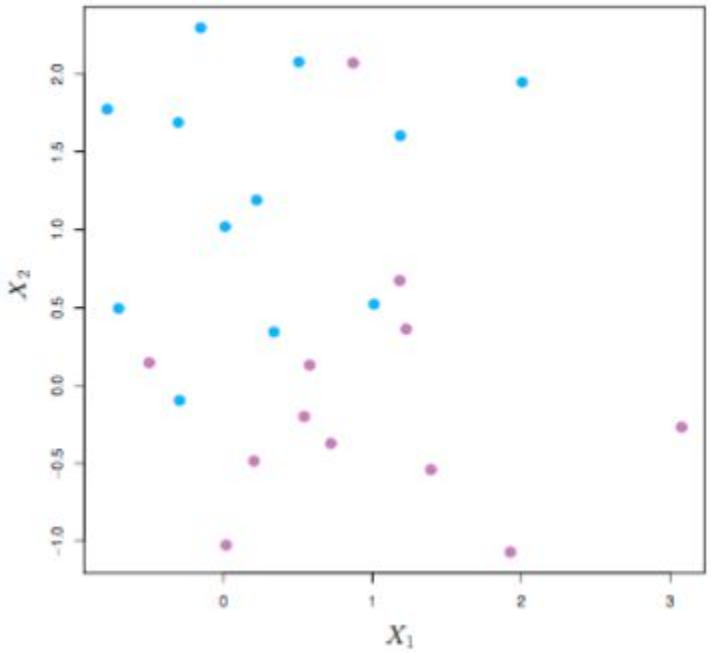
Noisy Data

- The technique for constructing an optimal separating hyperplane can be applied to cases of two perfectly separated classes.
- However, sometimes the data can be noisy, which can lead to a poor solution for the maximal margin classifier. (Note the one additional blue point on the right.)



Non-separable Data

- Even worse, quite often the data is not separable by a linear boundary.



- What shall we do?

The Support Vector Classifier

- To tolerate noise and errors, we still maximize *M* but meanwhile allow some points to be on the wrong side of the hyperplane.
- We introduce "slack" variables $\epsilon = (\epsilon_1, \ldots \epsilon_N)$ with constraints $\epsilon_i \geq 0$ and $\sum_i \epsilon_i \leq \text{Const}$, and modify the optimization problem to be:

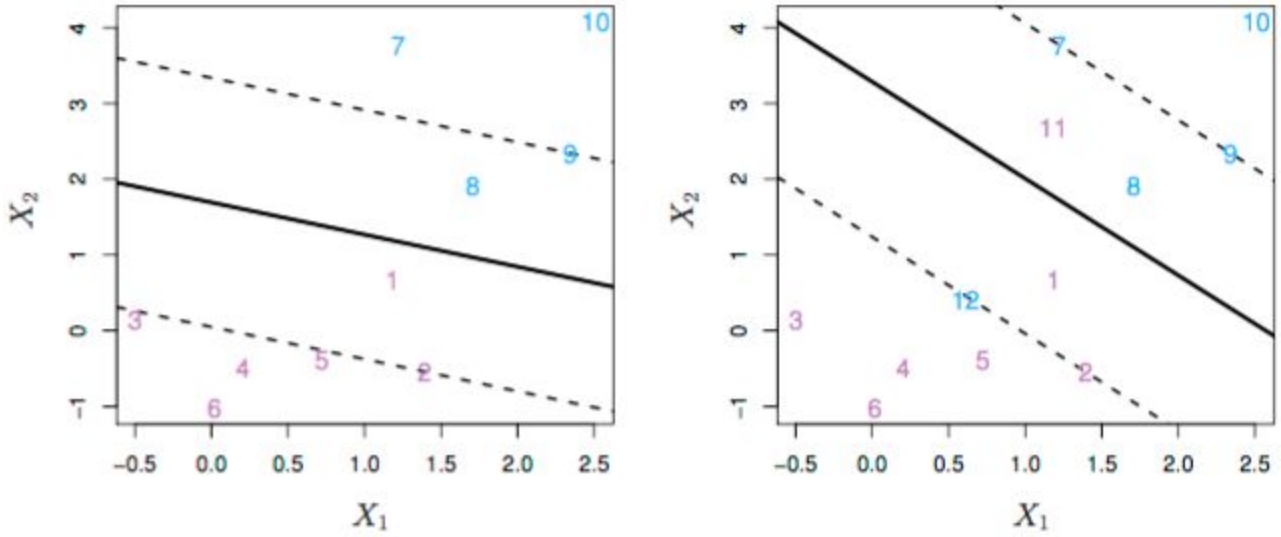
$$\max_{\beta_0, \epsilon, |\beta|=1} M$$

