

# Gradient Boosting

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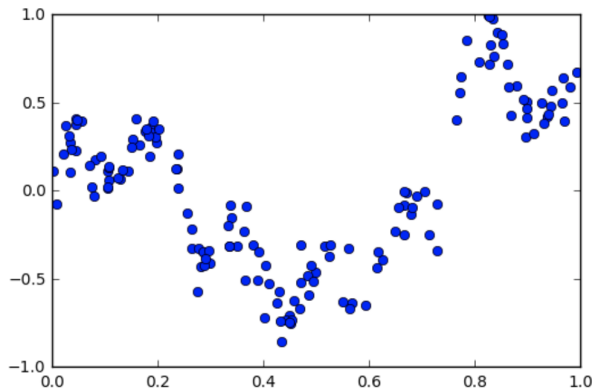
# Contents

- 1 Introduction
- 2 Forward Stagewise Additive Modeling
- 3 Example:  $L^2$  Boosting
- 4 Example: AdaBoost
- 5 Gradient Boosting / “Anyboost”
- 6 Example: BinomialBoost
- 7 Gradient Tree Boosting
- 8 GBM Regression with Stumps
- 9 Variations on Gradient Boosting

# Introduction

# Nonlinear Regression

- Suppose we have the following regression problem:



- What are some options?
- basis functions, kernel methods, trees, neural nets, ...

# Linear Model with Basis Functions

- Choose some basis functions on input space  $\mathcal{X}$ :

$$g_1, \dots, g_M : \mathcal{X} \rightarrow \mathbb{R}$$

- Predict with linear combination of basis functions:

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

- Can fit this using standard methods for linear models (e.g. least squares, lasso, ridge, etc.)
- In ML parlance, basis functions are called **features** or **feature functions**.

# Not Limited to Regression

- Linear combination of basis functions:

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

- $f(x)$  is a number — for regression, it's exactly what we're looking for.
- Otherwise,  $f(x)$  is often called a **score** function.
- It can be
  - thresholded to get a classification
  - transformed to get a probability
  - transformed to get a parameter of a probability distribution (e.g. Poisson regression)
  - used for ranking search results

# Adaptive Basis Function Model

- Let's “learn” the basis functions.
- **Base hypothesis space**  $\mathcal{H}$  consisting of functions  $h: \mathcal{X} \rightarrow \mathbf{R}$ .
  - We will choose our “basis functions” or “features” from this set of functions.
- An **adaptive basis function expansion** over  $\mathcal{H}$  is

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

where  $v_m \in \mathbf{R}$  and  $h_m \in \mathcal{H}$  are chosen based on training data.

# Adaptive Basis Function Model

- Base hypothesis space:  $\mathcal{H}$  of real-valued functions
- Combined hypothesis space:  $\mathcal{F}_M$ :

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

- Suppose we're given some data  $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n))$ .
- Learning is choosing  $v_1, \dots, v_M \in \mathbf{R}$  and  $h_1, \dots, h_M \in \mathcal{H}$  to fit  $\mathcal{D}$ .



# Empirical Risk Minimization

- We'll consider learning by **empirical risk minimization**:

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

for some **loss function**  $\ell(y, \hat{y})$ .

- Write ERM objective function as

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

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

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

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

- Can we differentiate  $J$  w.r.t.  $v_m$ 's and  $\theta_m$ 's? Optimize with SGD?
- 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?
- Can we even parameterize trees with  $\Theta = \mathbf{R}^b$ ?
- Even if we could for some set of trees,
  - predictions would not change continuously w.r.t.  $\theta \in \Theta$ ,
  - and so certainly not differentiable.
- Today we'll discuss **gradient boosting**. 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  $\mathcal{H}$  (e.g. regression trees).

- Forward stagewise additive modeling (FSAM)
  - example:  $L^2$  Boosting
  - example: exponential loss gives AdaBoost
  - Not clear how to do it with many other losses, including logistic loss
- Gradient Boosting
  - example: logistic loss gives BinomialBoost
- Variations on Gradient Boosting
  - step size selection
  - stochastic row/column selection
  - Newton step direction
  - XGBoost

## Forward Stagewise Additive Modeling

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# Forward Stagewise Additive Modeling (FSAM)

- FSAM is an iterative optimization algorithm for fitting adaptive basis function models.
- Start with  $f_0 \equiv 0$ .
- After  $m-1$  stages, we have

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

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

$$f_m = f_{m-1} + \nu_i h_m$$

improves objective function value by as much as possible.

