Decision Trees and Boosting

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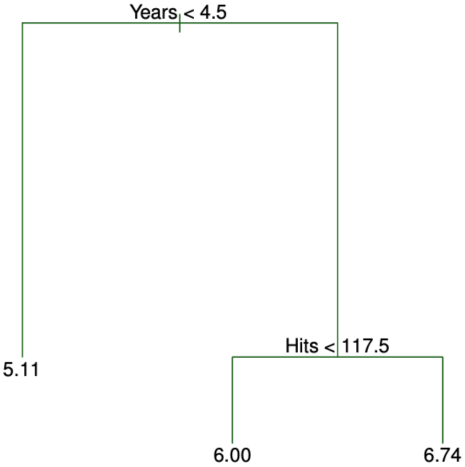
Nov 14, 2023

Overview

- 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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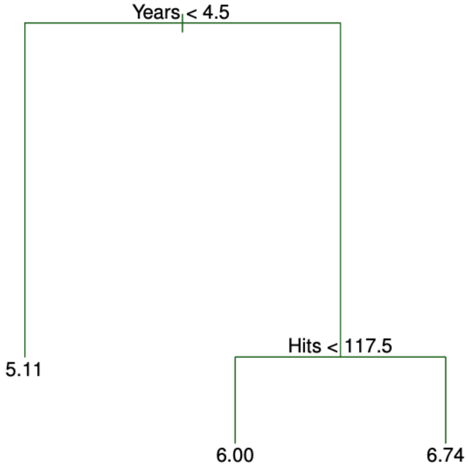

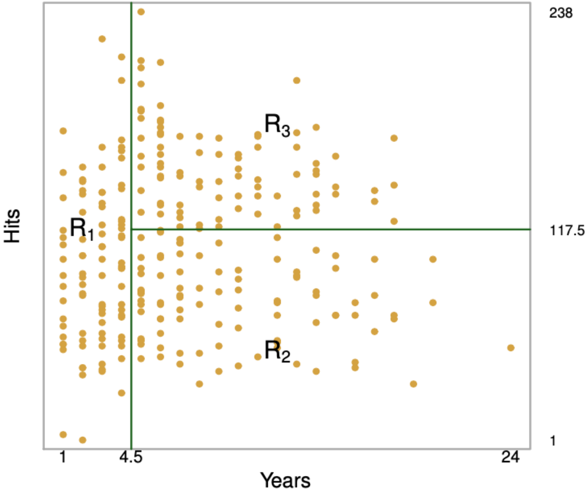

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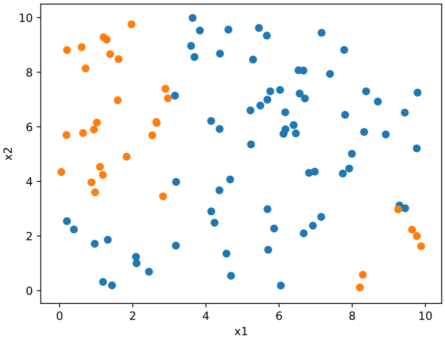

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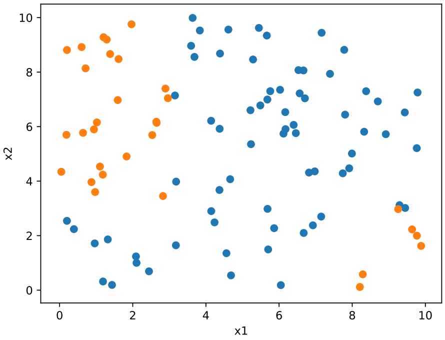

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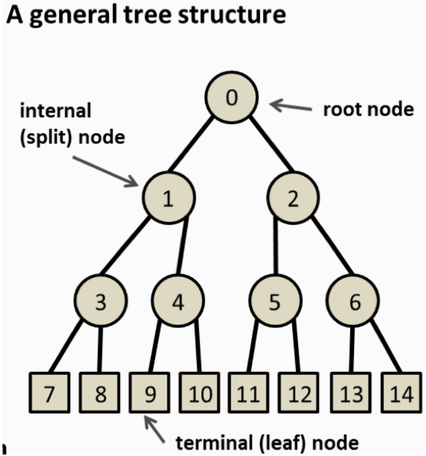
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



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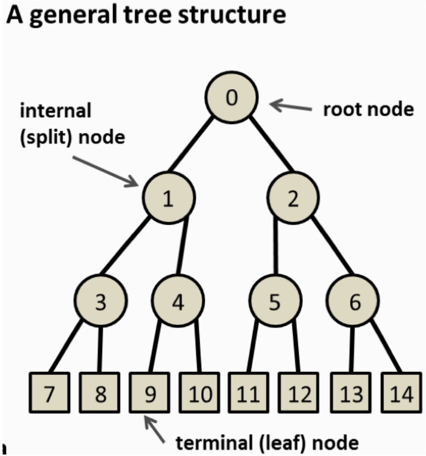

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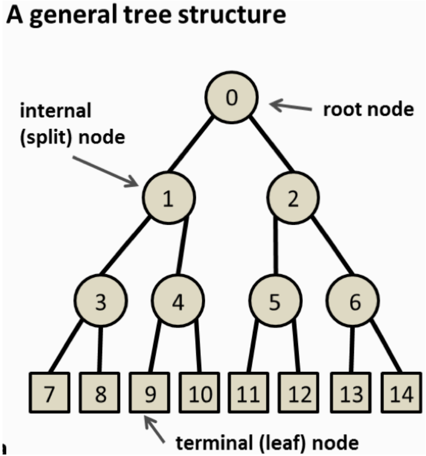

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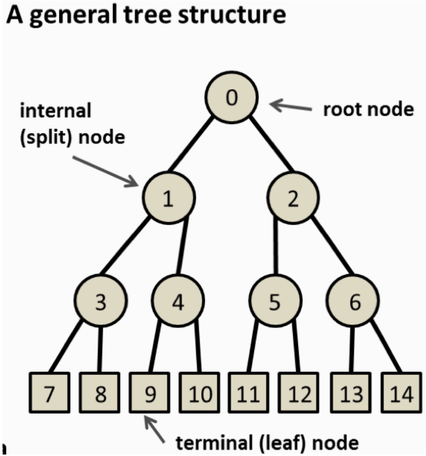

