Boosting Methods

Jeremy Cohen

Princeton University

3 May 2018

Overview

AdaBoost

Original boosting algorithm designed for the binary classification problem.

- Given an output variable, $Y \in \{-1, 1\}$ and a vector of predictor variables, X, a classifier $G(X)$ produces a prediction taking one of the two values of Y

[1] A weak classifier is one that performs only slightly better than random guessing.

AdaBoost

Original boosting algorithm designed for the binary classification problem.

- Given an output variable, $Y \in \{-1, 1\}$ and a vector of predictor variables, X, a classifier $G(X)$ produces a prediction taking one of the two values of Y
- We begin with a "weak" classifier fit to the data.[1]

[1] A weak classifier is one that performs only slightly better than random guessing.

AdaBoost

Original boosting algorithm designed for the binary classification problem.

- Given an output variable, $Y \in \{-1, 1\}$ and a vector of predictor variables, X, a classifier $G(X)$ produces a prediction taking one of the two values of Y
- We begin with a "weak" classifier fit to the data.[1]
- We then reweight the observations so that those that were misclassified in this round, $y_i \neq G(x_i)$*areupweighted*

[1] A weak classifier is one that performs only slightly better than random guessing.

AdaBoost

Original boosting algorithm designed for the binary classification problem.

- Given an output variable, $Y \in \{-1, 1\}$ and a vector of predictor variables, X, a classifier $G(X)$ produces a prediction taking one of the two values of Y
- We begin with a "weak" classifier fit to the data.[1]
- We then reweight the observations so that those that were misclassified in this round, $y_i \neq G(x_i) \mathit{areupweighted}$
- We then fit a new classifier and repeat this M times.

[1] A weak classifier is one that performs only slightly better than random guessing.

AdaBoost

Original boosting algorithm designed for the binary classification problem.

- Given an output variable, $Y \in \{-1, 1\}$ and a vector of predictor variables, X, a classifier $G(X)$ produces a prediction taking one of the two values of Y
- We begin with a "weak" classifier fit to the data.[1]
- We then reweight the observations so that those that were misclassified in this round, $y_i \neq G(x_i) \mathit{areupweighted}$
- We then fit a new classifier and repeat this M times.
- The final classification is given by a weighted vote of all classifiers, with those $G_m(x)$ that are more accurate receiving higher weights.

[1] A weak classifier is one that performs only slightly better than random guessing.

AdaBoost, Visually

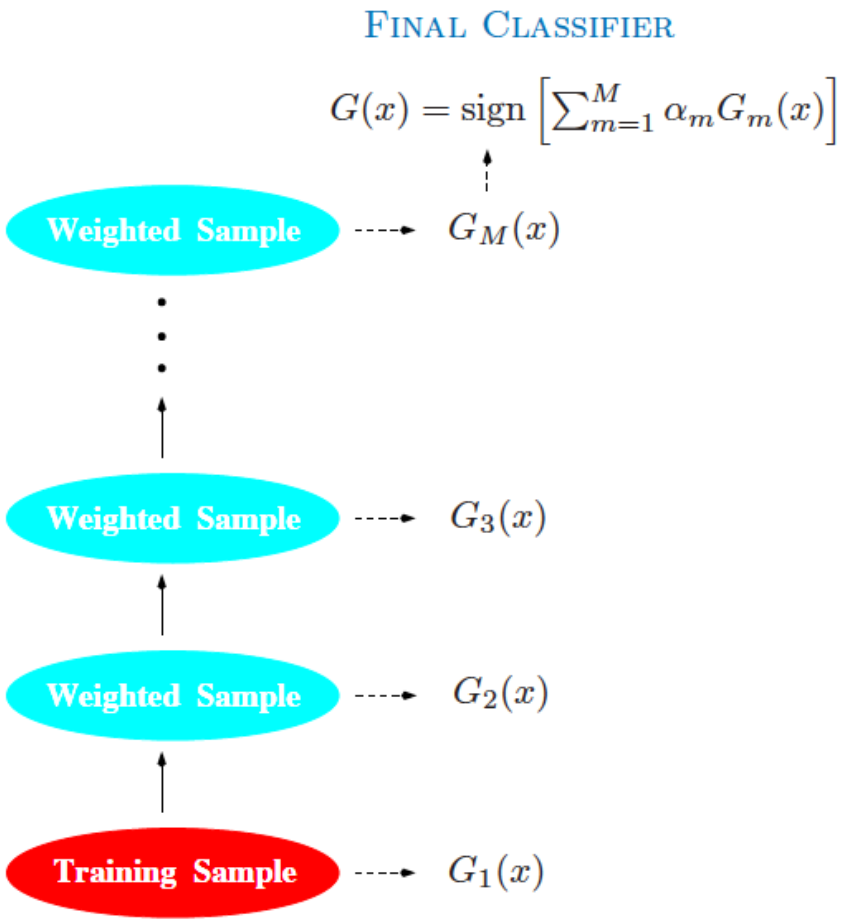


Figure 1: (Hastie et al. 2009:338)

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:
   - Fit a classifier $G_m(x)$ to the training data using weights w_i

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:
   - Fit a classifier $G_m(x)$ to the training data using weights w_i
   - Compute the error of the classifier as

$$err_m = \frac{\sum_{i=1}^{N} w_i \mathbf{1}(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$$

