Random Forest and Boosting

Mengye Ren

(Slides credit to David Rosenberg, He He, et al.)

NYU

Nov 12, 2024

Slides

Announcement

- HW4 release soon. Due Dec 3, 2024 Noon.
- Next week guest lecture on Neural Networks I.

Scientific Writing II

How to avoid sound like ChatGPT?

Shallow content, making the focus too broad

Understanding long video-language interactions represents a transformative challenge in multimodal learning, where models must navigate extensive visual and linguistic content to extract meaningful, coherent interpretations. Unlike short clips or single-image tasks, long videos embody intricate sequences of events, evolving contexts, and complex interactions that require sustained comprehension and nuanced understanding across time. This level of interpretation demands models capable of navigating high-dimensional data streams, maintaining contextual awareness, and preserving coherence as they bridge connections between video frames and corresponding language across prolonged durations. Achieving proficiency in long video-language understanding would unlock significant advancements in applications ranging from deep narrative analysis and sports commentary to educational content summarization and assistive technologies for enhanced accessibility.

Recent advances in multimodal architectures offer glimpses of what is possible, yet long-form video comprehension introduces unique challenges that require innovation in model design, memory retention, and temporal reasoning. This paper explores methodologies to elevate models' capabilities in understanding complex, continuous video narratives, emphasizing temporal alignment, memory management, and contextual coherence. By addressing these challenges, we aim to bridge the gap between machine processing and human-like comprehension, enabling models to deliver richer, more consistent insights from the layered, evolving narratives found in long-form video content.

How to avoid sound like ChatGPT?

Grandiose word choices

In the contemporary technological landscape, Large Language Models (LLMs) are emerging as revolutionary tools, driving innovations in various sectors from healthcare to finance, and from entertainment to academia. These models, with their unprecedented ability to understand and generate human-like text, hold significant promise for reshaping the dynamics of human-computer interaction. However, as LLMs become more ingrained in everyday applications, there arises a pertinent challenge: ensuring their alignment with human values, especially when subjected to third-party finetuning.

A few tips on how to properly use AI tools

- Brainstorm ideas
- Polishing, fixing grammatical mistakes, etc.
- "Please help me do some light editing (only when necessary)."
- "Please use scientific language and stick to fact."
- Exercise a high degree of caution.
  - Do I really need to write about this? Do I really mean it?
  - Be critical. Always give feedback to chat bot and do another round.

Bagging and Random Forests

Review: Decision Trees

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- Interpretable, up to certain depth.
- Greedy algorithm – maximizing the purity of nodes.
- Can overfit – need to limit the capacity.

Recap: Statistics and Point Estimators

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  - E.g., sample mean, sample variance, histogram, empirical data distribution
- A statistic $\hat{\theta} = \hat{\theta}(\mathcal{D})$ is a **point estimator** of θ if $\hat{\theta} \approx \theta$

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- Statistics are random, so they have probability distributions.
- The distribution of a statistic is called a **sampling distribution**.
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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: $\mathbb{E}\left[\hat{\theta}\right] = \theta$, $\mathrm{Var}(\hat{\theta}) = \sigma^2$.
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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):

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

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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!

The Bootstrap Sample

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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)

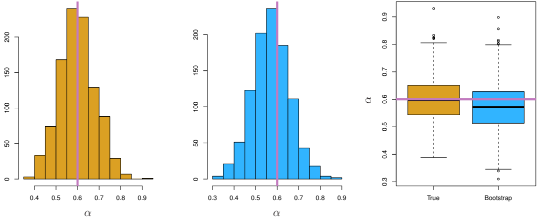

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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- 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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- Increasing the number of trees we use in bagging does not lead to overfitting
- Is there a downside, compared to having a single decision tree?
- Yes: if we have many trees, the bagged predictor is much less interpretable

