Forward Stagewise Additive Modeling

He He
Slides based on Lecture 11c from David Rosenberg's course materials
(https://github.com/davidrosenberg/mlcourse)

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Gradient Boosting / "Anyboost"

FSAM with squared loss

- Objective function at m'th round:

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

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

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

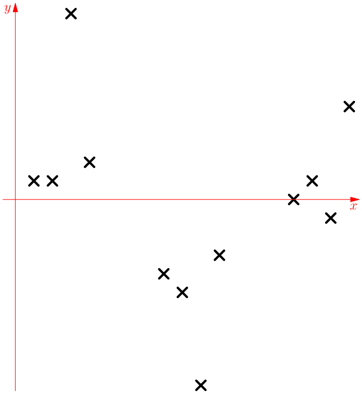
① Dataset: $\{(x_i, \text{residual})\}$

② Learn $h \in$ regression stump

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

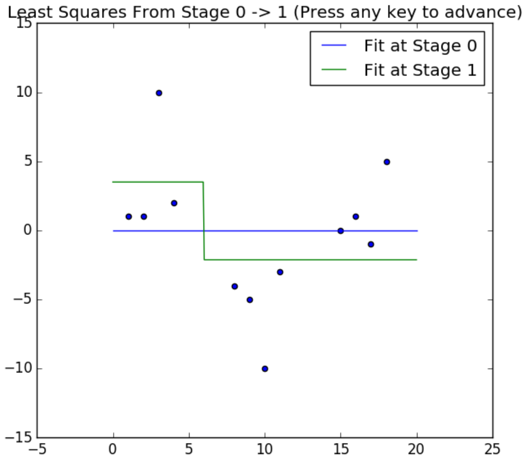
L^2 Boosting with Decision Stumps: Demo

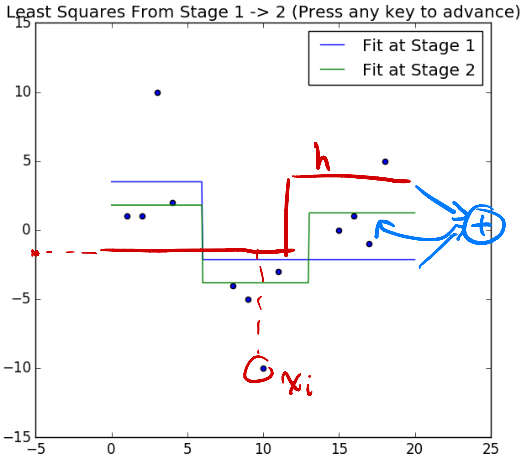
- Consider FSAM with L^2 loss (i.e. L^2 Boosting)
- For base hypothesis space of **regression stumps**



Plot courtesy of Brett Bernstein.

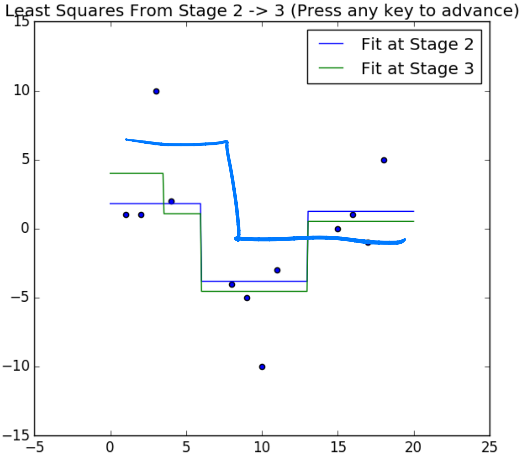
L^2 Boosting with Decision Stumps: Results

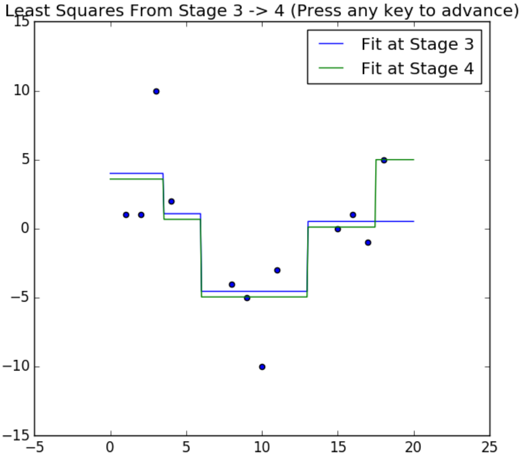




Plots and code courtesy of Brett Bernstein.