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:
   - Fit a classifier $G_m(x)$ to the training data using weights w_i
   - Compute the error of the classifier as

$$err_m = \frac{\sum_{i=1}^{N} w_i \mathbf{1}(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$$

   - Compute $\alpha_m = log(\frac{1-err_m}{err_m})$

AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:
   - Fit a classifier $G_m(x)$ to the training data using weights w_i
   - Compute the error of the classifier as

$$err_m = \frac{\sum_{i=1}^{N} w_i \mathbf{1}(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$$

   - Compute $\alpha_m = log(\frac{1-err_m}{err_m})$
   - Set $w_i \leftarrow w_i \cdot exp\left[\alpha_m \cdot G_m(x_i)\right]$

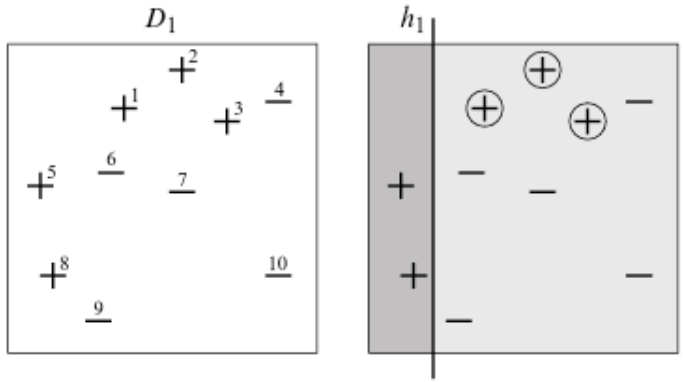
AdaBoost, More Formally

1. Initialize the observation weights $w_i = \frac{1}{N}$, for $i = 1, 2, ..., N$
2. For $m = 1$ to M:
   - Fit a classifier $G_m(x)$ to the training data using weights w_i
   - Compute the error of the classifier as

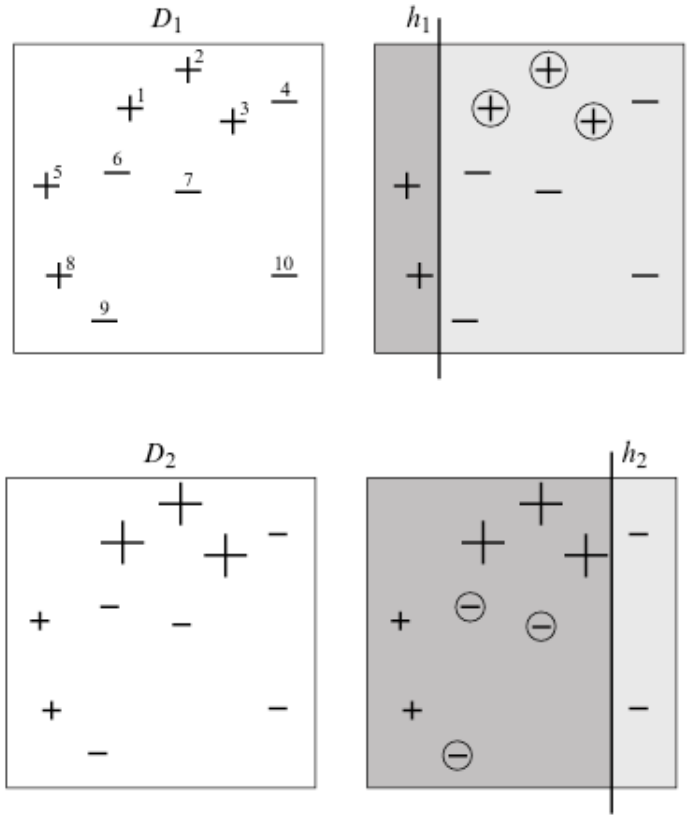
$$err_m = \frac{\sum_{i=1}^{N} w_i \mathbf{1}(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$$

   - Compute $\alpha_m = log(\frac{1-err_m}{err_m})$
   - Set $w_i \leftarrow w_i \cdot exp\left[\alpha_m \cdot G_m(x_i)\right]$
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$

