Decision Trees

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Slides based on Lecture 10 from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

CDS, NYU

April 5, 2022

Today's lecture

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

Decision Trees

Regression trees: Predicting basketball players' salaries

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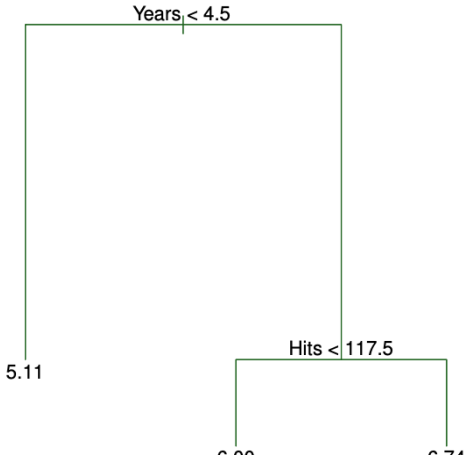
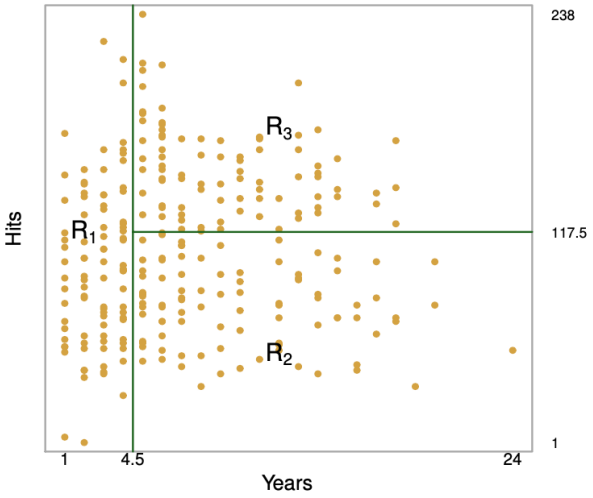
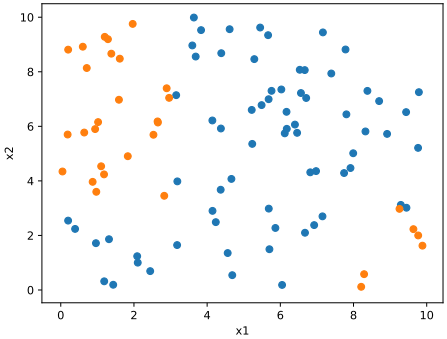




Classification trees



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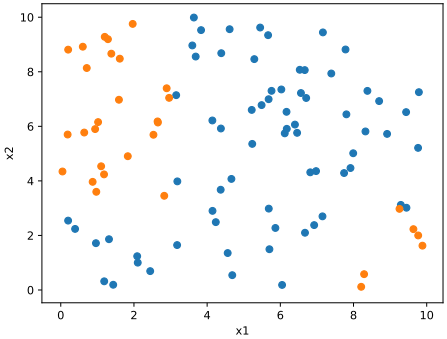
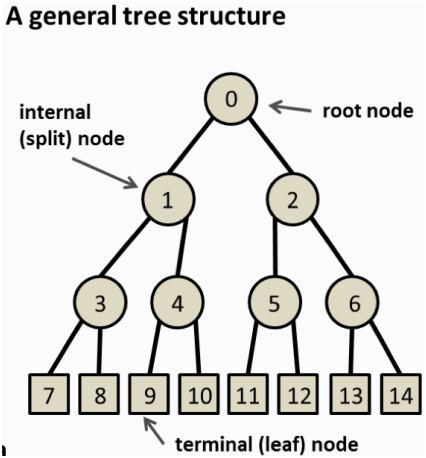


- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



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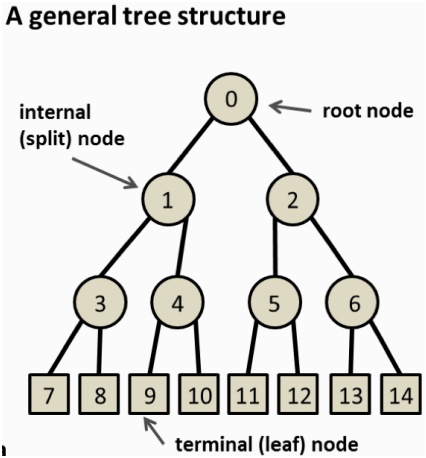

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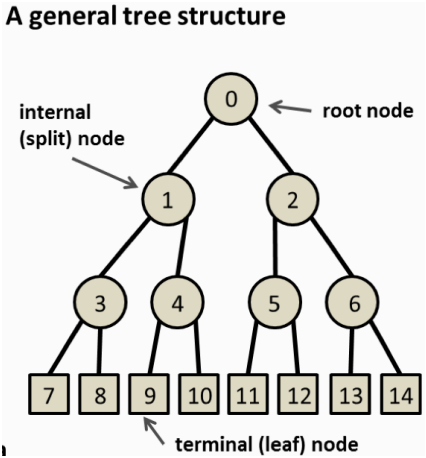

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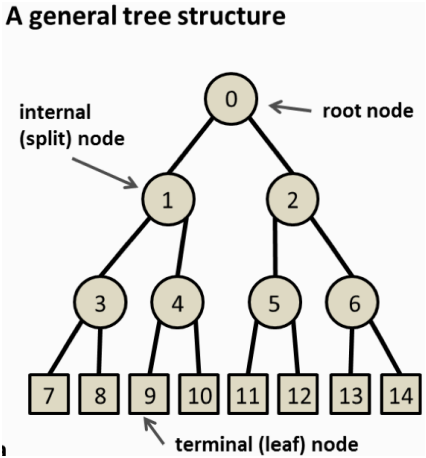

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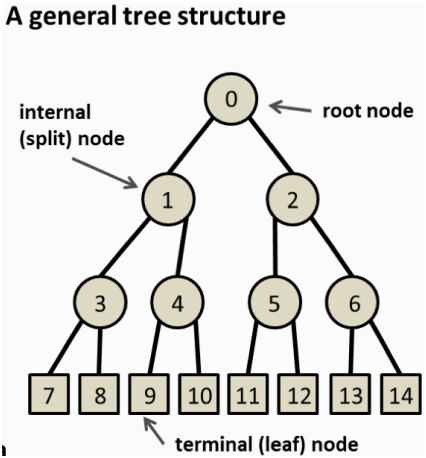

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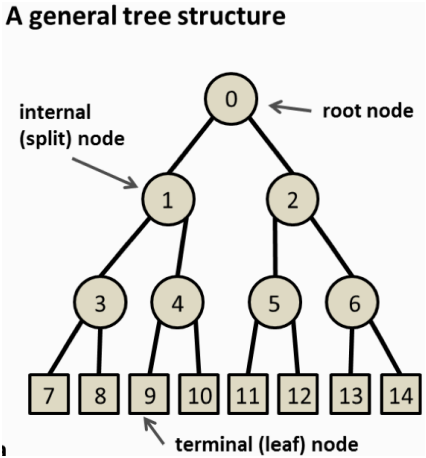

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- Predictions are made in terminal nodes

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.

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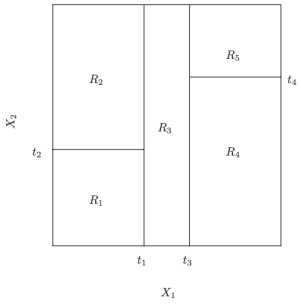
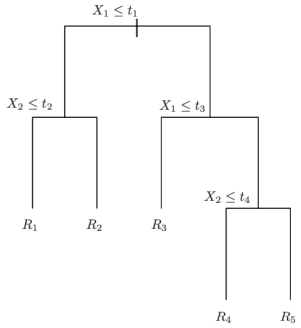
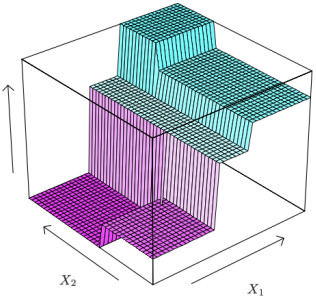
- A greedy algorithm is the one that make the best **local** decisions, without lookahead to evaluate their downstream consequences
- This procedure is not very likely to result in the globally optimal tree

