Decision Trees and Boosting

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- Can overfit – need to limit the capacity.

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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- 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):

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

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- We will define the average prediction function as:

$$\hat{f}_{\text{avg}} \stackrel{\text{def}}{=} \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b \tag{2}$$

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!

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- For large n,

$$\left(1-\frac{1}{n}\right)^n \approx \frac{1}{e} \approx .368. \tag{3}$$

- 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)

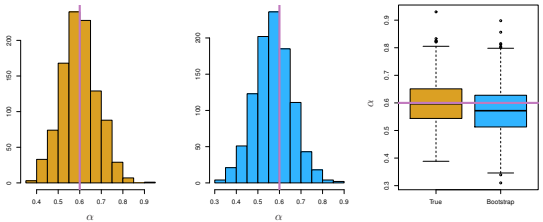

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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Key ideas:

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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

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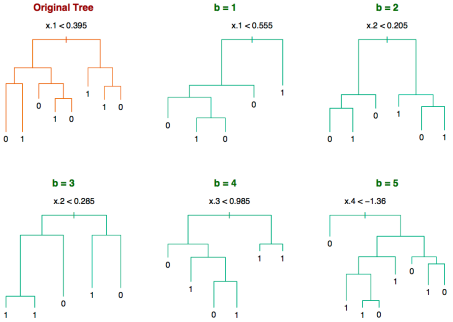
- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

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



From HTF Figure 8.9

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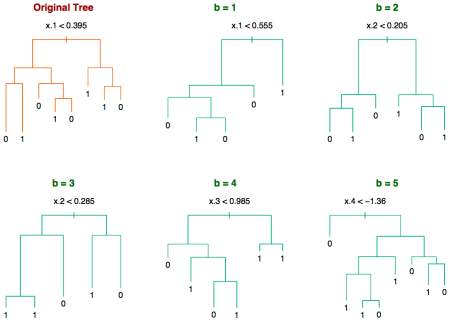

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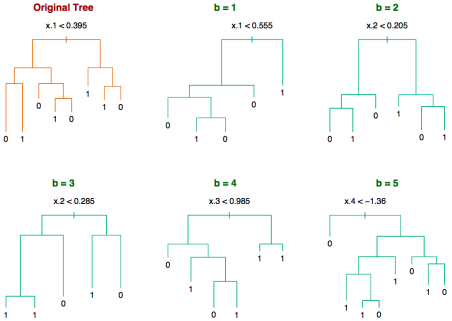

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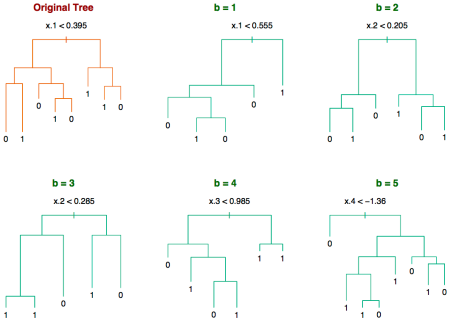

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- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

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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- We typically choose $m \approx \sqrt{p}$, where p is the number of features (or we can choose m using cross validation)

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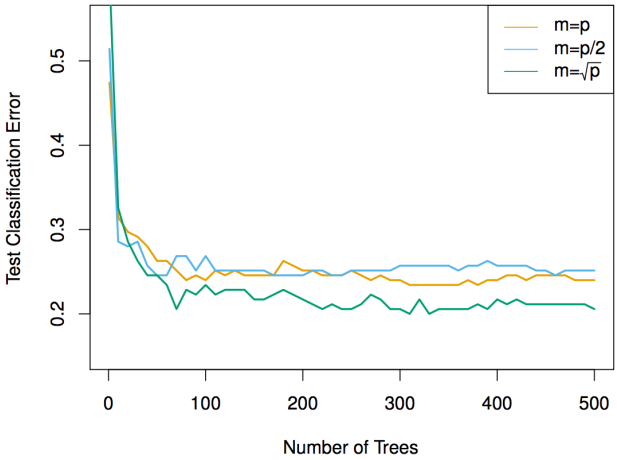
- When constructing each tree node, restrict choice of splitting variable to a randomly chosen subset of features of size m
  - This prevents a situation where all trees are dominated by the same small number of strong features (and are therefore too similar to each other)
- We typically choose $m \approx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

