Boosting and Additive Trees

Chapter 10 of

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    b. AdaBoost
    c. Boosting as Forward Stagewise Additive Modeling
    d. Loss functions robustness
2. Boosting trees:
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Boosting

Intuition

Boosting is one of the most powerful learning ideas introduced in last 30 years. It can be used both for classification and regression (we will focus on two-class classification with classes {-1, 1}).

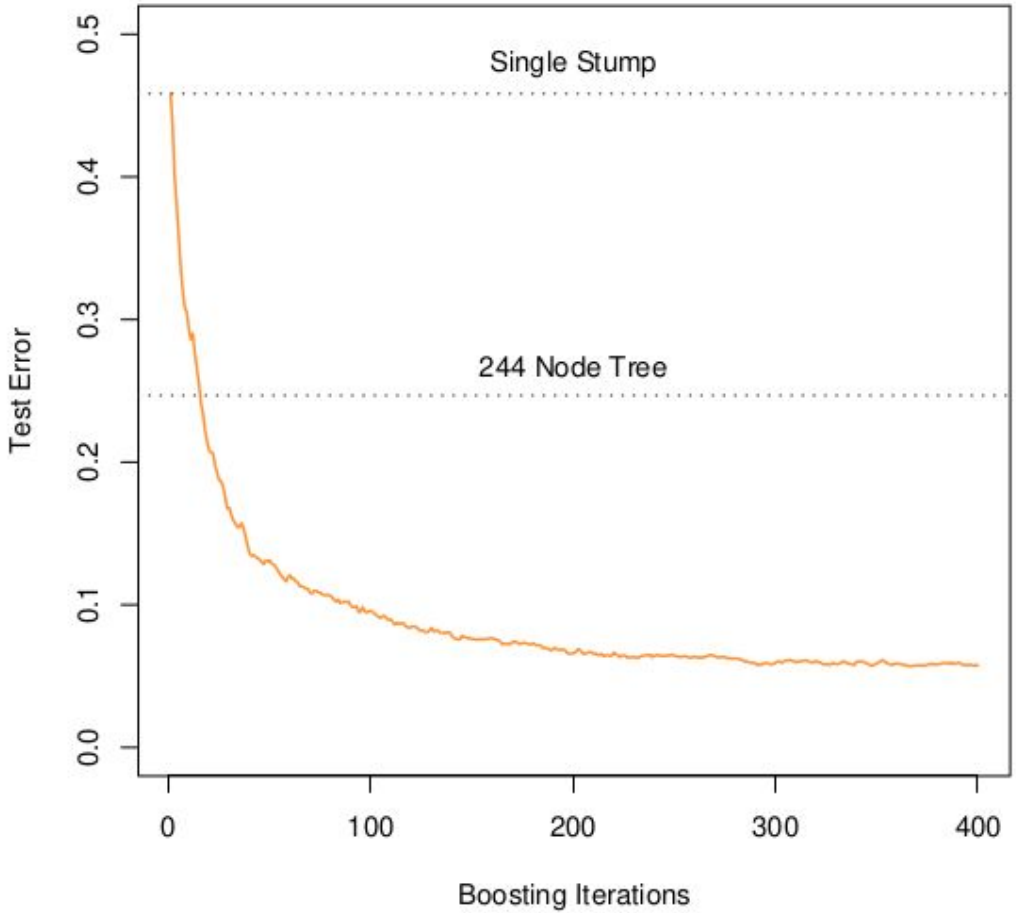
How does it work?:

- Combination of weak classifiers into powerful committee
- Sequential application of weak classificator on repeatedly modified versions of data
- At each step, weight of previously misclassified samples are increased
- Predictions of weak classifiers are combined through majority vote

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

Algorithm 10.1 *AdaBoost.M1.*

1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))],\ i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.


