

Decision Trees and Boosting

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- Can overfit – need to limit the capacity.

Bagging and Random Forests

Recap: Statistics and Point Estimators

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

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- 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 : $\mathbb{E}[\hat{\theta}] = \theta$, $\text{Var}(\hat{\theta}) = \sigma^2$.
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- The average has the same expected value but smaller standard error (recall that $\text{Var}(cX) = c^2 \text{Var}(X)$, and that the $\hat{\theta}_i$ -s are uncorrelated):

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

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- We will define the average prediction function as:

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

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 ,

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

- 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, \dots, 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)

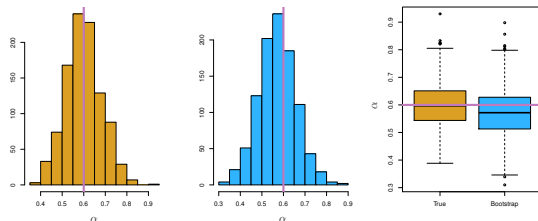


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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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 $\hat{f}_1, \hat{f}_2, \dots, \hat{f}_B$ be the prediction functions resulting from training on D^1, \dots, D^B , respectively
- The **bagged prediction function** is a *combination* of these:

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

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

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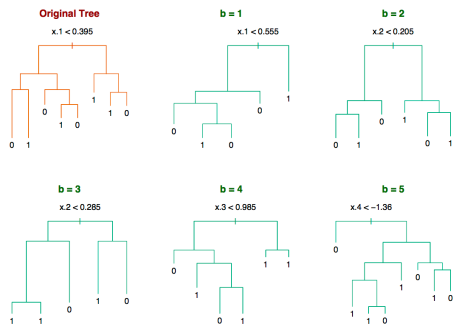
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- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

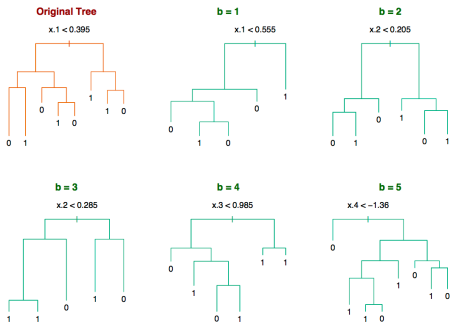
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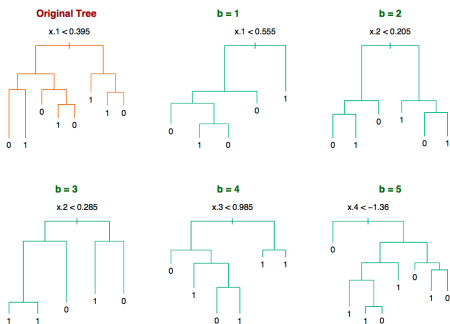


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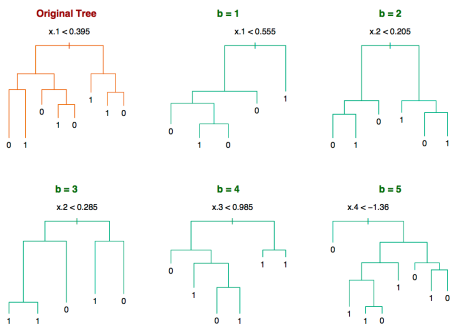


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- High variance:** small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

Motivating Random Forests: Correlated Prediction Functions

Recall the motivating principle of bagging:

- For $\hat{\theta}_1, \dots, \hat{\theta}_n$ *i.i.d.* with $\mathbb{E}[\hat{\theta}] = \theta$ and $\text{Var}[\hat{\theta}] = \sigma^2$,