Random Forests: Effect of m



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

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- Use bootstrap to simulate many data samples from one dataset
  - $\Longrightarrow$ Bagged decision trees
- 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:
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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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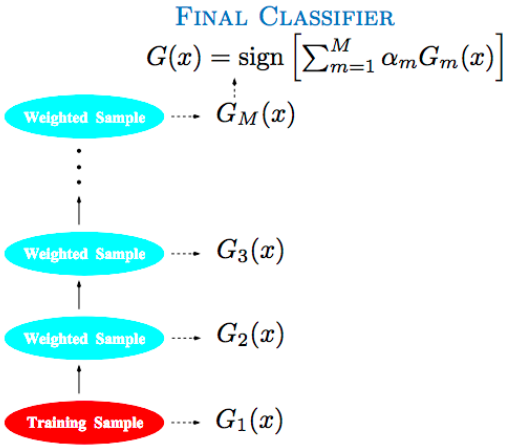
- **Weighted empirical risk**:

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

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- 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

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

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

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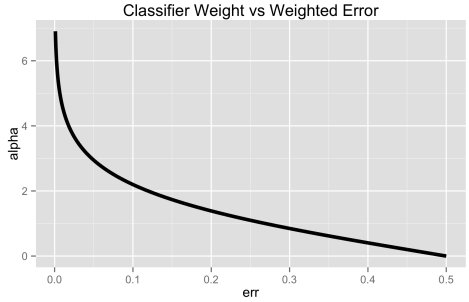

- Higher weighted error $\implies$ lower weight

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

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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:

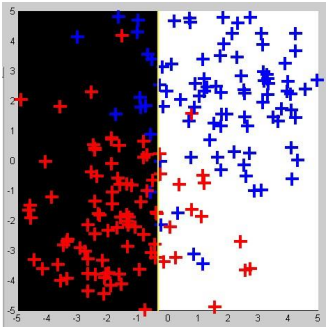


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:

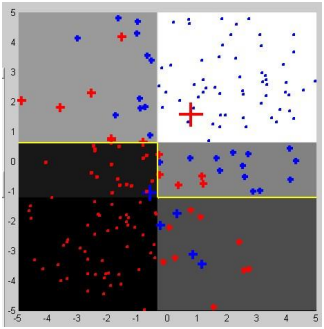
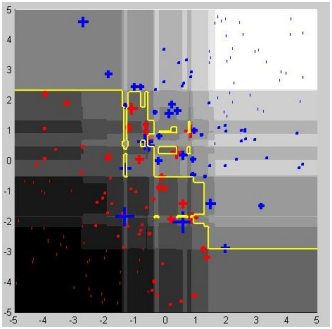


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:



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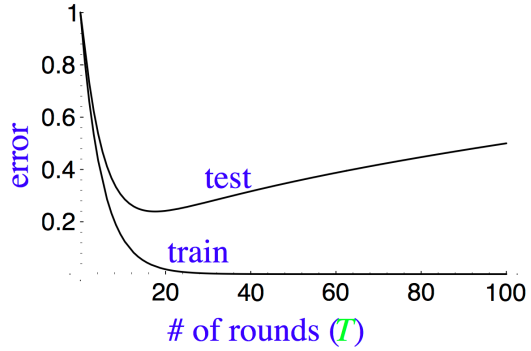
KPM Figure 16.10

Does AdaBoost overfit?