Single Stump
244 Node Tree
Test Error
0.0
0.1
0.2
0.3
0.4
0.5
0
100
200
300
400
Boosting Iterations

Boosting as Additive Model

Basis function expansion:

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

Boosting:

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

To train this kind of model, we need to find:

$$\min_{\{\beta_m, \gamma_m\}_1^M} \sum_{i=1}^{N} L\left(y_i, \sum_{m=1}^{M} \beta_m b(x_i; \gamma_m)\right)$$

Problem: This is very computationally intensive!

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

Examples of Forward Stagewise

Squared error loss:

$$L(y, f(x)) = (y - f(x))^2$$

Loss at m-th iteration of Forward Stagewise algorithm:

$$\begin{aligned} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)) &= (y_i - f_{m-1}(x_i) - \beta b(x_i; \gamma))^2 \\ &= (r_{im} - \beta b(x_i; \gamma))^2, \end{aligned}$$

New term added to the expansion is fitted to current residuals.

Examples of Forward Stagewise

Exponential loss:

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

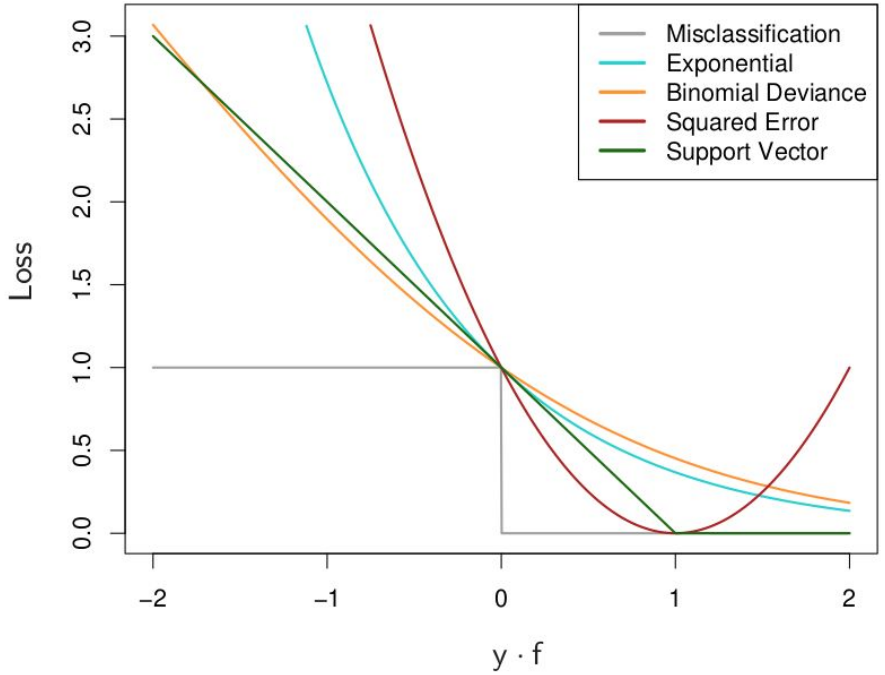
Fact 1: It can be proven that AdaBoost is minimizing the exponential loss criterion via a Forward Stagewise additive modeling approach.

Fact 2: Population minimizer for exponential loss is:

$$f^*(x) = \arg\min_{f(x)} \mathrm{E}_{Y|x}(e^{-Yf(x)}) = \frac{1}{2}\log\frac{\Pr(Y=1|x)}{\Pr(Y=-1|x)}$$

Fact 3: Population minimizer for binominal cross-entropy is the same.

Loss functions and robustness



y - classes: {-1, 1}
f - prediction, class prediction is sign(f)
Conclusions:

- Exponential and squared error loss are sensitive to outliers
- Squared error is bad for classification: it penalizes correctly classified examples

Boosting trees

Motivation

- Decision trees have some useful characteristics: handling missing data and mixed data types, ability to deal with irrelevant inputs but have low predictive power
- AdaBoost increases accuracy, but is implementing exponential loss which is not ideal
- We would like to be able to boost decision trees using different loss functions

Decision trees

Decision tree can be expressed as:

$$T(x;\Theta) = \sum_{j=1}^{J} \gamma_j I(x \in R_j)$$

where R_j - region corresponding to leaf j and γ_j - label assigned to leaf j.

