## Lecture 11: Boosting STATS 202: Data Mining and Analysis

# Linh Tran

tranlm@stanford.edu



Department of Statistics Stanford University

August 2, 2023



- Kaggle predictions due in 11 days.
- Homework 4 is out (due in 9 days)
- Final exam details TBD
- Final project review this Friday.

## Outline



- Boosting introduction
- Boosting vs bagging
- Boosting remarks
- AdaBoost
- Boosting training error
- Gradient boosting
- Regularization
- Random tips



- Decision trees partition our feature space and make predictions within each partitioned region.
- Bagging reduces the high variability of decision trees.
- Random forest further reduces variance via random variable selection.



- Decision trees partition our feature space and make predictions within each partitioned region.
- Bagging reduces the high variability of decision trees.
- Random forest further reduces variance via random variable selection.

**Question**: Is there another way of improving the performance of decision trees?



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.

The general algorithm is:

1. Fit an initial  $\hat{f}_n^0$  to the data and compute residuals  $r_i$ .



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.

The general algorithm is:

- 1. Fit an initial  $\hat{f}_n^0$  to the data and compute residuals  $r_i$ .
- 2. For b = 1, ..., B:
  - Fit a weak leaner  $\hat{f}_n^b$  on the residuals.



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.

The general algorithm is:

- 1. Fit an initial  $\hat{f}_n^0$  to the data and compute residuals  $r_i$ .
- 2. For b = 1, ..., B:
  - Fit a weak leaner  $\hat{f}_n^b$  on the residuals.
  - With learning rate  $\lambda_b$ , update prediction to:

$$\hat{f}_n \leftarrow \hat{f}_n + \lambda_b \hat{f}_n^b. \tag{1}$$



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.

The general algorithm is:

- 1. Fit an initial  $\hat{f}_n^0$  to the data and compute residuals  $r_i$ .
- 2. For b = 1, ..., B:
  - Fit a weak leaner  $\hat{f}_n^b$  on the residuals.
  - With learning rate  $\lambda_b$ , update prediction to:

$$\hat{f}_n \leftarrow \hat{f}_n + \lambda_b \hat{f}_n^b. \tag{1}$$

Update the residuals

$$r_i \leftarrow r_i - \lambda_b \hat{f}_n^b(x_i). \tag{2}$$



Boosting uses a set of weak learners (e.g. decision trees) to create a strong one.

The general algorithm is:

- 1. Fit an initial  $\hat{f}_n^0$  to the data and compute residuals  $r_i$ .
- 2. For b = 1, ..., B:
  - Fit a weak leaner  $\hat{f}_n^b$  on the residuals.
  - With learning rate  $\lambda_b$ , update prediction to:

$$\hat{f}_n \leftarrow \hat{f}_n + \lambda_b \hat{f}_n^b. \tag{1}$$

- Update the residuals
- 3. Output prediction, e.g.  $r_i \leftarrow r_i \lambda_b \hat{f}_n^b(x_i)$ . (2)

$$\hat{f}_n(x) = \sum_{b=1}^B \lambda_b \hat{f}_n^b(x).$$
(3)

STATS 202: Data Mining and Analysis



Hyper-parameters to consider when applying a boosting model:

- ▶ The number of learners (aka trees) *B* to use.
- The shrinkage parameter  $\lambda_b$ .
- ▶ The parameters of the learner (e.g. splits in each tree).

Typically, these are found via *cross-validation*.

# Boosting vs bagging

**Bagging**: For  $b = 1, \ldots, B$ :

- 1. Created a bootstrapped sample,  $P_n^b$ .
- 2. Get estimate  $\hat{f}_n^b(x)$  using  $P_n^b$ .

Average the estimates, i.e.

$$\hat{f}_n^{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}_n^b(x).$$

- $\triangleright$   $P_n$  is varied for each fit.
- Designed to reduce variance.

L. Tran



# Boosting vs bagging



#### **Bagging**: For $b = 1, \ldots, B$ :

- 1. Created a bootstrapped sample,  $P_n^b$ .
- 2. Get estimate  $\hat{f}_n^b(x)$  using  $P_n^b$ .

Average the estimates, i.e.

$$\hat{f}_n^{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}_n^b(x).$$

*P<sub>n</sub>* is varied for each fit.
 Designed to reduce variance.

**Boosting**: For  $b = 1, \ldots, B$ :

- 1. Get estimate  $\hat{f}_n^b(x)$  for the residuals  $r^{b-1}$ .
- 2. Update residuals  $r_i^b = r_i^{b-1} - \lambda_b \hat{f}_n^b(x_i).$

Sum the estimates, i.e.

$$\hat{f}_n^{\text{boost}}(x) = \sum_{b=1}^B \lambda_b \hat{f}_n^b(x).$$

'Y' is varied for each fit.
Designed to reduce bias.