L^2 Boosting with Decision Stumps: Results





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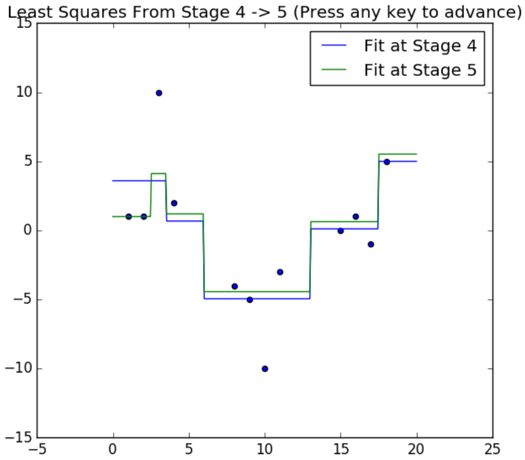
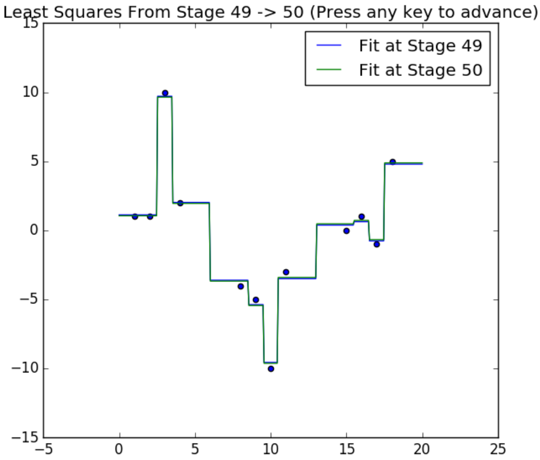
L^2 Boosting with Decision Stumps: Results





Plots and code courtesy of Brett Bernstein.

Interpret the residual

- Objective: $J(f) = \frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2$.
- What is the residual at $x = x_i$?

$$\frac{\partial}{\partial f(x_i)} J(f) = -2\underbrace{(y_i - f(x_i))}_{\text{residual}} \tag{1}$$

  - Gradient w.r.t. f: how should the output of f change to minimize the squared loss.
  - *Residual is the negative gradient* (differ by some constant).
- At each boosting round, we learn a function $h \in \mathcal{H}$ to fit the residual.

$v \in \mathbb{R}$
$h \in \mathcal{H}$
(e.g. regression tree)

$$f \leftarrow f + vh \rightarrow \text{residual} \qquad \text{FSAM / boosting} \tag{2}$$

$$f \leftarrow f - \alpha \nabla_f J(f) \qquad \text{gradient descent} \tag{3}$$

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

"Functional" Gradient Descent

- We want to minimize
$$J(f) = \sum_{i=1}^{n} \ell\left(y_i, f(x_i)\right).$$
- In some sense, we want to take the gradient w.r.t. f.
- $J(f)$ only depends on f at the n training points.
- 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

- Consider gradient descent on
$$J(\mathrm{f}) = \sum_{i=1}^{n} \ell\left(y_i, \mathrm{f}_i\right).$$
- The negative gradient step direction at f is
$$\begin{aligned} -\mathrm{g} &= -\nabla_{\boldsymbol{f}} J(\mathrm{f}) \\ &= -\left(\partial_{\mathrm{f}_1} \ell\left(y_1, \mathrm{f}_1\right), \ldots, \partial_{\mathrm{f}_n} \ell\left(y_n, \mathrm{f}_n\right)\right) \end{aligned}$$
  which we can easily calculate.
- $-\mathrm{g} \in \mathrm{R}^n$ is the direction we want to change each of our n predictions on training data.
- With gradient descent, our final predictor will be an additive model: $f_0 + \sum_{m=1}^{M} v_t(-\mathrm{g}_t)$.

Functional Gradient Descent: Projection Step

- Unconstrained step direction is

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

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

- 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):

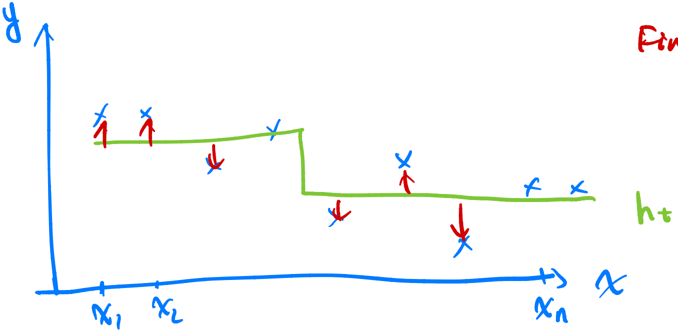
Projection

$$\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \left(\underbrace{-\mathbf{g}_i}_{\mathbb{R}^n} - \underbrace{h(x_i)}_{\in \mathcal{H} \text{ (regression tree)}}\right)^2. \qquad \text{least square regression} \tag{4}$$

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

projected gradient

Explain by figure



Find h that min. $\ell(x, y, h)$.