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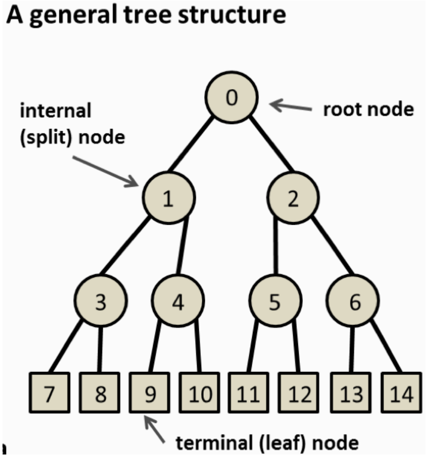

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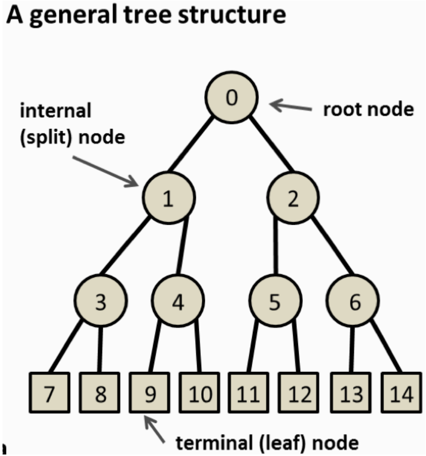

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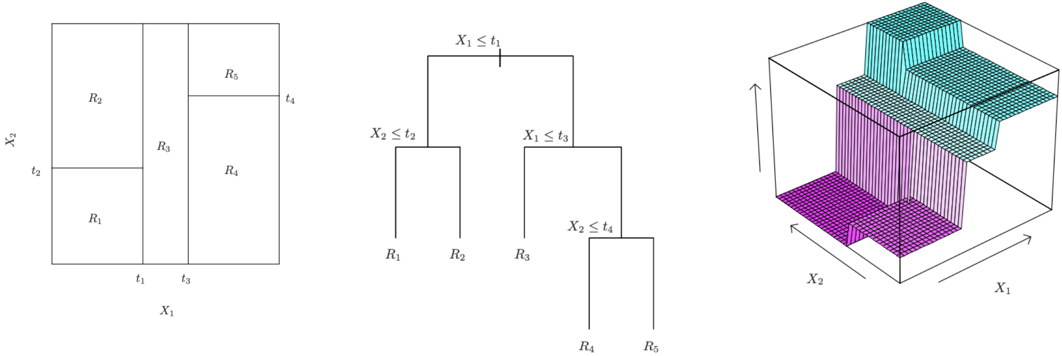
- This procedure is not very likely to result in the globally optimal tree

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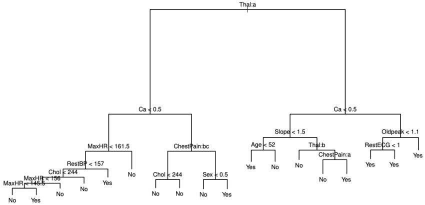
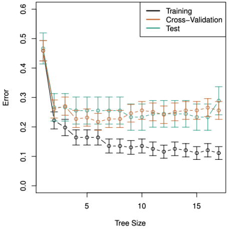
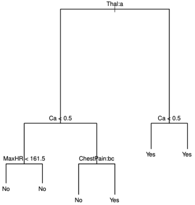
    2. *Prune* the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

Pruning: Example







What Makes a Good Split for Classification?

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.

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- We predict the majority class in node m:

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

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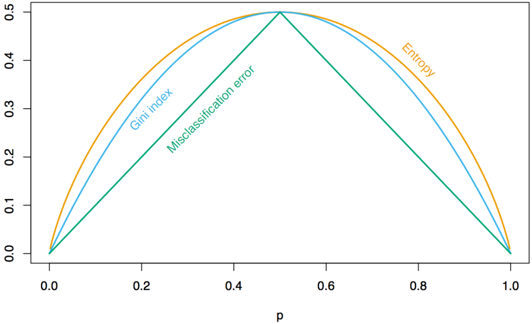
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

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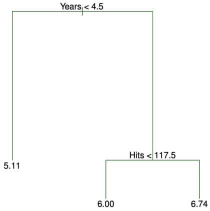
- We aim to find a split that minimizes the *weighted average of node impurities*:

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

Discussion: Interpretability of Decision Trees



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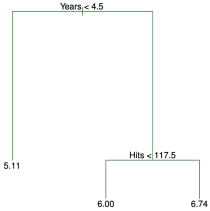

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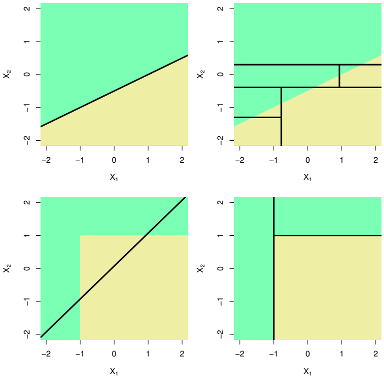
- Small trees are interpretable – large trees, maybe not so much

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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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 θ if $\hat{\theta} \approx \theta$

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Variance $\text{Var}(\hat{\theta}) \overset{\text{def}}{=} \mathbb{E}\left[\hat{\theta}^2\right] - \mathbb{E}^2\left[\hat{\theta}\right].$

- Why does variance matter if an estimator is unbiased?
  - $\hat{\theta}(\mathcal{D}) = x_1$ is an unbiased estimator of the mean of a Gaussian, but would be farther away from θ than the sample mean.

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

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

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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.

