

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 : $\mathbb{E}[\hat{\theta}] = \theta$, $\text{Var}(\hat{\theta}) = \sigma^2$.
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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)

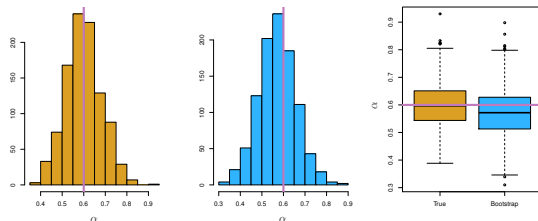


Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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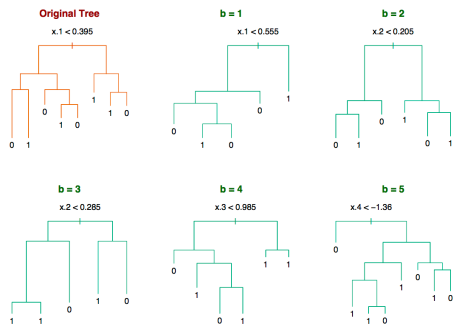
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- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

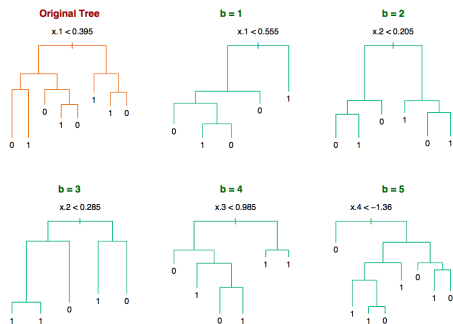
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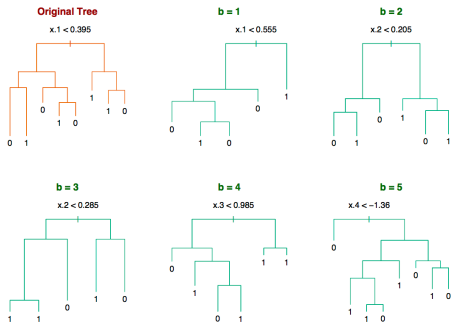


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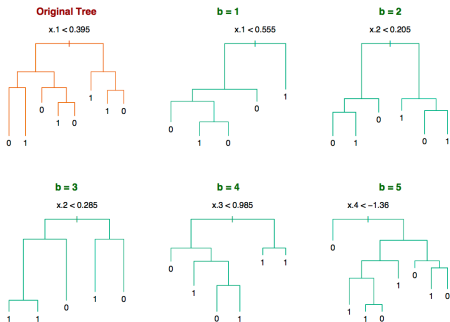


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- High variance:** small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

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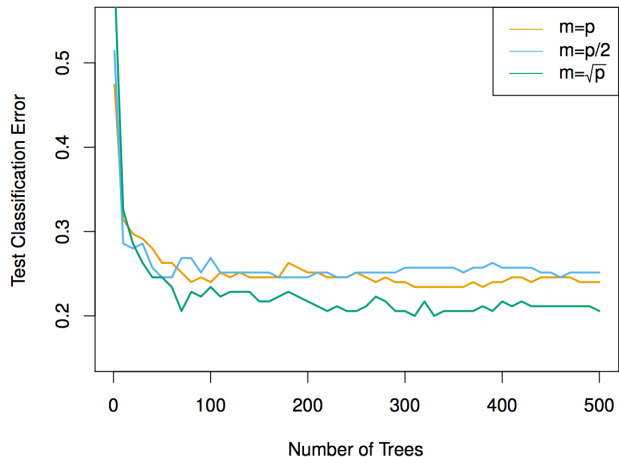
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- If $m = p$, this is just bagging

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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Boosting Reduce the error rate of a high bias estimator by ensembling many estimators trained in sequence (without bootstrapping).

