Decision Trees

CDS, NYU

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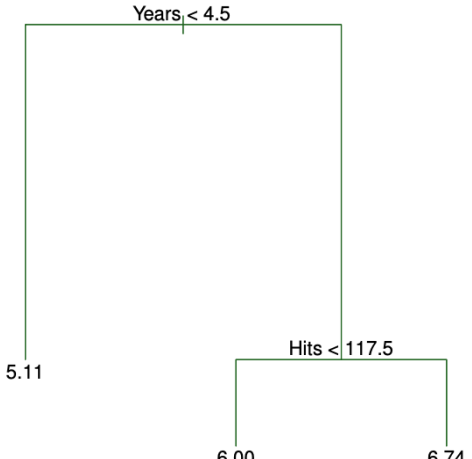
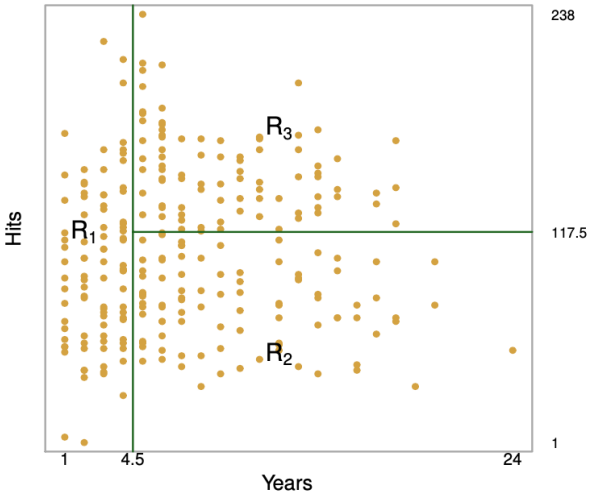
Today's lecture

- Our first inherently non-linear classifier: decision trees.
- Ensemble methods: bagging and boosting.

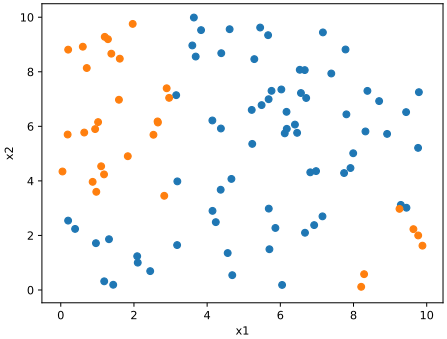
Decision Trees

Regression trees: Predicting basketball players' salaries



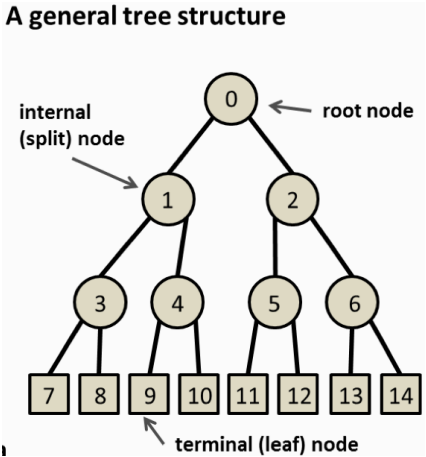


Classification trees



- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



From Criminisi et al. MSR-TR-2011-114, 28 October 2011.

- We focus on *binary* trees (as opposed to multiway trees where nodes can have more than two children)
- Each node contains a subset of data points
- The data splits created by each node involve only a *single* feature
- For continuous variables, the splits are always of the form $x_i \leqslant t$
- For discrete variables, we partition values into two sets (not covered today)
- Predictions are made in terminal nodes

Constructing the tree

Goal Find boxes $R_1, \ldots, R_J$ that minimize $\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$, subject to complexity constraints.

Problem Finding the optimal binary tree is computationally intractable.