# Forward Stagewise Additive Modeling for ERM

① Initialize  $f_0(x) = 0$ .

② For  $m = 1$  to  $M$ :

① Compute:

$$(\nu_m, h_m) = \arg \min_{\nu \in \mathbf{R}, h \in \mathcal{H}} \frac{1}{n} \sum \ell \left( y_i, f_{m-1}(x_i) + \underbrace{\nu h(x_i)}_{\text{new piece}} \right).$$

② Set  $f_m = f_{m-1} + \nu_m h$ .

③ Return:  $f_M$ .

## Example: $L^2$ Boosting



## Example: $L^2$ Boosting

- Suppose we use the **square loss**. Then in each step we minimize

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

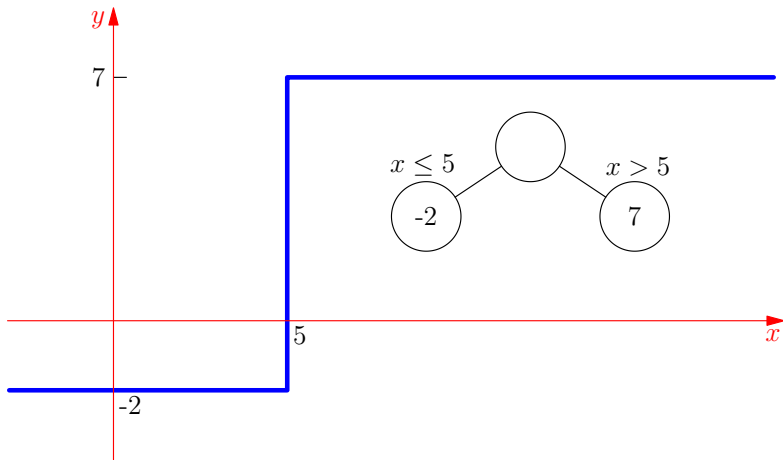
- If  $\mathcal{H}$  is closed under rescaling (i.e. if  $h \in \mathcal{H}$ , then  $vh \in \mathcal{H}$  for all  $h \in \mathbf{R}$ ), then don't need  $v$ .
- Take  $v = 1$  and minimize

$$J(h) = \frac{1}{n} \sum_{i=1}^n ([y_i - f_{m-1}(x_i)] - h(x_i))^2$$

- This is just fitting the residuals with least-squares regression!
- If we can do regression with our base hypothesis space  $\mathcal{H}$ , then we're set!

## Recall: Regression Stumps

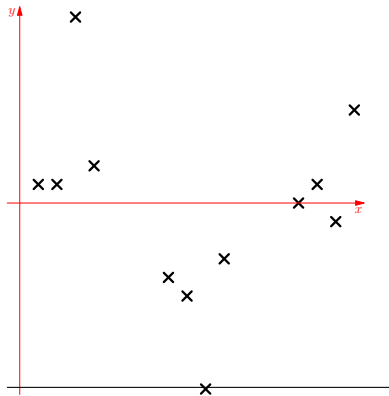
- A **regression stump** is a function of the form  $h(x) = a1(x_i \leq c) + b1(x_i > c)$



Plot courtesy of Brett Bernstein.

# $L^2$ Boosting with Decision Stumps: Demo

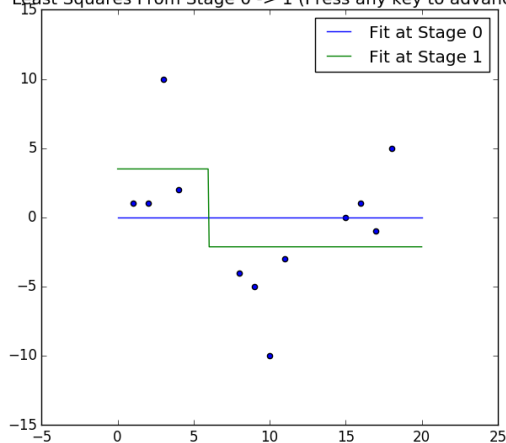
- Consider FSAM with  $L^2$  loss (i.e.  $L^2$  Boosting)
- For base hypothesis space of **regression stumps**
- Data we'll fit with **code**:



Plot courtesy of Brett Bernstein.