Prediction in a Regression Tree







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- It is common to split half way between two adjacent values:

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

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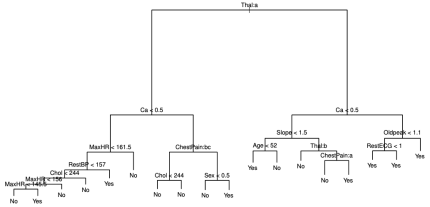
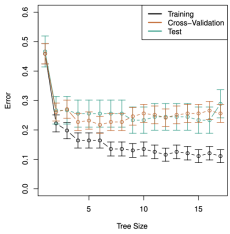
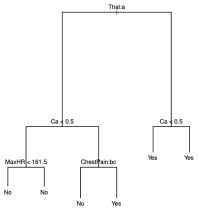
  - Every data point will be in its own region—overfitting.
- When should we stop splitting? (Controlling the complexity of the hypothesis space)
  - Limit total number of nodes.
  - Limit number of terminal nodes.
  - Limit tree depth.
  - Require minimum number of data points in a terminal node.
  - **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?

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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:

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

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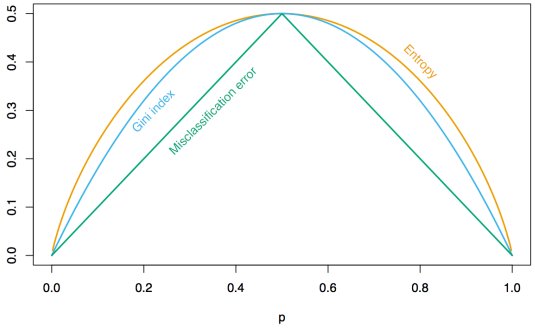
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

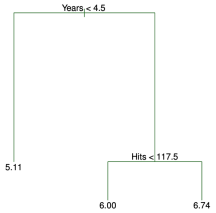
Quantifying the Impurity of a Split

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



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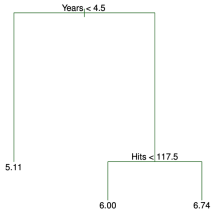
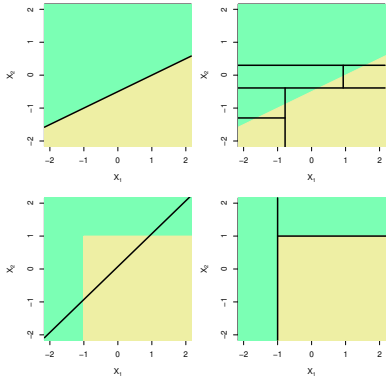


- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

Discussion: Trees vs. Linear Models

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



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Decision trees are:

- Non-linear: the decision boundary that results from splitting may end up being quite complicated
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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

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- A statistic $\hat{\theta} = \hat{\theta}(\mathcal{D})$ is a **point estimator** of θ if $\hat{\theta} \approx \theta$

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- Statistics are random, so they have probability distributions.
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- Why does variance matter if an estimator is unbiased?

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- 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 ($\mathcal{D} \sim p(\cdot \mid \theta)$).

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- 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
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- 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?