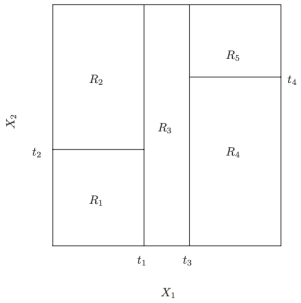
Solution Greedy algorithm: starting from the root, and repeating until a stopping criterion is reached (e.g., max depth), find the non-terminal node that results in the "best" split

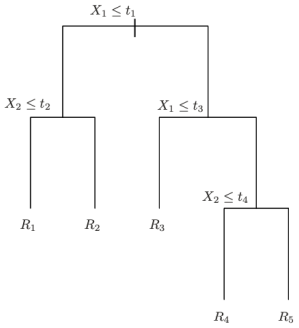
- We only split regions defined by previous non-terminal nodes

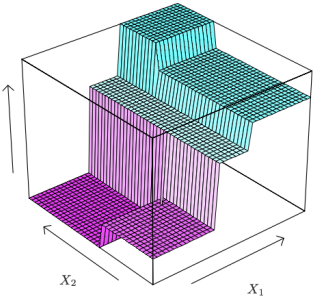
Prediction Our prediction is the mean value of a terminal node: $\hat{y}_{R_m} = \text{mean}(y_i \mid x_i \in R_m)$

- A greedy algorithm is the one that make the best **local** decisions, without lookahead to evaluate their downstream consequences
- This procedure is not very likely to result in the globally optimal tree

Prediction in a Regression Tree







Finding the Best Split Point

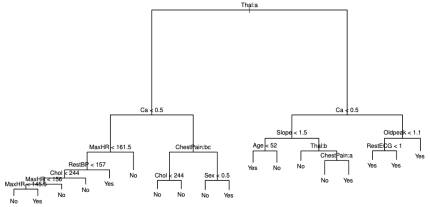
- We enumerate all features and all possible split points for each feature. There are infinitely many split points, but...
- Suppose we are now considering splitting on the j-th feature x_j, and let $x_{j(1)}, \ldots, x_{j(n)}$ be the sorted values of the j-th feature.
- We only need to consider split points between two adjacent values, and any split point in the interval $(x_{j(r)}, x_{(j(r+1)})$ will result in the same loss
- It is common to split half way between two adjacent values:

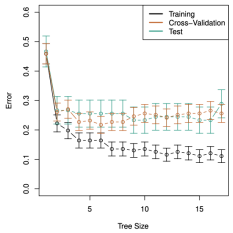
$$s_j \in \left\{ \frac{1}{2}\left(x_{j(r)} + x_{j(r+1)}\right) \mid r = 1, \ldots, n-1 \right\}. \qquad n-1 \text{ splits} \qquad (1)$$

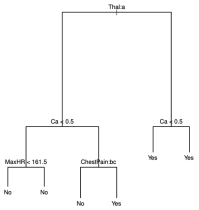
Decision Trees and Overfitting

- What will happen if we keep splitting the data into more and more regions?
  - Every data point will be in its own region—overfitting.
- When should we stop splitting? (Controlling the complexity of the hypothesis space)
  - Limit total number of nodes.
  - Limit number of terminal nodes.
  - Limit tree depth.
  - Require minimum number of data points in a terminal node.
  - **Backward pruning** (the approach used in **CART**; Breiman et al 1984):
    1. Build a really big tree (e.g. until all regions have $\leqslant 5$ points).
    2. *Prune* the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

Pruning: Example







What Makes a Good Split for Classification?

Our plan is to predict the **majority label** in each region.

Which of the following splits is better?

Split 1 $R_1 : 8+/2-$ $R_2 : 2+/8-$

Split 2 $R_1 : 6+/4-$ $R_2 : 4+/6-$

How about here?

Split 1 $R_1 : 8+/2-$ $R_2 : 2+/8-$

Split 2 $R_1 : 6+/4-$ $R_2 : 0+/10-$

Intuition: we want to produce *pure* nodes, i.e. nodes where most instances have the same class.