$$\text{subject to } \begin{cases} y_i(x_i^T \beta + \beta_0) \geq M(1 - \epsilon_i) \\ \epsilon_i \geq 0, \text{ and } \sum_i \epsilon_i \leq \text{Const} \end{cases}$$

  - ϵ_i are proportional to the amount by which the prediction is on the wrong side of their margin.
  - Misclassifications occur when $\epsilon_i > 1$.

The Support Vector Classifier

- The effect of the data points that fall into the margin will be penalized by the slack variable ϵ.



The Support Vector Classifier

- Computationally, it's convenient to use the equivalent form:

$$\min_{\beta_0,\beta}\left(\frac{1}{2}|\beta|^2 + C\sum_{i=1}^{N}\epsilon_i\right)$$

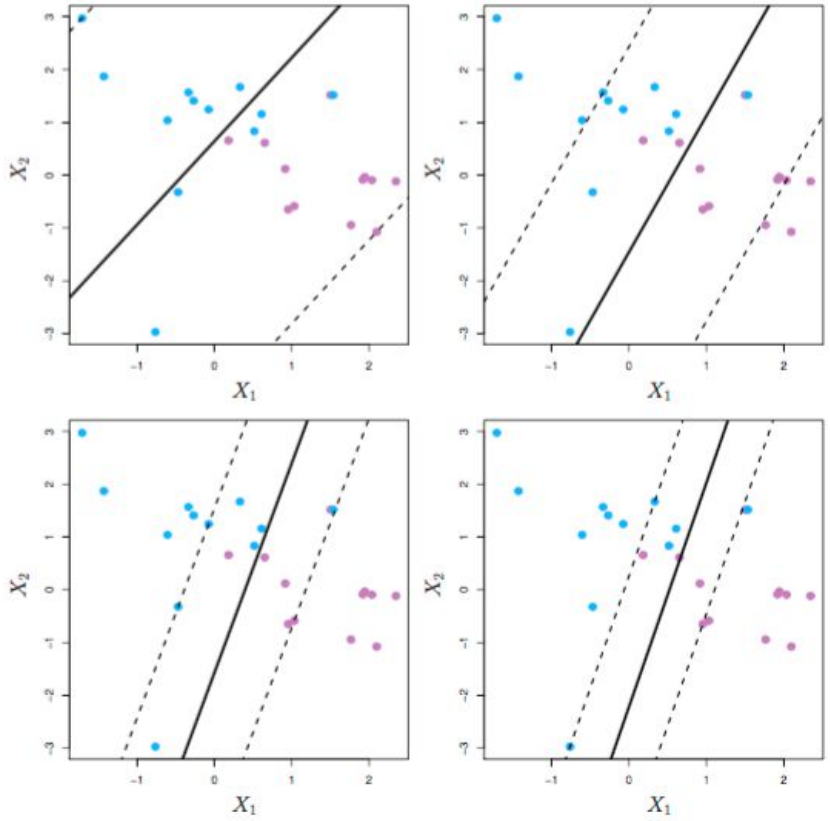
$$\text{subject to } \begin{cases} y_i(x_i^T\beta + \beta_0) \geq 1 - \epsilon_i \\ \epsilon_i \geq 0 \end{cases}$$

  where *C* is the penalty parameter of the error term.

- The maximum margin classifier corresponds to $C = \infty$.

The Support Vector Classifier

- If *C* is close to 0 then we have a *wide*, *soft margin*.
- If *C* is large then we are close to the *hard-margin* formulation.



