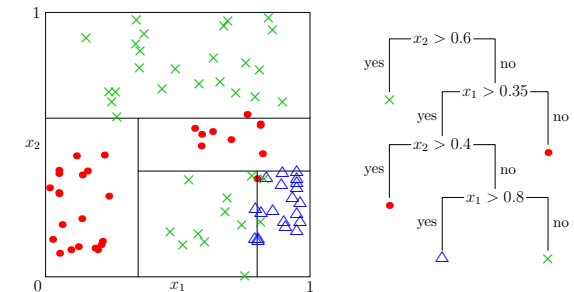


Decision Trees, Averaging, Bagging

1. Decision Trees
2. Bagging



Removing Variance By Averaging

- We can reduce the variance and hence improve our generalisation error by averaging over different learning machines
- There are a number of different techniques for doing this that go by the name of **ensemble methods** or **ensemble learning**
- This trick can be used with many different learning machines, but is clearly most practical for machine that can be trained quickly
- (nevertheless, even for deep learning taking the average response of many machines is usually done to win competitions)

Ensembling of Decision Trees

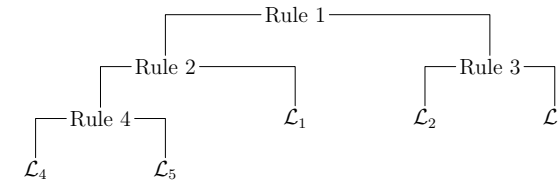
- One set of algorithms where ensembling are common place are decision trees
- These are particularly good for handling messy data
 - ★ categorical data
 - ★ mixture of data types
 - ★ missing data
 - ★ large data sets
 - ★ multiclass
- In many competitions ensembled trees, particularly *random forests* and *gradient boosting* beat all other techniques

Decision Trees

- A decision tree builds a binary tree to partition the data, $\mathcal{D} = \{(\mathbf{x}_i, y_i) | i = 1, \dots, m\}$, into the leaves of the tree
- Each decision rule depends on a single feature
- At each step the rule is chosen that maximises the “purity” of the leaf nodes
- Decisions can be made on numerical values or categories

Partitioning

- Consider a classification problem with examples (\mathbf{x}, y) belonging to some classes $y \in \mathcal{C}$
- The data is partitioned by the tree into leaves



- The proportion of data points in leaf \mathcal{L} belonging to class c is

$$p_c(\mathcal{L}) = \frac{1}{|\mathcal{L}|} \sum_{(\mathbf{x}, y) \in \mathcal{L}} \mathbb{I}[y = c]$$

where $\mathbb{I}[y = c] = 1$ if $y = c$ and 0 otherwise

Leaf Purity

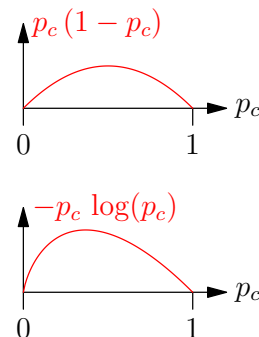
- Two different purity measures, $Q_m(\mathcal{L})$, for a leaf node \mathcal{L} are commonly used

★ Gini index

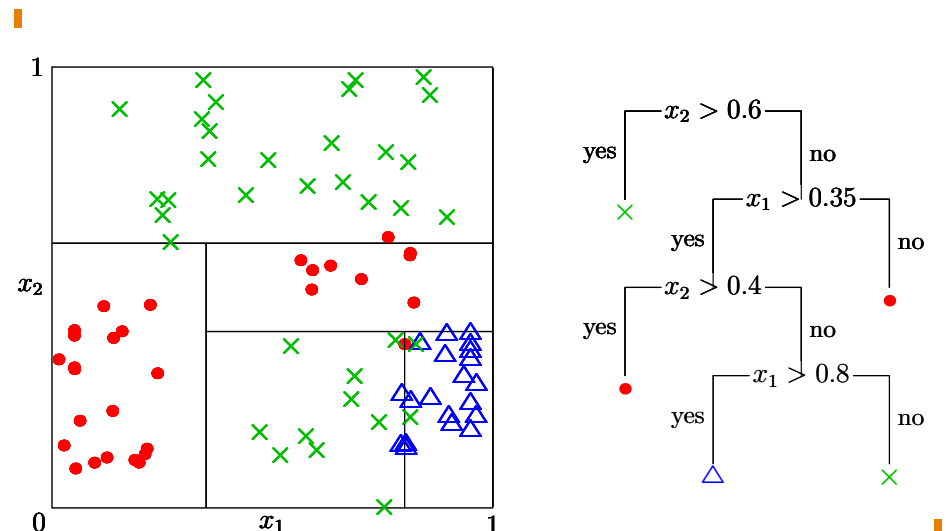
$$Q_m^g(\mathcal{L}) = \sum_{c \in \mathcal{C}} p_c(\mathcal{L}) (1 - p_c(\mathcal{L}))$$

★ Cross-entropy

$$Q_m^e(\mathcal{L}) = - \sum_{c \in \mathcal{C}} p_c(\mathcal{L}) \log(p_c(\mathcal{L}))$$