# $L^2$ Boosting with Decision Stumps: Results

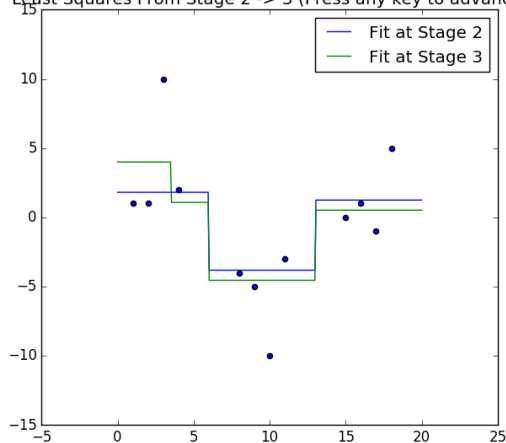
Least Squares From Stage 0 -> 1 (Press any key to advance)



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

# $L^2$ Boosting with Decision Stumps: Results

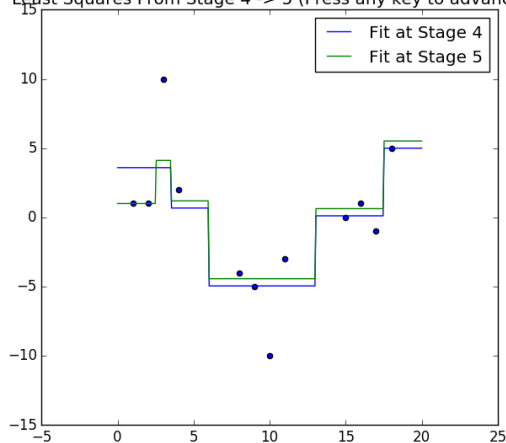
Least Squares From Stage 2 -> 3 (Press any key to advance)



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)

## Example: AdaBoost

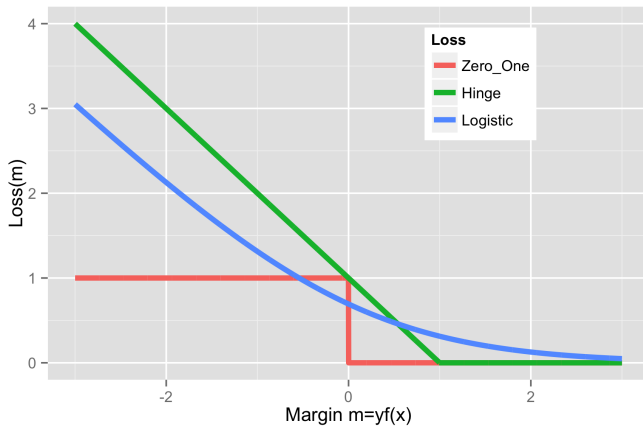
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# The Classification Problem

- Outcome space  $\mathcal{Y} = \{-1, 1\}$
- Action space  $\mathcal{A} = \mathbf{R}$
- Score function  $f : \mathcal{X} \rightarrow \mathcal{A}$ .
- Margin for example  $(x, y)$  is  $m = yf(x)$ .
  - $m > 0 \iff$  classification correct
  - Larger  $m$  is better.

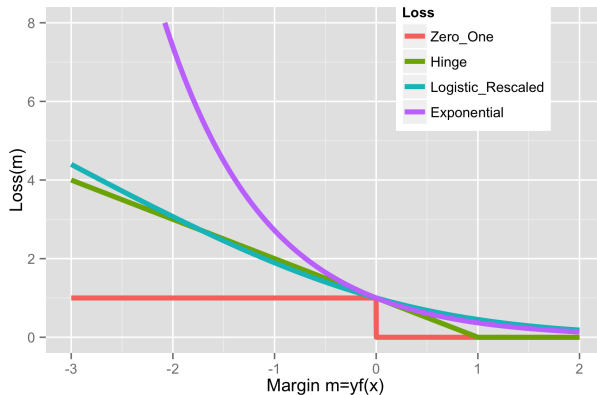


# Margin-Based Losses for Classification



# Exponential Loss

- Introduce the **exponential loss**:  $\ell(y, f(x)) = \exp(-yf(x))$ .