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

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

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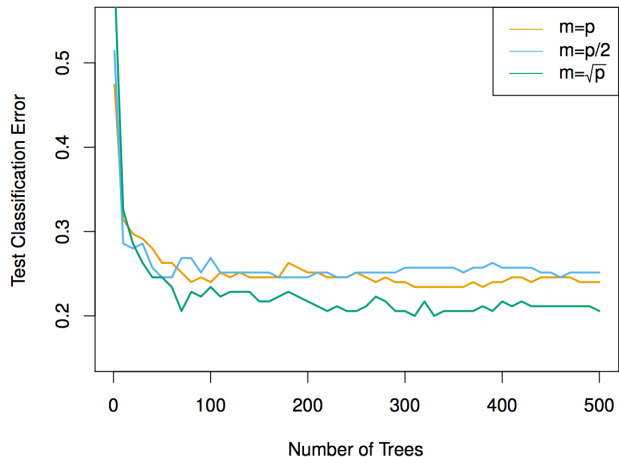
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- If $m = p$, this is just bagging

Random Forests: Effect of m



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

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- But bootstrap samples (and the induced models) are correlated

- The usual approach is to build very deep trees—low bias but **high variance**
- Ensembling many models reduces variance
 - Motivation: Mean of i.i.d. estimates has smaller variance than single estimate
- Use bootstrap to simulate many data samples from one dataset
 - \implies Bagged decision trees
- But bootstrap samples (and the induced models) are correlated
- Ensembling works better when we combine a diverse set of prediction functions
 - \implies Random forests: select a random subset of features for each decision tree

Boosting

Bagging Reduce variance of a low bias, high variance estimator by ensembling many estimators trained in parallel (on different datasets obtained through sampling).

Boosting: Overview

- 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).

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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)

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- Base hypothesis space $\mathcal{H} = \{h : \mathcal{X} \rightarrow \{-1, 1\}\}$.
- 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 $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n))$.
- Weights (w_1, \dots, w_n) associated with each example.

Weighted Training Set

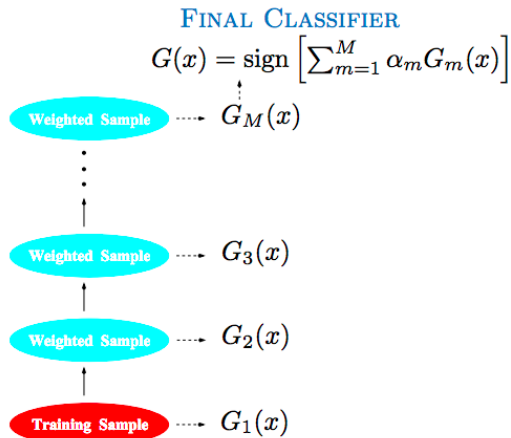
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- **Weighted empirical risk:**

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

AdaBoost: Sketch of the Algorithm

- Start with equal weights for all training points: $w_1 = \dots = w_n = 1$

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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

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

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

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

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

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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:

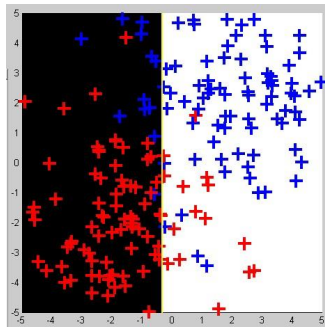


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

AdaBoost with Decision Stumps

- After 3 rounds:

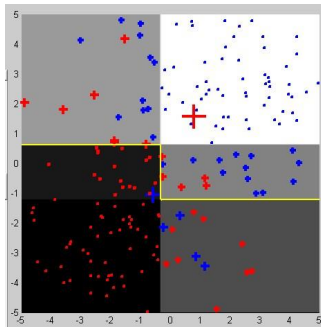


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AdaBoost with Decision Stumps

- After 120 rounds:

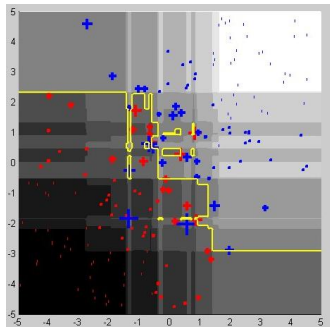
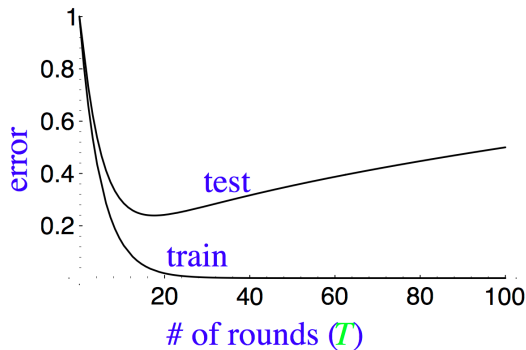


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Does AdaBoost overfit?