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- 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)

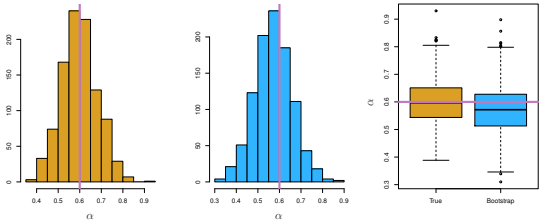

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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Key ideas:

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- 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

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- 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:

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

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- 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

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- Recall that each bagged predictor was trained on about 63% of the data.
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- For ith training point, let

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

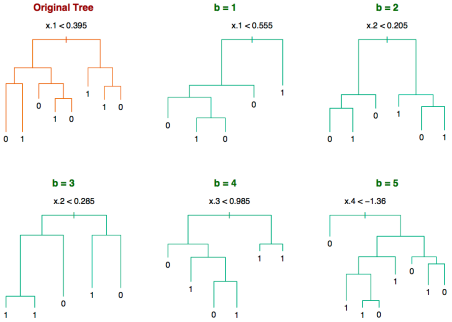
- The **OOB prediction** on x_i is

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

- 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 $n = 30$.



From HTF Figure 8.9

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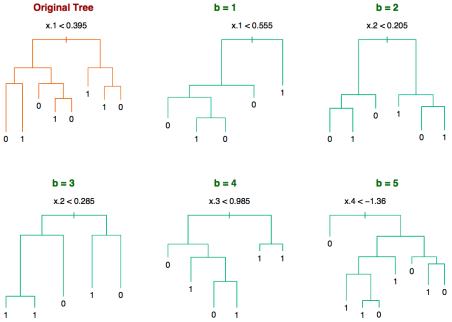

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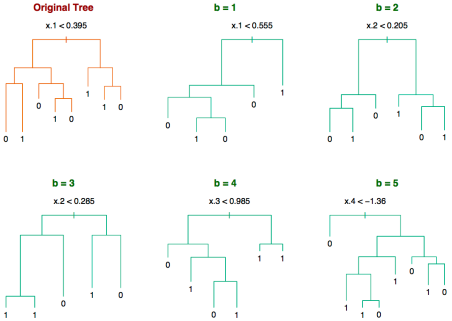

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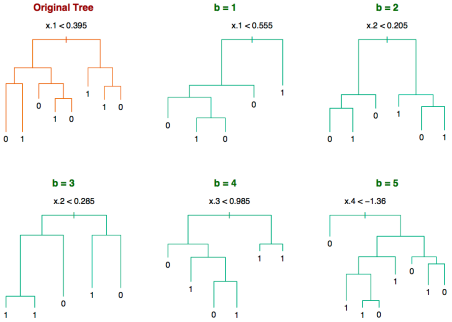

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- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively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

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 $\mathrm{Var}\left[\hat{\theta}\right] = \sigma^2$,

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

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- Can we reduce the dependence between $\hat{f}_i$'s?

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

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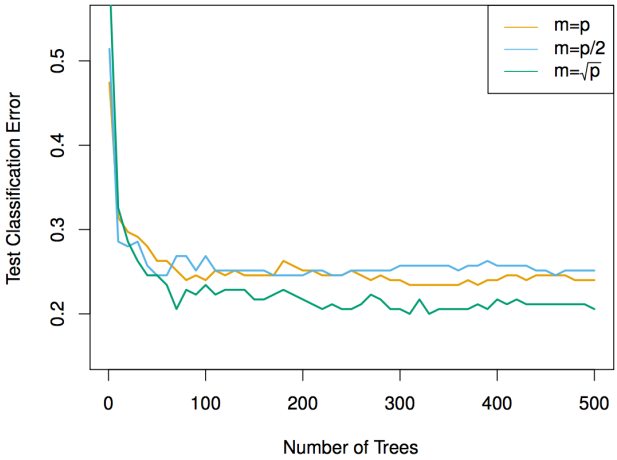
- If $m = p$, this is just bagging

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.

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- But bootstrap samples (and the induced models) are correlated
- Ensembling works better when we combine a diverse set of prediction functions
  - $\Longrightarrow$ Random forests: select a random subset of features for each decision tree

Boosting

Boosting: Overview

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- 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
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- We'll focus on a specific implementation, AdaBoost (Freund & Schapire, 1997)

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- 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.