- Like bagging, boosting is a general method that is particularly popular with decision trees.
- Main intuition: instead of fitting the data very closely using a large decision tree, train gradually, using a sequence of simpler trees

Boosting: Overview

- A **weak/base learner** is a classifier that does slightly better than chance.
- Weak learners are like rules of thumb:
 - “Inheritance” \implies spam
 - From a friend \implies not spam

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- We'll focus on a specific implementation, AdaBoost (Freund & Schapire, 1997)

AdaBoost: Setting

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

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

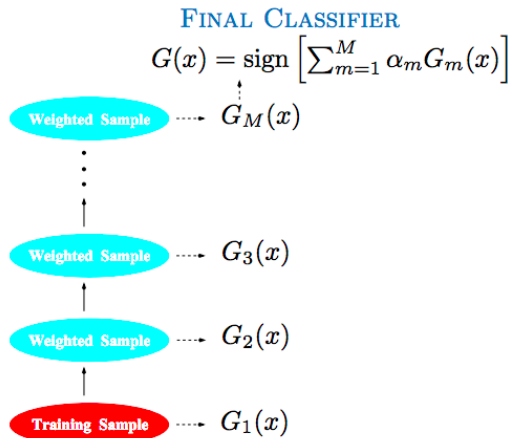
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- Training set $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n))$.
- Weights (w_1, \dots, w_n) associated with each example.
- **Weighted empirical risk:**

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

AdaBoost: Sketch of the Algorithm

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

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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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- The weight of classifier $G_m(x)$ is $\alpha_m = \ln \left(\frac{1 - \text{err}_m}{\text{err}_m} \right)$

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- Higher weighted error \implies lower weight

AdaBoost: Example Reweighting

- We train G_m to minimize weighted error; the resulting error rate is err_m
- Then $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$ is the weight of G_m in the final ensemble

We want the next base learner to focus more on examples misclassified by the previous learner.

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

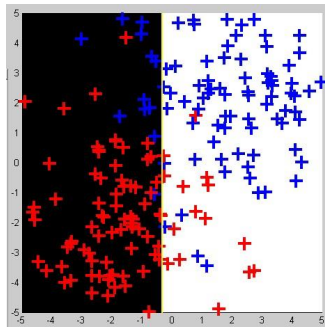


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

AdaBoost with Decision Stumps

- After 3 rounds:

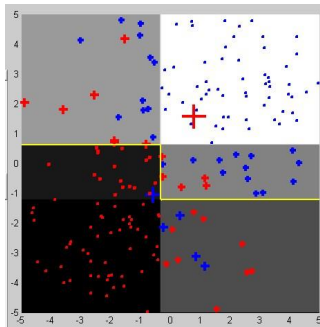


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AdaBoost with Decision Stumps

- After 120 rounds:

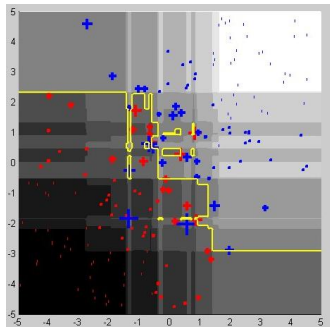
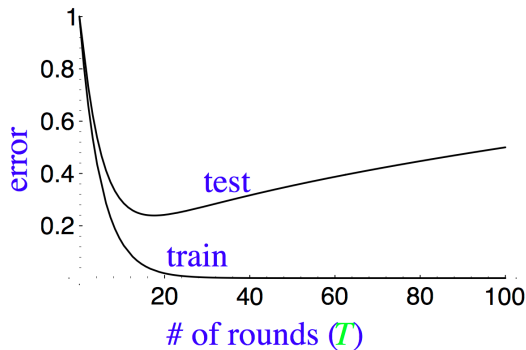


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Does AdaBoost overfit?

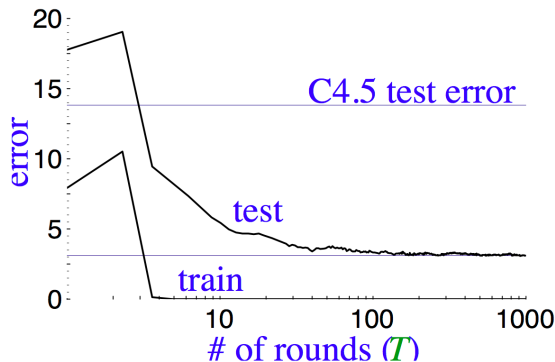
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



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

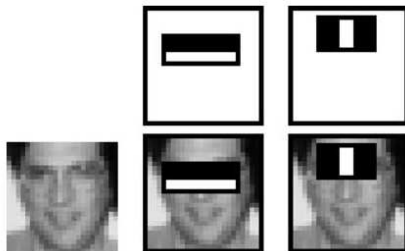
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AdaBoost for Face Detection