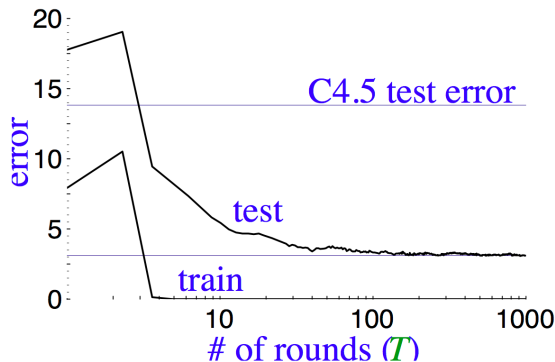
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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!



From Rob Schapire's NIPS 2007 Boosting tutorial.

AdaBoost for Face Detection

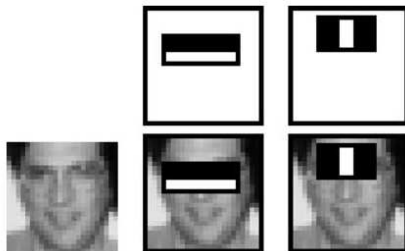
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- A few twists on standard algorithm
 - Pre-define weak classifiers, so optimization=selection
 - Smart way to do inference in real-time (in 2001 hardware)



Harr wavelet basis functions

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

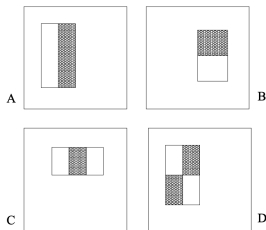
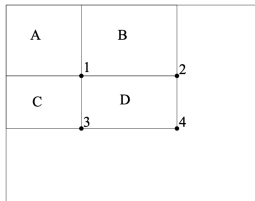


Figure 1: Example rectangle features shown relative to the enclosing detection window. The sum of the pixels which lie within the white rectangles are subtracted from the sum of pixels in the grey rectangles. Two-rectangle features are shown in (A) and (B). Figure (C) shows a three-rectangle feature,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

Integral image

- How to efficiently compute $[\text{image} * \text{weights}]$ (hint: the sum of an area of the image).
- Compute an “integral image”
- Store a 2-D array: $S[i, j] = \text{Sum of the image from } (0,0) \text{ to } (i,j)$.
- $D = ABCD - AB - AC + A$



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- Review AdaBoost again here, with a slightly different but equivalent setup.
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 - ⑤ Final classifier
$$h(x) = \begin{cases} 1 & \text{if } \sum_t \alpha_t h_t(x) > \frac{1}{2} \sum_t \alpha_t \\ 0 & \text{otherwise,} \end{cases} \quad \alpha_t = -\log \beta_t$$

Cascaded Processing for Faster Speed

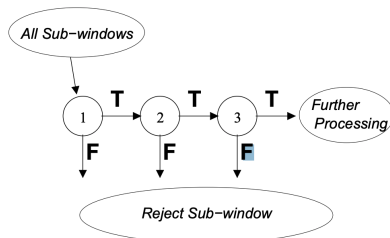
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- False positive is ok. We can reject the windows later.
- Stop processing if one weak classifier says no.