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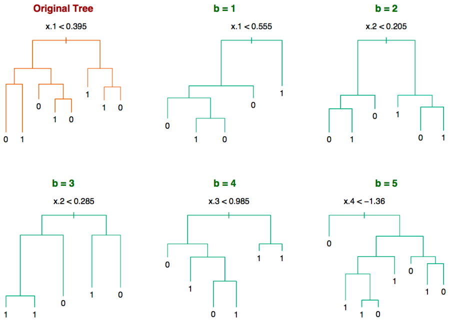
- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

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



From HTF Figure 8.9

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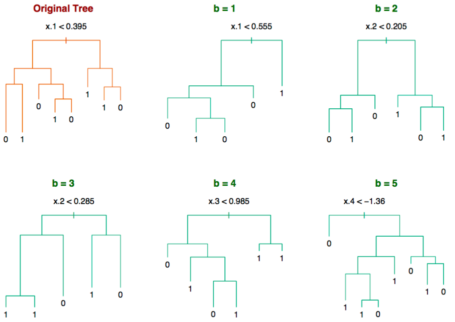

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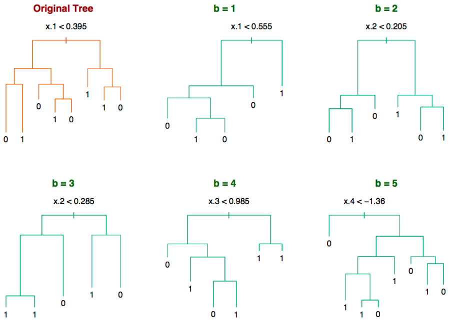

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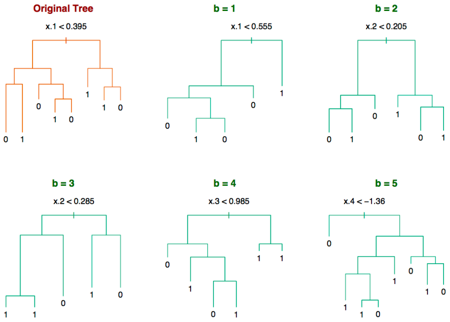

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- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

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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- For large n, the covariance term dominates, limiting the benefits of averaging
- Bootstrap samples are
  - independent samples from the training set, but
  - not independent samples from $P_{\mathcal{X}\times\mathcal{Y}}$
- Can we reduce the dependence between $\hat{f}_i$'s?

Random Forests

Key idea

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

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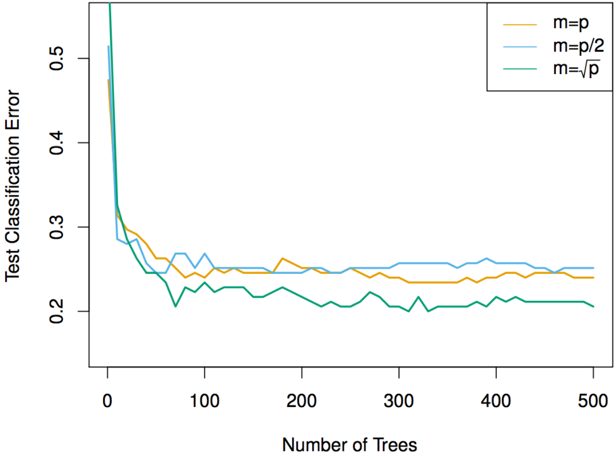
- We typically choose $m \approx \sqrt{p}$, where p is the number of features (or we can choose m using cross validation)
- If $m = p$, this is just bagging

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

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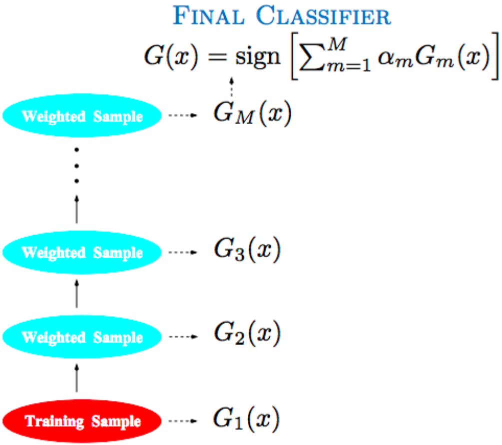
- **Weighted empirical risk**:

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

- Examples with larger weights affect the loss more.

