Chapter 10: Boosting and Additive Trees

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Boosting Methods

Overview of boosting

- Boosting is a procedure to combine the output of many **weak** classifiers to produce a powerful **committee**.
- A weak classifier is one whose error rate is only slightly better than random guessing.
- Boosting produces a sequence of weak classifiers $G_m(x)$ for $m = 1, \ldots, M$ whose predictions are then combined

  $$G(x) = \mathrm{sgn}\left(\sum_{m=1}^{M} \alpha_m \, G_m(x)\right)$$

  through a weighted majority to produce the final prediction.
- Each $\alpha_m > 0$ is computed by the boosting algorithm and reflects how accurately G_m classified the data.

Most popular boosting algorithm: AdaBoost.M1

"**AdaBoost.M1**" algorithm of *Freund and Schapire* (1997)

- Have training data $(x_i, y_i), i = 1, 2, \ldots, n$
- Introduce a weight $w_i = 1/n$ for each training example.
- for $m = 1, \ldots, M$
  - ⋆ Let G_m be the weak classifier with minimum error:

    $$\text{err}_m = \sum_{i=1}^{n} w_i \, \text{Ind}(y_i \neq G_m(x_i))$$

  - ⋆ Set $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
  - ⋆ Set

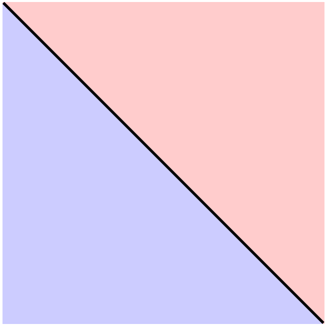
    $$w_i \leftarrow w_i \, e^{\alpha_m \text{Ind}(y_i \neq G_m(x_i))} \quad \text{for } i = 1, \ldots, n$$

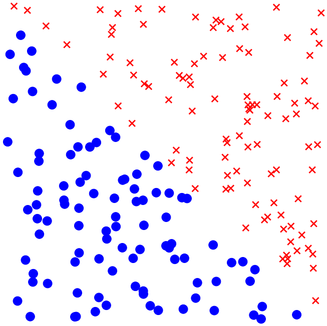
    This increases (decreases) w_i for x_i misclassified (correctly classified) by G_M
  - ⋆ Normalize the w_i's so that they sum to one.

What AdaBoost.M1 does

- As iterations proceed, observations difficult to classify correctly receive more influence.
- Each successive classifier is forced to concentrate on training observations missed by previous ones in the sequence

Binary classification example

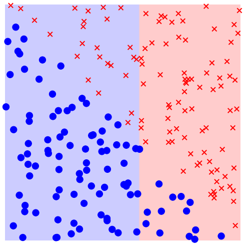

True decision boundary


Training data

$\mathcal{H}$ is the set of all possible oriented vertical and horizontal lines.