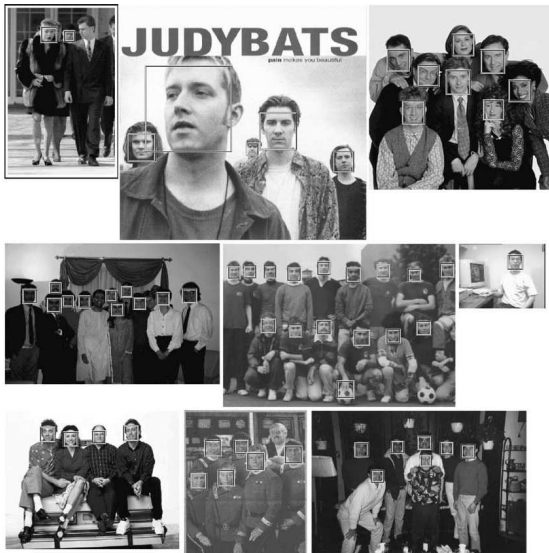
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- A few twists on standard algorithm
 - Pre-define weak classifiers, so optimization=selection
 - Smart way to do inference in real-time (in 2001 hardware)



AdaBoost Face Detection Results



- Boosting is used to reduce bias from shallow decision trees

Interim Summary

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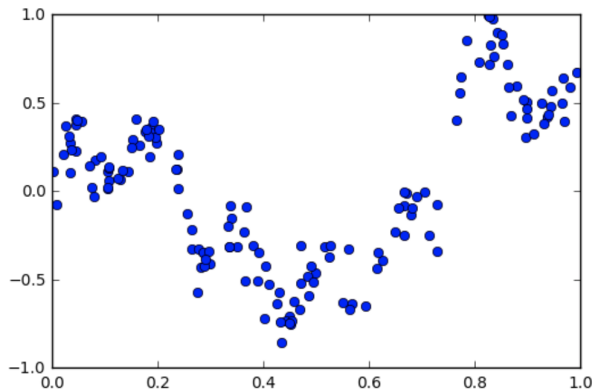
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 - Generalizations to other loss functions
 - Gradient Boosting

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):

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

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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?

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

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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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 - Can we differentiate J w.r.t. v_m 's and θ_m 's?

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

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

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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 :

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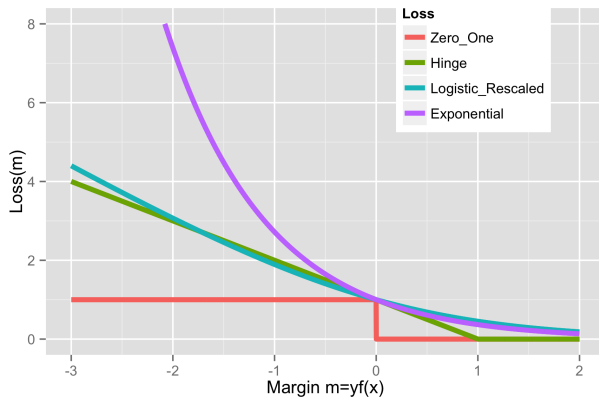
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❷ Set $f_m = f_{m-1} + v_m h_m$.

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

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

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

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

FSAM with Exponential Loss: basis function

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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:

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

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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:

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

(18)

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- $2v_m = \alpha_m$ in Adaboost.

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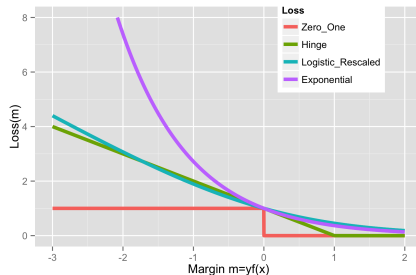
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- How is it different from other losses?



- Exponential loss puts a high penalty on misclassified examples.

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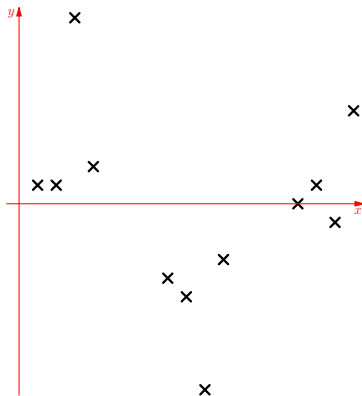
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- This is just fitting the residuals with least-squares regression!
- Example base hypothesis space: regression stumps.