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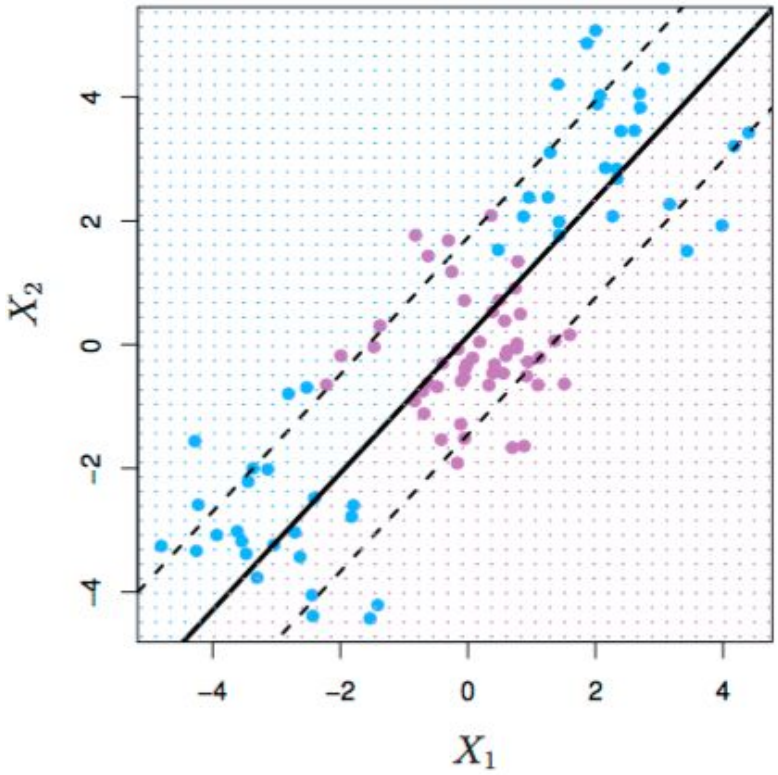
Beyond Linearity

- The support vector classifier described so far finds linear boundaries in the feature space.
- In reality, it's very unlikely that the true boundary is actually linear in *X*.