# FSAM with Exponential Loss

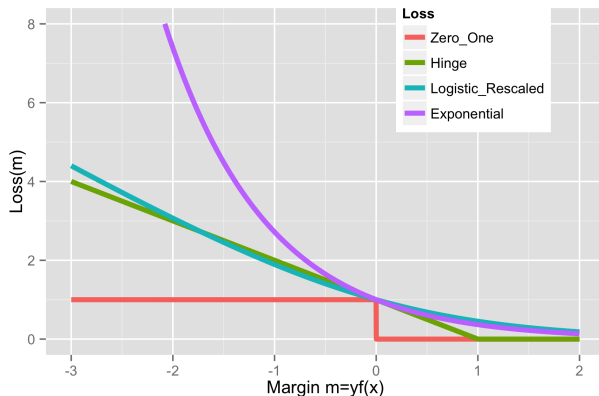
- Consider classification setting:  $\mathcal{Y} = \{-1, 1\}$ .
- Take loss function to be the **exponential loss**:

$$\ell(y, f(x)) = \exp(-yf(x)).$$

- Let  $\mathcal{H}$  be a base hypothesis space of classifiers  $h: \mathcal{X} \rightarrow \{-1, 1\}$ .
- Then Forward Stagewise Additive Modeling (FSAM) reduces to a version of **AdaBoost**.
- Proof on [Spring 2017 Homework #6, Problem 4](#) (and see HTF Section 10.4).

# Exponential Loss

- Note that exponential loss puts a very large weight on bad misclassifications.



- When Bayes error rate is high (e.g.  $\mathbb{P}(f^*(X) \neq Y) = 0.25$ )
  - e.g. there's some intrinsic randomness in the label
  - e.g. training examples with same input, but different classifications.
- Best we can do is predict the most likely class for each  $X$ .
- Some training predictions **should be wrong**,
  - because example doesn't have majority class
  - AdaBoost / exponential loss puts a lot of focus on getting those right
- Empirically, AdaBoost has degraded performance in situations with
  - high Bayes error rate, or when there's
  - high “**label noise**”
- Logistic loss performs better in settings with high Bayes error

# FSAM for Other Loss Functions

- We know how to do FSAM for certain loss functions
  - e.g square loss, absolute loss, exponential loss,...
- In each case, happens to reduce to another problem we know how to solve.
- However, not clear how to do FSAM in general.
- For example, logistic loss / cross-entropy loss?

## Gradient Boosting / “Anyboost”

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# FSAM Is Iterative Optimization

- The FSAM step

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

- Hard part: finding the **best step direction**  $h$ .
- What if we looked for the **locally best** step direction?
  - like in gradient descent



# “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. “ $f$ ”, whatever that means.
- $J(f)$  only depends on  $f$  at the  $n$  training points.
- Define

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

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

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

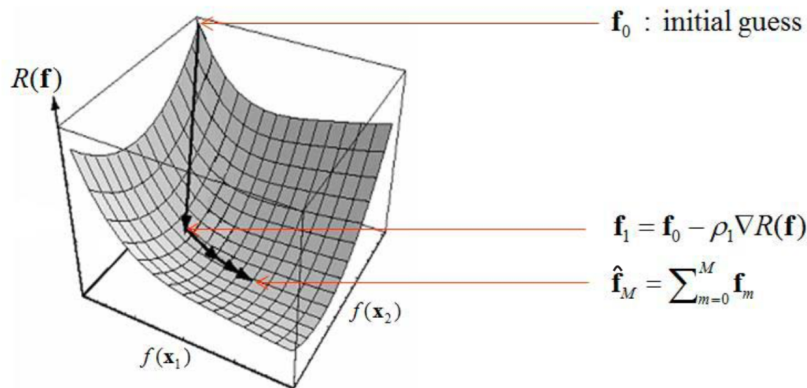
- The **negative gradient step direction** at  $\mathbf{f}$  is

$$\begin{aligned} -\mathbf{g} &= -\nabla_{\mathbf{f}} J(\mathbf{f}) \\ &= -(\partial_{\mathbf{f}_1} \ell(y_1, \mathbf{f}_1), \dots, \partial_{\mathbf{f}_n} \ell(y_n, \mathbf{f}_n)) \end{aligned}$$

which we can easily calculate.