AdaBoost: Schematic



From ESL Figure 10.1

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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 $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
- We would like α_m to be:
  - Nonnegative
  - Larger when G_m fits its weighted training data well
- The **weighted 0-1 error** of $G_m(x)$ is

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

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

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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 $\Longrightarrow$ lower weight

AdaBoost: Example Reweighting

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

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  - If G_m is a strong classifier overall, then its α_m will be large; this means that if x_i is misclassified, w_i will increase to a greater extent

AdaBoost: Algorithm

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

AdaBoost with Decision Stumps

- After 1 round:

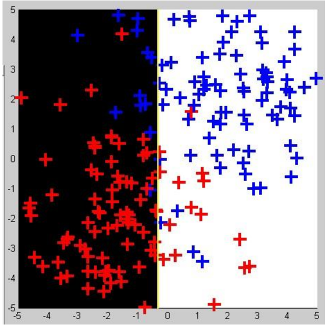
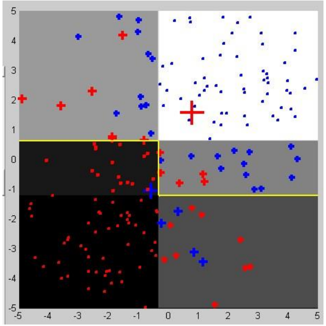


Figure: Size of plus sign represents weight of example. Blackness represents preference for red class; whiteness represents preference for blue class.

KPM Figure 16.10

- After 3 rounds:



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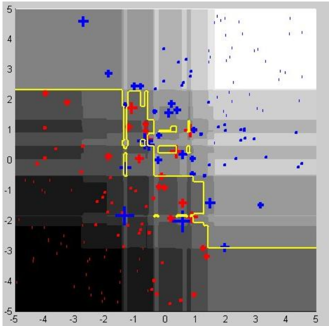
KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:



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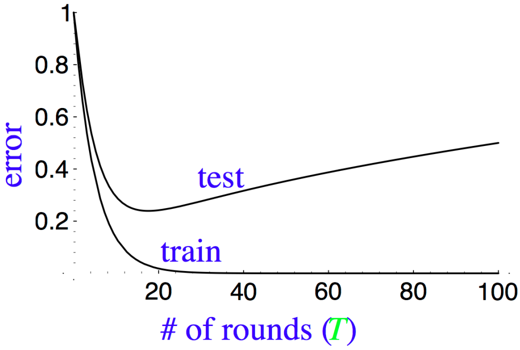
KPM Figure 16.10

Does AdaBoost overfit?

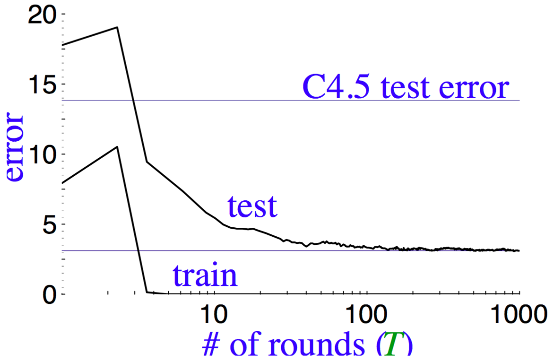
- Does a large number of rounds of boosting lead to overfitting?
- If we were overfitting, the learning curves would look like:



From Rob Schapire's NIPS 2007 Boosting tutorial.

Learning Curves for AdaBoost

- AdaBoost is usually quite resistant to overfitting
- The test error continues to decrease even after the training error drops to zero!