AdaBoost Face Detection Results



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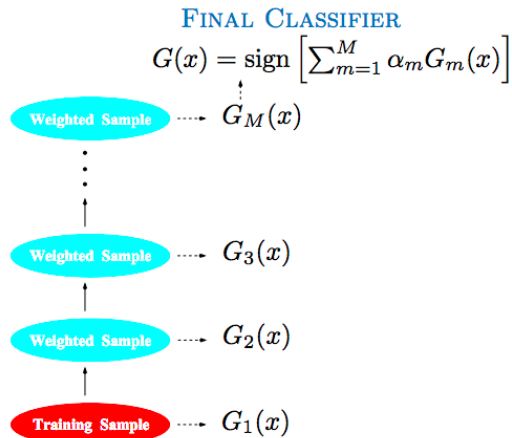
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 - Gradient Boosting

- 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



From ESL Figure 10.1

AdaBoost: Algorithm

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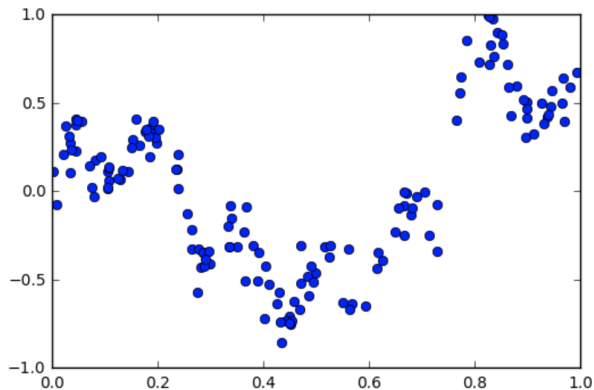
- ① Initialize observation weights $w_i = 1, i = 1, 2, \dots, n$.
- ② For $m = 1$ to M :
 - ① Base learner fits weighted training data and returns $G_m(x)$
 - ② Compute *weighted empirical 0-1 risk*:

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

- ③ Compute *classifier weight*: $\alpha_m = \ln \left(\frac{1 - \text{err}_m}{\text{err}_m} \right)$.
 - ④ Update *example weight*: $w_i \leftarrow w_i \cdot \exp[\alpha_m \mathbb{1}[y_i \neq G_m(x_i)]]$
- ③ Return *voted classifier*: $G(x) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x) \right]$. 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):

$$h_1, \dots, h_M : \mathcal{X} \rightarrow \mathbb{R}$$

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- Can fit this using standard methods for linear models (e.g. least squares, lasso, ridge, etc.)
 - *Note that h_m 's are fixed and known, i.e. chosen ahead of time.*

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- What if we want to learn the basis functions? (hence *adaptive*)

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- Base hypothesis space \mathcal{H} consisting of functions $h : \mathcal{X} \rightarrow \mathbb{R}$.
- An **adaptive basis function expansion** over \mathcal{H} is an ensemble model:

$$f(x) = \sum_{m=1}^M v_m h_m(x), \quad (4)$$

where $v_m \in \mathbb{R}$ and $h_m \in \mathcal{H}$.

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- Combined hypothesis space:

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

- What are the learnable?

Empirical Risk Minimization

- What's our learning objective?

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

for some loss function ℓ .

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

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

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Gradient-Based Methods

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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, \dots, h_M are neurons of last hidden layer.)

What if Gradient Based Methods Don't Apply?

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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} .

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

- 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.

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

Forward Stagewise Additive Modeling for ERM

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

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

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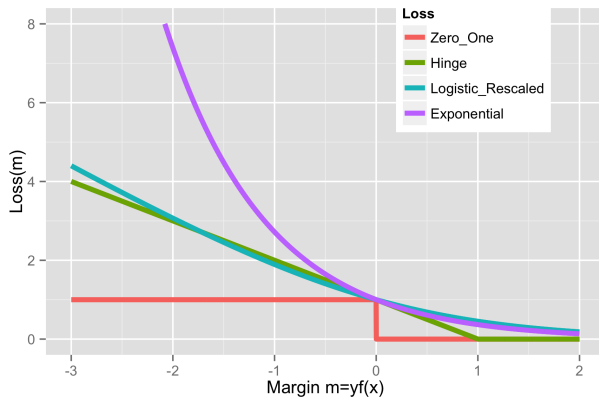
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❷ Set $f_m = f_{m-1} + v_m h_m$.