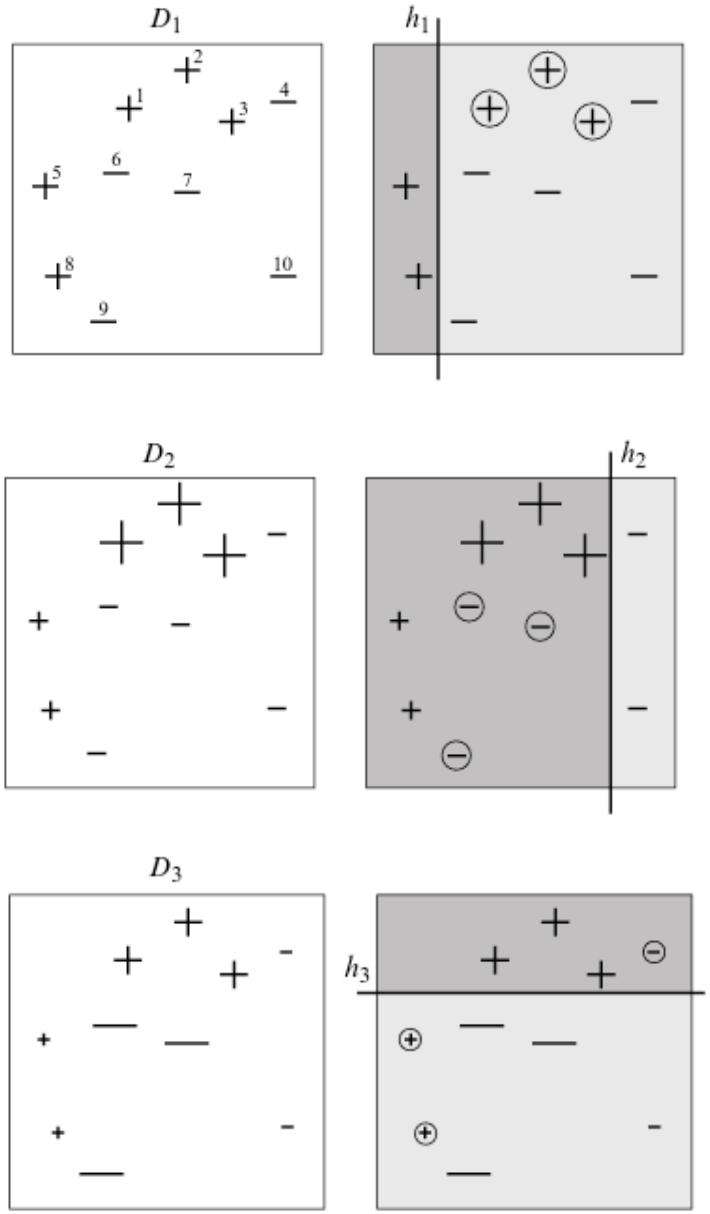
AdaBoost, Visually in More Detail



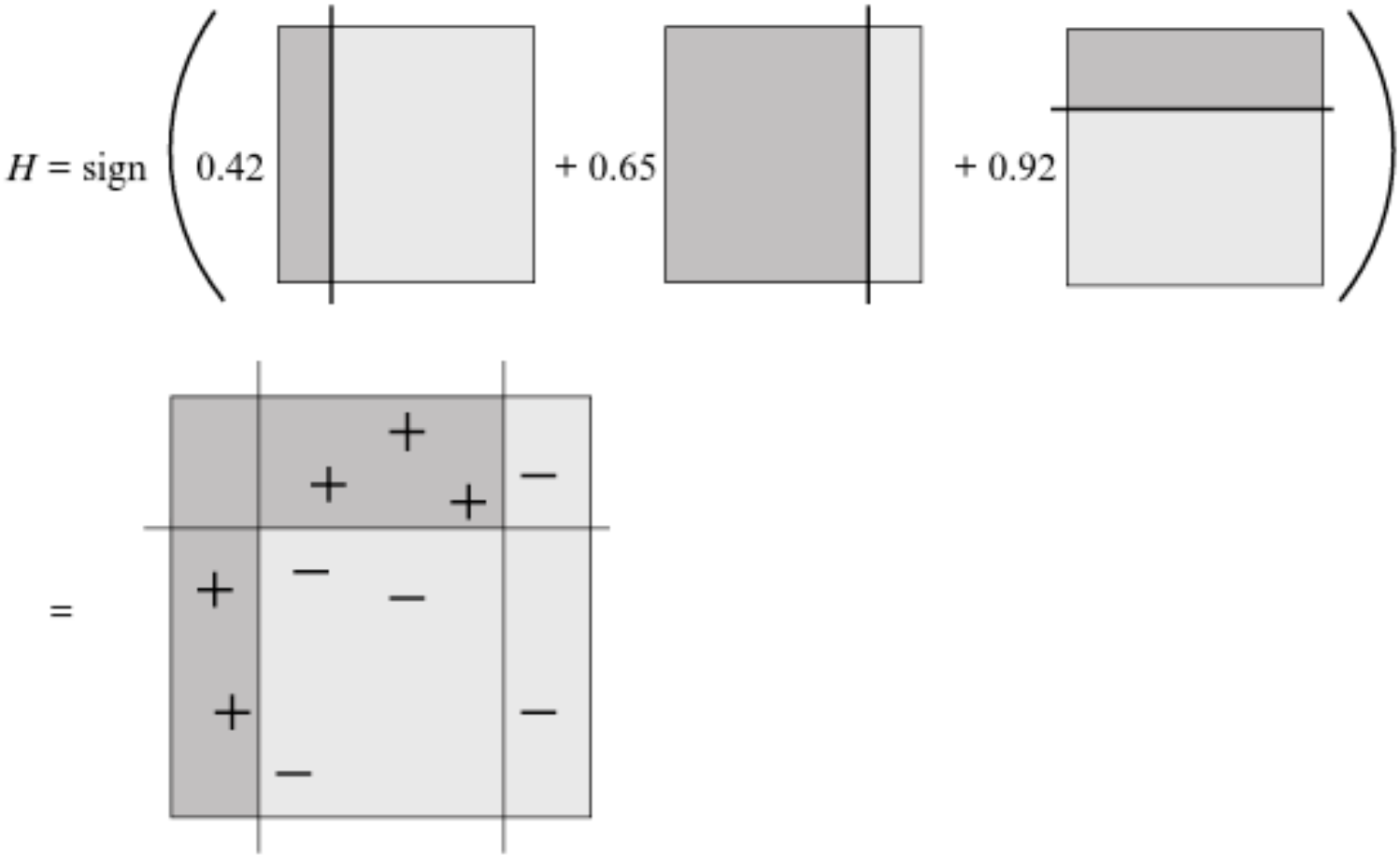
AdaBoost, Visually in More Detail



AdaBoost, Visually in More Detail



AdaBoost, Visually in More Detail



Boosting Implements an Additive Model

- What is AdaBoost doing and how can we generalize it to other classification problems and to regression?