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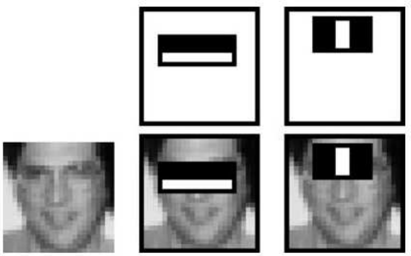
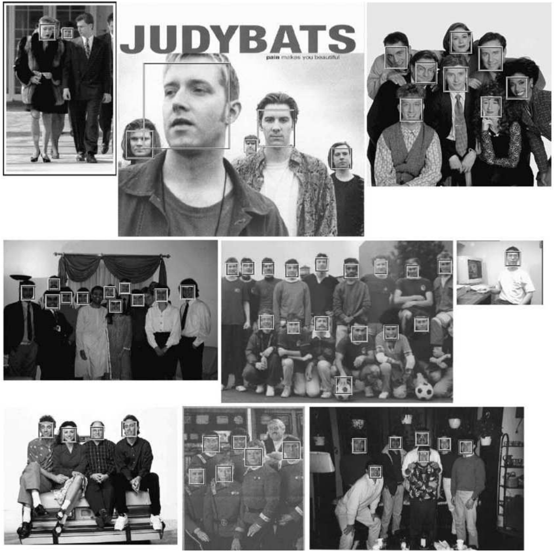
- A few twists on standard algorithm
  - Pre-define weak classifiers, so optimization=selection
  - Smart way to do inference in real-time (in 2001 hardware)



AdaBoost Face Detection Results



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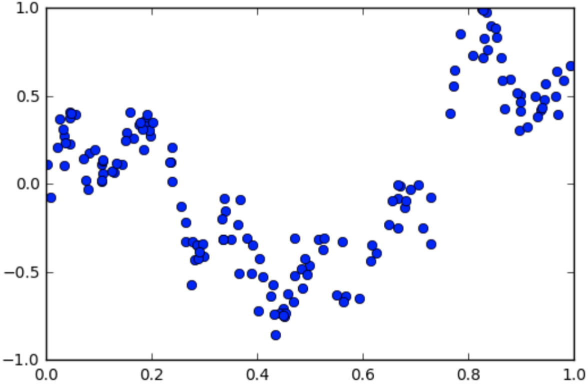
    - Generalizations to other loss functions
    - Gradient Boosting

- 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):

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

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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.

Adaptive Basis Function Model

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

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

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

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- Combined hypothesis space:

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

- What are the learnable?

Empirical Risk Minimization

- What's our learning objective?

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

for some loss function ℓ.

Empirical Risk Minimization

- What's our learning objective?

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

  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 $\Theta = \mathbb{R}^b$:

$$J(v_1, \ldots, v_M, \theta_1, \ldots, \theta_M) = \frac{1}{n}\sum_{i=1}^{n} \ell\left(y_i, \sum_{m=1}^{M} v_m h(x; \theta_m)\right).$$

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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?

What if base hypothesis space $\mathcal{H}$ consists of decision trees?

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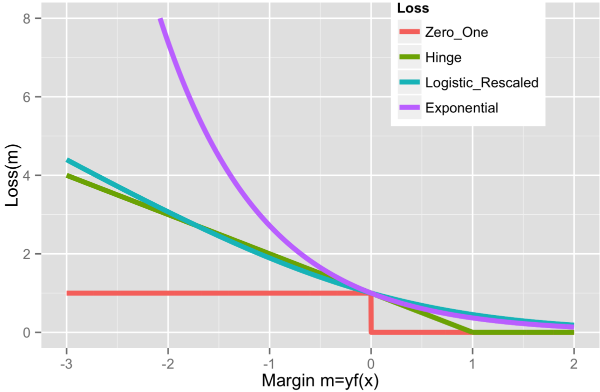
    2. Set $f_m = f_{m-1} + v_m h_m$.
3. Return: f_M.