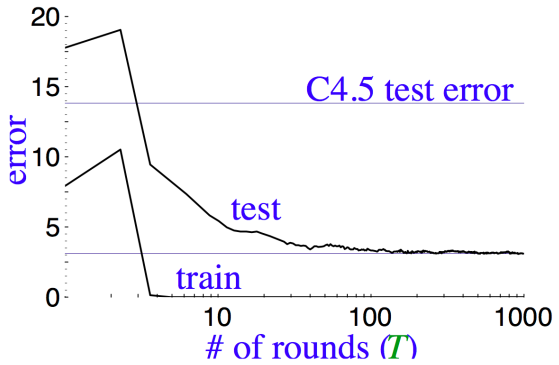
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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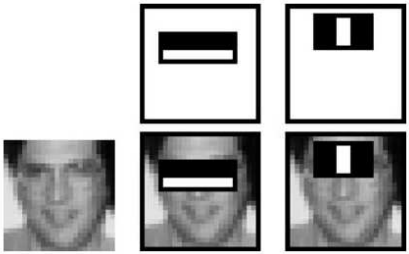
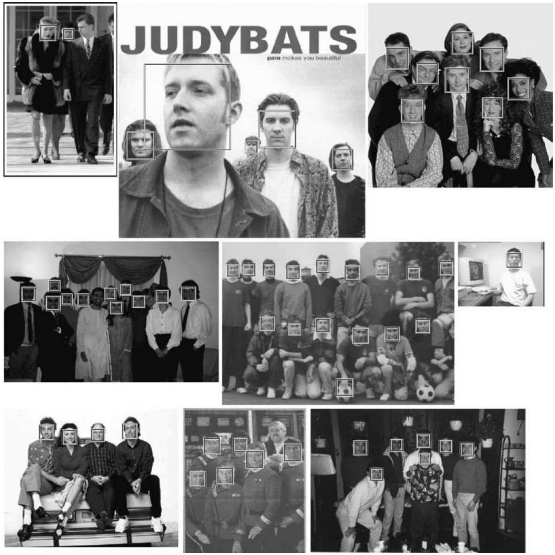
  - Pre-define weak classifiers, so optimization=selection
  - Smart way to do inference in real-time (in 2001 hardware)



AdaBoost Face Detection Results



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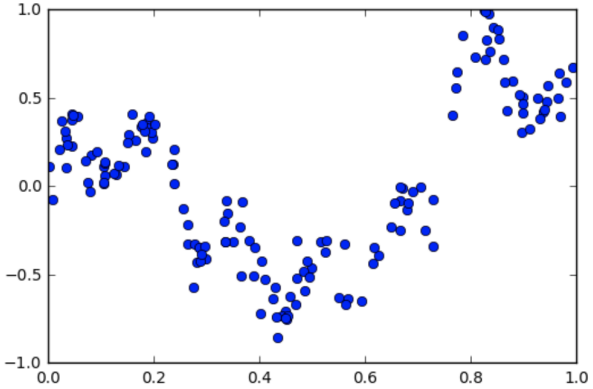
Nonlinear Regression

- How do we fit the following data?
- Another way to get non-linear models in a linear form—adaptive basis function models.



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):

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

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- An **adaptive basis function expansion** over $\mathcal{H}$ is an ensemble model:

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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?

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

for some loss function ℓ.

Empirical Risk Minimization

- What's our learning objective?

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

  for some loss function ℓ.

- Write ERM objective function as

$$J(v_1, \ldots, v_M, h_1, \ldots, h_M) = \frac{1}{n} \sum_{i=1}^{n} \ell\left(y_i, \sum_{m=1}^{M} v_m h_m(x)\right).$$

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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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- Can we optimize it with SGD?
  - Can we differentiate J w.r.t. v_m's and θ_m's?
- 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?

Gradient Boosting

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 $\mathcal{H}$.

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".

- After $m-1$ stages, we have

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- 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.

1. Initialize $f_0(x) = 0$.
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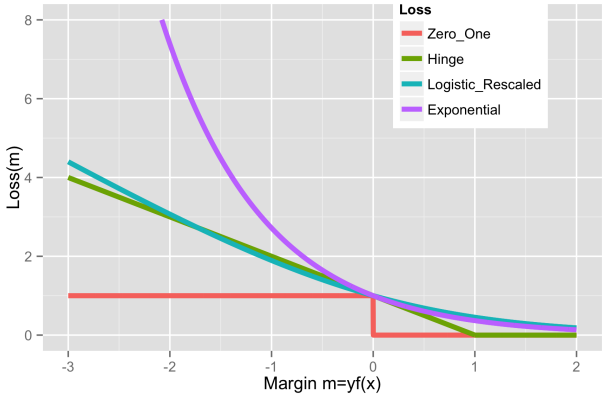
   2. Set $f_m = f_{m-1} + v_m h_m$.
3. Return: f_M.

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.

