Decision Trees

CDS, NYU

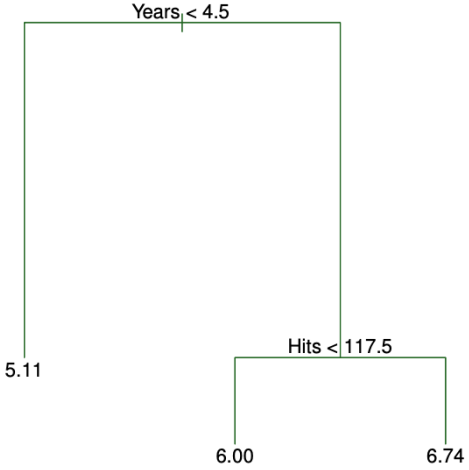
April 4, 2022

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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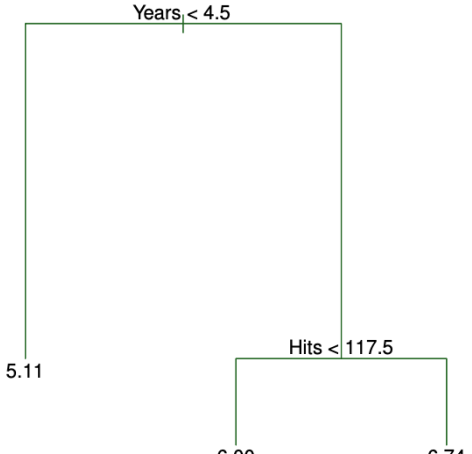

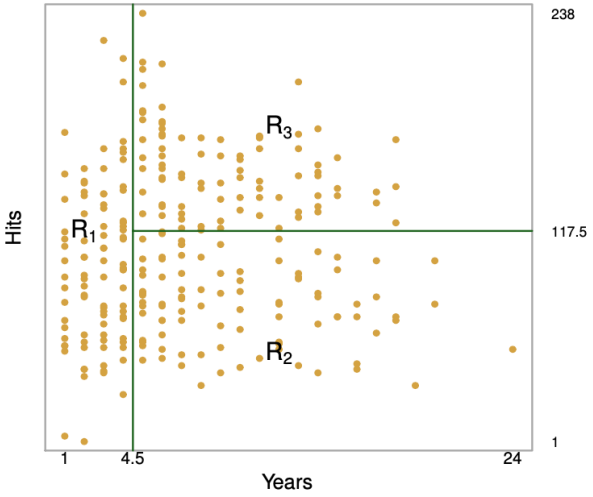

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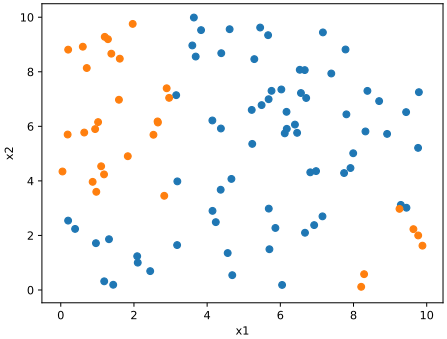

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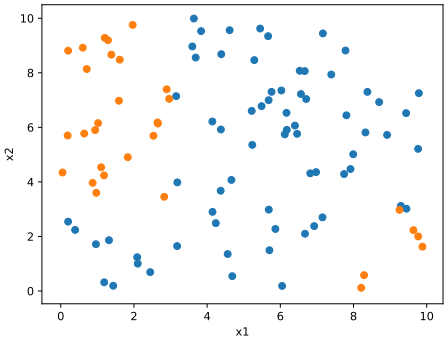
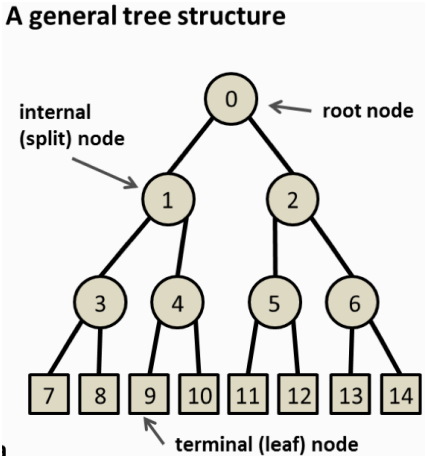


- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



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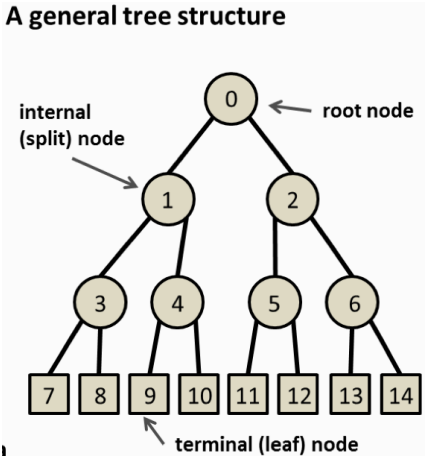

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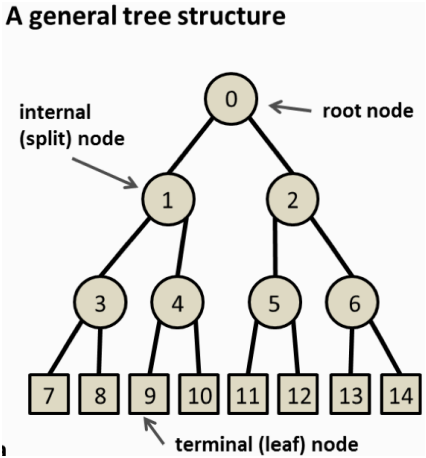

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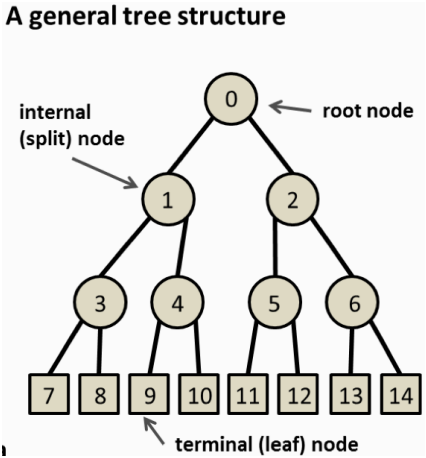

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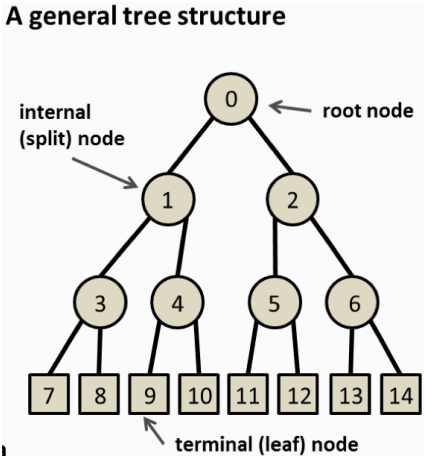

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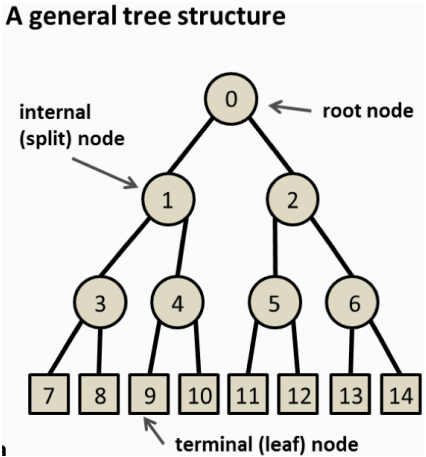

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- Predictions are made in terminal nodes