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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2. For $m = 1$ to M:
    1. Compute:
    $$(v_m, h_m) = \underset{v \in \mathbb{R}, h \in \mathcal{H}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \ell_{\text{exp}} \left(y_i, f_{m-1}(x_i) \underbrace{+ v h(x_i)}_{\text{new piece}} \right).$$
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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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\begin{aligned}
J(v,h) &= \sum_{i=1}^{n} \exp\left[-y_i\left(f_{m-1}(x_i) + vh(x_i)\right)\right] && (5)\\
&= \sum_{i=1}^{n} w_i^m \exp\left[-y_i v h(x_i)\right] && w_i^m \stackrel{\text{def}}{=} \exp\left[-y_i f_{m-1}(x_i)\right] \quad (6)\\
&= \sum_{i=1}^{n} w_i^m \left[\mathbb{I}\left(y_i = h(x_i)\right) e^{-v} + \mathbb{I}\left(y_i \neq h(x_i)\right) e^{v}\right] && h(x_i) \in \{1, -1\} \quad (7)\\
&= \sum_{i=1}^{n} w_i^m \left[\left(e^{v} - e^{-v}\right)\mathbb{I}\left(y_i \neq h(x_i)\right) + e^{-v}\right] && \mathbb{I}\left(y_i = h(x_i)\right) = 1 - \mathbb{I}\left(y_i \neq h(x_i)\right) \quad (8)
\end{aligned}
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FSAM with Exponential Loss: basis function

- Objective function in the m'th round:

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

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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:

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

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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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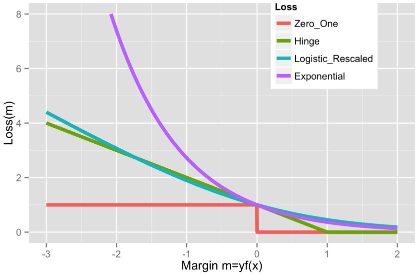
- How is it different from other losses?



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AdaBoost / Exponential Loss: Robustness Issues

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  - $\implies$ not robust to outliers / noise.
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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:

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

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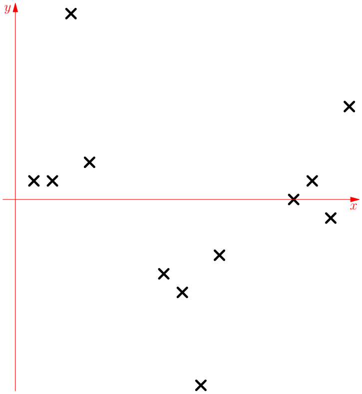
- This is just fitting the residuals with least-squares regression!
- Example base hypothesis space: regression stumps.