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   1. Compute:
   $$(v_m, h_m) = \underset{v \in \mathbb{R}, h \in \mathcal{H}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell_{\exp} \left(y_i, f_{m-1}(x_i) \underbrace{+ v h(x_i)}_{\text{new piece}} \right).$$
   2. Set $f_m = f_{m-1} + v_m h_m$.
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FSAM with Exponential Loss: objective function

- Base hypothesis: $\mathcal{H} = \{h \colon \mathcal{X} \to \{-1, 1\}\}$.
- Objective function in the m'th round:

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$$J(v, h) = \sum_{i=1}^{n} \exp\left[-y_i \left(f_{m-1}(x_i) + v h(x_i)\right)\right] \tag{5}$$

$$= \sum_{i=1}^{n} w_i^m \exp\left[-y_i v h(x_i)\right] \qquad w_i^m \stackrel{\text{def}}{=} \exp\left[-y_i f_{m-1}(x_i)\right] \tag{6}$$

$$= \sum_{i=1}^{n} w_i^m \left[\mathbb{I}(y_i = h(x_i))\, e^{-v} + \mathbb{I}(y_i \neq h(x_i))\, e^{v}\right] \qquad h(x_i) \in \{1, -1\} \tag{7}$$

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

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:

$$\text{err}_m = \frac{\sum_{i=1}^{n} w_i^m \mathbb{I}(y_i \neq h(x_i))}{\sum_{i=1}^{n} w_i^m}. \tag{13}$$

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  - Same as the classifier weights in Adaboost (differ by a constant).
  - If $\text{err}_m < 0.5$ (better than chance), then $v_m > 0$.

FSAM with Exponential Loss: example weights

- Weights in the next round:

$$w_i^{m+1} \stackrel{\text{def}}{=} \exp\left[-y_i f_m(x_i)\right] \tag{15}$$

(18)

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- $2v_m = \alpha_m$ in Adaboost.

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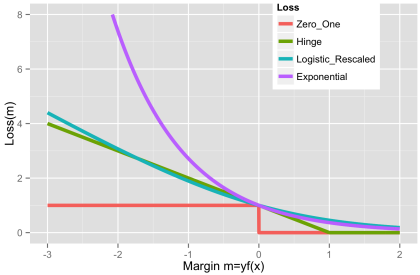
- How is it different from other losses?



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- 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.

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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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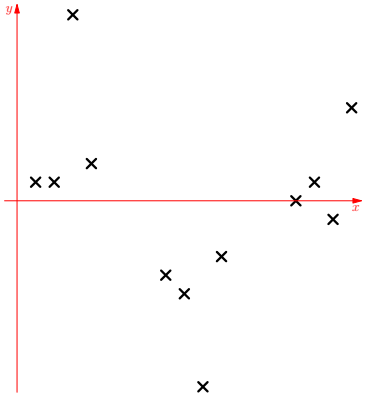
- This is just fitting the residuals with least-squares regression!
- Example base hypothesis space: regression stumps.

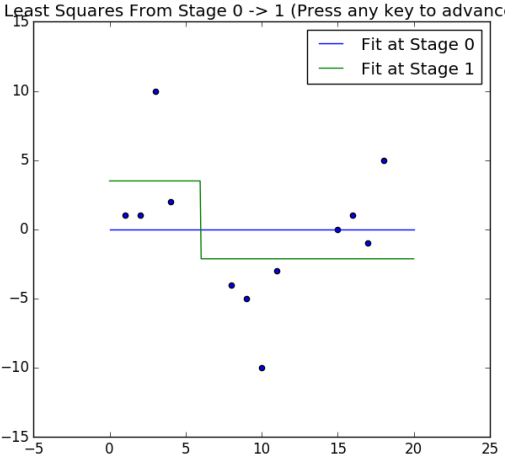
L^2 Boosting with Decision Stumps: Demo

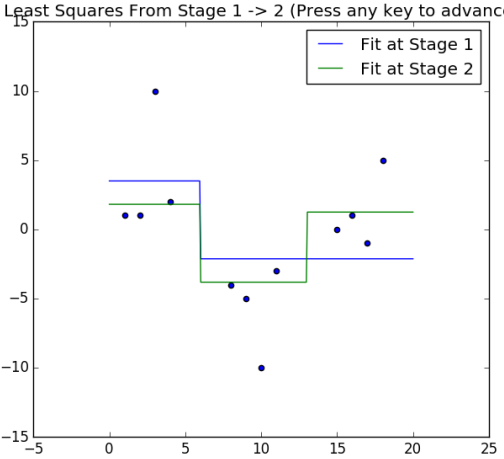
- Consider FSAM with L^2 loss (i.e. L^2 Boosting)
- For base hypothesis space of **regression stumps**