Boosting has been called the "best off-the-shelf classifier in the world".



- Boosting has been called the "best off-the-shelf classifier in the world".
- Boosting (generally) works by upweighing points at each iteration which are misclassified.



- Boosting has been called the "best off-the-shelf classifier in the world".
- Boosting (generally) works by upweighing points at each iteration which are misclassified.
- Boosting can use any classifier as its weak learner (base classifier) but decision trees are by far the most popular.



- Boosting has been called the "best off-the-shelf classifier in the world".
- Boosting (generally) works by upweighing points at each iteration which are misclassified.
- Boosting can use any classifier as its weak learner (base classifier) but decision trees are by far the most popular.
- Boosting learns slowly, first using the samples that are easiest to predict, then slowly down weigh these cases, moving on to harder samples.



- Boosting has been called the "best off-the-shelf classifier in the world".
- Boosting (generally) works by upweighing points at each iteration which are misclassified.
- Boosting can use any classifier as its weak learner (base classifier) but decision trees are by far the most popular.
- Boosting learns slowly, first using the samples that are easiest to predict, then slowly down weigh these cases, moving on to harder samples.
- Boosting can give zero training error, but rarely overfits.



- Boosting has been called the "best off-the-shelf classifier in the world".
- Boosting (generally) works by upweighing points at each iteration which are misclassified.
- Boosting can use any classifier as its weak learner (base classifier) but decision trees are by far the most popular.
- Boosting learns slowly, first using the samples that are easiest to predict, then slowly down weigh these cases, moving on to harder samples.
- Boosting can give zero training error, but rarely overfits.
- Can be thought of as fitting a model on multiple data sets.



1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.



- 1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.
- 2. For b = 1, ..., B:

a Fit a classifier  $G^{b}(x)$  to the training data using weights  $w_{i}$ .



- 1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.
- 2. For b = 1, ..., B:
  - a Fit a classifier  $G^{b}(x)$  to the training data using weights  $w_{i}$ .
  - **b** Compute

$$err_b = \frac{\sum_{i=1}^n w_i \mathbb{I}(y_i \neq G^b(x_i))}{\sum_{i=1}^n w_i}$$
(4)



- 1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.
- 2. For b = 1, ..., B:

a Fit a classifier  $G^{b}(x)$  to the training data using weights  $w_{i}$ .

**b** Compute

$$err_{b} = \frac{\sum_{i=1}^{n} w_{i} \mathbb{I}(y_{i} \neq G^{b}(x_{i}))}{\sum_{i=1}^{n} w_{i}}$$
(4)

c Compute  $\lambda_b = \log((1 - err_b)/err_b)$ 



- 1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.
- 2. For b = 1, ..., B:

a Fit a classifier  $G^{b}(x)$  to the training data using weights  $w_{i}$ .

**b** Compute

$$err_{b} = \frac{\sum_{i=1}^{n} w_{i} \mathbb{I}(y_{i} \neq G^{b}(x_{i}))}{\sum_{i=1}^{n} w_{i}}$$
(4)

c Compute  $\lambda_b = \log((1 - err_b)/err_b)$ d Set  $w_i \leftarrow w_i \cdot \exp[\lambda_b \mathbb{I}(y_i \neq G^b(x_i))] : i = 1, ..., n.$ 



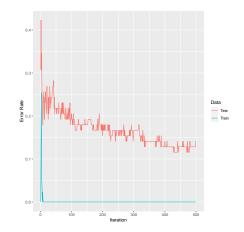
- 1. Initialize the observation weights  $w_i = 1/n$ : i = 1, ..., n.
- 2. For b = 1, ..., B:
  - a Fit a classifier  $G^{b}(x)$  to the training data using weights  $w_{i}$ .
  - **b** Compute

$$err_{b} = \frac{\sum_{i=1}^{n} w_{i}\mathbb{I}(y_{i} \neq G^{b}(x_{i}))}{\sum_{i=1}^{n} w_{i}}$$
(4)

c Compute  $\lambda_b = \log((1 - err_b)/err_b)$ d Set  $w_i \leftarrow w_i \cdot \exp[\lambda_b \mathbb{I}(y_i \neq G^b(x_i))] : i = 1, ..., n.$ 3. Output  $G_B(x) = \operatorname{sign}\left(\sum_{b=1}^B \lambda_b G^b(x)\right).$ 

### AdaBoost example





AdaBoost applied to the *Sonar Data*.



Question: What happens after the training error reaches 0?



