# Decision Trees

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

CDS, NYU

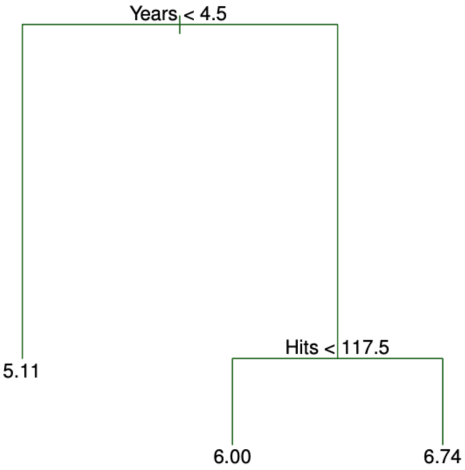
April 5, 2022

# 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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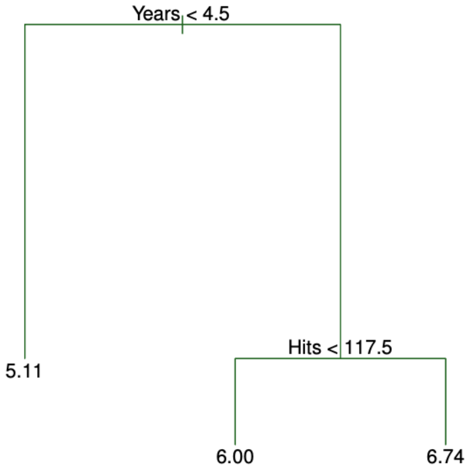


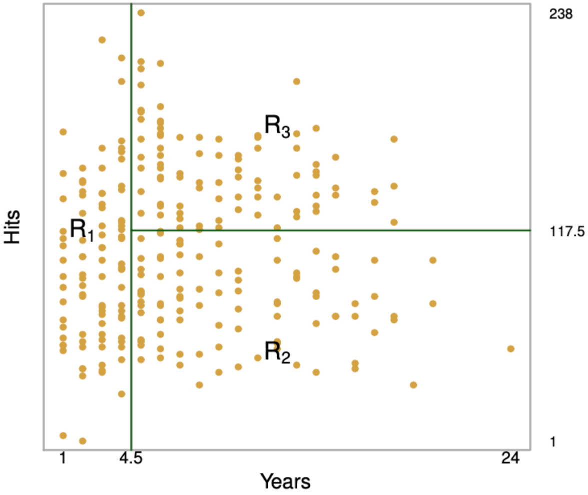

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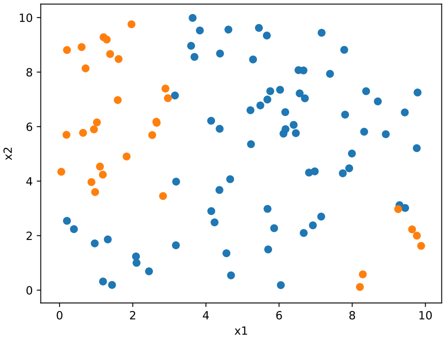


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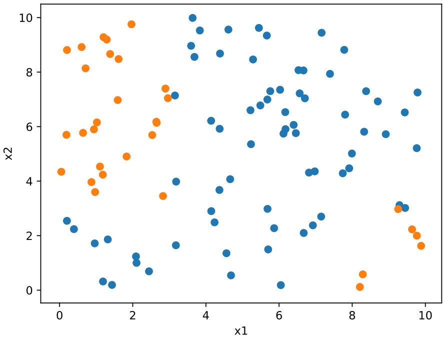
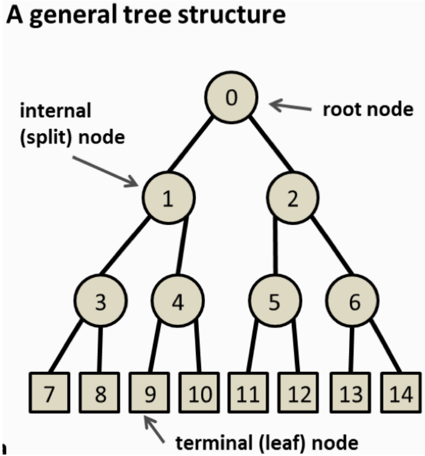



- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

# Decision trees setup

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

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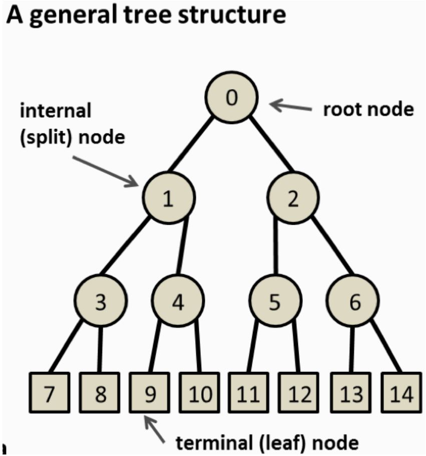