- $-\mathbf{g} \in \mathbf{R}^n$  is the direction we want to change each of our  $n$  predictions on training data.
- Eventually we need more than just  $\mathbf{f}$ , which is just predictions on training.

# Unconstrained Functional Gradient Stepping



$R(\mathbf{f})$  is the empirical risk, where  $\mathbf{f} = (f(x_1), f(x_2))$  are predictions on training set.  
Issue:  $\hat{\mathbf{f}}_M$  only defined at training points.

From Seni and Elder's *Ensemble Methods in Data Mining*, Fig B.1.

# Functional Gradient Descent: Projection Step

- Unconstrained step direction is

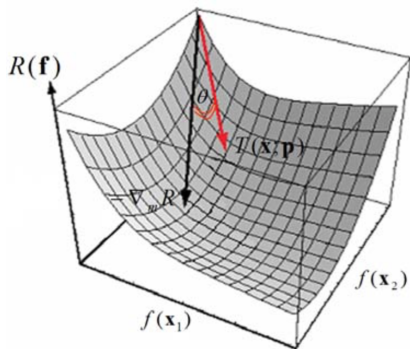
$$-\mathbf{g} = -\nabla_{\mathbf{f}} J(\mathbf{f}) = -(\partial_{\mathbf{f}_1} \ell(y_1, \mathbf{f}_1), \dots, \partial_{\mathbf{f}_n} \ell(y_n, \mathbf{f}_n)).$$

- Also called the “**pseudo-residuals**”
  - (for square loss, they’re exactly the residuals)
- Find the closest base hypothesis  $h \in \mathcal{H}$  (in the  $\ell^2$  sense):

$$\min_{h \in \mathcal{H}} \sum_{i=1}^n (-\mathbf{g}_i - h(x_i))^2.$$

- This is a least squares regression problem over hypothesis space  $\mathcal{H}$ .
- Take the  $h \in \mathcal{H}$  that best approximates  $-\mathbf{g}$  as our step direction.

# “Projected” Functional Gradient Stepping



$T(\mathbf{x}; \mathbf{p}) \in \mathcal{H}$  is our actual step direction – like the projection of  $-\mathbf{g} = -\nabla R(\mathbf{f})$  onto  $\mathcal{H}$ .

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From Seni and Elder's *Ensemble Methods in Data Mining*, Fig B.2.

# Functional Gradient Descent: Step Size

- Finally, we choose a stepsize.
- Option 1 (Line search):

$$\nu_m = \arg \min_{\nu > 0} \sum_{i=1}^n \ell\{y_i, f_{m-1}(x_i) + \nu h_m(x_i)\}.$$

- Option 2: (Shrinkage parameter – **more common**)
  - We consider  $\nu = 1$  to be the full gradient step.
  - Choose a fixed  $\nu \in (0, 1)$  – called a **shrinkage parameter**.
  - A value of  $\nu = 0.1$  is typical – optimize as a hyperparameter .

# The Gradient Boosting Machine Ingredients (Recap)

- Take any [sub]differentiable loss function.
- 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!

## Example: BinomialBoost

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# BinomialBoost: Gradient Boosting with Logistic Loss

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

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

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

$$\begin{aligned} r_i &= -\partial_{f(x_i)} \left[ \log(1 + e^{-y_i f(x_i)}) \right] \\ &= \frac{y_i e^{-y_i f(x_i)}}{1 + e^{-y_i f(x_i)}} \\ &= \frac{y_i}{1 + e^{y_i f(x_i)}} \end{aligned}$$

# BinomialBoost: Gradient Boosting with Logistic Loss

- Pseudoresidual for  $i$ th example:

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

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

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

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

# Gradient Tree Boosting

# Gradient Tree Boosting

- One common form of gradient boosting machine takes

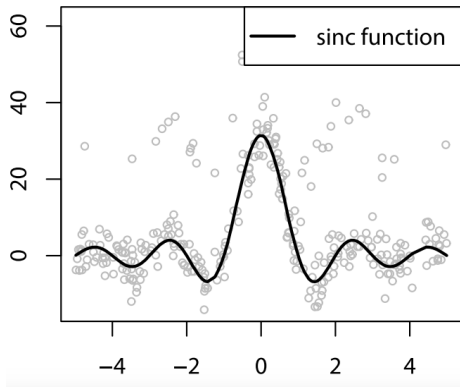
$$\mathcal{H} = \{\text{regression trees of size } J\},$$

where  $J$  is the number of terminal nodes.