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- 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)

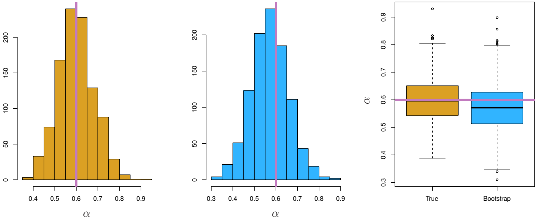

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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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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- Yes: if we have many trees, the bagged predictor is much less interpretable

Aside: Out-of-Bag Error Estimation

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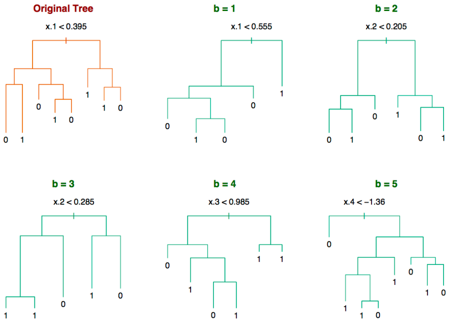
- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

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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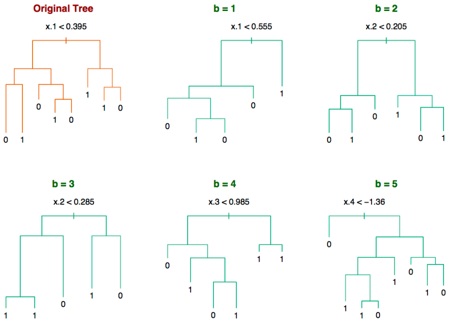

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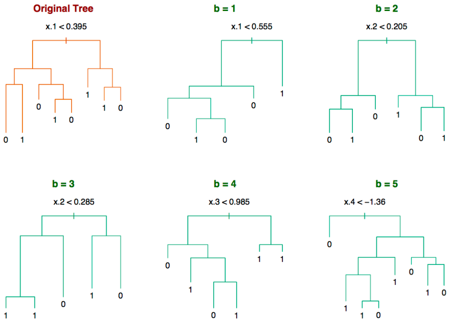

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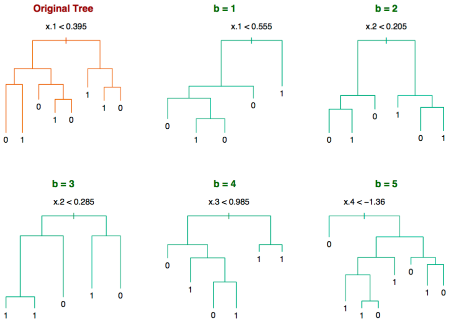

- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for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

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Key idea

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

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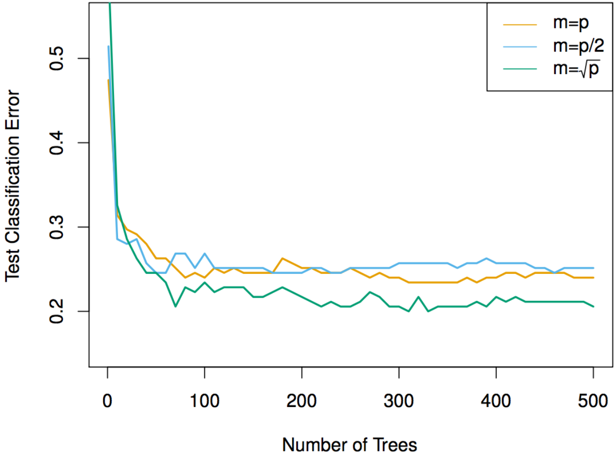
- If $m = p$, this is just bagging

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

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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.

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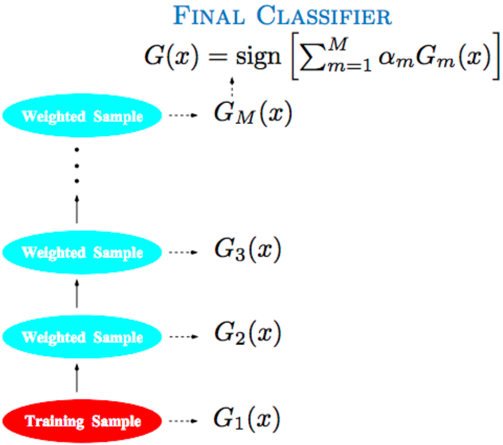
- **Weighted empirical risk**:

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

- 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 $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
- 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

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

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

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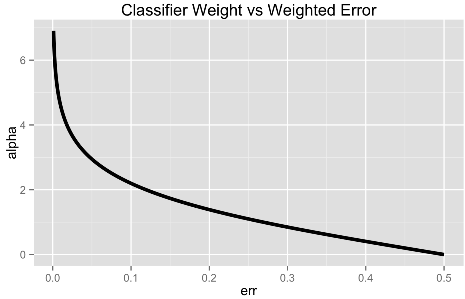

- Higher weighted error $\Longrightarrow$ lower weight

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

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AdaBoost with Decision Stumps

- After 1 round:

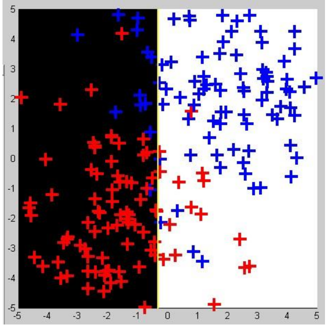
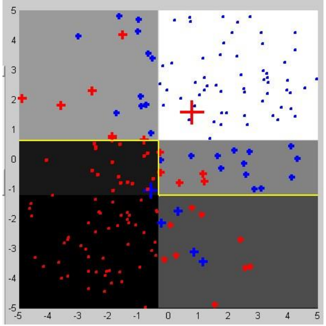


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:



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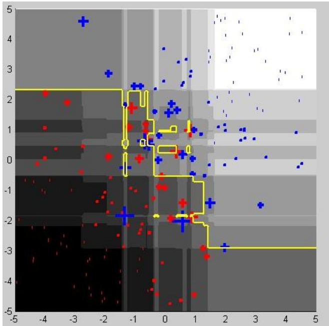
KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:



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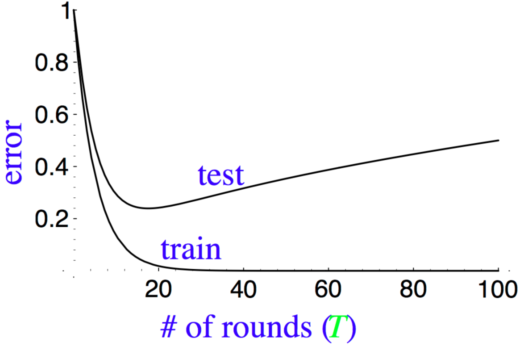
KPM Figure 16.10

Does AdaBoost overfit?