❸ 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.

❶ Initialize $f_0(x) = 0$.

❷ For $m = 1$ to M :

❶ Compute:

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

❷ Set $f_m = f_{m-1} + v_m h_m$.

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FSAM with Exponential Loss: objective function

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

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

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

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

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

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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:

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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:

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

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- $2v_m = \alpha_m$ in Adaboost.

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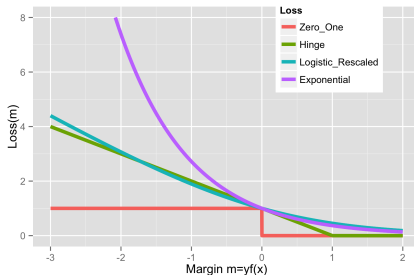
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- How is it different from other losses?



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AdaBoost / Exponential Loss: Robustness Issues

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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)

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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.

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.
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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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- Take $v = 1$ and minimize

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

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

FSAM with squared loss

- Objective function at m 'th round:

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

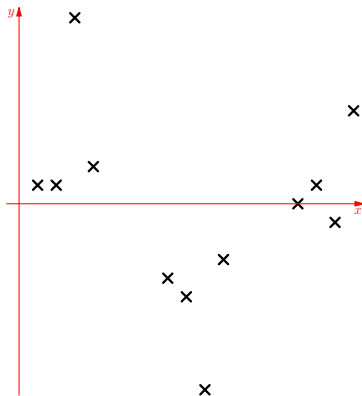
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- This is just fitting the residuals with least-squares regression!
- Example base hypothesis space: regression stumps.

L^2 Boosting with Decision Stumps: Demo

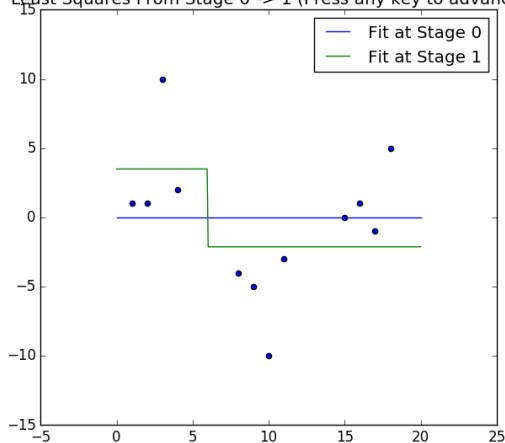
- Consider FSAM with L^2 loss (i.e. L^2 Boosting)
- For base hypothesis space of **regression stumps**



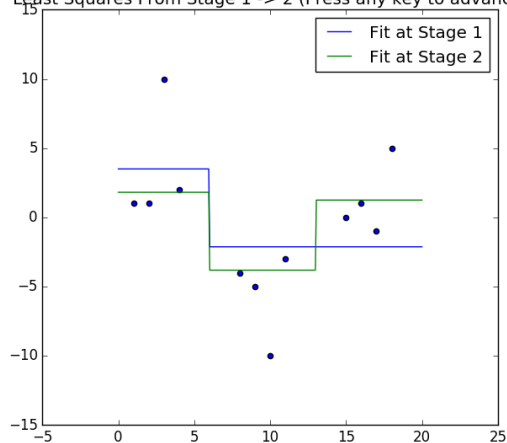
Plot courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results

Least Squares From Stage 0 -> 1 (Press any key to advance)

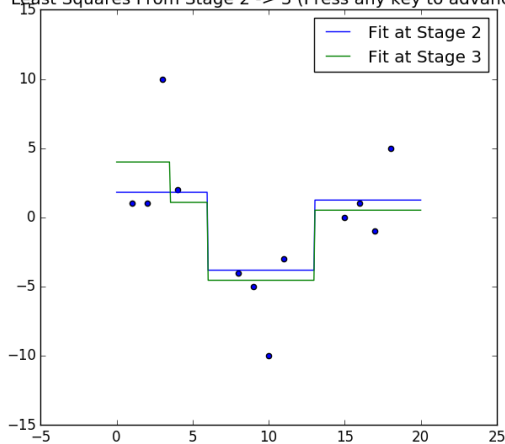


Least Squares From Stage 1 -> 2 (Press any key to advance)