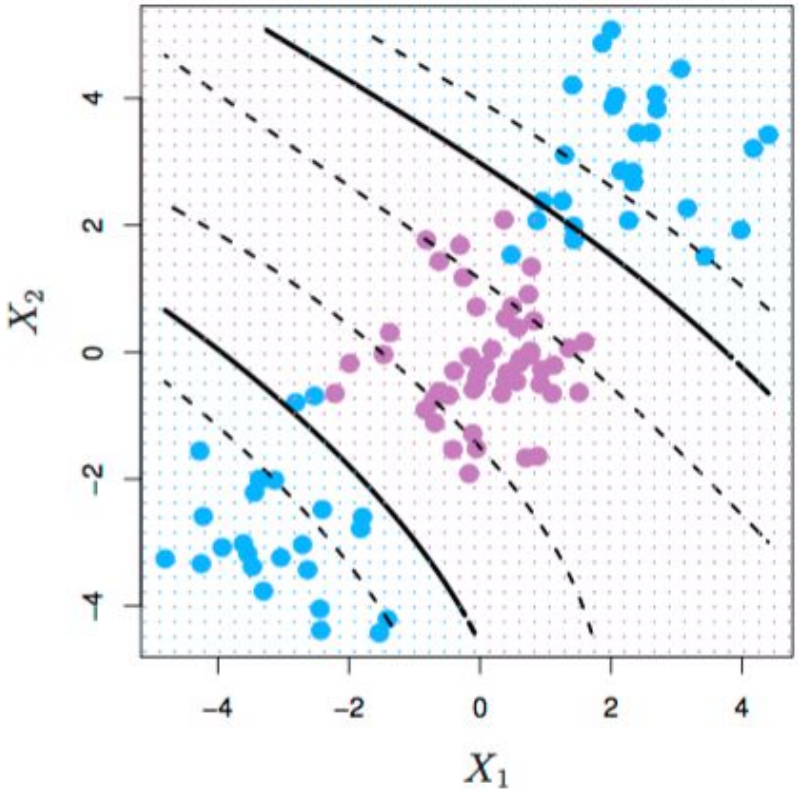
Basis Expansions

- If a linear boundary fails, we need to move beyond linearity.
- The core idea can be summarized as:
  - enlarge the features *X* using basis expansions such as polynomials,
  - use linear models in the enlarged space of derived input features,
  - then translate to nonlinear boundaries in the original space.
- Example:
  - We enlarge the feature space (X_1, X_2) to $(X_1, X_2, X_1^2, X_2^2, X_1X_2)$
  - The boundary is then determined by:

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

Basis Expansions

- Back to the previous example, a basis expansion of cubic polynomials will create a nonlinear boundary in the lower-dimensional feature space.



Kernels

- In general, the idea for nonlinearity is to map the feature *X* to a high dimensional space by some mapping functions *h*(*X*).
- Notice that only the inner-products of the input vectors play a role in the optimization problem. A more elegant and controlled way to have nonlinear boundaries is to use kernels.

  (The proof of this requires us to derive a so called *Lagrangian dual function* which is beyond the scope of this course.)
- We first introduce the notation for inner product of two vectors:

$$\langle x, x' \rangle = \sum_{i=1}^{p} x_i x'_i$$

Kernels

- It can be mathematically proven that the linear vector classifier can be represented as:

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

where α_i are parameters subject to $0 < \alpha_i < C$. For the data points that are not support vectors, their α_i are equal to 0.

- Since the support vector classifiers involve the mapping $h(X)$ only through inner products, instead of specifying the transformation, we only need to provide a kernel function

$$K(x, x') = \langle h(x), h(x') \rangle$$

Kernels

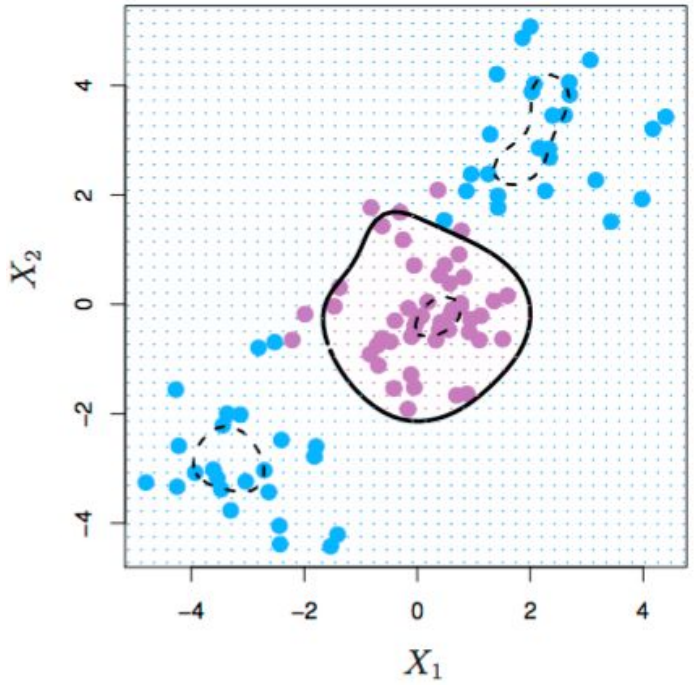
- Some popular choices for kernel functions for SVMs are:
  - *d*th-Degree polynomial: $K(x, x') = (1 + \langle x, x' \rangle)^d$
  - Radial basis: $K(x, x') = \exp(-\gamma |x - x'|)^2$
- Using the kernel function, the solution now can be written as:

$$f(x) = \beta_0 + \sum_{i=1}^{N} \alpha_i y_i K(x, x_i)$$

- The parameter *C*, which gives the upper bound of α_i, is now in an enlarged feature space, since perfect separation is often achievable.

Kernels

- The figure below shows the solution with Radial Kernel.



Hands-on Session

- Please go to the **"SVM in Scikit Learn"** in the lecture code.