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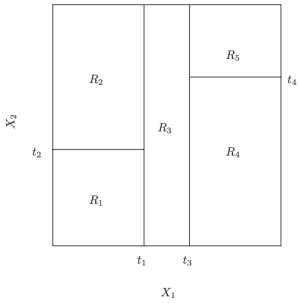
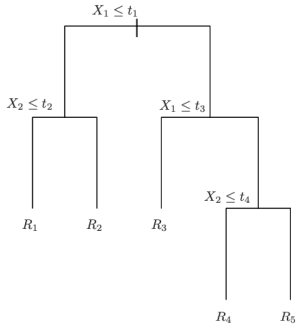
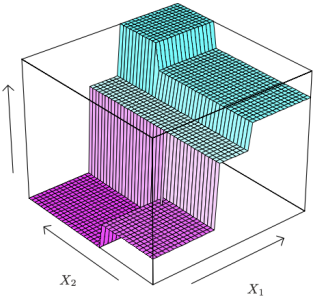
- This procedure is not very likely to result in the globally optimal tree

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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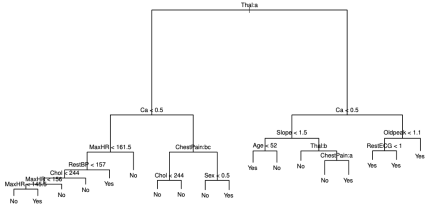
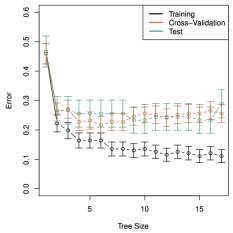
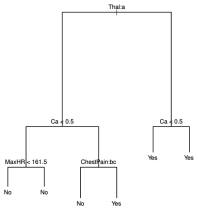
    2. *Prune* the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

Pruning: Example







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

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- We predict the majority class in node m:

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

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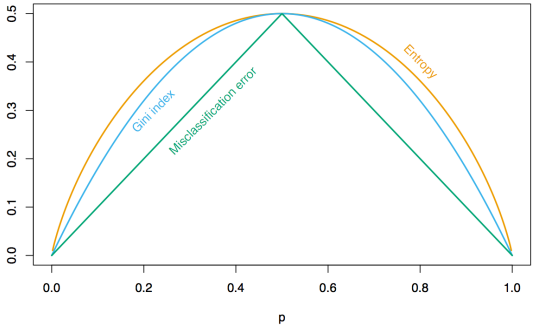
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

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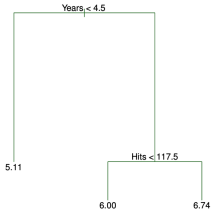
- We aim to find a split that minimizes the *weighted average of node impurities*:

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

Discussion: Interpretability of Decision Trees



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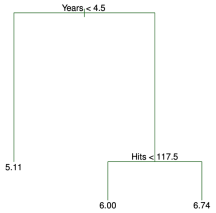
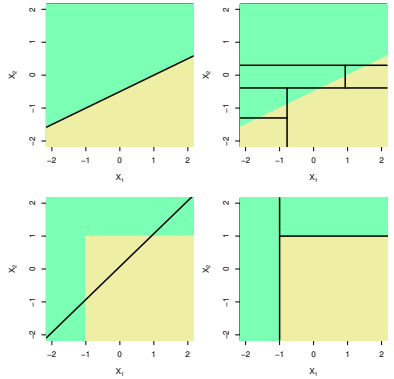


- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

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

Recap: Statistics and Point Estimators

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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 σ^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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- 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

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- 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)

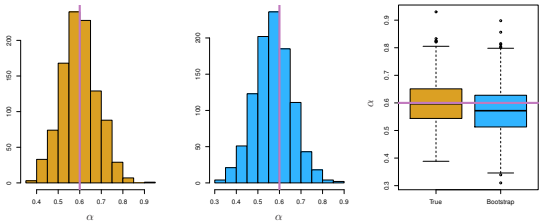

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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- Sequential ensemble (e.g., boosting): models are built sequentially
  - We try to find new learners that do well where previous learners fall short

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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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- 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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- For ith training point, let