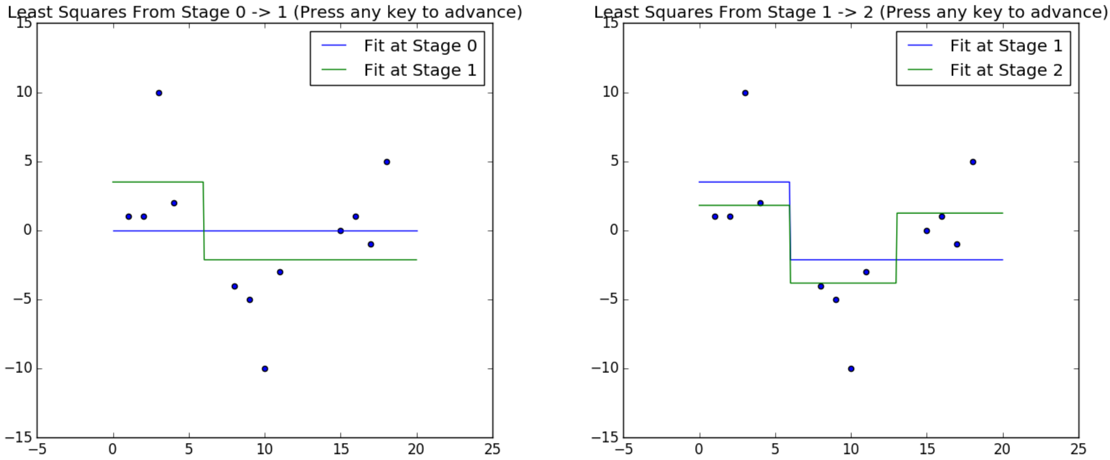
L^2 Boosting with Decision Stumps: Demo

- 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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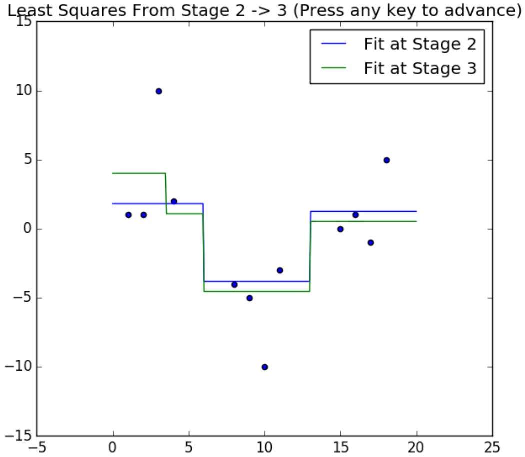

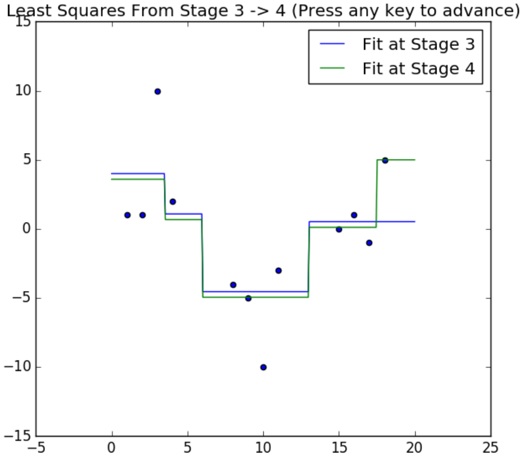

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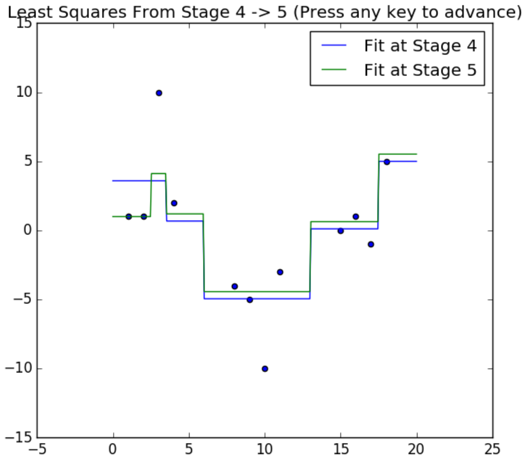

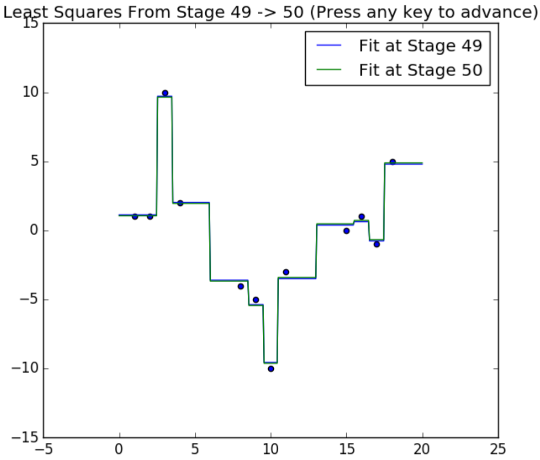

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Interpret the residual

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$$\frac{\partial}{\partial f(x_i)} J(f) = \tag{20}$$

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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

- We want to minimize
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- Define "parameters"

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

and write the objective function as

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

Functional Gradient Descent: Unconstrained Step Direction

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  which we can easily calculate.

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

Functional Gradient Descent: Projection Step

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  - Also called the "**pseudo-residuals**". (For squared loss, they're exactly the residuals.)