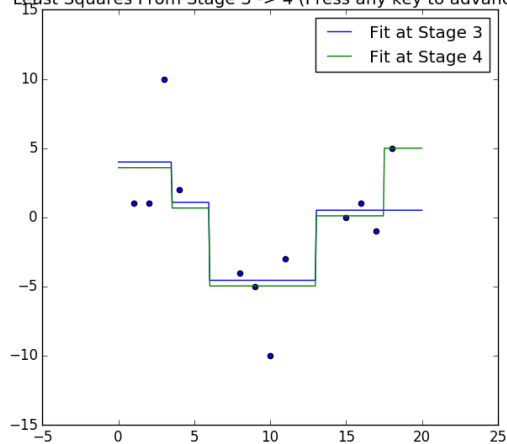


L^2 Boosting with Decision Stumps: Results

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

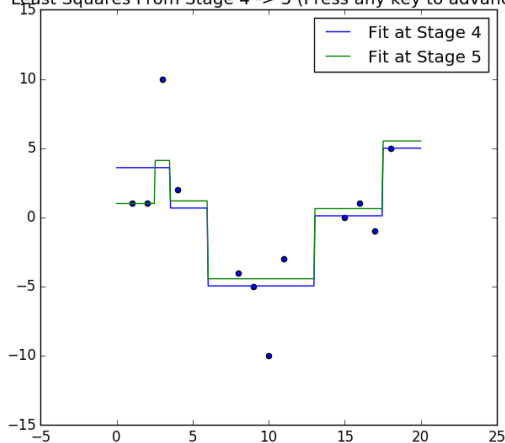


Least Squares From Stage 3 -> 4 (Press any key to advance)

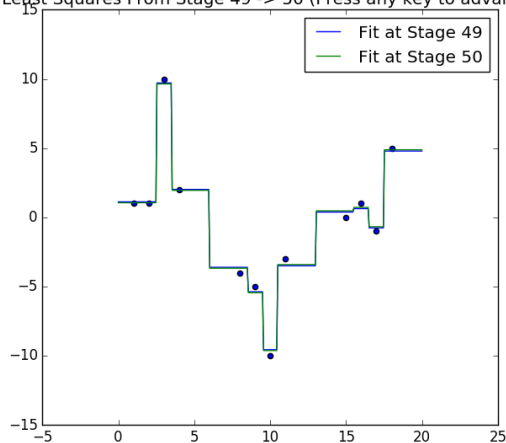


L^2 Boosting with Decision Stumps: Results

Least Squares From Stage 4 -> 5 (Press any key to advance)



Least Squares From Stage 49 -> 50 (Press any key to advance)



Interpret the residual

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$$f \leftarrow f + \textcolor{red}{v} \textcolor{green}{h} \quad \text{FSAM / boosting} \quad (21)$$

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$$f \leftarrow f + \nu h \quad \text{FSAM / boosting} \quad (21)$$

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

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

“Functional” Gradient Descent

- We want to minimize

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- $J(f)$ only depends on f at the n training points.
- Define “parameters”

$$\mathbf{f} = (f(x_1), \dots, f(x_n))^T$$

and write the objective function as

$$J(\mathbf{f}) = \sum_{i=1}^n \ell(y_i, \mathbf{f}_i).$$

Functional Gradient Descent: Unconstrained Step Direction

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which we can easily calculate.

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which we can easily calculate.

- $-g \in \mathbb{R}^n$ 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: $f_0 + \sum_{m=1}^M v_t(-g_t)$.

Functional Gradient Descent: Projection Step

- Unconstrained step direction is

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- Also called the “**pseudo-residuals**”. (For squared loss, they’re exactly the residuals.)