Boosting Implements an Additive Model

- What is AdaBoost doing and how can we generalize it to other classification problems and to regression?
- It turns out that AdaBoost implements Forward Stagewise Additive Modeling (FSAM) using an exponential loss function. Let's take these one at a time.

Forward Stagewise Additive Modeling

1. Initialize $f_0(x) = 0$

Forward Stagewise Additive Modeling

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

Forward Stagewise Additive Modeling

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

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

Forward Stagewise Additive Modeling

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

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

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

Forward Stagewise Additive Modeling

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

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

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

At each iteration, we fit the optimal basis function and corresponding coefficient β_m to add to the current expansion, $f_{m-1}(x)$. We do not update the parameters of previously estimated functions

The Loss Function

- AdaBoost minimizes an exponential loss function. But let's look at the more familiar case of squared-error loss familiar from linear regression

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

The Loss Function

- AdaBoost minimizes an exponential loss function. But let's look at the more familiar case of squared-error loss familiar from linear regression

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

- So the basis function that best fits the residuals from the *last* iteration will minimize the loss and be added to the model.

Selecting a Loss Function

- Will depend on the problem at hand.

Loss Functions for Classification

- In the binary classification situation outlined above, the margin, $yf(x)$, plays a role analogous to the residuals $y - f(x)$ in regression. Positive margins are classified correctly; negative margins are misclassified.
- We want a loss function that penalizes negative margins more heavily than positive ones.

Loss Functions for Classification

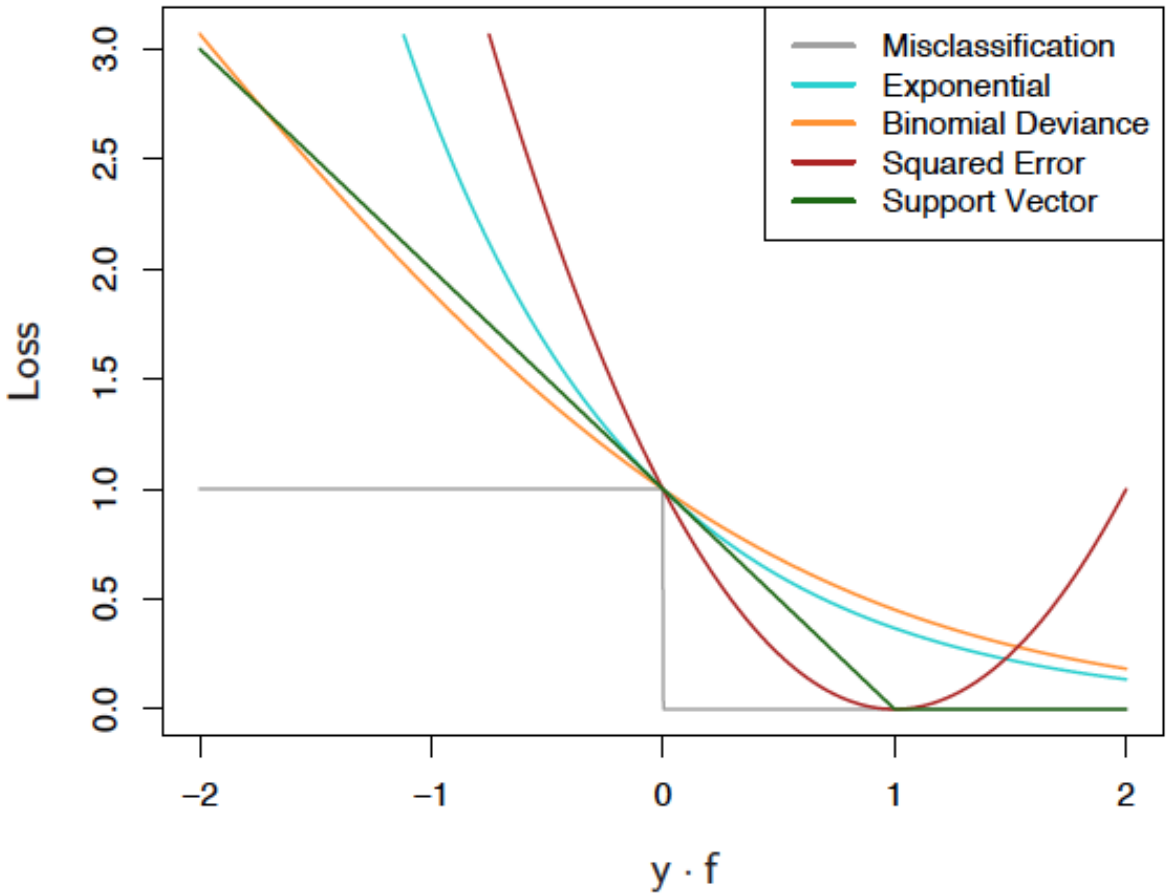


Figure 2: (Hastie et al. 2009:347)