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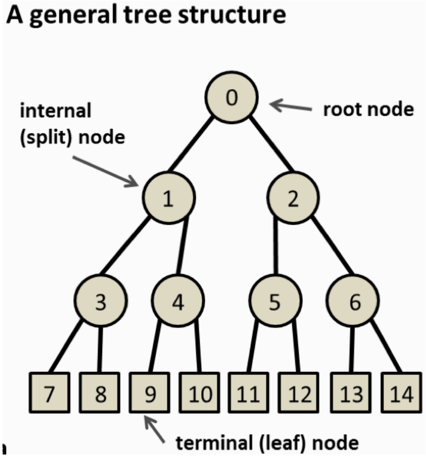


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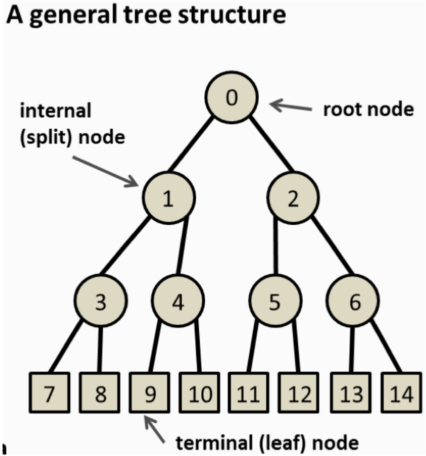


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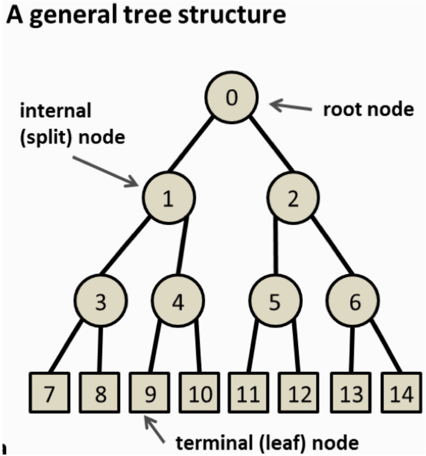


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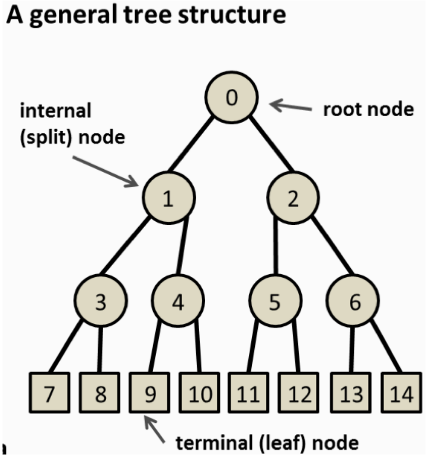


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- Predictions are made in terminal nodes

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# Constructing the tree

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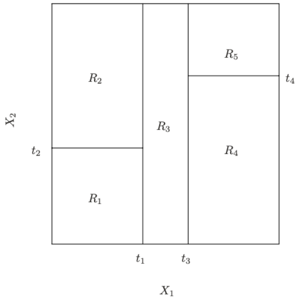
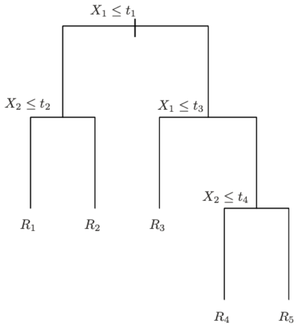
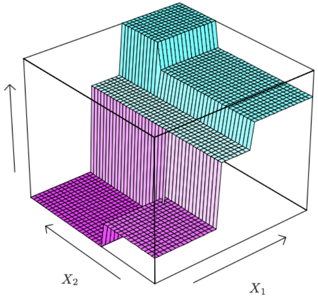
- This procedure is not very likely to result in the globally optimal tree

# Prediction in a Regression Tree



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

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

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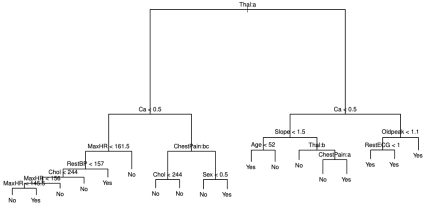
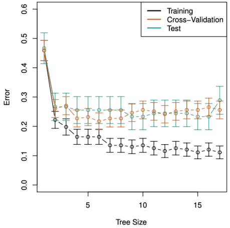
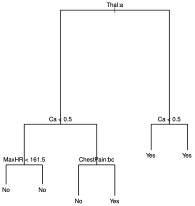
  - Every data point will be in its own region—overfitting.
- When should we stop splitting? (Controlling the complexity of the hypothesis space)
  - Limit total number of nodes.
  - Limit number of terminal nodes.
  - Limit tree depth.
  - Require minimum number of data points in a terminal node.
  -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