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- Also called the “**pseudo-residuals**”. (For squared loss, they’re exactly the residuals.)
- **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):

$$\min_{h \in \mathcal{H}} \sum_{i=1}^n (-g_i - h(x_i))^2. \quad \text{least square regression} \quad (23)$$

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

Recap

- Objective function:

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- Gradient descent:

$$f \leftarrow f + \textcolor{red}{\alpha} h \quad (27)$$

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**:

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

- 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):

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

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

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

BinomialBoost: Gradient Boosting with Logistic Loss

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

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

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

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

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

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

BinomialBoost: Gradient Boosting with Logistic Loss

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

Gradient Tree Boosting

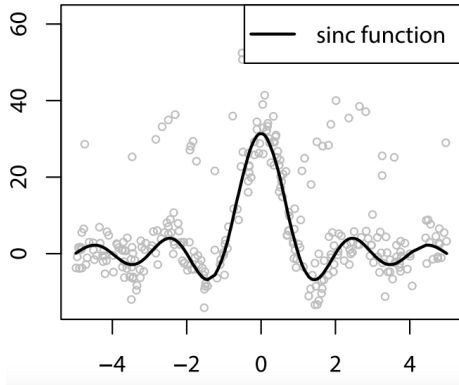
- One common form of gradient boosting machine takes

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

where S is the number of terminal nodes.

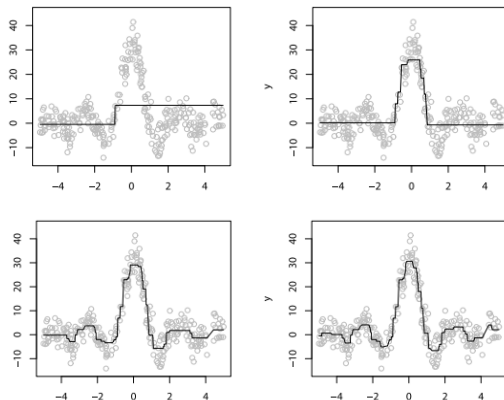
- $S = 2$ gives decision stumps
- HTF recommends $4 \leq S \leq 8$ (but more recent results use much larger trees)
- Software packages:
 - Gradient tree boosting is implemented by the `gbm` package for R
 - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in `sklearn`
 - `xgboost` and `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 $\lambda = 1$.

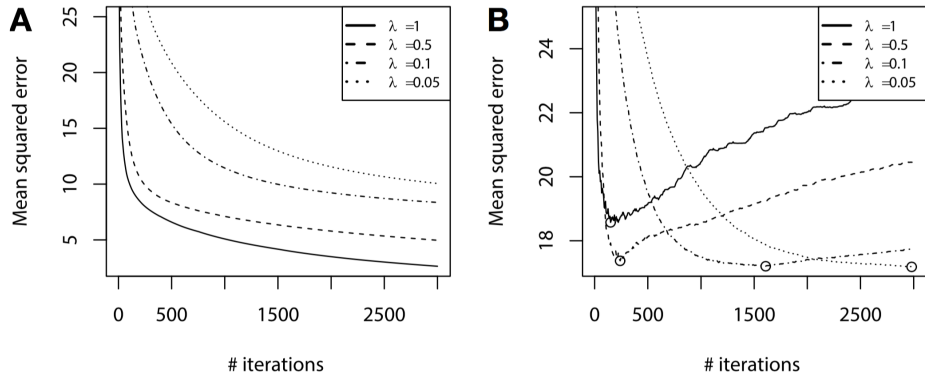
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

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.

Stochastic Gradient Boosting

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 - choose random *subset of data* for computing projected gradient step.
- Why do this?
 - Introduce randomization thus may help overfitting.
 - Faster; often better than gradient descent given the same computation resource.

Introduced by Friedman (1999) in [Stochastic Gradient Boosting](#).

Stochastic Gradient Boosting

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 - choose random *subset of data* for computing projected gradient step.
- Why do this?
 - Introduce randomization thus may help overfitting.
 - 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.

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