While creating such tree, we want to find:

$$\hat{\Theta} = \arg\min_{\Theta} \sum_{j=1}^{J} \sum_{x_i \in R_j} L(y_i, \gamma_j)$$

Given the regions, calculating their optimal labels is easy, but finding these regions is much more difficult (we use greedy top-down strategy).

Boosted trees

Boosted trees are a sum of decision trees:

$$f_M(x) = \sum_{m=1}^{M} T(x; \Theta_m)$$

We induce them in forward stagewise manner:

$$\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} L\left(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)\right)$$

Finding labels is easy:

$$\hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma_{jm}\right)$$

Finding regions is more difficult than for single tree. **We can do it for exponential and squared-error loss, but we can't do it for more robust loss functions (but we want!).**

How does gradient descent help?

We want to minimize loss with respect to predict function.

Imagine that that function is a simple mapping between inputs and outputs (we lose the constraint that the predictor must be a tree/forest).

$$\mathbf{f} = \{f(x_1), f(x_2), \ldots, f(x_N)\}^T$$

For a forest:

$$\mathbf{f}_M = \sum_{m=0}^{M} \mathbf{h}_m\,, \quad \mathbf{h}_m \in \mathbb{R}^N$$

Solving is easy using gradient descent:

$$\mathbf{f}_m = \mathbf{f}_{m-1} - \rho_m \mathbf{g}_m$$

where ρ_m - step length, $\mathbf{g}_m$ is gradient of loss with respect to $\mathbf{f}_m$

Gradient boosting

We need to deal with the constraint that predictor must be a tree, not a simple mapping.

Hack:

1. Calculate the gradient of loss (it can be any differentiable loss) as in previous slide
2. Induct a tree minimizing square loss between the gradient and the tree's predictions (we can induct a tree for square loss):

$$\tilde{\Theta}_m = \arg\min_{\Theta} \sum_{i=1}^{N} \left(-g_{im} - T(x_i; \Theta)\right)^2$$

This allows us to create boosted forests using any loss function!

Algorithm 10.3 *Gradient Tree Boosting Algorithm.*

1. Initialize $f_0(x) = \arg\min_\gamma \sum_{i=1}^{N} L(y_i, \gamma)$.
2. For $m = 1$ to M:
   (a) For $i = 1, 2, \ldots, N$ compute
   $$r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}.$$
   (b) Fit a regression tree to the targets r_{im} giving terminal regions R_{jm}, $j = 1, 2, \ldots, J_m$.
   (c) For $j = 1, 2, \ldots, J_m$ compute
   $$\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma\right).$$
   (d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
3. Output $\hat{f}(x) = f_M(x)$.

Regularization techniques: sizes of trees

Small trees are desired - they are less prone to overfitting.

We can prune them one by one (poor results) or limit size of all the trees to a constant J (number of leaves).

How to chose J:

- J-1 limits the level of interactions between input features
- too big value leads to overfitting
- sensible values are normally between 4 and 8

Regularization techniques: other

- limiting number of boosting rounds (size of forest): early stopping
- shrinkage (learning rate):

$$f_m(x) = f_{m-1}(x) + \nu \cdot \sum_{j=1}^{J} \gamma_{jm} I(x \in R_{jm})$$

- subsampling: training each tree on randomly selected η fraction of training data

Often using all of that techniques at once leads to good results, but introduce new hyperparameters to optimize.