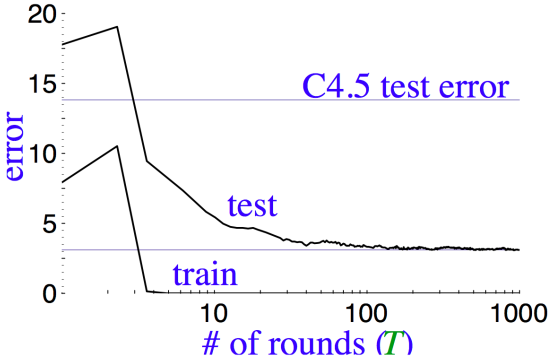
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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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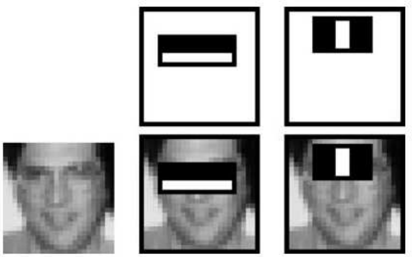
  - Pre-define weak classifiers, so optimization=selection
  - Smart way to do inference in real-time (in 2001 hardware)



Harr wavelet basis functions

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

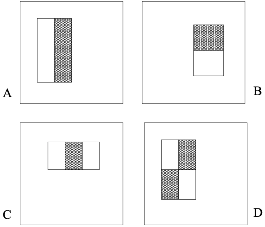
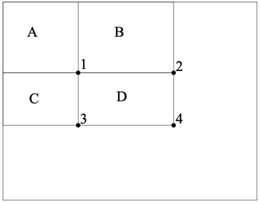


Figure 1: Example rectangle features shown relative to the enclosing detection window. The sum of the pixels which lie within the white rectangles are subtracted from the sum of pixels in the grey rectangles. Two-rectangle features are shown in (A) and (B). Figure (C) shows a three-rectangle feature,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

Integral image

- How to efficiently compute [image * weights] (hint: 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



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  5. Final classifier $h(x) = \begin{cases} 1 \text{ if } \sum_t \alpha_t h_t(x) > \frac{1}{2} \sum_t \alpha_t \\ 0 \text{ otherwise,} \end{cases}$ $\quad \alpha_t = -\log \beta_t$

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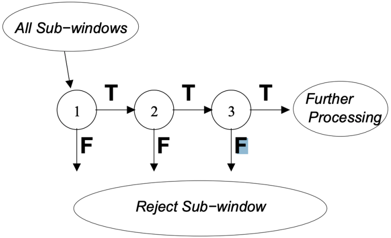
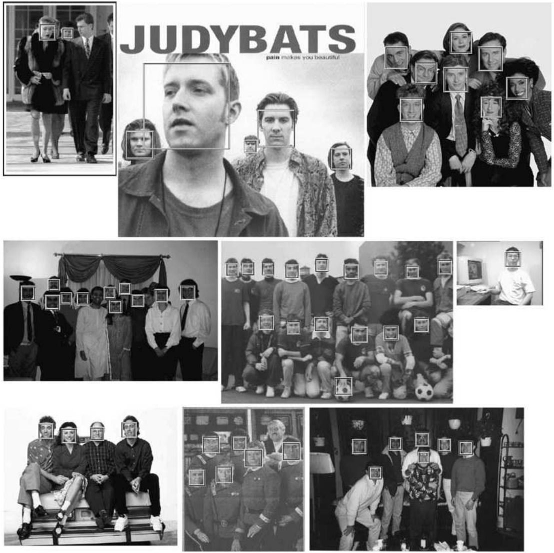
- Stop processing if one weak classifier says no.



AdaBoost Face Detection Results



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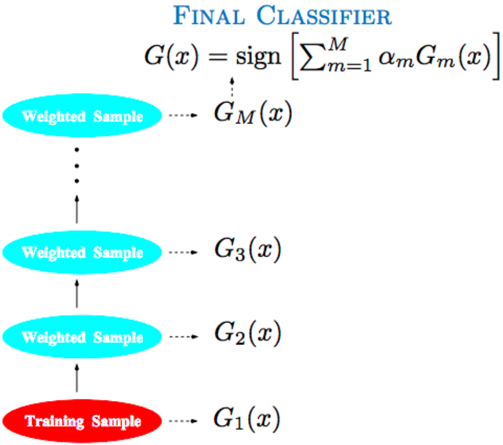
  - Gradient Boosting

Gradient Boosting

- Another way to get non-linear models in a linear form—adaptive basis function models.
- A general algorithm for greedy function approximation—gradient boosting machine.
    - Adaboost is a special case.

Motivation

Recap: Adaboost



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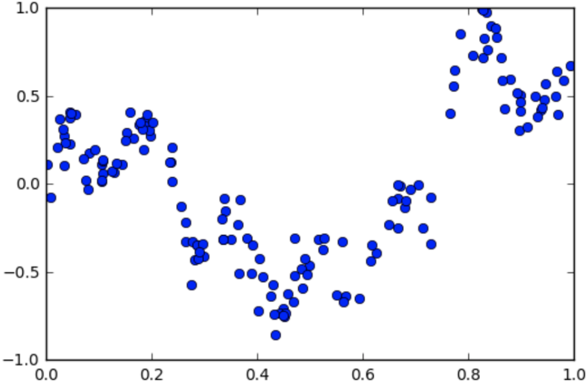
3. Return *voted classifier*: $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

Why not learn $G(x)$ directly?