Plot courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results





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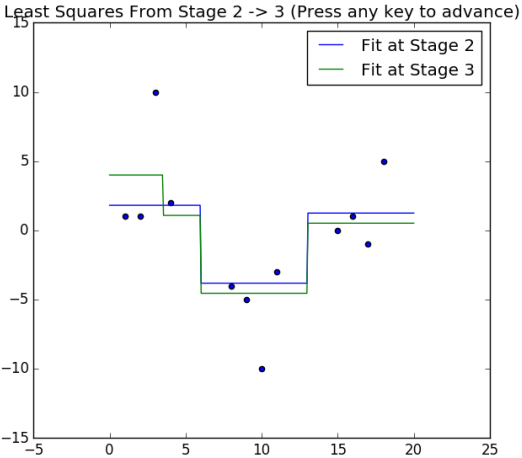
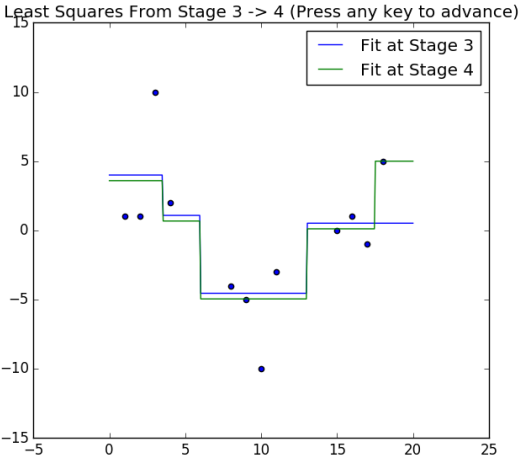
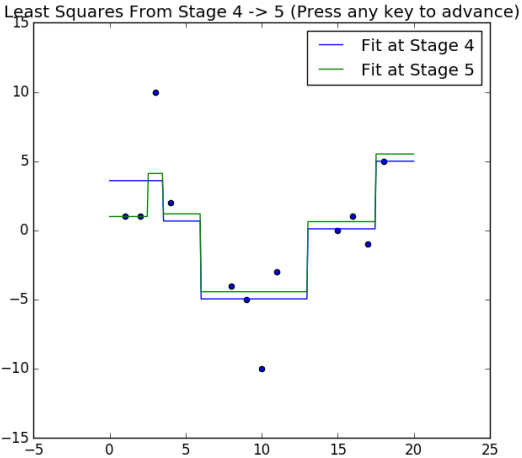
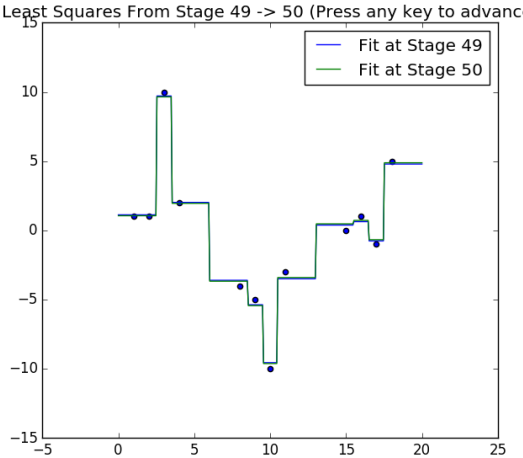




Plots and code courtesy of Brett Bernstein

L^2 Boosting with Decision Stumps: Results





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$$f \leftarrow f + vh \qquad \text{FSAM / boosting} \tag{21}$$

$$f \leftarrow f - \alpha \nabla_f J(f) \qquad \text{gradient descent} \tag{22}$$

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

"Functional" Gradient Descent

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- $J(f)$ only depends on f at the n training points.
- Define "parameters"
$$\mathsf{f} = (f(x_1), \ldots, f(x_n))^T$$
and write the objective function as
$$J(\mathsf{f}) = \sum_{i=1}^{n} \ell(y_i, \mathsf{f}_i).$$

Functional Gradient Descent: Unconstrained Step Direction

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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: $f_0 + \sum_{m=1}^{M} v_t(-\mathrm{g}_t)$.

Functional Gradient Descent: Projection Step

- Unconstrained step direction is

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- Problem: only know how to update at n points. How do we take a gradient step in $\mathcal{H}$?