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

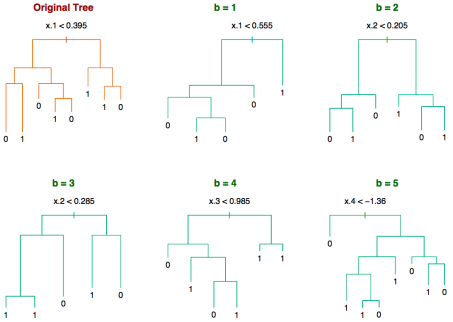
- The **OOB prediction** on x_i is

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

- 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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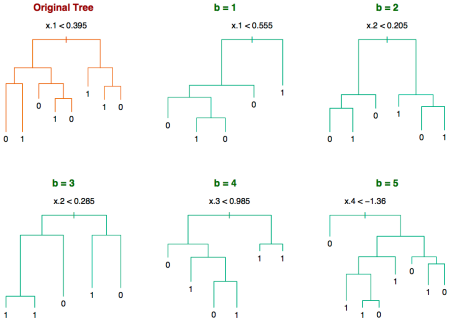

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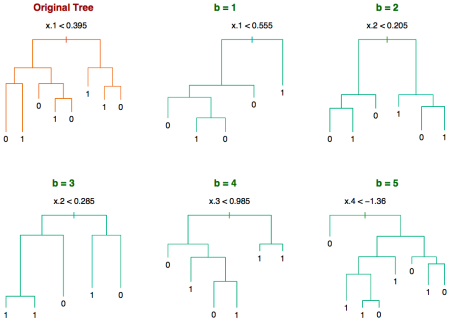

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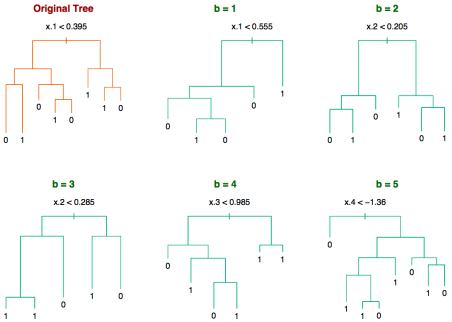

- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for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

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Key idea

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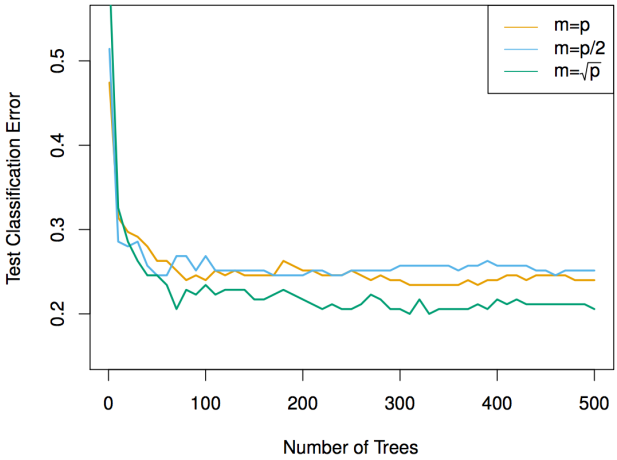
- If $m = p$, this is just bagging

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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- 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

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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

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- A set of smaller, simpler trees may improve interpretability
- We'll focus on a specific implementation, AdaBoost (Freund & Schapire, 1997)

AdaBoost: Setting

- Binary classification: $\mathcal{Y} = \{-1, 1\}$

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

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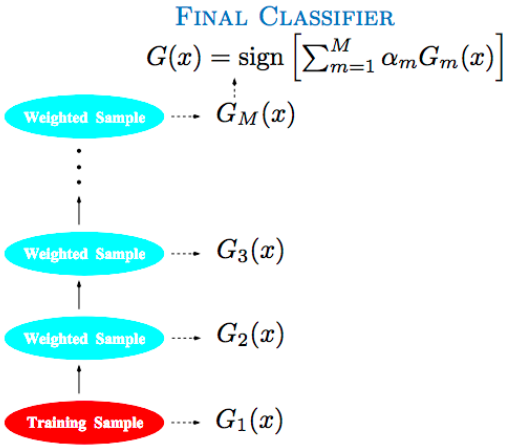
- **Weighted empirical risk**:

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

AdaBoost: Sketch of the Algorithm

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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

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

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

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- 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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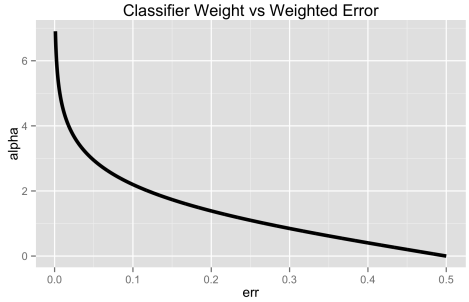

- Higher weighted error $\implies$ lower weight

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: Algorithm

Given training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.

1. Initialize observation weights $w_i = 1,\ i = 1, 2, \ldots, n$.

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3. Return *voted classifier*: $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

AdaBoost with Decision Stumps

- After 1 round:

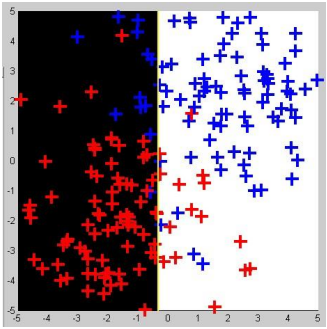
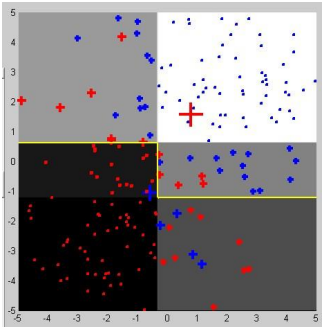


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:



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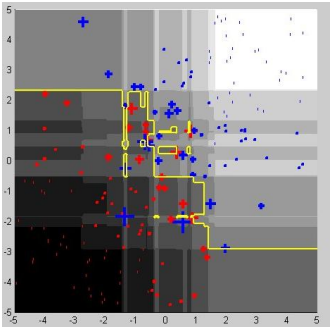
KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:



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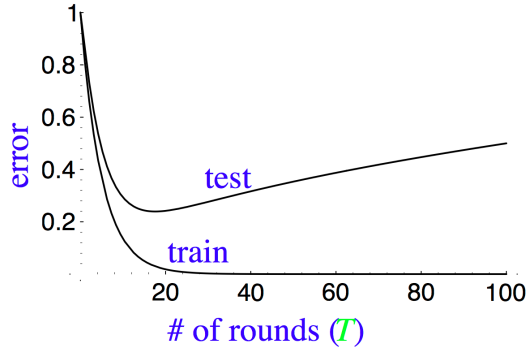
KPM Figure 16.10

Does AdaBoost overfit?

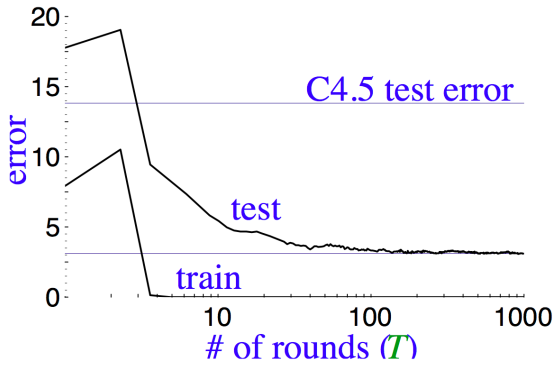
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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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AdaBoost for Face Detection

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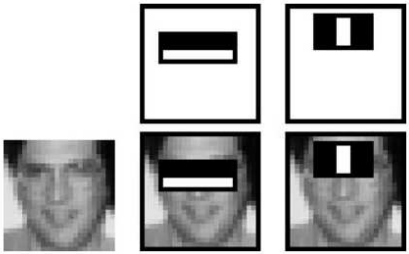
- A few twists on standard algorithm
  - Pre-define weak classifiers, so optimization=selection
  - Smart way to do inference in real-time (in 2001 hardware)



Harr wavelet basis functions

- A simple way to generate rectangular weights.
- Over 180,000 filters on a small image (subwindow) of 24x24.