Misclassification error in a node

- Let's consider the multiclass classification case: $\mathcal{Y} = \{1, 2, \ldots, K\}$.
- Let node m represent region R_m, with N_m observations
- We denote the proportion of observations in R_m with class k by

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{\{i: x_i \in R_m\}} 1(y_i = k).$$

- We predict the majority class in node m:

$$k(m) = \arg\max_k \hat{p}_{mk}$$

Node Impurity Measures

- Three measures of **node impurity** for leaf node m:

  Misclassification error

  $$1 - \hat{p}_{mk(m)}.$$

  The Gini index encourages $\hat{p}_{mk}$ to be close to 0 or 1

  $$\sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

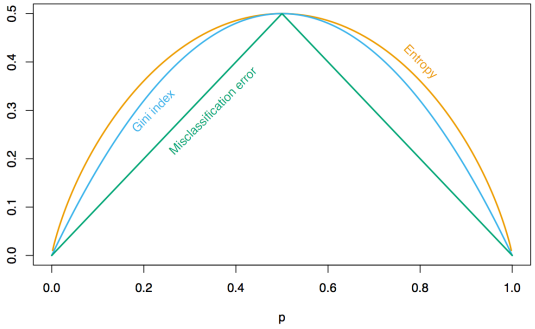
  Entropy / Information gain

  $$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$$

- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

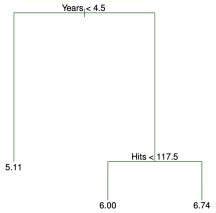
Quantifying the Impurity of a Split

Scoring a potential split that produces the nodes R_L and R_R:

- Suppose we have N_L points in R_L and N_R points in R_R.
- Let $Q(R_L)$ and $Q(R_R)$ be the node impurity measures for each node.
- We aim to find a split that minimizes the *weighted average of node impurities*:

$$\frac{N_L Q(R_L) + N_R Q(R_R)}{N_L + N_R}$$

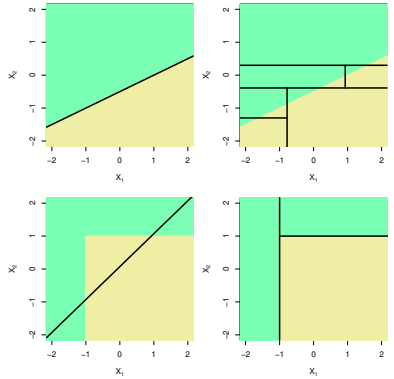
Discussion: Interpretability of Decision Trees



- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

Discussion: Trees vs. Linear Models

Trees may have to work hard to capture linear decision boundaries, but can easily capture certain nonlinear ones:



Discussion: Review

Decision trees are:

- Non-linear: the decision boundary that results from splitting may end up being quite complicated
- Non-metric: they do not rely on the geometry of the space (inner products or distances)
- Non-parametric: they make no assumptions about the distribution of the data

Additional pros:

- Interpretable and simple to understand

Cons:

- Struggle to capture linear decision boundaries
- They have high variance and tend to overfit: they are sensitive to small changes in the training data (The ensemble techniques we discuss next can mitigate these issues)

Bagging and Random Forests

Recap: Statistics and Point Estimators

- We observe data $\mathcal{D} = (x_1, x_2, \ldots, x_n)$ sampled i.i.d. from a parametric distribution $p(\cdot \mid \theta)$
- A **statistic** $s = s(\mathcal{D})$ is any function of the data:
  - E.g., sample mean, sample variance, histogram, empirical data distribution
- A statistic $\hat{\theta} = \hat{\theta}(\mathcal{D})$ is a **point estimator** of θ if $\hat{\theta} \approx \theta$

Recap: Bias and Variance of an Estimator

- Statistics are random, so they have probability distributions.
- The distribution of a statistic is called a **sampling distribution**.
- The standard deviation of the sampling distribution is called the **standard error**.
- Some parameters of the sampling distribution we might be interested in:

  Bias $\text{Bias}(\hat{\theta}) \stackrel{\text{def}}{=} \mathbb{E}\left[\hat{\theta}\right] - \theta.$

  Variance $\text{Var}(\hat{\theta}) \stackrel{\text{def}}{=} \mathbb{E}\left[\hat{\theta}^2\right] - \mathbb{E}^2\left[\hat{\theta}\right].$
- Why does variance matter if an estimator is unbiased?