Nonlinear Regression

- How do we fit the following data?



Linear Model with Basis Functions

- Fit a linear combination of transformations of the input:

$$f(x) = \sum_{m=1}^{M} v_m h_m(x),$$

where h_m's are called **basis functions** (or feature functions in ML):

$$h_1, \ldots, h_M : \mathcal{X} \to \mathrm{R}$$

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  - *Note that h_m's are fixed and known*, i.e. chosen ahead of time.

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- Base hypothesis space $\mathcal{H}$ consisting of functions $h : \mathcal{X} \to R$.
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- Combined hypothesis space:

$$\mathcal{F}_M = \left\{ \sum_{m=1}^{M} v_m h_m(x) \mid v_m \in \mathrm{R},\, h_m \in \mathcal{H},\, m = 1, \ldots, M \right\}$$

- What are the learnable?

Empirical Risk Minimization

- What's our learning objective?

$$\hat{f} = \arg\min_{f \in \mathcal{F}_M} \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, f\left(x_i\right)\right),$$

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- How to optimize J? i.e. how to learn?

Gradient-Based Methods

- Suppose our base hypothesis space is parameterized by $\Theta = \mathrm{R}^b$:

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- For some hypothesis spaces and typical loss functions, yes!
  - Neural networks fall into this category! ($h_1, \ldots, h_M$ are neurons of last hidden layer.)

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What about a greedy algorithm similar to Adaboost?

- Applies to non-parametric or non-differentiable basis functions.
- But is it optimizing our objective using some loss function?

Today we'll discuss **gradient boosting**.

- Gradient descent in the *function space*.
- It applies whenever
  - our loss function is [sub]differentiable w.r.t. training predictions $f(x_i)$, and
  - we can do regression with the base hypothesis space $\mathcal{H}$.

History

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Friedman, Hastie, Tibshirani (2000): Actually, boosting fits an additive model.

Friedman (2001): Furthermore, it can be considered as gradient descent in the function space.

Forward Stagewise Additive Modeling

Forward Stagewise Additive Modeling (FSAM)

Goal fit model $f(x) = \sum_{m=1}^{M} v_m h_m(x)$ given some loss function.

Approach Greedily fit one function at a time without adjusting previous functions, hence "forward stagewise".

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$$f_{m-1} = \sum_{i=1}^{m-1} v_i h_i.$$

- In m'th round, we want to find $h_m \in \mathcal{H}$ (i.e. a basis function) and $v_m > 0$ such that

$$f_m = \underbrace{f_{m-1}}_{\text{fixed}} + v_m h_m$$

improves objective function value by as much as possible.

Forward Stagewise Additive Modeling for ERM

Let's plug in our objective function.

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    2. Set $f_m = f_{m-1} + v_m h_m$.
3. Return: f_M.

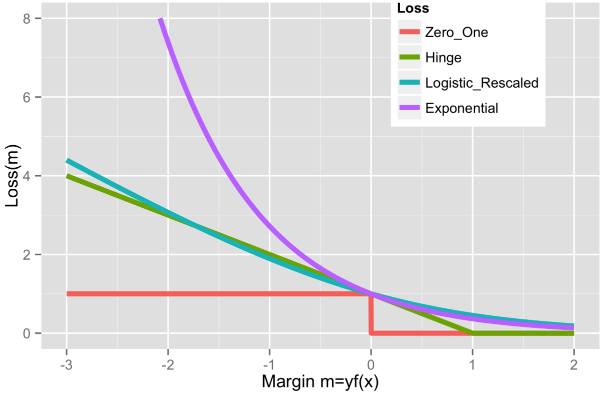
Recap: margin-based classifier

Binary classification

- Outcome space $\mathcal{Y} = \{-1, 1\}$
- Action space $\mathcal{A} = \mathrm{R}$ (model outoput)
- Score function $f : \mathcal{X} \to \mathcal{A}$.
- Margin for example (x, y) is $m = yf(x)$.
    - $m > 0 \iff$ classification correct
    - Larger m is better.
- Concept check: What are margin-based loss functions we've seen?

Exponential Loss

- Introduce the **exponential loss**: $\ell(y, f(x)) = \exp\left(-\underbrace{yf(x)}_{\text{margin}}\right)$.



Forward Stagewise Additive Modeling with exponential loss

Recall that we want to do FSAM with exponential loss.

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
    1. Compute:

$$(v_m, h_m) = \underset{v \in \mathrm{R}, h \in \mathcal{H}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell_{\text{exp}} \left(y_i, f_{m-1}(x_i) \underbrace{+ v h(x_i)}_{\text{new piece}} \right).$$

    2. Set $f_m = f_{m-1} + v_m h_m$.
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FSAM with Exponential Loss: objective function

- Base hypothesis: $\mathcal{H} = \{h \colon \mathcal{X} \to \{-1, 1\}\}$.
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$$J(v,h) = \sum_{i=1}^{n} \exp\left[-y_i\left(f_{m-1}(x_i) + vh(x_i)\right)\right] \tag{6}$$

$$= \sum_{i=1}^{n} w_i^m \exp\left[-y_i vh(x_i)\right] \qquad w_i^m \overset{\text{def}}{=} \exp\left[-y_i f_{m-1}(x_i)\right] \tag{7}$$

$$= \sum_{i=1}^{n} w_i^m \left[\mathbb{I}\left(y_i = h(x_i)\right)e^{-v} + \mathbb{I}\left(y_i \neq h(x_i)\right)e^{v}\right] \qquad h(x_i) \in \{1, -1\} \tag{8}$$

$$= \sum_{i=1}^{n} w_i^m \left[(e^{v} - e^{-v})\mathbb{I}\left(y_i \neq h(x_i)\right) + e^{-v}\right] \qquad \mathbb{I}\left(y_i = h(x_i)\right) = 1 - \mathbb{I}\left(y_i \neq h(x_i)\right) \tag{9}$$

FSAM with Exponential Loss: basis function

- Objective function in the m'th round:

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i.e. h_m is the minimizer of the weighted zero-one loss.