- $J = 2$  gives decision stumps
- HTF recommends  $4 \leq J \leq 8$  (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

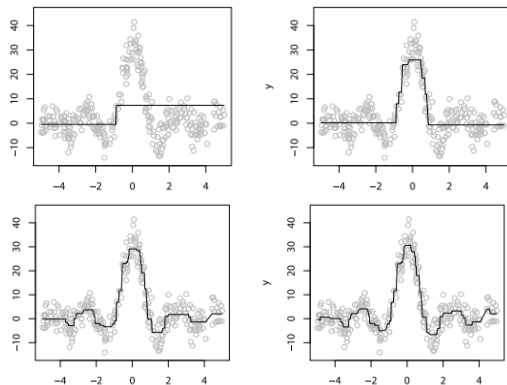
## GBM Regression with Stumps

# Sinc Function: Our Dataset



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

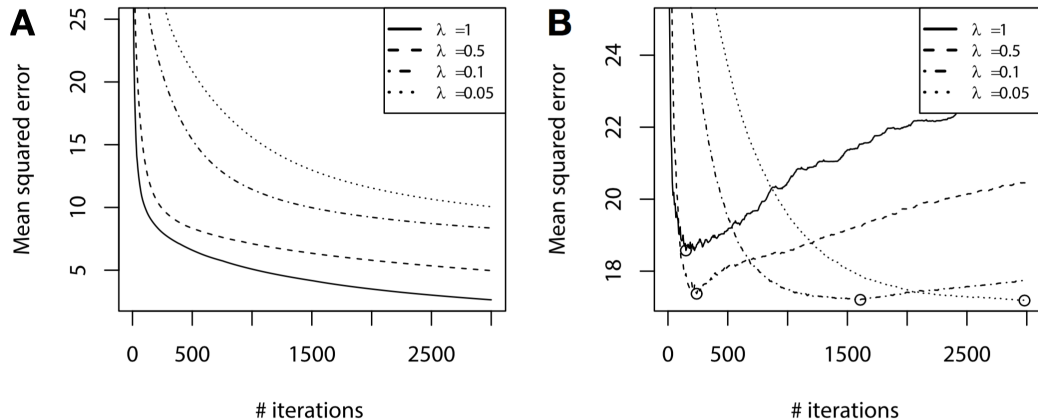
# Minimizing Square Loss with Ensemble of Decision Stumps



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

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

# Step Size as Regularization



Performance vs rounds of boosting and step size. (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.

## Variations on Gradient Boosting

# Stochastic Gradient Boosting

- For each stage,
  - choose random subset of data for computing projected gradient step.
  - “Typically, about 50% of the dataset size, can be much smaller for large training set.”
  - Fraction is called the **bag fraction**.
- Why do this?
  - Subsample percentage is additional regularization parameter – may help overfitting.
  - Faster.
- We can view this is a **minibatch method**.
  - we’re estimating the “true” step direction (the projected gradient) using a subset of data

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

# Bag as Minibatch

- Just as we argued for minibatch SGD,
  - sample size needed for a good estimate of step direction is independent of training set size
- Minibatch size should depend on
  - the complexity of base hypothesis space
  - the complexity of the target function (Bayes decision function)
- Seems like an interesting area for both practical and theoretical pursuit.

## Column / Feature Subsampling for Regularization

- 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.”
- Zhao Xing (top Kaggle competitor) finds optimal percentage to be 20%-100%

# Newton Step Direction

- For GBM, we find the closest  $h \in \mathcal{F}$  to the negative gradient

$$-\mathbf{g} = -\nabla_{\mathbf{f}} J(\mathbf{f}).$$

- This is a “first order” method.
- Newton’s method is a “second order method”:
  - Find 2nd order (quadratic) approximation to  $J$  at  $\mathbf{f}$ .
    - Requires computing gradient and Hessian of  $J$ .
  - Newton step direction points towards minimizer of the quadratic.
  - Minimizer of quadratic is easy to find in closed form
- Boosting methods with projected Newton step direction:
  - LogitBoost (logistic loss function)
  - XGBoost (any loss – uses regression trees for base classifier)