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

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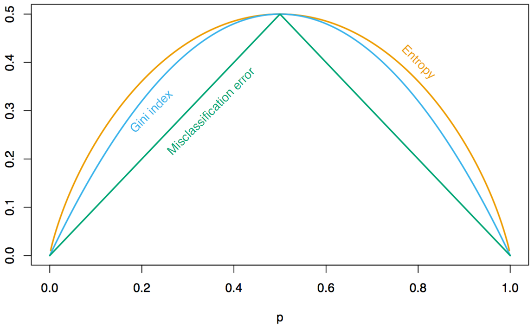
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

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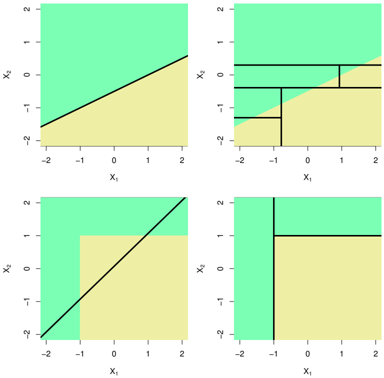
- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

# 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:

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Additional pros:

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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

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

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- Why does variance matter if an estimator is unbiased?

# Variance of a Mean

- Let $\hat{\theta}(\mathcal{D})$ be an unbiased estimator with variance $\sigma^2$: $\mathbb{E}\left[\hat{\theta}\right] = \theta$, $\text{Var}(\hat{\theta}) = \sigma^2$.
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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):

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

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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
- $\hat{f}_{\text{avg}}(x_0)$ has smaller variance:

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

# 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:

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

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

# The Bootstrap Sample

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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)

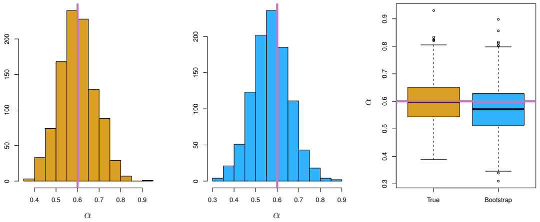


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

# Ensemble Methods

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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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- 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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- 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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- The remaining 37% are called **out-of-bag (OOB)** observations.
- For $i$th training point, let

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

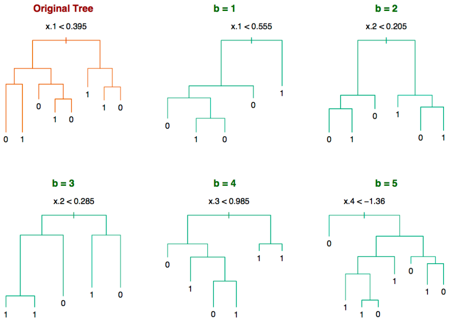
- The **OOB prediction** on $x_i$ is

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

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




From HTF Figure 8.9

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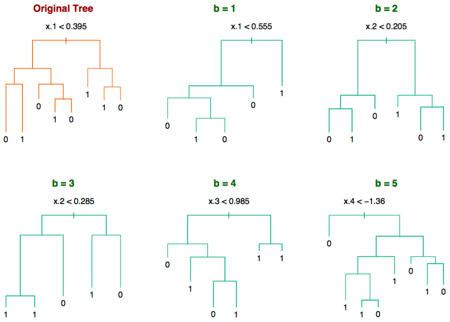


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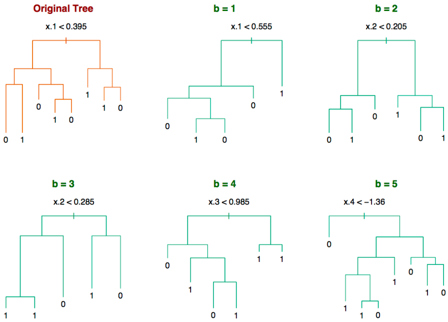


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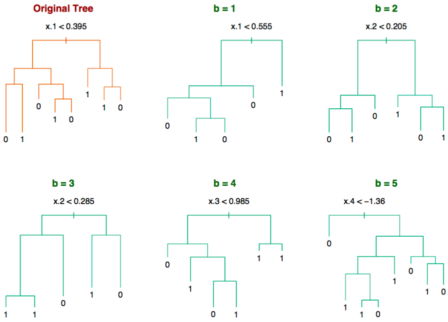


- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for 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 $\mathrm{Var}\left[\hat{\theta}\right] = \sigma^2$,

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

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- 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.