L^2 Boosting with Decision Stumps: Demo

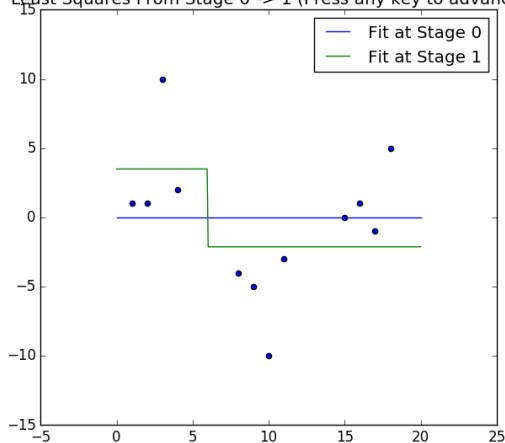
- Consider FSAM with L^2 loss (i.e. L^2 Boosting)
- For base hypothesis space of **regression stumps**



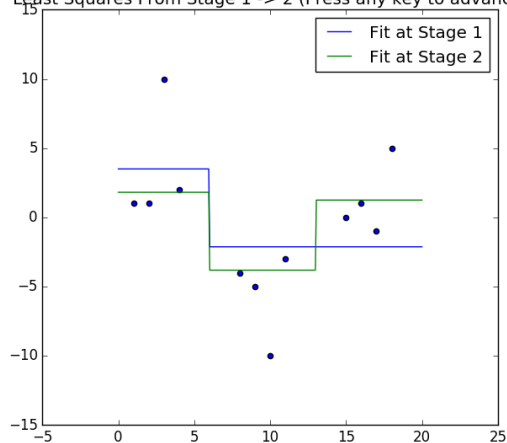
Plot courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results

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

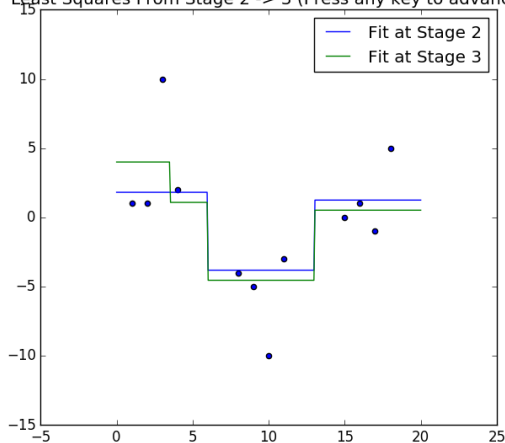


Least Squares From Stage 1 -> 2 (Press any key to advance)

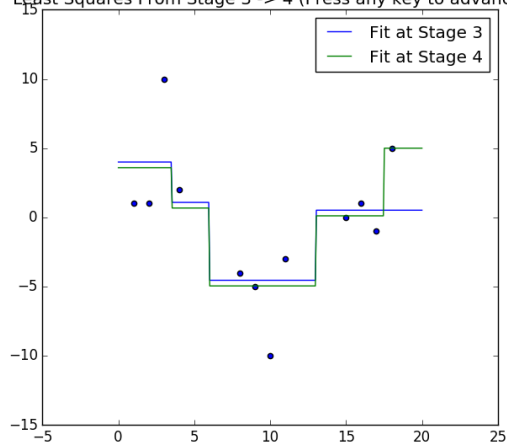


L^2 Boosting with Decision Stumps: Results

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

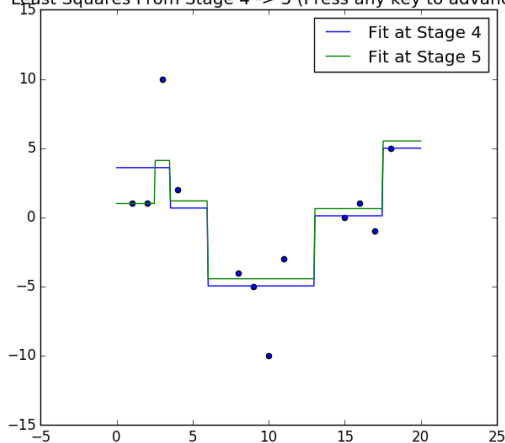


Least Squares From Stage 3 -> 4 (Press any key to advance)