Variance of a Mean

- Let $\hat{\theta}(\mathcal{D})$ be an unbiased estimator with variance σ^2: $\mathbb{E}\left[\hat{\theta}\right] = \theta$, $\text{Var}(\hat{\theta}) = \sigma^2$.
- So far we have used a single statistic $\hat{\theta} = \hat{\theta}(\mathcal{D})$ to estimate θ.
- Its standard error is $\sqrt{\text{Var}(\hat{\theta})} = \sigma$
- Consider a new estimator that takes the average of i.i.d. $\hat{\theta}_1, \ldots, \hat{\theta}_n$ where $\hat{\theta}_i = \hat{\theta}(\mathcal{D}^i)$.
- The average has the same expected value but smaller standard error (recall that $Var(cX) = c^2 Var(X)$, and that the $\hat{\theta}_i$-s are uncorrelated):

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \theta \qquad \text{Var}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \frac{\sigma^2}{n} \tag{2}$$

Averaging Independent Prediction Functions

- Suppose we have B independent training sets, all drawn from the same distribution ($\mathcal{D} \sim p(\cdot \mid \theta)$).
- Our learning algorithm gives us B prediction functions: $\hat{f}_1(x), \hat{f}_2(x), \ldots, \hat{f}_B(x)$
- We will define the average prediction function as:

$$\hat{f}_{\text{avg}} \stackrel{\text{def}}{=} \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b \tag{3}$$

Averaging Reduces Variance of Predictions

- The average prediction for x_0 is

$$\hat{f}_{\text{avg}}(x_0) = \frac{1}{B}\sum_{b=1}^{B} \hat{f}_b(x_0).$$

- $\hat{f}_{\text{avg}}(x_0)$ and $\hat{f}_b(x_0)$ have the same expected value, but
- $\hat{f}_{\text{avg}}(x_0)$ has smaller variance:

$$\text{Var}(\hat{f}_{\text{avg}}(x_0)) = \frac{1}{B}\text{Var}\left(\hat{f}_1(x_0)\right)$$

- Problem: in practice we don't have B independent training sets!

The Bootstrap Sample

How do we simulate multiple samples when we only have one?

- A **bootstrap sample** from $\mathcal{D}_n = (x_1, \ldots, x_n)$ is a sample of size n drawn *with replacement* from $\mathcal{D}_n$
- Some elements of $\mathcal{D}_n$ will show up multiple times, and some won't show up at all
- Each x_i has a probability of $(1-1/n)^n$ of not being included in a given bootstrap sample
- For large n,

$$\left(1-\frac{1}{n}\right)^n \approx \frac{1}{e} \approx .368. \tag{4}$$

- So we expect ~63.2% of elements of $\mathcal{D}_n$ will show up at least once.

The Bootstrap Method

Definition

A **bootstrap method** simulates B independent samples from P by taking B bootstrap samples from the sample $\mathcal{D}_n$.

- Given original data $\mathcal{D}_n$, compute B bootstrap samples $D_n^1, \ldots, D_n^B$.
- For each bootstrap sample, compute some function

$$\phi(D_n^1), \ldots, \phi(D_n^B)$$

- Use these values as though $D_n^1, \ldots, D_n^B$ were i.i.d. samples from P.
- This often ends up being very close to what we'd get with independent samples from P!

Independent Samples vs. Bootstrap Samples

- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100, for a synthetic case where the data generating distribution is known
- Histograms of $\hat{\alpha}$ based on
  - 1000 independent samples of size 100 (left), vs.
  - 1000 bootstrap samples of size 100 (right)

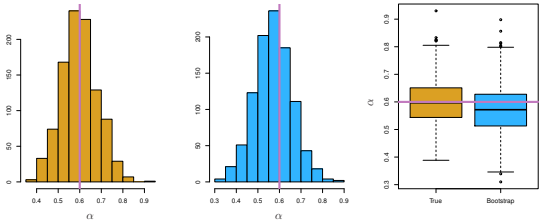


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Ensemble Methods

Key ideas:

- In general, **ensemble methods** combine multiple weak models into a single, more powerful model
- Averaging i.i.d. estimates reduces variance without changing bias
- We can use bootstrap to simulate multiple data samples and average them
- Parallel ensemble (e.g., bagging): models are built independently
- Sequential ensemble (e.g., boosting): models are built sequentially
  - We try to find new learners that do well where previous learners fall short