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Tree-Based Methods

- Tree based methods partition the feature space into a set of rectangular regions and then fit a simple model (usually the mean in that region) in each subregion.
- Methods we'll talk about include
  - Decision Trees
  - Bagging and Random Forests

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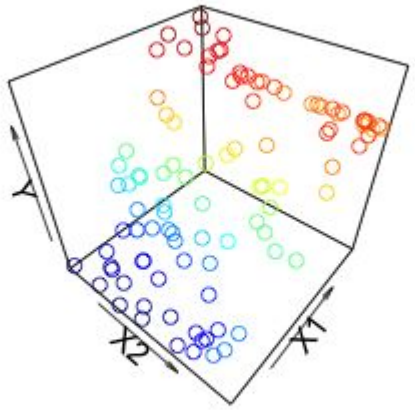
Decision Trees

- Decision trees partition the feature space into a set of simple rectangular regions.
- **Decision trees** can be used for both regression and classification problems.
- We'll first consider a regression problem and then focus on classification.

Decision Trees - Regression

- Let's consider a regression problem with predictors X_1 and X_2 and continuous response Y.



- To fit a decision tree, we divide the feature space into non-overlapping regions and in each region R_j we model the response by its mean $\hat{y}_{Rj}$.
- The goal is to find rectangular regions that minimize the RSS:

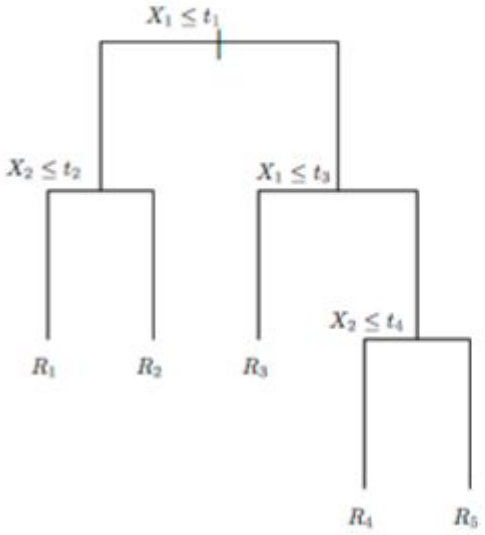
$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

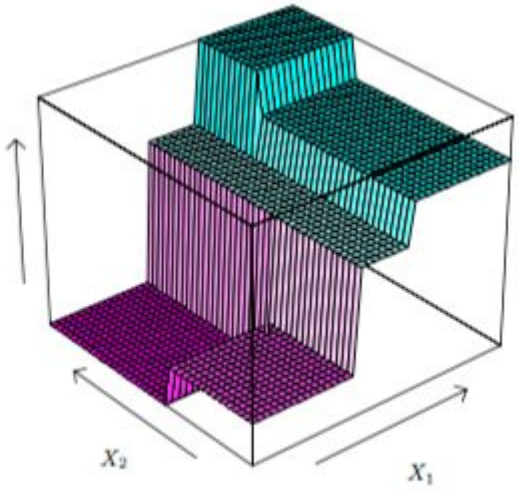
Decision Trees - Regression

- To simplify the process, we restrict the partition to recursive binary splitting.
- We first select the predictor X_j and the cutpoint that splits the dataset to the greatest reduction in *RSS*.
- Then we repeat the process within each resulting region (not the entire predictor space) to reduce the overall *RSS*.
- We continue the process recursively until we reach a stopping criterion.
- Finally the decision tree partitions the feature space into a set of regions, each of which is modeled by the mean responses of the data points that fall in that region.

Decision Trees - Regression

- A five-region splitting is achieved.
  1. split the overall dataset at $X_1 = t_1$;
  2. split the region $X_1 < t_1$ at $X_2 = t_2$ and the region $X_1 > t_1$ at $X_1 = t_3$;
  3. split the region $X_1 > t_3$ at $X_2 = t_4$.





