Lecture 10: Boosting

STATS 202: Statistical Learning and Data Science

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July 28, 2025

Announcements



- ► Midterm grades will be out soon
- Homework 3 due today
 - Homework 4 is posted
- Final predictions due in 2 weeks
- Section this Friday goes into more final project details

Outline



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

Recall



- Decision trees partition our feature space and make predictions within each partitioned region.
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Question: Is there another way of improving the performance of decision trees?



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Update the residuals

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

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



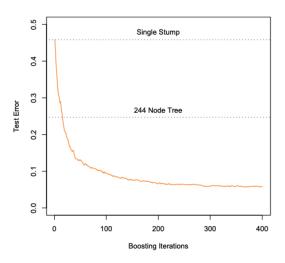


Figure 10.2

Boosting hyperparameters



Hyper-parameters to consider when applying a boosting model:

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

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

Boosting vs bagging



Bagging: For $b = 1, \dots, B$:

- 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.

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

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Boosting: For $b = 1, \dots, B$:

- 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.



Remarks:

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- 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.



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- 3. Output $G_B(x) = \operatorname{sign}\left(\sum_{b=1}^B \alpha_b G^b(x)\right)$.



FINAL CLASSIFIER

$$G(x) = \operatorname{sign} \left[\sum_{m=1}^{M} \alpha_m G_m(x) \right]$$

Weighted Sample $\longrightarrow G_3(x)$

Weighted Sample $\longrightarrow G_2(x)$

Training Sample $\longrightarrow G_1(x)$

Figure 10.1

AdaBoost example



Features

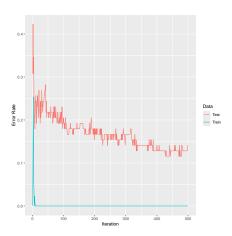
Measured energy level within one of 60 frequency bands

Label

▶ Indicator object is a Mine (1) vs Rock (0)

AdaBoost example





AdaBoost applied to the Sonar Data.



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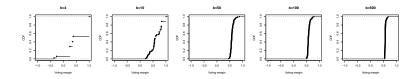
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$$margin(x) = y * G_B^*(x)$$
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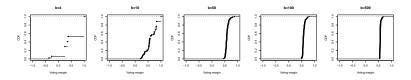
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n.b. Letting $err_b \leq 1/2 - \gamma$, then $Error_{train} \leq (\sqrt{1 - 4\gamma^2})^B$

Weak learners



Question: How "weak" should our learners be?

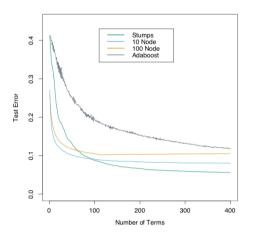
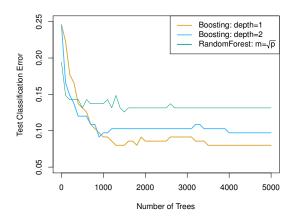


Figure 10.9

Boosting vs. random forests



Example: Applied to 15-class gene expression data (Figure 8.11).





Boosting can be viewed as an additive model, i.e.

$$f(\mathbf{X}) = \sum_{m=1}^{M} \beta_m b(\mathbf{X}; \gamma_m)$$
 (7)

for \emph{M} basis functions characterized by $\gamma_{\emph{m}}$



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Algorithm 10.2 Forward Stagewise Additive Modeling.

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

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

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$$L(y_{i}, f_{m-1}(x_{i}) + \beta b(x_{i}; \gamma)) = (y_{i} - (f_{m-1}(x_{i}) + \beta b(x_{i}; \gamma)))^{2}$$

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$$= (r_{im} - \beta b(x_{i}; \gamma))^{2}$$

Problem: RSS isn't a good loss for classification

Gradient Boosting



Define the following loss:

$$L(y, f(x)) = \exp(-yf(x)) \tag{8}$$

Applying the forward stagewise additive representation to Adaboost:

$$(\beta_m, G_m) = \arg \min_{\beta, G} \sum_{i=1}^n \exp\left(-y_i(f_{m-1}(x_i) + \beta G(x_i))\right)$$
$$= \arg \min_{\beta, G} \sum_{i=1}^n w_i^{(m)} \exp\left(-\beta y_i G(x_i)\right)$$

where $w_i^{(m)} = \exp(-y_i f_{m-1}(x_i))$ It can be shown that

$$w_i^{(m+1)} = w_i^{(m)} \cdot \exp(\alpha_m \mathbb{I}(y_i \neq G_m(x_i))) \cdot \exp(-\beta_m)$$

Gradient Boosting



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

Some common loss functions:

TABLE 10.2. Gradients for commonly used 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) $	$sign[y_i - f(x_i)]$	
Regression	Huber	$ \begin{vmatrix} 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) \} $	
Classification	Deviance	kth component: $I(y_i = G_k) - p_k(x_i)$	



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- c For $j = 1, ..., J^b$, compute

$$\gamma_i^b = \arg\min_{\gamma} \sum_{x_i \in R_j^b} L(y_i, f^{b-1}(x_i) + \gamma)$$
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3. Output $\hat{f}_n(x) = f^B(x)$.



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- Random splitting: at each iteration a subsample of the training data is drawn at random (without replacement).
- ▶ Penalized learning: Apply *L*1 or *L*2 regularization to the terminal nodes.



Example: Shrinkage (ν)

$$f^{b}(x) = f^{b-1}(x) + \nu \sum_{j=1}^{J^{b}} \gamma_{j}^{b} \mathbb{I}(x \in R_{j}^{b})$$
 (11)

Further trades off slower / longer learning.

Shrinkage



Example: Comparing shrinkage vs not.

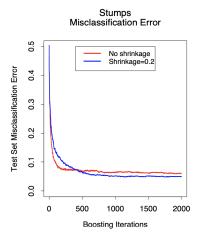


Figure 10.11

Sub-sampling



Example: Shrinkage with sub-sampling.

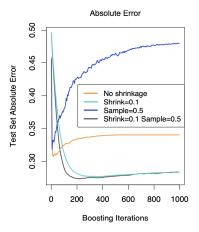


Figure 10.12

Gradient boosting tips



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

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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: https://github.com/tqchen/xqboost by **Tianqi Chen** (U of Washington)



References



- [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.