**Question**: What happens after the training error reaches 0? Define:  $\square B$ 

$$G_B^*(x) = \frac{\sum_{b=1}^B \lambda_b G^b(x)}{\sum_{b=1}^B \lambda_b}$$
(5)

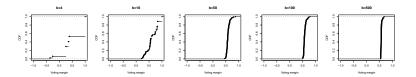


**Question**: What happens after the training error reaches 0? Define:

$$G_B^*(x) = \frac{\sum_{b=1}^B \lambda_b G^b(x)}{\sum_{b=1}^B \lambda_b}$$
(5)

We can look at voting margins for our training data, i.e.

$$margin(x) = y * G_B^*(x)$$
(6)



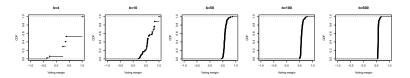


**Question**: What happens after the training error reaches 0? Define:

$$G_B^*(x) = \frac{\sum_{b=1}^B \lambda_b G^b(x)}{\sum_{b=1}^B \lambda_b}$$
(5)

We can look at voting margins for our training data, i.e.

$$margin(x) = y * G_B^*(x)$$
(6)



n.b. Letting  $err_b \leq 1/2 - \gamma$ , then  $\operatorname{Error}_{train} \leq (\sqrt{1 - 4\gamma^2})^B$ 



# AdaBoost can be framed as Forward Stagewise Additive Modeling:

Algorithm 10.2 Forward Stagewise Additive Modeling.

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

$$(\beta_m, \gamma_m) = \arg \min_{\beta, \gamma} \sum_{i=1}^N L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$

(b) Set  $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$ .

where  $L(y, f_{m-1}(x) + \beta b(x; \gamma))$  is the exponential loss, i.e.

$$L(y, f(x)) = \exp(-yf(x))$$
(7)



# Gradient boosting generalizes L(y, f(x)) to any smooth loss function.

#### Some common loss functions:

Setting	Loss Function	$-\partial L(y_i, f(x_i))/\partial f(x_i)$
Regression	$\frac{1}{2}[y_i - f(x_i)]^2$	$y_i - f(x_i)$
Regression	$ y_i - f(x_i) $	$\operatorname{sign}[y_i - f(x_i)]$
Regression	Huber	$\begin{split} y_i - f(x_i) \text{ for }  y_i - f(x_i)  &\leq \delta_m \\ \delta_m \text{sign}[y_i - f(x_i)] \text{ for }  y_i - f(x_i)  > \delta_m \\ \text{where } \delta_m &= \alpha \text{th-quantile}\{ y_i - f(x_i) \} \end{split}$
Classification	Deviance	kth component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

TABLE 10.2. Gradients for commonly used loss functions.

## Gradient Boosting algorithm



1. Initialize 
$$f_n^0(x) = \arg\min_{\gamma} \sum_{i=1}^n L(y_i, \gamma)$$
.

# Gradient Boosting algorithm



- 1. Initialize  $f_n^0(x) = \underset{\gamma}{\arg\min \sum_{i=1}^n L(y_i, \gamma)}$ . 2. For b = 1, ..., B:
  - a Compute the residuals/gradients:

$$r_i^b = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f^{b-1}} : i = 1, ..., n$$
(8)

# Gradient Boosting algorithm



- 1. Initialize  $f_n^0(x) = \underset{\gamma}{\arg\min \sum_{i=1}^n L(y_i, \gamma)}$ . 2. For b = 1, ..., B:
  - a Compute the residuals/gradients:

$$r_{i}^{b} = -\left[\frac{\partial L(y_{i}, f(x_{i}))}{\partial f(x_{i})}\right]_{f=f^{b-1}} : i = 1, ..., n$$
(8)

b Fit a regression tree to  $r_i^b$ , giving terminal regions  $R_j^b: j = 1, ..., J^b$ 

# Gradient Boosting algorithm



- 1. Initialize  $f_n^0(x) = \underset{\gamma}{\arg\min \sum_{i=1}^n L(y_i, \gamma)}$ . 2. For b = 1, ..., B:
  - a Compute the residuals/gradients:

$$r_{i}^{b} = -\left[\frac{\partial L(y_{i}, f(x_{i}))}{\partial f(x_{i})}\right]_{f=f^{b-1}} : i = 1, ..., n$$
(8)

b Fit a regression tree to  $r_i^b$ , giving terminal regions  $R_j^b: j = 1, ..., J^b$ c For  $j = 1, ..., J^b$ , compute  $\gamma_i^b = \arg\min_{\gamma} \sum_{x_i \in R_i^b} L(y_i, f^{b-1}(x_i) + \gamma)$  (9)