Decision Trees - Classification

- Similar to regression, we use the same procedure to fit a classification tree.
- For regression we used the *RSS* to determine the splitting, what should we use for classification? Two commonly used metrics are:
  - **Gini impurity**: the probability a randomly chosen item from the set would be incorrectly labeled if it were randomly labeled according to the distribution of labels in the subset.

$$I_G(f) = \sum_{i=1}^{m} f_i(1 - f_i)$$

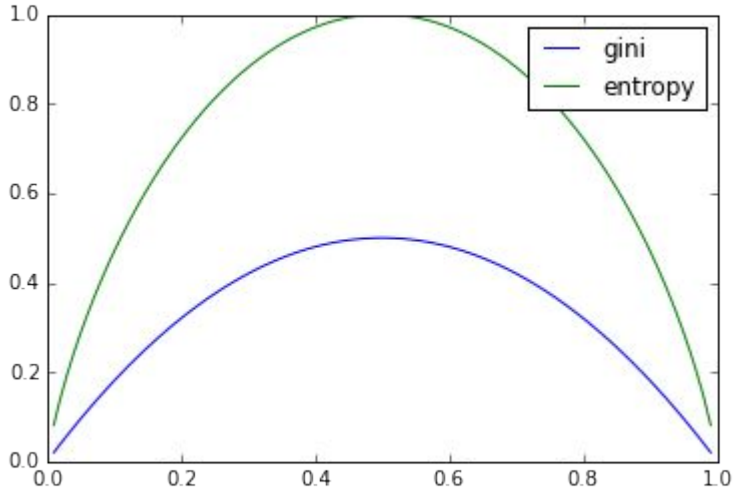
  - **Information gain** which is based on the concept of *entropy*

$$I_E(f) = -\sum_{i=1}^{m} f_i \log_2(f_i)$$

where f_i is the fraction of items labeled with i in the set and $\sum f_i = 1$.

Decision Trees - Gini impurity and Information Gain

- For a binary classification problem, the gini impurity and entropy can be visualized as:



where the horizontal axis refers to the proportion of one of the classes.

Decision Trees - Gini impurity and Information Gain

- Gini impurity is a measure of node purity.
- When using gini impurity as the metric for splitting, our goal is to have two subregions as pure as possible by reducing the weighted sum of gini impurities.
- Similarly, when using entropy we want the information gain as great as possible after the splitting.
- In practice, the behavior of the two metrics are very similar.

Decision Trees

- If we keep splitting the regions until there's only one class in each region, we may end up with *overfitting*: high accuracy on the training dataset, but poor prediction performance.
- A decision tree with fewer splits may lead to lower variance and better interpretation.
- To prevent overfitting, we can set the threshold to:
  - the max depth of the tree,
  - the minimum number of observations to split, or
  - the minimum number of observations in each region.

Hands-on Session

- Please go to the **"Decision Tree in Scikit Learn"** in the lecture code.

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Decision Trees Pros and Cons

- Pros:
  - Interpretability: easier to explain than most other regression methods.
  - Easy to handle qualitative predictors.
  - Can be displayed graphically.
- Cons:
  - Instability: a small change in the data may result in very different splits.
  - Predictive accuracy usually not as good as other approaches.
- By aggregating many decision trees, the predictive performance can be improved substantially.

Bagging on Decision Trees

- By averaging a collection of bootstrap (repeated) samples from the training data set, we can dramatically reduce the variance of trees, leading to improved prediction. This is called **bagging**.
  - Generate *B* bootstrapped training datasets.
  - For each test observation, we record the class predicted by each of the B trees, and choose the majority.
  - The overall prediction is the most commonly occurring class among the B predictions.

Random Forests

- The idea for bagging of decision trees is to average many noisy trees and hence reduce the variance.
- However, since each tree generated in bagging is identically distributed, the expectation of the averages is the same as the expectation of any one of them. This means the bias will not be improved.
- Random forests is a modification of bagging that builds a large collection of de-correlated trees, and then averages them.

Random Forest Algorithm

1. Build bootstrapped training samples of size *N* from the training data.
2. For each sample select *m* out of *p* variables randomly.
3. Train a random-forest tree to each of the bootstrapped datasets with only the *m* selected variables.
4. To use the ensemble of trees for classification prediction, we pick the majority vote from the *N* trees.

Hands-on Session

- Please go to the **"Random Forest in Scikit Learn"** in the lecture code.