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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):

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

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

Recap

- Objective function:

$$J(f) = \sum_{i=1}^{n} \ell(y_i, f(x_i)). \tag{24}$$

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- Gradient descent:

$$f \leftarrow f + {\color{red}v} h \tag{27}$$

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 $v_m = \arg\min_v \sum_{i=1}^n \ell\left(yi, f_{m-1}(x_i) + vh_m(x_i)\right)$.
    4. Update $f_m = f_{m-1} + \lambda v_m h_m$
3. Return $f_M(x)$.

The Gradient Boosting Machine Ingredients (Recap)

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

BinomialBoost: Gradient Boosting with Logistic Loss

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

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

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

$$\begin{aligned}
r_i &= -\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)) && (30)\\
&= -\frac{\partial}{\partial f(x_i)} \left[\log\left(1 + e^{-y_i f(x_i)}\right)\right] && (31)\\
&= \frac{y_i e^{-y_i f(x_i)}}{1 + e^{-y_i f(x_i)}} && (32)\\
&= \frac{y_i}{1 + e^{y_i f(x_i)}} && (33)
\end{aligned}$$

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

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

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

Gradient Tree Boosting

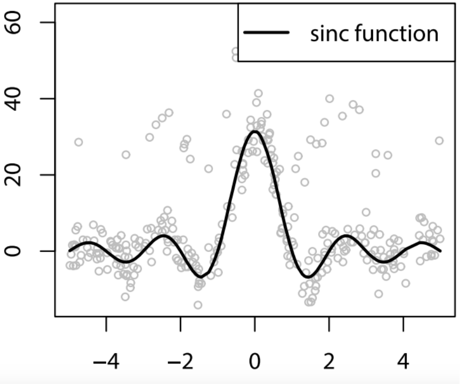
- One common form of gradient boosting machine takes

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

  where S is the number of terminal nodes.

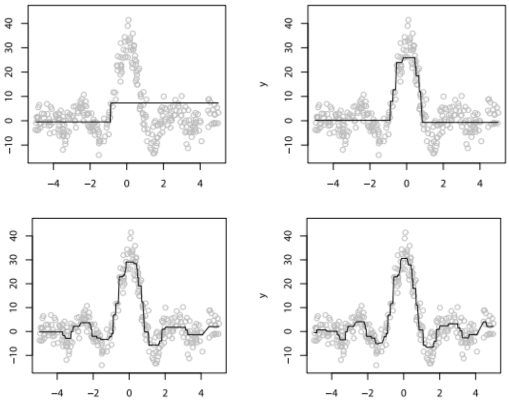
- $S = 2$ gives decision stumps
- Common choice: $4 \leqslant S \leqslant 8$
- Software packages:
  - Gradient tree boosting is implemented by the gbm package for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in sklearn
  - xgboost and lightGBM are state of the art for speed and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

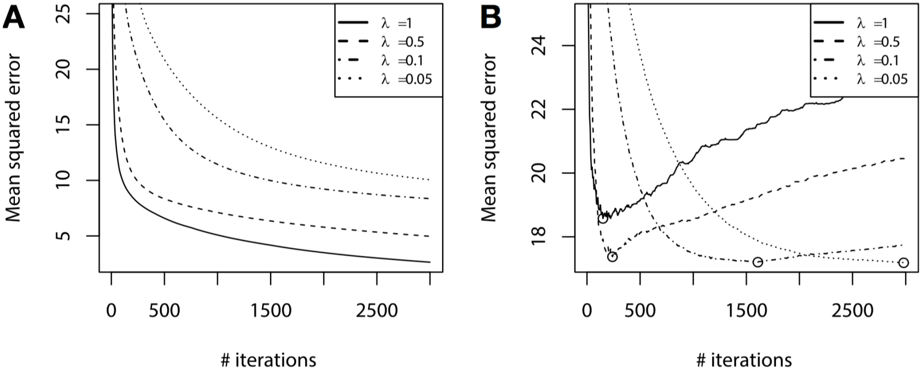
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

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

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- 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.

Introduced by Friedman (1999) in Stochastic Gradient Boosting.

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