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

$$\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \left(-\mathrm{g}_i - h(x_i)\right)^2. \qquad \text{least square regression} \qquad (23)$$

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

Recap

- Objective function:

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- Gradient descent:

$$f \leftarrow f + \nu h \tag{27}$$

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**:

$$f_m \leftarrow f_{m-1} + \lambda v_m h_m \quad \text{where } \lambda \in [0, 1]. \tag{28}$$

  - 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):

$$r_{im} = -\left[\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)\right]_{f(x_i)=f_{m-1}(x_i)} \tag{29}$$

   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 $v_m = \arg\min_v \sum_{i=1}^n \ell\left(yi, f_{m-1}(x_i) + v h_m(x_i)\right)$.
   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 $\mathcal{Y} = \{-1, 1\}$:

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

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

$$r_i = -\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)) \tag{30}$$

$$= -\frac{\partial}{\partial f(x_i)} \left[\log\left(1 + e^{-y_i f(x_i)}\right)\right] \tag{31}$$

$$= \frac{y_i e^{-y_i f(x_i)}}{1 + e^{-y_i f(x_i)}} \tag{32}$$

$$= \frac{y_i}{1 + e^{y_i f(x_i)}} \tag{33}$$

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

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

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

Gradient Tree Boosting

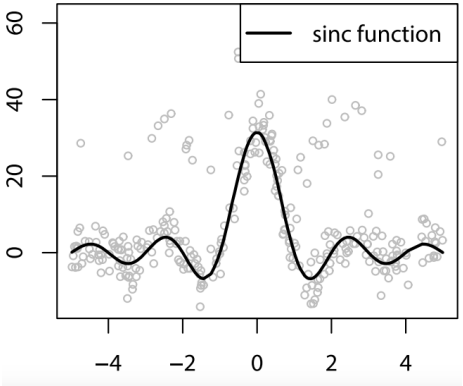
- One common form of gradient boosting machine takes

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

  where S is the number of terminal nodes.

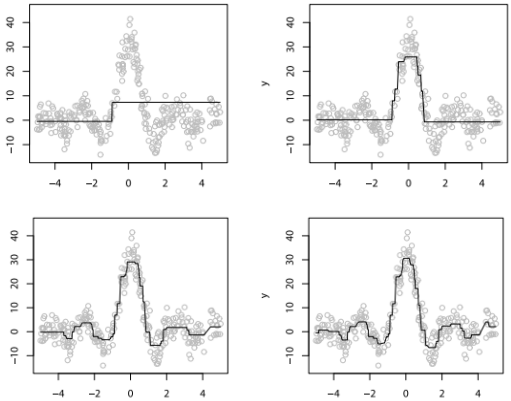
- $S = 2$ gives decision stumps
- Common choice: $4 \leqslant S \leqslant 8$
- Software packages:
  - Gradient tree boosting is implemented by the gbm package for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in sklearn
  - xgboost and lightGBM are state of the art for speed and 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 $\lambda = 1$.

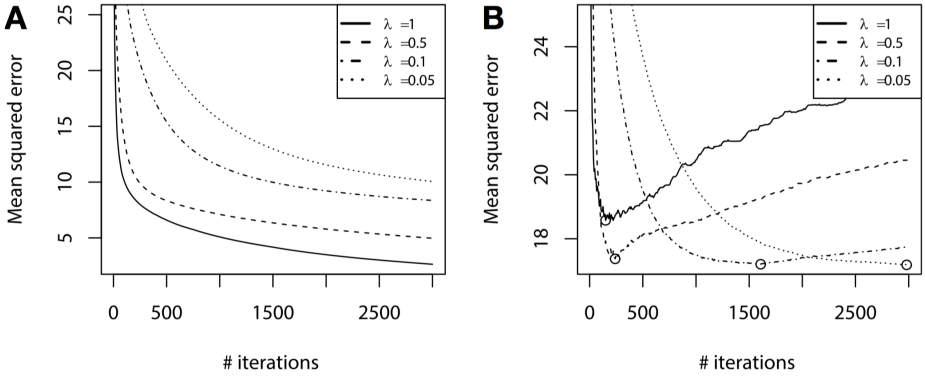
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

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"

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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  - Introduce randomization thus may help overfitting.
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  - Faster; often better than gradient descent given the same computation resource.
- 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