Loss Functions for Regression

- In the regression setting we can look at squared error loss (seen above) or absolute loss, $L(y, f(x)) = |y - f(x)|$
- We can also use the Huber loss criterion used in robust regression to address the strengths of each

Loss Functions for Regression

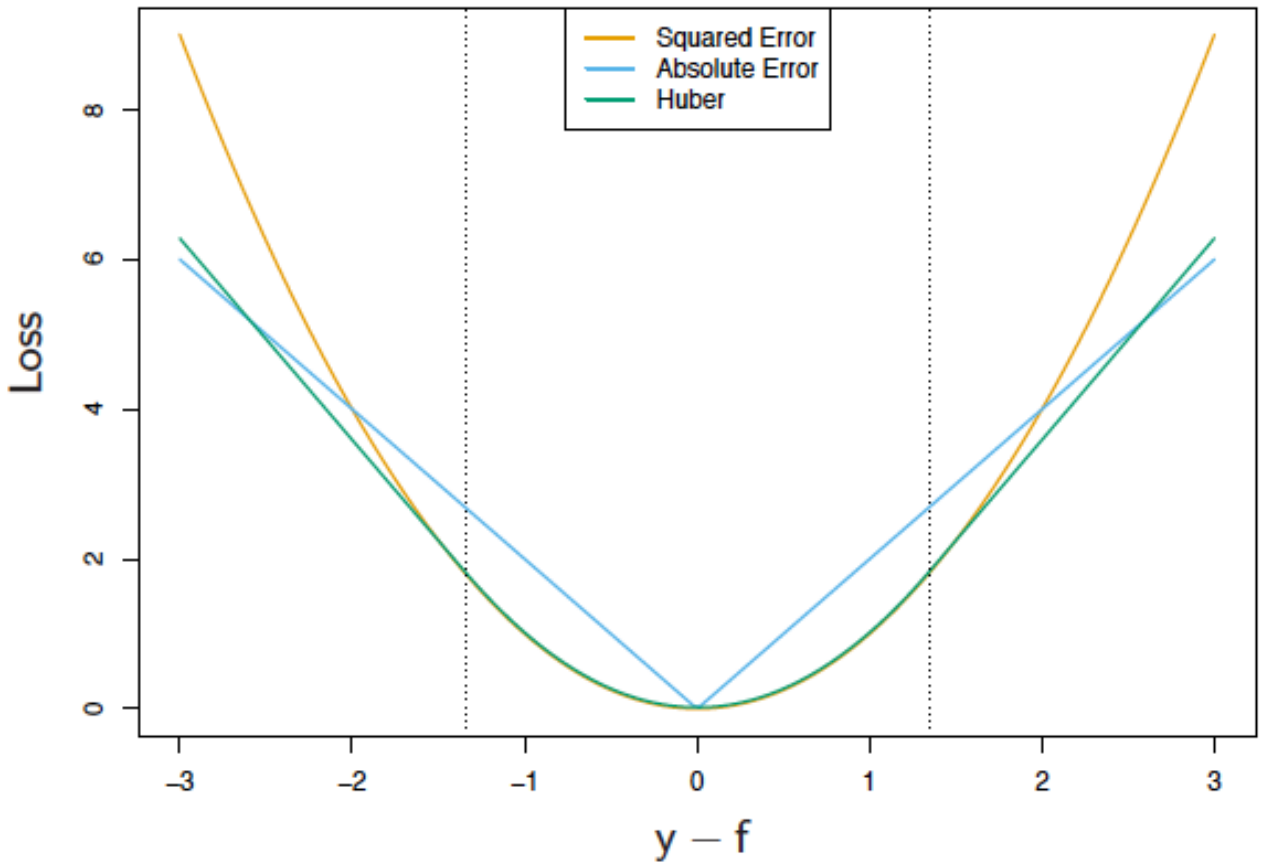


Figure 3: (Hastie et al. 2009:350)

Boosting Trees

Let's boost some trees!

What is a Classification/Regression Tree?

- Trees partition the space of all joint predictor variable values into disjoint regions R_j as represented by the terminal nodes of the tree. A constant γ_j is assigned to each such reagion and the predictive rule is $x \in R_j \Rightarrow f(x) = \gamma_j$

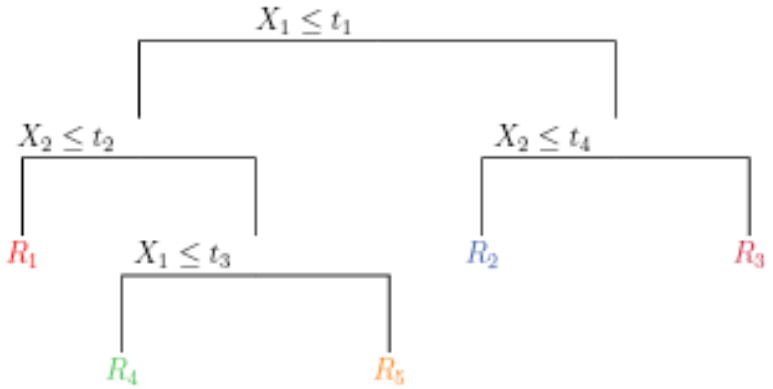
What is a Classification/Regression Tree?