Bagging: Bootstrap Aggregation

- We draw B bootstrap samples $D^1, \ldots, D^B$ from original data $\mathcal{D}$
- Let $\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_B$ be the prediction functions resulting from training on $D^1, \ldots, D^B$, respectively
- The **bagged prediction function** is a *combination* of these:

$$\hat{f}_{\text{avg}}(x) = \text{Combine}\left(\hat{f}_1(x), \hat{f}_2(x), \ldots, \hat{f}_B(x)\right)$$

Bagging: Bootstrap Aggregation

- Bagging is a general method for variance reduction, but it is particularly useful for decision trees
- For classification, averaging doesn't make sense; we can take a **majority vote** instead
- Increasing the number of trees we use in bagging does not lead to overfitting
- Is there a downside, compared to having a single decision tree?
- Yes: if we have many trees, the bagged predictor is much less interpretable

Aside: Out-of-Bag Error Estimation

- Recall that each bagged predictor was trained on about 63% of the data.
- The remaining 37% are called **out-of-bag (OOB)** observations.
- For ith training point, let

$$S_i = \left\{ b \mid D^b \text{ does not contain } i\text{th point} \right\}$$

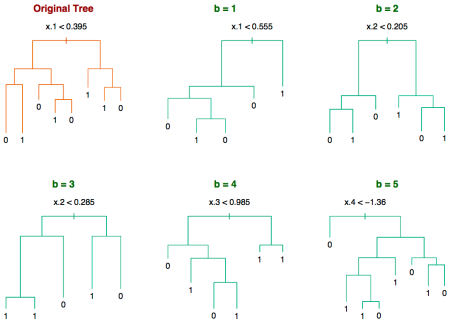
- The **OOB prediction** on x_i is

$$\hat{f}_{\text{OOB}}(x_i) = \frac{1}{|S_i|} \sum_{b \in S_i} \hat{f}_b(x_i)$$

- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

- Input space $\mathcal{X} = \mathrm{R}^5$ and output space $\mathcal{Y} = \{-1, 1\}$. Sample size $n = 30$.



- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

From HTF Figure 8.9

Motivating Random Forests: Correlated Prediction Functions

Recall the motivating principle of bagging:

- For $\hat{\theta}_1, \ldots, \hat{\theta}_n$ *i.i.d.* with $\mathbb{E}\left[\hat{\theta}\right] = \theta$ and $\mathrm{Var}\left[\hat{\theta}\right] = \sigma^2$,

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \mu \qquad \mathrm{Var}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \frac{\sigma^2}{n}.$$

- What if $\hat{\theta}$'s are correlated?
- For large n, the covariance term dominates, limiting the benefits of averaging
- Bootstrap samples are
  - independent samples from the training set, but
  - not independent samples from $P_{\mathcal{X}\times\mathcal{Y}}$
- Can we reduce the dependence between $\hat{f}_i$'s?

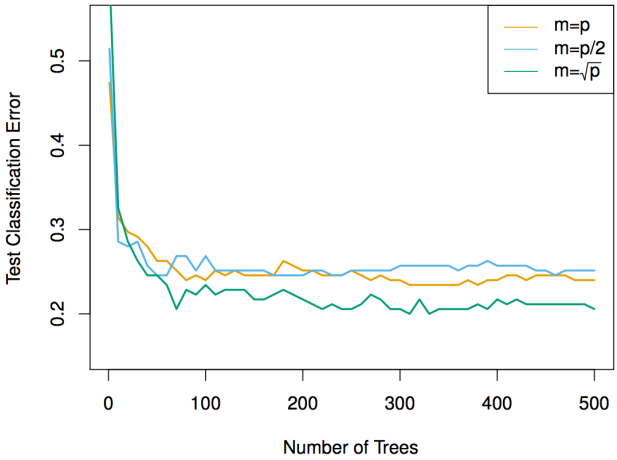
Random Forests

Key idea

Use bagged decision trees, but modify the tree-growing procedure to reduce the dependence between trees.