FSAM with Exponential Loss: classifier weights

- Define the weighted zero-one error:

$$\mathrm{err}_m = \frac{\sum_{i=1}^{n} w_i^m \mathbb{I}\left(y_i \neq h(x_i)\right)}{\sum_{i=1}^{n} w_i^m}. \tag{14}$$

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  - If $\text{err}_m < 0.5$ (better than chance), then $v_m > 0$.

FSAM with Exponential Loss: example weights

- Weights in the next round:

$$w_i^{m+1} \overset{\text{def}}{=} \exp\left[-y_i f_m(x_i)\right] \tag{16}$$

(19)

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- $2v_m = \alpha_m$ in Adaboost.

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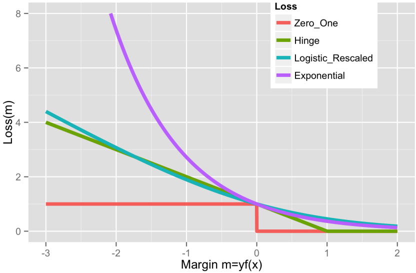
- How is it different from other losses?



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    - $\implies$ not robust to outliers / noise.
- Empirically, AdaBoost has degraded performance in situations with
    - high Bayes error rate (intrinsic randomness in the label)
- Logistic/Log loss performs better in settings with high Bayes error.
- Exponential loss has some computational advantages over log loss though.

Review

We've seen

- Use basis function to obtain *nonlinear* models: $f(x)=\sum_{i=1}^{M} v_m h_m(x)$ with known h_m's.
- *Adaptive* basis function models: $f(x)=\sum_{i=1}^{M} v_m h_m(x)$ with unknown h_m's.
- Forward stagewise additive modeling: greedily fit h_m's to minimize the average loss.

Review

We've seen

- Use basis function to obtain *nonlinear* models: $f(x) = \sum_{i=1}^{M} v_m h_m(x)$ with known h_m's.
- *Adaptive* basis function models: $f(x) = \sum_{i=1}^{M} v_m h_m(x)$ with unknown h_m's.
- Forward stagewise additive modeling: greedily fit h_m's to minimize the average loss.

But,

- We only know how to do FSAM for certain loss functions.
- Need to derive new algorithms for different loss functions.

Next, how to do FSAM in general.

Gradient Boosting / “Anyboost”

FSAM with squared loss

- Objective function at m'th round:

$$J(v,h) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \left[f_{m-1}(x_i) \underbrace{+vh(x_i)}_{\text{new piece}}\right]\right)^2$$

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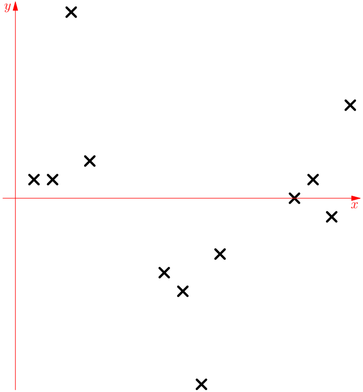
- This is just fitting the residuals with least-squares regression!

- Example base hypothesis space: regression stumps.

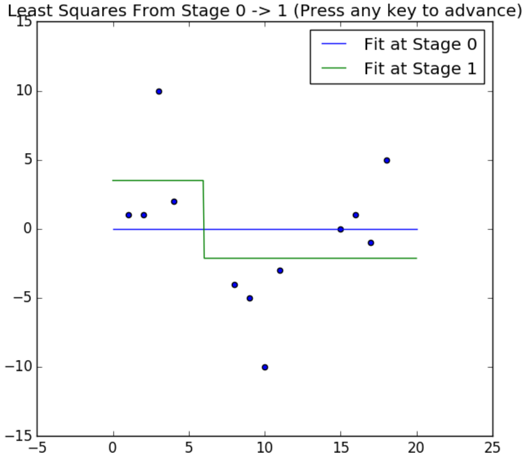
L^2 Boosting with Decision Stumps: Demo

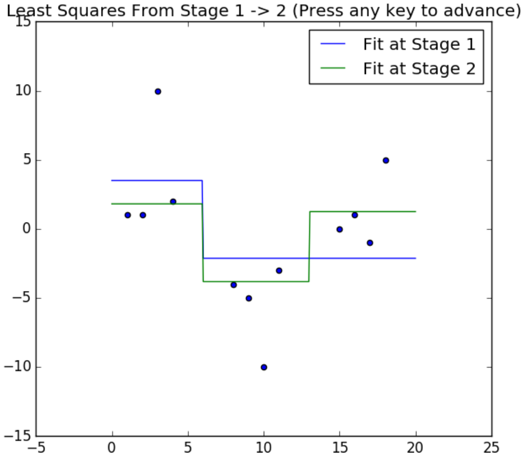
- Consider FSAM with L^2 loss (i.e. L^2 Boosting)
- For base hypothesis space of **regression stumps**



Plot courtesy of Brett Bernstein.

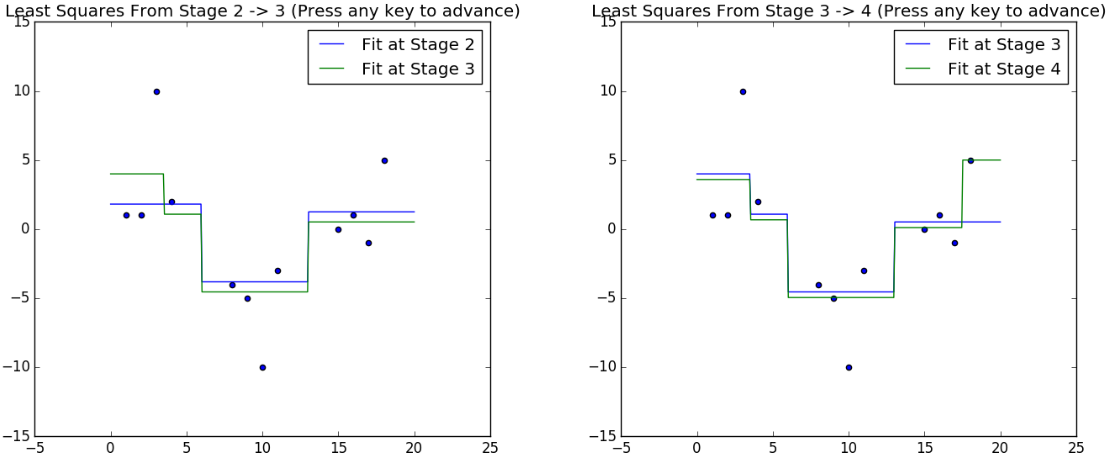
L^2 Boosting with Decision Stumps: Results