Interpretation: relative importance of predictor variables

To compare importance of predictor variables, we can calculate how much of an improvement in loss splits based on them gives us:

$$\mathcal{I}_\ell^2(T) = \sum_{t=1}^{J-1} \hat{\imath}_t^2 \, I(v(t) = \ell)$$

For forests we can average:

$$\mathcal{I}_\ell^2 = \frac{1}{M} \sum_{m=1}^{M} \mathcal{I}_\ell^2(T_m)$$

Interpretation: partial dependence plots

To analyze how value of one predictor value affects prediction, we can calculate partial dependence on that value (or set of values):

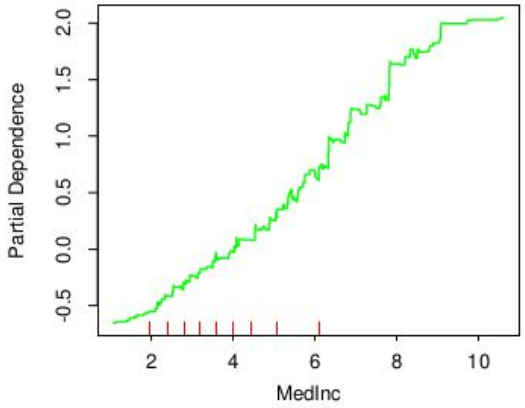
$$f_S(X_S) = \mathrm{E}_{X_C} f(X_S, X_C)$$

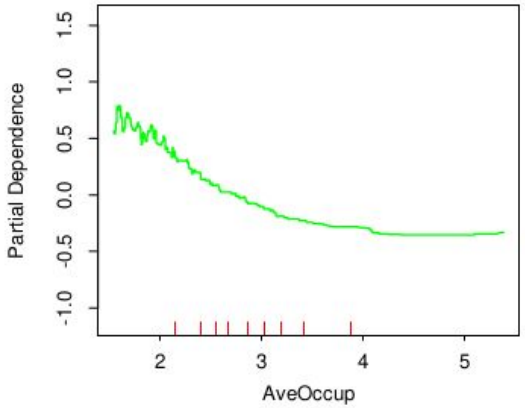
This “averages” the contribution of other values.

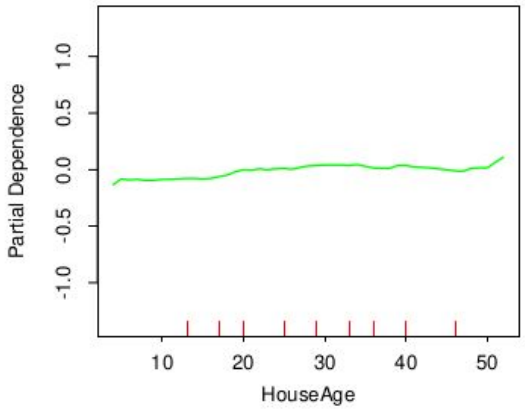
We can also ignore the other values:

$$\tilde{f}_S(X_S) = \mathrm{E}(f(X_S, X_C)|X_S)$$

These approaches lead to different results, example: $f(a, b) = a^b$


Partial Dependence
-0.5
0.0
0.5
1.0
1.5
2.0
2
4
6
8
10
MedInc


Partial Dependence
-1.0
-0.5
0.0
0.5
1.0
1.5
2
3
4
5
AveOccup


Partial Dependence
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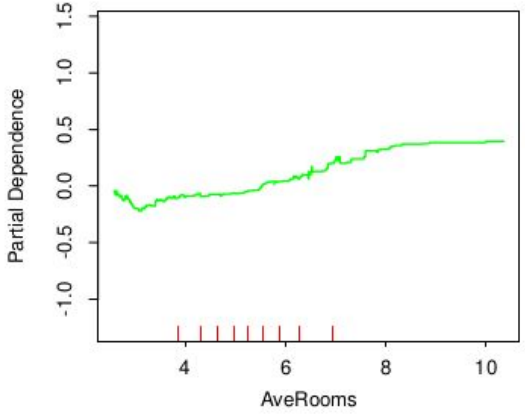
0.0
0.5
1.0
10
20
30
40
50
HouseAge


Partial Dependence
-1.0
-0.5
0.0
0.5
1.0
1.5
4
6
8
10
AveRooms

Thanks for your attention!