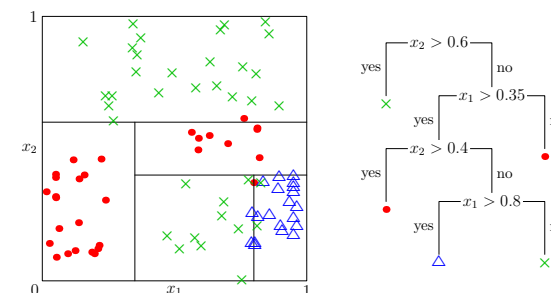


Building Decision Trees



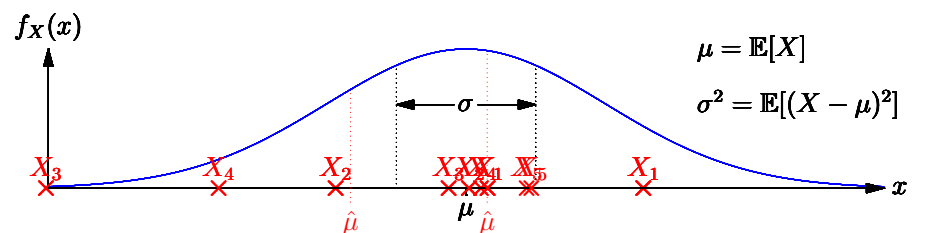
- Decision trees are very useful for exploring new data sets—the tree shows what features are most important
- Decision trees can also be used for regression problems
 - ★ Approximate function by a series of rules
 - ★ Reduce variance between data points assigned to leaf nodes
- CART is a classic implementation that builds **C**lassification **A**nd **R**egression **T**rees
- Decision trees depend strongly on the early decisions and so vary a lot for slightly different data sets—high variance

- Decision Trees
- Bagging



Error In The Means

- By taking the mean over many samples we can reduce the variance and thus improve our generalisation performance
- To get a feel for this consider estimating the mean of a random variable, X , from a number of samples ($n = 5$ in the example below)



Mean and Variance

- The expected value of the mean, $\hat{\mu}_n$, of n random **independent** variables, X_i , is the expected value $\mu = \mathbb{E}[X_i]$

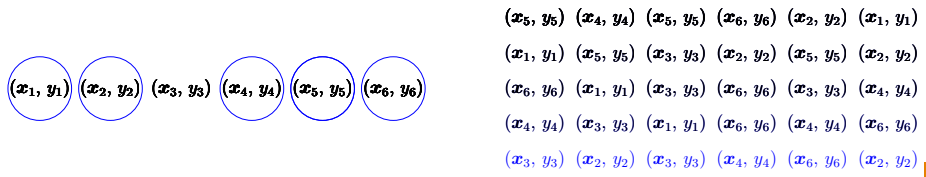
$$\mathbb{E}[\hat{\mu}_n] = \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n X_i\right] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[X_i] = \frac{1}{n} \sum_{i=1}^n \mu = \mu$$

- The variance is $\mathbb{E}[(\hat{\mu}_n - \mu)^2]$ or equivalently

$$\begin{aligned} \frac{1}{n^2} \mathbb{E}\left[\left(\sum_{i=1}^n (X_i - \mu)\right)^2\right] &= \frac{1}{n^2} \mathbb{E}\left[\sum_{i=1}^n (X_i - \mu)^2 + \sum_{i=1}^n \sum_{\substack{j=1 \\ j \neq i}}^n (X_i - \mu)(X_j - \mu)\right] \\ &= \frac{1}{n^2} \sum_{i=1}^n \left(\mathbb{E}[(X_i - \mu)^2] + \sum_{\substack{j=1 \\ j \neq i}}^n \mathbb{E}[X_i - \mu] \mathbb{E}[X_j - \mu]\right) \\ &= \frac{1}{n^2} \sum_{i=1}^n \sigma^2 = \frac{1}{n} \sigma^2 \end{aligned}$$

Bootstrap Aggregation (Bagging)

- To reduce the variance in a learning machine (such as a decision tree) we can average over many machines
- To average many machines they must learn something different
- We only have one data set, but we can resample from the data set to make them look a bit different—this is known as **bootstrapping**



Performance of Bagging

- Bootstrapping is an early form of data augmentation
- For classification we get our different machines to vote
- For regression we can average the prediction of different machines
- Bagging improves the performance of decision trees
- However, we can usually do better using Boosting
- This is because our decision trees are correlated

Variance of Positive Correlated Variables

- If we calculate the variance of the mean of positively correlated variables with correlation ρ we find

$$\frac{1}{n^2} \mathbb{E} \left[\left(\sum_{i=1}^n X_i - n\mu \right)^2 \right] = \rho\sigma^2 + \frac{1-\rho}{n}\sigma^2$$

$$(\rho = \mathbb{E}[(X_i - \mu)(X_j - \mu)] / \sigma^2)$$

- As $n \rightarrow \infty$ the second term vanishes, but we are left with the first term
- If we want to do well we need our learning machines to be unbiased and decorrelated

Random Forest

- In random forests we average much less correlated trees
- To do this for each tree we choose a subset of $p' \ll p$ of the features on which to split the tree
- Typically p' can range from 1 to \sqrt{p}
- The trees aren't that good, but are very decorrelated
- By averaging over a huge number of trees (order of 1000) we typically get good results
- Random Forest won (wins?) many competitions

Lessons

- Ensemble methods have proved themselves to be very powerful■
- They work by averaging over different machines, trying to reduce their variance■
- Here the variance comes from forcing the machines to learn different functions using Bootstrap Aggregation■
- Tend to work best with very simple models (true of random forest and boosting)■—seems to reduce over-fitting■
- Random forest is very powerful, but gradient boosting is competitive■