# Newton Step Direction for GBM

- Generically, second order Taylor expansion of  $J$  at  $\mathbf{f}$  in direction  $\mathbf{r}$

$$J(\mathbf{f} + \mathbf{r}) = J(\mathbf{f}) + [\nabla_{\mathbf{f}} J(\mathbf{f})]^T \mathbf{r} + \frac{1}{2} \mathbf{r}^T [\nabla_{\mathbf{f}}^2 J(\mathbf{f})] \mathbf{r}$$

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

$$J(\mathbf{f} + \mathbf{r}) = \sum_{i=1}^n \left[ \ell(y_i, \mathbf{f}_i) + g_i \mathbf{r}_i + \frac{1}{2} h_i \mathbf{r}_i^2 \right],$$

where  $g_i = \partial_{\mathbf{f}_i} \ell(y_i, \mathbf{f}_i)$  and  $h_i = \partial_{\mathbf{f}_i}^2 \ell(y_i, \mathbf{f}_i)$ .

- Can find  $\mathbf{r}$  that minimizes  $J(\mathbf{f} + \mathbf{r})$  in closed form.
- Can take step direction to be “projection” of  $\mathbf{r}$  into base hypothesis space  $\mathcal{H}$ .

# XGBoost: Objective Function with Tree Penalty Term

- Adds explicit penalty term on tree complexity to the empirical risk:

$$\Omega(r) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2,$$

where  $r \in \mathcal{H}$  is a regression tree from our base hypothesis space and

- $T$  is the number of leaf nodes and
- $w_j$  is the prediction in the  $j$ 'th node
- Objective function at step  $m$ :

$$J(r) = \sum_{i=1}^n \left[ g_i r(x_i) + \frac{1}{2} h_i r(x_i)^2 \right] + \Omega(r)$$

- In XGBoost, they also use this objective to decide on tree splits
- See [XGBoost Introduction](#) for a nice introduction.



## XGBoost: Rewriting objective function

- For a given tree, let  $q(x_i)$  be  $x_i$ 's node assignment and  $w_j$  the prediction for node  $j$ .
- In each step of XGBoost we're looking for a tree that minimizes

$$\begin{aligned} & \sum_{i=1}^n \left[ g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2 \\ &= \sum_{\text{leaf node } j=1}^T \left[ \left( \underbrace{\sum_{i \in I_j} g_i}_{G_j} \right) w_j + \frac{1}{2} \left( \underbrace{\sum_{i \in I_j} h_i + \lambda}_{H_j} \right) w_j^2 \right] + \gamma T, \end{aligned}$$

where  $I_j = \{i \mid q(x_i) = j\}$  is set of training example indices landing in leaf  $j$ .

# XGBoost: Simple Expression for Tree Penalty/Loss

- Simplifies to

$$\sum_{j=1}^T \left[ G_j w_j + \frac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T$$

- For fixed  $q(x)$  (i.e. fixed tree partitioning), objective minimized when leaf node values are

$$w_j^* = -G_j / (H_j + \lambda).$$

- Plugging  $w_j^*$  back in, this objective reduces to

$$-\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T,$$

which we can think of as the loss for tree partitioning function  $q(x)$ .

- If time were no issue, we could search over all trees to minimize this objective.

# XGBoost: Building Tree Using Objective Function

- Expression to evaluate a tree's node assignment function  $q(x)$ :

$$-\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T,$$

where  $G_j = \sum_{i \in I_j} g_i$  for examples  $i$  assigned to leaf node  $j$ . And  $H_j = \sum_{i \in I_j} h_i$ .

- Suppose we're considering splitting some data into two nodes:  $L$  and  $R$ .
- Loss of tree with this one split is

$$-\frac{1}{2} \left[ \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} \right] + 2\gamma.$$

- Without the split – i.e. a tree with a single leaf node, loss is

$$-\frac{1}{2} \left[ \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] + \gamma.$$

# XGBoost: Node Splitting Criterion

- We can define the **gain** of a split to be the reduction in objective between tree with and without split:

$$\text{Gain} = \frac{1}{2} \left[ \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] - \gamma.$$

- Tree building method:
  - recursively choose split that maximizes the gain.