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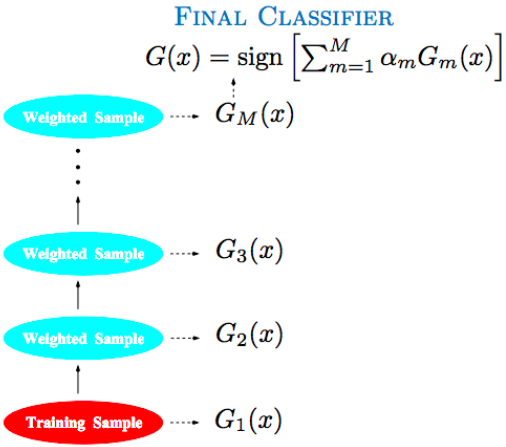
- **Weighted empirical risk**:

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

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  - Increase the weight of the points misclassified by $G_m(x)$ (this is the key idea of boosting!)

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 $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$

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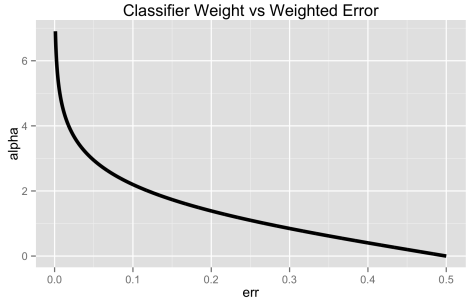

- Higher weighted error $\implies$ lower weight

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

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  - 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:

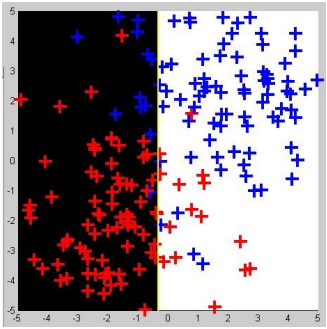


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:

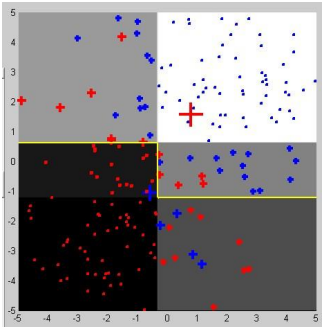
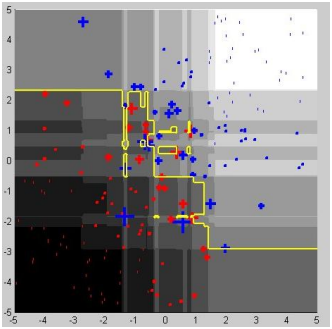


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:



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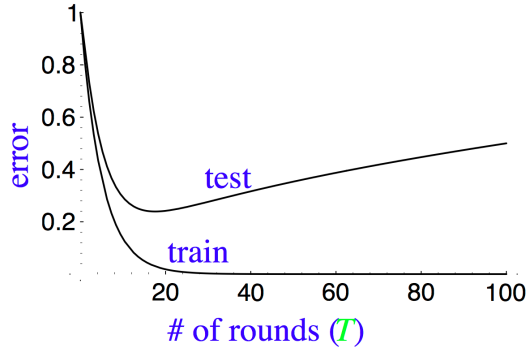
KPM Figure 16.10

Does AdaBoost overfit?

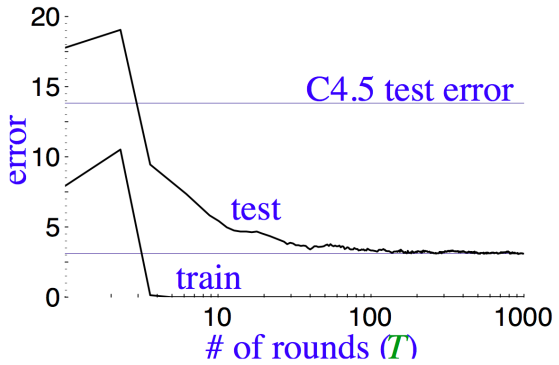
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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!



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