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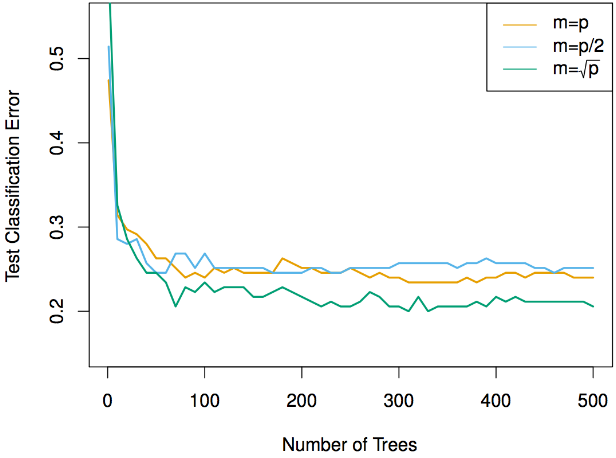
- If $m = p$, this is just bagging

# 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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  - $\implies$ 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

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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

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- Weak learners are like rules of thumb:
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- We'll focus on a specific implementation, AdaBoost (Freund & Schapire, 1997)

# AdaBoost: Setting

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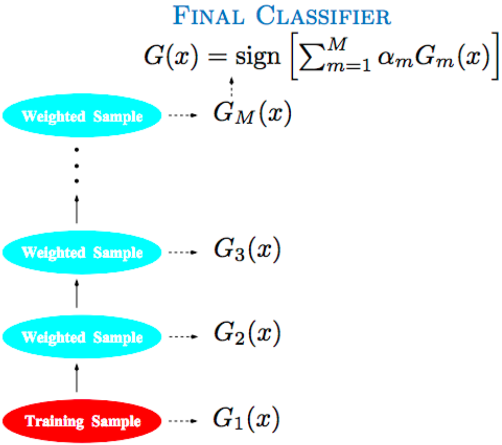
- Weights $(w_1, \dots, w_n)$ associated with each example.
- **Weighted empirical risk**:

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

- Examples with larger weights affect the loss more.

# AdaBoost: Schematic




From ESL Figure 10.1

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# AdaBoost: Classifier Weights

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

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

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

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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 $\text{err}_m$
- 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.

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    - If $G_m$ is a strong classifier overall, then its $\alpha_m$ 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:

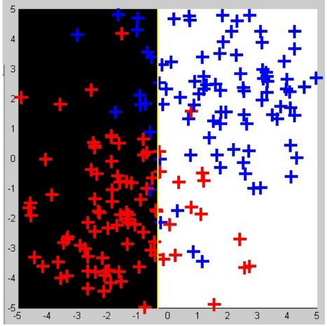



Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

# AdaBoost with Decision Stumps

- After 3 rounds:

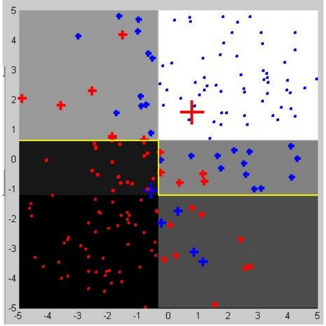
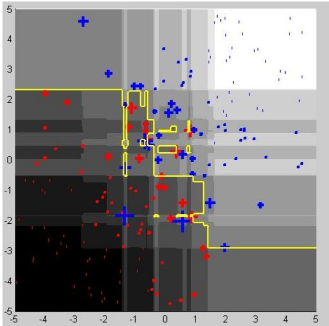



Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

# AdaBoost with Decision Stumps

- After 120 rounds:

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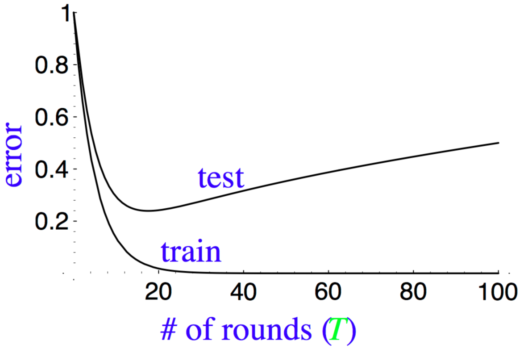
KPM Figure 16.10

# Does AdaBoost overfit?

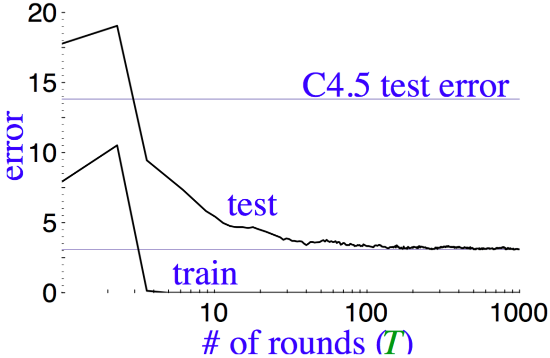
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:




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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