Plots and code courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results

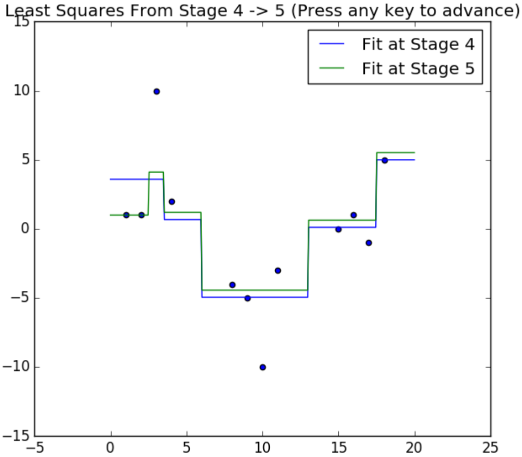


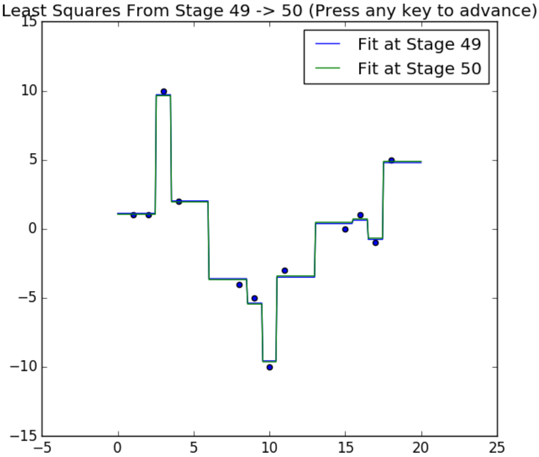
Least Squares From Stage 2 -> 3 (Press any key to advance)

Least Squares From Stage 3 -> 4 (Press any key to advance)

Plots and code courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results





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Interpret the residual

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- At each boosting round, we learn a function $h \in \mathcal{H}$ to fit the residual.

$$f \leftarrow f + \nu h \qquad \text{FSAM / boosting} \tag{22}$$

$$f \leftarrow f - \alpha \nabla_f J(f) \qquad \text{gradient descent} \tag{23}$$

  - h approximates the gradient (step direction).
  - ν is the step size.

“Functional” Gradient Descent

- We want to minimize

$$J(f) = \sum_{i=1}^{n} \ell\left(y_i, f(x_i)\right).$$

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- Define "parameters"

$$\mathrm{f}=\left(f\left(x_1\right),\dots,f\left(x_n\right)\right)^T$$

and write the objective function as

$$J(\mathrm{f})=\sum_{i=1}^{n}\ell\left(y_{i,}\mathrm{f}_i\right).$$

Functional Gradient Descent: Unconstrained Step Direction

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  which we can easily calculate.

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- $-\mathrm{g} \in \mathrm{R}^n$ is the direction we want to change each of our n predictions on training data.
- With gradient descent, our final predictor will be an additive model: $f_0 + \sum_{m=1}^{M} v_t\left(-\mathrm{g}_t\right)$.

Functional Gradient Descent: Projection Step

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- *Solution*: approximate by the closest base hypothesis $h \in \mathcal{H}$ (in the ℓ^2 sense):

$$\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \left(-\mathrm{g}_i - h(x_i)\right)^2. \qquad \text{least square regression} \qquad (24)$$

- Take the $h \in \mathcal{H}$ that best approximates $-\mathrm{g}$ as our step direction.

Recap

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- Gradient descent:

$$f \leftarrow f + {\color{red}v} h \tag{28}$$

Functional Gradient Descent: hyperparameters

- Choose a step size by **line search**.

$$v_m = \arg\min_v \sum_{i=1}^{n} \ell\{y_i, f_{m-1}(x_i) + v h_m(x_i)\}.$$

  - Not necessary. Can also choose a fixed hyperparameter v.

- Regularization through **shrinkage**:

$$f_m \leftarrow f_{m-1} + \lambda v_m h_m \quad \text{where } \lambda \in [0, 1]\,. \tag{29}$$

  - Typically choose $\lambda = 0.1$.

- Choose M, i.e. when to stop.
  - Tune on validation set.

Gradient boosting algorithm

1. Initialize f to a constant: $f_0(x) = \arg\min_\gamma \sum_{i=1}^n \ell(y_i, \gamma)$.
2. For m from 1 to M:
    1. Compute the pseudo-residuals (negative gradient):

$$r_{im} = -\left[\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)\right]_{f(x_i)=f_{m-1}(x_i)} \tag{30}$$

    2. Fit a base learner h_m with squared loss using the dataset $\{(x_i, r_{im})\}_{i=1}^n$.
    3. [Optional] Find the best step size $v_m = \arg\min_v \sum_{i=1}^n \ell\left(yi, f_{m-1}(x_i) + vh_m(x_i)\right)$.
    4. Update $f_m = f_{m-1} + \lambda v_m h_m$
3. Return $f_M(x)$.

The Gradient Boosting Machine Ingredients (Recap)

- Take any loss function [sub]differentiable w.r.t. the prediction $f(x_i)$
- Choose a base hypothesis space for regression.
- Choose number of steps (or a stopping criterion).
- Choose step size methodology.
- Then you're good to go!