- Build a collection of trees independently (in parallel), as before
- When constructing each tree node, restrict choice of splitting variable to a randomly chosen subset of features of size m
  - This prevents a situation where all trees are dominated by the same small number of strong features (and are therefore too similar to each other)
- We typically choose $m \approx \sqrt{p}$, where p is the number of features (or we can choose m using cross validation)
- If $m = p$, this is just bagging

Random Forests: Effect of m



From *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Review

- The usual approach is to build very deep trees—low bias but high variance
- Ensembling many models reduces variance
  - Motivation: Mean of i.i.d. estimates has smaller variance than single estimate
- Use bootstrap to simulate many data samples from one dataset
  - $\implies$ Bagged decision trees
- But bootstrap samples (and the induced models) are correlated
- Ensembling works better when we combine a diverse set of prediction functions
  - $\implies$ Random forests: select a random subset of features for each decision tree

Boosting

Boosting: Overview

Bagging Reduce variance of a low bias, high variance estimator by ensembling many estimators trained in parallel (on different datasets obtained through sampling).

Boosting Reduce the error rate of a high bias estimator by ensembling many estimators trained in sequence (without bootstrapping).

- Like bagging, boosting is a general method that is particularly popular with decision trees.
- Main intuition: instead of fitting the data very closely using a large decision tree, train gradually, using a sequence of simpler trees

Boosting: Overview

- A **weak/base learner** is a classifier that does slightly better than chance.
- Weak learners are like rules of thumb:
  - "Inheritance" $\implies$ spam
  - From a friend $\implies$ not spam
- **Key idea**:
  - Each weak learner focuses on different training examples (*reweighted data*)
  - Weak learners make different contributions to the final prediction (*reweighted classifier*)
- A set of smaller, simpler trees may improve interpretability
- We'll focus on a specific implementation, AdaBoost (Freund & Schapire, 1997)

AdaBoost: Setting

- Binary classification: $\mathcal{Y} = \{-1, 1\}$
- Base hypothesis space $\mathcal{H} = \{h : \mathcal{X} \to \{-1, 1\}\}$.
- Typical base hypothesis spaces:
  - **Decision stumps** (tree with a single split)
  - Trees with few terminal nodes
  - Linear decision functions

Weighted Training Set

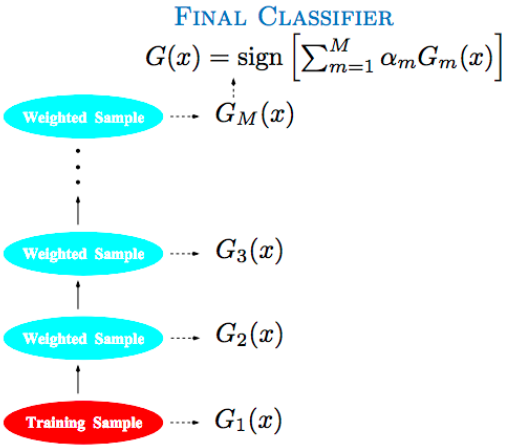
Each base learner is trained on weighted data.

- Training set $\mathcal{D} = ((x_1, y_1), \ldots, (x_n, y_n))$.
- Weights $(w_1, \ldots, w_n)$ associated with each example.
- **Weighted empirical risk**:

$$\hat{R}_n^w(f) \stackrel{\text{def}}{=} \frac{1}{W} \sum_{i=1}^{n} w_i \ell(f(x_i), y_i) \quad \text{where } W = \sum_{i=1}^{n} w_i$$

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

AdaBoost: Sketch of the Algorithm

- Start with equal weights for all training points: $w_1 = \cdots = w_n = 1$
- Repeat for $m = 1, \ldots, M$ (where M is the number of classifiers we plan to train):
  - Train base classifier $G_m(x)$ on the weighted training data; this classifier may not fit the data well
  - Increase the weight of the points misclassified by $G_m(x)$ (this is the key idea of boosting!)
- Our final prediction is $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$

AdaBoost: Classifier Weights

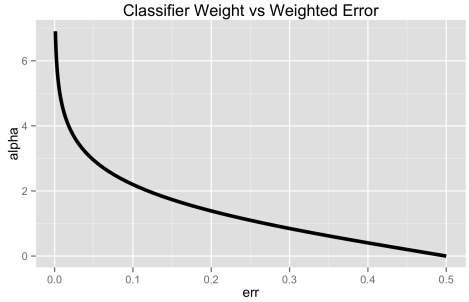
- Our final prediction is $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
- We would like α_m to be:
  - Nonnegative
  - Larger when G_m fits its weighted training data well
- The **weighted 0-1 error** of $G_m(x)$ is

$$\text{err}_m = \frac{1}{W} \sum_{i=1}^{n} w_i 1(y_i \neq G_m(x_i)) \quad \text{where } W = \sum_{i=1}^{n} w_i.$$