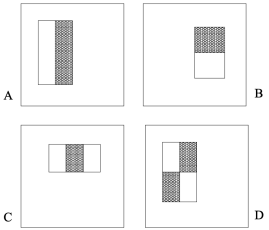
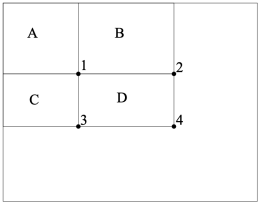


Figure 1: Example rectangle features shown relative to the enclosing detection window. The sum of the pixels which lie within the white rectangles are subtracted from the sum of pixels in the grey rectangles. Two-rectangle features are shown in (A) and (B). Figure (C) shows a three-rectangle feature, and (D) a four-rectangle feature.

Integral image

- Harr Filter * Image means compute the sum of an area of the image.
- Compute an "integral image"
- Store a 2-D array: S[i, j] = Sum of the image from (0,0) to (i,j).
- D = ABCD - AB - AC + A

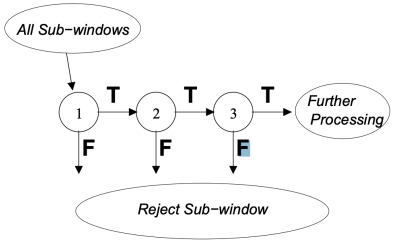


Learning Procedure (AdaBoost)

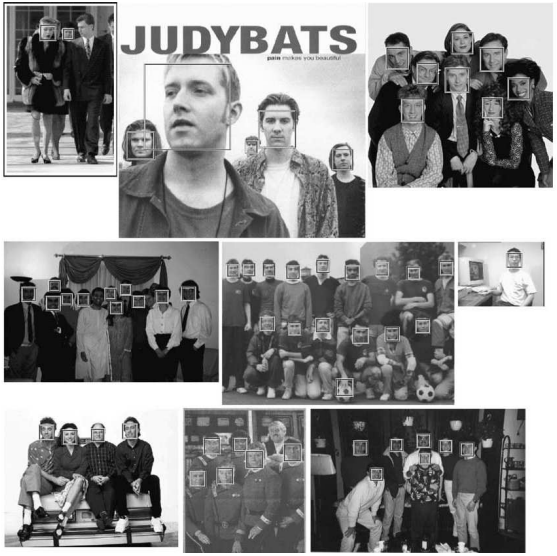
- Review AdaBoost again here, with a slightly different but equivalent setup.
- Given example images $(x_1, y_1), \ldots, (x_n, y_n)$ where $y_i = 0, 1$ for negative and positive.
- Initialize example weights $w_{1,i} = \frac{1}{2m}, \frac{1}{2l}$ for $y_i = 0, 1$ respectively, where m and l are the number of negatives and positives.
- For $t = 1, \ldots, T$:
  1. Normalize the example weights, $w_{t,i} \leftarrow \frac{w_{t,i}}{\sum_{i'=1}^{n} w_{t,i'}}$
  2. For each feature j, train a classifier h_j. Evaluate weighted error $\epsilon_j = \sum_i w_i |h_j(x_i) - y_i|$.
  3. Choose the classifier h_t, with the lowest error ϵ_t.
  4. Update the example weights: $w_{t+1} = w_{t,i} \beta_t^{1-e_i}$, $\beta_t = \frac{\epsilon_t}{1-\epsilon_t}$, $e_i = 0$ if correct else 1,
  5. Final classifier $h(x) = \begin{cases} 1 \text{ if } \sum_t \alpha_t h_t(x) > \frac{1}{2} \sum_t \alpha_t \\ 0 \text{ otherwise,} \end{cases}$ $\alpha_t = -\log \beta_t$

Cascaded Processing for Faster Speed

- Object detection: A large number of subwindows to process.
- Do we need to run all the weak classifiers at test time?
- Threshold can be adjusted so that there is almost no false negative.
- False positive is ok. We can reject the windows later.
- Stop processing if one weak classifier says no.



AdaBoost Face Detection Results



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