$h \in$ regression trees.

$$g = \left[\frac{\partial \ell}{\partial h(x_1)} \ \cdots \ \frac{\partial \ell}{\partial h(x_n)} \right] \in R^n$$

$$h_t \leftarrow h_t - \alpha g \qquad g \in R^n$$

$\downarrow$ projection

$g' \in$ regression tree

$$x_i \longmapsto \frac{\partial \ell}{\partial h(x_i)} = g_i$$

$\{(x_i, g_i)\}_{i=1}^n$ dataset $\xrightarrow{\text{learn}}$ $g' \in$ regression tree

Recap

- Objective function:

$$J(f) = \sum_{i=1}^{n} \ell(y_i, f(x_i)). \tag{5}$$

- Unconstrained gradient $\mathrm{g} \in \mathrm{R}^n$ w.r.t. $\boldsymbol{f} = (f(x_1), \ldots, f(x_n))^T$:

$$\mathrm{g} = \nabla_{\boldsymbol{f}} J(\mathrm{f}) = (\partial_{\mathrm{f}_1} \ell(y_1, \mathrm{f}_1), \ldots, \partial_{\mathrm{f}_n} \ell(y_n, \mathrm{f}_n)). \tag{6}$$

- Projected negative gradient $h \in \mathcal{H}$:

$$h = \operatorname*{arg\,min}_{h \in \mathcal{H}} \sum_{i=1}^{n} (\underbrace{-\mathrm{g}_i}^{\in \mathbb{R}^n} - h(x_i))^2. \tag{7}$$

- Gradient descent:

$$f \leftarrow f + {\color{red}v} h \tag{8}$$

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**:

$$f_m \leftarrow f_{m-1} + \lambda v_m h_m \quad \text{where } \lambda \in [0, 1]. \tag{9}$$

  - 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):

$$r_{im} = -\left[\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i))\right]_{f(x_i)=f_{m-1}(x_i)} \tag{10}$$

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

$D = \{(x_i, y_i)\}_{i=1}$

inputs

$\begin{cases} x_i \in \mathbb{R}^? & \text{— input} \\ r_{im} \in \mathbb{R} & \text{— target} \end{cases}$

$? \, 0.1$

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

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

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

$$\begin{aligned}
r_i &= -\frac{\partial}{\partial f(x_i)} \ell(y_i, f(x_i)) && (11)\\
&= -\frac{\partial}{\partial f(x_i)} \left[\log\left(1 + e^{-y_i f(x_i)}\right)\right] && (12)\\
&= \frac{y_i e^{-y_i f(x_i)}}{1 + e^{-y_i f(x_i)}} && (13)\\
&= \frac{y_i}{1 + e^{y_i f(x_i)}} && (14)
\end{aligned}$$

BinomialBoost: Gradient Boosting with Logistic Loss

- Pseudoresidual for ith example:

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

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

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

$\{(x_i, r_i)\}_{i=1}^{n}$

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

Gradient Tree Boosting

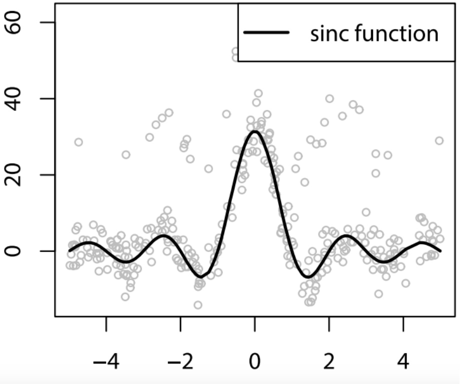
- One common form of gradient boosting machine takes

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

  where S is the number of terminal nodes.

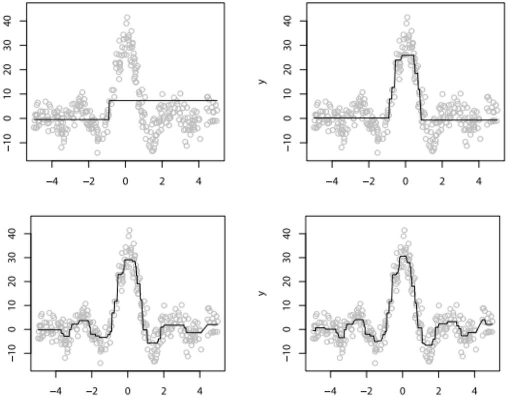
- $S = 2$ gives decision stumps
- HTF recommends $4 \leqslant S \leqslant 8$ (but more recent results use much larger trees)
- Software packages:
  - Gradient tree boosting is implemented by the gbm package for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in sklearn
  - xgboost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

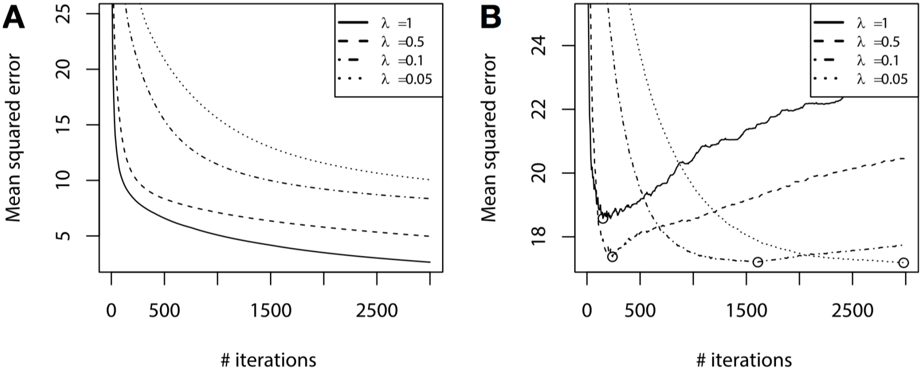
Figure 3 from Natekin and Knoll's "Gradient boosting machines, a tutorial"

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.
- 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