- Trees partition the space of all joint predictor variable values into disjoint regions R_j as represented by the terminal nodes of the tree. A constant γ_j is assigned to each such reagion and the predictive rule is $x \in R_j \Rightarrow f(x) = \gamma_j$
- So a tree can be formally expressed as:

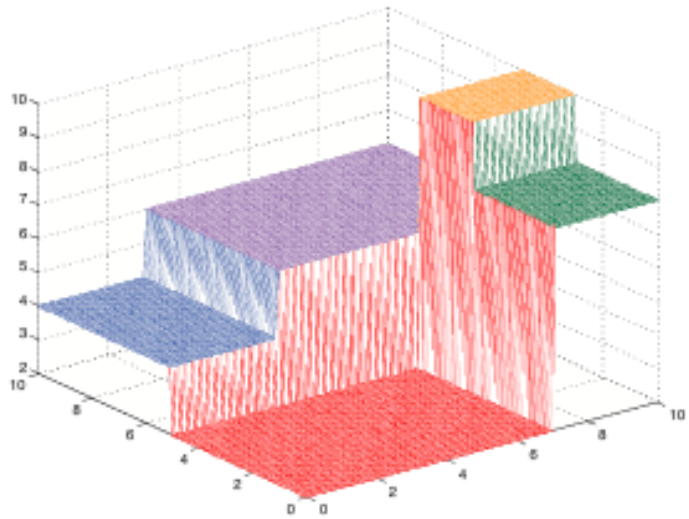
$$T(x; \Theta) = \sum_{j=1}^{J} \gamma_j \mathbf{1}(x \in R_j)$$

with $\Theta = \{R_j, \gamma_j\}_1^J$

What is a Classification/Regression Tree



(a)



(b)

Figure 4: (Murphy 2012:545)

Boosting Trees

- The boosted tree model is a sum of trees

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

Boosting Trees

- The boosted tree model is a sum of trees

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

- We will grow our trees in a FSAM. At each step we must solve:

$$\hat{\Theta}_m = \underset{\Theta_m}{\operatorname{argmin}} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m))$$

Boosting Trees

- The boosted tree model is a sum of trees

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

- We will grow our trees in a FSAM. At each step we must solve:

$$\hat{\Theta}_m = \underset{\Theta_m}{\operatorname{argmin}} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m))$$

- Finding the optimal constants γ_{jm} is easy if we know the regions R_{jm}. But finding the regions is difficult.

Boosting Trees

Two cases where the problem simplifies

1. For **squared-error loss** the solution will be to grow a tree that best predicts the current residuals, and $\hat{\gamma}_{jm}$ is the mean of the residuals in each corresponding region.

But recall that neither exponential nor squared-error loss are robust. Choosing other loss criteria, though, make the solution to the problem more difficult.

Boosting Trees

Two cases where the problem simplifies

1. For **squared-error loss** the solution will be to grow a tree that best predicts the current residuals, and $\hat{\gamma}_{jm}$ is the mean of the residuals in each corresponding region.
2. For **two-class classification with exponential loss** then (under certain conditions) this gives rise to the AdaBoost method for boosting classification trees. In general, the $\hat{\gamma}_j m$ will be the weighted log-odds in each corresponding region.

But recall that neither exponential nor squared-error loss are robust. Choosing other loss criteria, though, make the solution to the problem more difficult.

Gradient Boosting

In order to solve this complex problem (for any differentiable loss function) we will implement a solution known as gradient boosting.

Steepest Descent

The solution we will implement is analogous to the steepest descent numerical optimization procedure.

- At any point in the procedure we evaluate the gradient ($\mathbf{g}_m$) of the function $L(\mathbf{f})$ at the last update:

$$g_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i)=f_{m-1}(x_i)}$$

Steepest Descent

The solution we will implement is analogous to the steepest descent numerical optimization procedure.

- At any point in the procedure we evaluate the gradient ($\mathbf{g}_m$) of the function $L(\mathbf{f})$ at the last update:

$$g_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i)=f_{m-1}(x_i)}$$

- and take a step of length ρ_m, which is the solution to

$$\rho_m = \underset{\rho}{\operatorname{argmin}}\, L(\mathbf{f}_{m-1} - \rho \mathbf{g}_m)$$

Steepest Descent

The solution we will implement is analogous to the steepest descent numerical optimization procedure.

- At any point in the procedure we evaluate the gradient ($\mathbf{g}_m$) of the function $L(\mathbf{f})$ at the last update:

$$g_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i)=f_{m-1}(x_i)}$$

- and take a step of length ρ_m, which is the solution to

$$\rho_m = \underset{\rho}{\operatorname{argmin}}\, L(\mathbf{f}_{m-1} - \rho \mathbf{g}_m)$$

- We then update by subtracting $\rho_m \mathbf{g}_m$ from the previous update.

Gradient Boosting

- Steepest descent chooses the direction in which the function is most rapidly decreasing

Gradient Boosting

- Steepest descent chooses the direction in which the function is most rapidly decreasing
- We would like to do the same thing but here our solution must be a tree. Also importantly, we don't want to simply minimize loss on the training set but generalize to new data.