# Gradient Boosting algorithm



- 1. Initialize  $f_n^0(x) = \underset{\gamma}{\arg\min \sum_{i=1}^n L(y_i, \gamma)}$ . 2. For b = 1, ..., B:
  - a Compute the residuals/gradients:

$$r_{i}^{b} = -\left[\frac{\partial L(y_{i}, f(x_{i}))}{\partial f(x_{i})}\right]_{f=f^{b-1}} : i = 1, ..., n$$
(8)

b Fit a regression tree to  $r_i^b$ , giving terminal regions  $R_j^b: j = 1, ..., J^b$ c For  $j = 1, ..., J^b$ , compute  $\gamma_i^b = \arg \min_{\gamma} \sum_{x_i \in R_j^b} L(y_i, f^{b-1}(x_i) + \gamma)$  (9)

d Update 
$$f^b(x) = f^{b-1}(x) + \sum_{j=1}^{J^b} \gamma_j^b \mathbb{I}(x \in R_j^b)$$

# Gradient Boosting algorithm



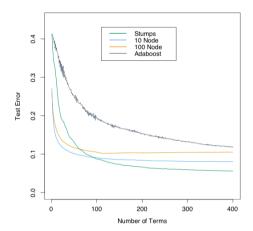
- 1. Initialize  $f_n^0(x) = \underset{\gamma}{\arg\min \sum_{i=1}^n L(y_i, \gamma)}$ . 2. For b = 1, ..., B:
  - a Compute the residuals/gradients:

$$r_{i}^{b} = -\left[\frac{\partial L(y_{i}, f(x_{i}))}{\partial f(x_{i})}\right]_{f=f^{b-1}} : i = 1, ..., n$$
(8)

b Fit a regression tree to  $r_i^b$ , giving terminal regions  $R_j^b: j = 1, ..., J^b$ c For  $j = 1, ..., J^b$ , compute  $\gamma_i^b = \arg \min_{\gamma} \sum_{x_i \in R_j^b} L(y_i, f^{b-1}(x_i) + \gamma)$  (9) d Update  $f^b(x) = f^{b-1}(x) + \sum_{j=1}^{J^b} \gamma_j^b \mathbb{I}(x \in R_j^b)$ 3. Output  $\hat{f}_n(x) = f^B(x)$ .

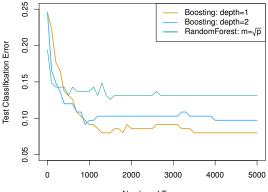


### Example: Applied to simulated data.





**Example**: Applied to 15-class gene expression data.



Number of Trees





### Regularization methods:

Tree constraints: for each tree, limiting the e.g. number of trees, depth, terminal nodes, obserations in a split, improvement made.



### Regularization methods:

- Tree constraints: for each tree, limiting the e.g. number of trees, depth, terminal nodes, obserations in a split, improvement made.
- Shrinkage: Each tree is weighted to slow down the learning by the algorithm.



### **Regularization methods**:

- Tree constraints: for each tree, limiting the e.g. number of trees, depth, terminal nodes, obserations in a split, improvement made.
- Shrinkage: Each tree is weighted to slow down the learning by the algorithm.
- Random splitting: at each iteration a subsample of the training data is drawn at random (without replacement).



### **Regularization methods**:

- Tree constraints: for each tree, limiting the e.g. number of trees, depth, terminal nodes, obserations in a split, improvement made.
- Shrinkage: Each tree is weighted to slow down the learning by the algorithm.
- Random splitting: at each iteration a subsample of the training data is drawn at random (without replacement).
- Penalized learning: Apply L1 or L2 regularization to the terminal nodes.



Gradient boosting wins most of the Kaggle competitions.

Trick is to fine tune the hyper-parameters during training.



Gradient boosting wins most of the Kaggle competitions.

Trick is to fine tune the hyper-parameters during training.

Some tips from Kaggle master *Owen Zhang*:

#### **GBDT Hyper Parameter Tuning**

Hyper Parameter	Tuning Approach	Range	Note
# of Trees	Fixed value	100-1000	Depending on datasize
Learning Rate	Fixed => Fine Tune	[2 - 10] / # of Trees	Depending on # trees
Row Sampling	Grid Search	[.5, .75, 1.0]	
Column Sampling	Grid Search	[.4, .6, .8, 1.0]	
Min Leaf Weight	Fixed => Fine Tune	3/(% of rare events)	Rule of thumb
Max Tree Depth	Grid Search	[4, 6, 8, 10]	
Min Split Gain	Fixed	0	Keep it 0

Best GBDT implementation today: <u>https://github.com/tqchen/xgboost</u>

by Tianqi Chen (U of Washington)





- [1] ISL. Chapter 8
- [2] ESL. Chapter 10
- [3] Schapire, RE. The Boosting Approach to Machine Learning An Overview. Nonlinear Estimation and Classification, Springer, 2003.