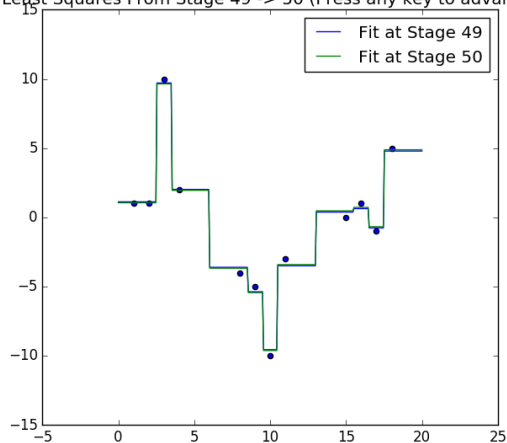


L^2 Boosting with Decision Stumps: Results

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



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



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

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

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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

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

- In some sense, we want to take the gradient w.r.t. f .

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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

- Consider gradient descent on

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which we can easily calculate.

- $-\mathbf{g} \in \mathbb{R}^n$ is the direction we want to change each of our n predictions on training data.

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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

$$-g = -\nabla_{\mathbf{f}} J(\mathbf{f}) = -(\partial_{f_1} \ell(y_1, f_1), \dots, \partial_{f_n} \ell(y_n, f_n)).$$

- 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} ?

Functional Gradient Descent: Projection Step

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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):

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

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

Recap

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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:

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

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

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

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

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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

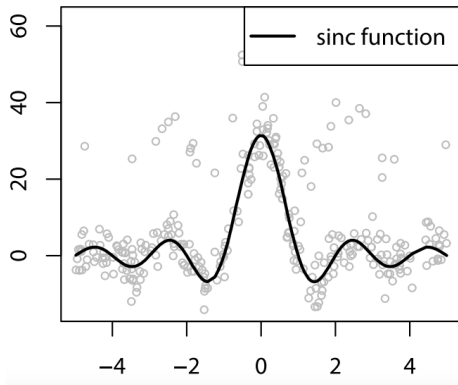
- One common form of gradient boosting machine takes

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

where S is the number of terminal nodes.

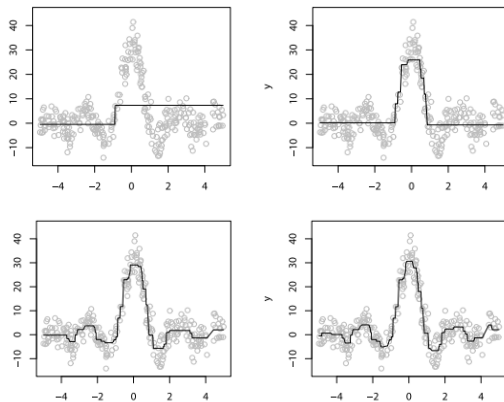
- $S = 2$ gives decision stumps
- HTF recommends $4 \leq S \leq 8$ (but more recent results use much larger trees)
- Software packages:
 - Gradient tree boosting is implemented by the `gbm` package for R
 - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in `sklearn`
 - `xgboost` and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

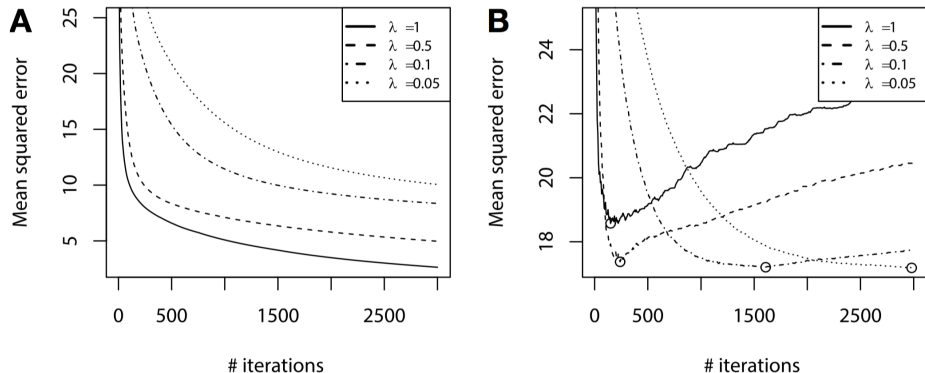
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

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

- For each stage,
 - 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