Gradient Boosting

- Steepest descent chooses the direction in which the function is most rapidly decreasing
- We would like to do the same thing but here our solution must be a tree. Also importantly, we don't want to simply minimize loss on the training set but generalize to new data.
- A potential solution is to induce a tree at the mth iteration whose predictions $\mathbf{t}_m$ are as close as possible to the negative gradient

$$\tilde{\Theta}_m = \underset{\Theta}{\operatorname{argmin}} \sum_{i=1}^{N} (-g_{im} - T(x_i; \Theta))^2$$

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute

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

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute

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

   - Fit a regression tree to the targets r_{im} giving terminal regions $R_{jm}, j = 1, 2, ..., J_m$

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute

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

   - Fit a regression tree to the targets r_{im} giving terminal regions $R_{jm}, j = 1, 2, ..., J_m$
   - For $j = 1, 2, ..., J_m$ compute

$$\gamma_{jm} = \underset{\gamma}{\text{argmin}} \sum_{x_i \in R_{jm}} L(Y - i, f_{m-1}(x_i) + \gamma)$$

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute

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

   - Fit a regression tree to the targets r_{im} giving terminal regions $R_{jm}, j = 1, 2, ..., J_m$
   - For $j = 1, 2, ..., J_m$ compute

$$\gamma_{jm} = \underset{\gamma}{\text{argmin}} \sum_{x_i \in R_{jm}} L(Y - i, f_{m-1}(x_i) + \gamma)$$

   - Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbf{1}(x \in R_{jm})$

Gradient Boosting

1. Initialize $f_0(x) = \underset{\gamma}{\text{argmin}} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to M:
   - For $i = 1, 2, ..., N$ compute

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

   - Fit a regression tree to the targets r_{im} giving terminal regions $R_{jm}, j = 1, 2, ..., J_m$
   - For $j = 1, 2, ..., J_m$ compute

$$\gamma_{jm} = \underset{\gamma}{\text{argmin}} \sum_{x_i \in R_{jm}} L(Y - i, f_{m-1}(x_i) + \gamma)$$

   - Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbf{1}(x \in R_{jm})$
3. Output $\hat{f}(x) = f_M(x)$

Tuning and Metaparameters

There are a number of parameters for the algorithm that we might be concerned about setting

- J_m, the number of terminal nodes in each tree
- M, the number of boosting iterations
- ν, a shrinkage parameter
- η, fraction of training observations to select at each iteration (stochastic gradient boosting)

Tree Size, J

- Set $J_m = J \, \forall m$
- Selection of J will affect the number of interactions you allow in your model as the interaction order for any tree is given by $J - 1$.
- HT&F recommend $J \simeq 6$

Regularization: Number of Iterations, M

- In setting the number of iterations we want to run enough to maximally reduce error on the test sample but not so much that we overfit to the training sample.
- This implies some optimal $M = M^*$ that HT&F recommend finding using an early stopping strategy.

Regularization: Shrinkage, ν

- The simplest implementation of shrinkage is to scale the contributions of each tree by a factor $0 < \nu < 1$
- Because smaller values of ν imply a slower learning, there is a tradeoff between M and ν
- HT&F suggest that the best results are found with $\nu < 0.1$