BinomialBoost: Gradient Boosting with Logistic Loss

- Recall the logistic loss for classification, with $\mathcal{Y} = \{-1, 1\}$:

$$\ell(y, f(x)) = \log\left(1 + e^{-yf(x)}\right)$$

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- Pseudoresidual for i'th example is negative derivative of loss w.r.t. prediction:

$$\begin{aligned}
r_i &= -\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)) && (31)\\
&= -\frac{\partial}{\partial f(x_i)} \left[\log\left(1 + e^{-y_i f(x_i)}\right)\right] && (32)\\
&= \frac{y_i e^{-y_i f(x_i)}}{1 + e^{-y_i f(x_i)}} && (33)\\
&= \frac{y_i}{1 + e^{y_i f(x_i)}} && (34)
\end{aligned}$$

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- So if $f_{m-1}(x)$ is prediction after $m-1$ rounds, step direction for m'th round is

$$h_m = \underset{h\in\mathcal{H}}{\arg\min} \sum_{i=1}^{n} \left[\left(\frac{y_i}{1+e^{y_i f_{m-1}(x_i)}}\right) - h(x_i)\right]^2 .$$

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- And $f_m(x) = f_{m-1}(x) + v h_m(x)$.

Gradient Tree Boosting

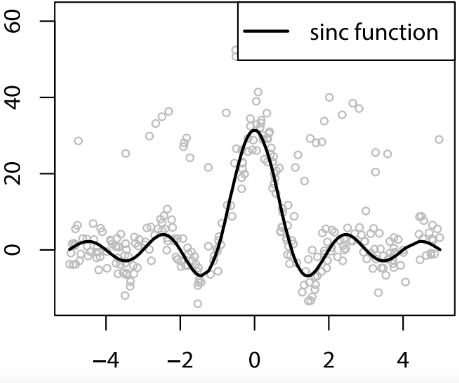
- One common form of gradient boosting machine takes

  $$\mathcal{H} = \{\text{regression trees of size } S\},$$

  where S is the number of terminal nodes.

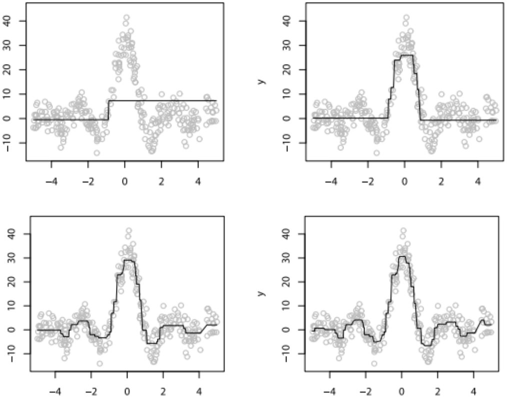
- $S = 2$ gives decision stumps
- HTF recommends $4 \leqslant S \leqslant 8$ (but more recent results use much larger trees)
- Software packages:
  - Gradient tree boosting is implemented by the gbm package for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in sklearn
  - xgboost and lightGBM are state of the art for speed and performance

Sinc Function: Our Dataset



From Natekin and Knoll's "Gradient boosting machines, a tutorial"

Minimizing Square Loss with Ensemble of Decision Stumps



Decision stumps with $1, 10, 50$, and 100 steps, shrinkage $\lambda = 1$.

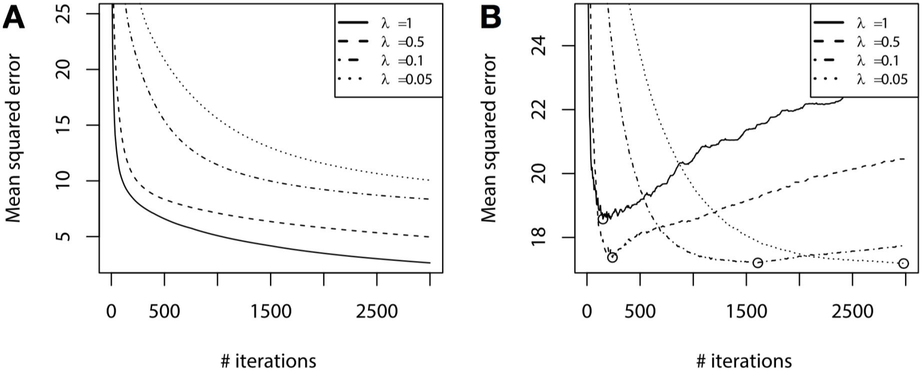
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

Gradient Boosting in Practice

Prevent overfitting

- Boosting is resistant to overfitting. Some explanations:
  - Implicit feature selection: greedily selects the best feature (weak learner)
  - As training goes on, impact of change is localized.
- But it can of course overfit. Common regularization methods:
  - Shrinkage (small learning rate)
  - Stochastic gradient boosting (row subsampling)
  - Feature subsampling (column subsampling)

Step Size as Regularization



- (continued) sinc function regression
- Performance vs rounds of boosting and shrinkage. (Left is training set, right is validation set)

Figure 5 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

Rule of Thumb

- The smaller the step size, the more steps you'll need.
- But never seems to make results worse, and often better.
- So set your step size as small as you have patience for.

Stochastic Gradient Boosting

- For each stage,
  - choose random *subset of data* for computing projected gradient step.

Introduced by Friedman (1999) in Stochastic Gradient Boosting.

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- Why do this?
  - Introduce randomization thus may help overfitting.
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- We can view this is a **minibatch method**.
  - Estimate the “true” step direction using a subset of data.

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Column / Feature Subsampling

- Similar to random forest, randomly choose *a subset of features* for each round.
- XGBoost paper says: "According to user feedback, using column sub-sampling prevents overfitting even more so than the traditional row sub-sampling."
- Speeds up computation.

Summary

- Motivating idea of boosting: combine weak learners to produce a strong learner.
- The statistical view: boosting is fitting an additive model (greedily).
- The numerical optimization view: boosting makes local improvement iteratively—gradient descent in the function space.
- Gradient boosting is a generic framework
  - Any differentiable loss function
  - Classification, regression, ranking, multiclass etc.
  - Scalable, e.g., XGBoost