- $\text{err}_m \in [0, 1]$

AdaBoost: Classifier Weights

- The weight of classifier $G_m(x)$ is $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$



- Higher weighted error $\implies$ lower weight

Adaboost: Example Reweighting

- We train G_m to minimize weighted error; the resulting error rate is err_m
- Then $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$ is the weight of G_m in the final ensemble

We want the next base learner to focus more on examples misclassified by the previous learner.

- Suppose w_i is the weight of example x_i before training:
  - If G_m classifies x_i correctly, keep w_i as is
  - Otherwise, increase w_i:

$$\begin{aligned} w_i &\leftarrow w_i e^{\alpha_m} \\ &= w_i \left(\frac{1-\text{err}_m}{\text{err}_m}\right) \end{aligned}$$

  - If G_m is a strong classifier overall, then its α_m will be large; this means that if x_i is misclassified, w_i will increase to a greater extent

AdaBoost with Decision Stumps

- After 1 round:

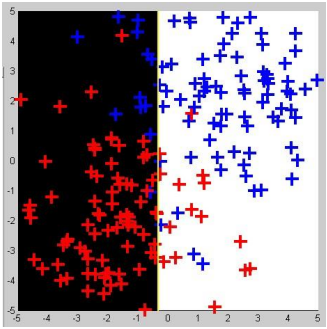


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:

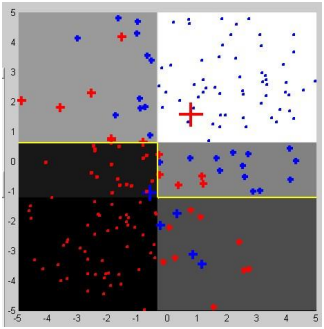


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:

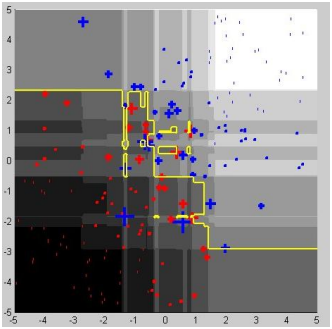
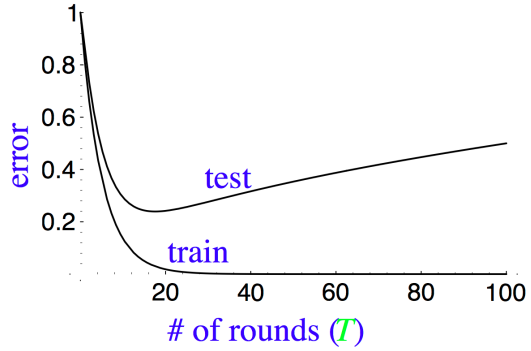


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

Does AdaBoost overfit?

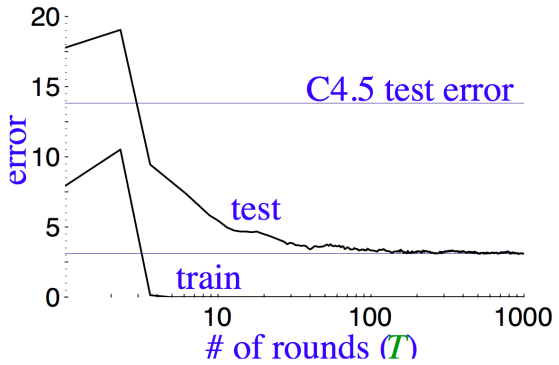
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



From Rob Schapire's NIPS 2007 Boosting tutorial.

Learning Curves for AdaBoost

- AdaBoost is usually quite resistant to overfitting
- The test error continues to decrease even after the training error drops to zero!



From Rob Schapire's NIPS 2007 Boosting tutorial.

Summary

- Boosting is used to reduce bias from shallow decision trees
- AdaBoost is a very powerful off-the-self classifier!
- Next week
  - What is the objective function of AdaBoost?
  - Generalizations to other loss functions