Regularization: Shrinkage, ν

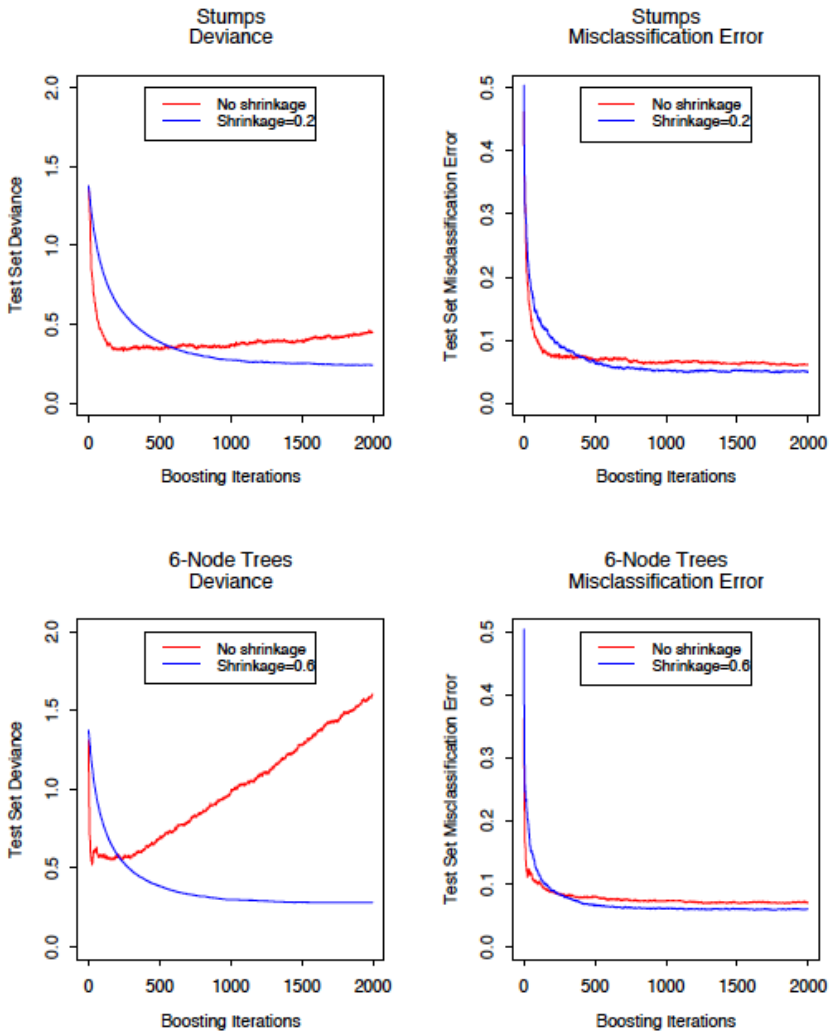


Figure 5: Hastie et al. 2009:366

Regularization: Subsampling, η

- Boootstrap averaging (bagging) can improve the performance of a noisy classifier. We can apply a similar logic here.
- At each iteration we sample without replacement some fraction η of the training observations. A typical value is $\eta = 0.5$. This reduces computational effort while also (often) improving accuracy.

Regularization: Subsampling, η

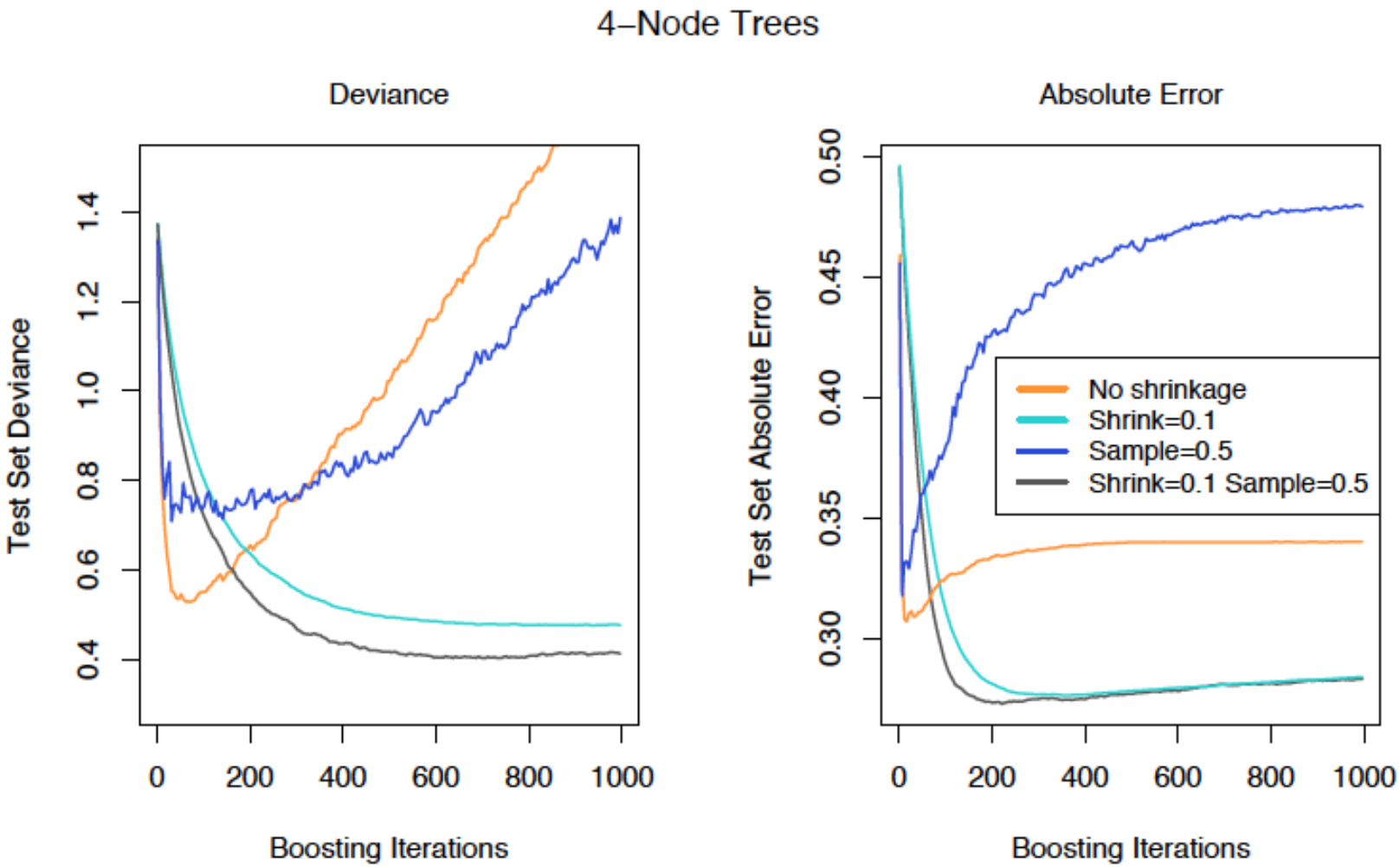


Figure 6: Hastie et al. 2009:367

xgboost package

- xgboost implements gradient boosting in R
- command xgboost allows you to control the depth of trees, regularization, subsampling, and the number of rounds of boosting
- also creates visualizations of variable importance plots