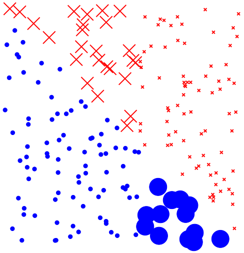
Example

Round 1



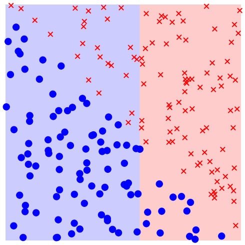
Chosen weak classifier

$\epsilon_1 = 0.19$, $\alpha_1 = 1.45$



Re-weight training points

$w_i^{(2)}$**'s**

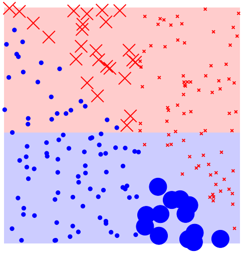


Current strong classifier

$G(\mathbf{x})$

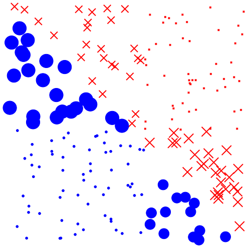
Example

Round 2



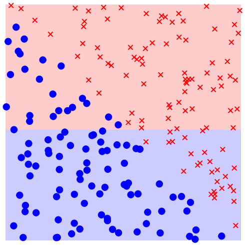
Chosen weak classifier

$\epsilon_2 = 0.1512$, $\alpha_2 = 1.725$



Re-weight training points

$w_i^{(3)}$**'s**

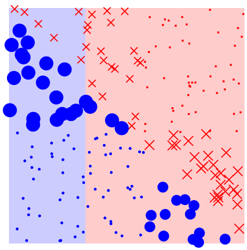


Current strong classifier

$G(\mathbf{x})$

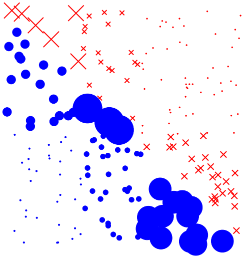
Example

Round 3



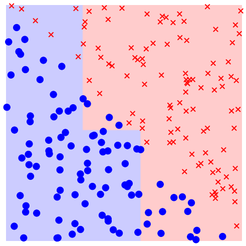
Chosen weak classifier

$\epsilon_3 = 0.2324$, $\alpha_3 = 1.1946$



Re-weight training points

$w_i^{(4)}$**'s**

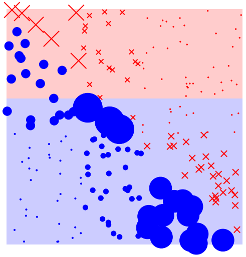


Current strong classifier

$G(\mathbf{x})$

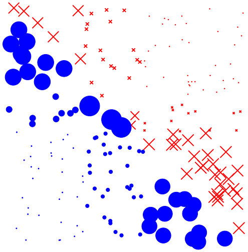
Example

Round 4



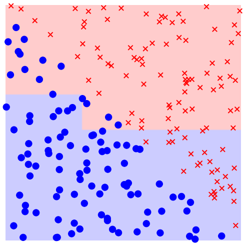
Chosen weak classifier

$\epsilon_4 = 0.2714$, $\alpha_4 = 0.9874$



Re-weight training points

$w_i^{(5)}$**'s**

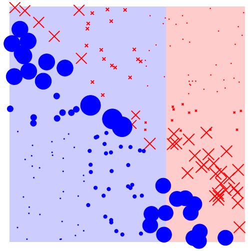


Current strong classifier

$G(\mathbf{x})$

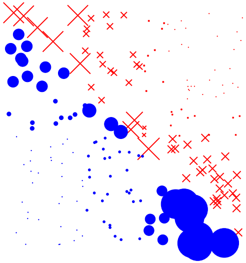
Example

Round 5



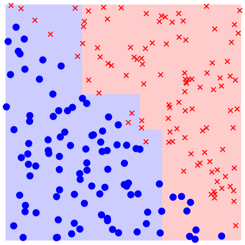
Chosen weak classifier

$\epsilon_5 = 0.2616$, $\alpha_5 = 1.0375$



Re-weight training points

$w_i^{(6)}$**'s**

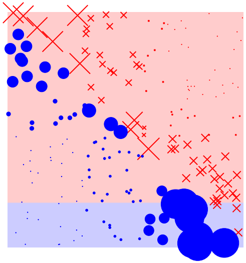


Current strong classifier

$G(\mathbf{x})$

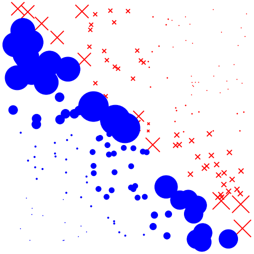
Example

Round 6



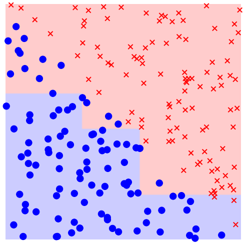
Chosen weak classifier

$\epsilon_6 = 0.2262$, $\alpha_6 = 1.2298$



Re-weight training points

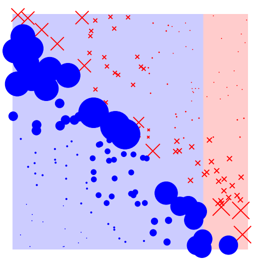
$w_i^{(7)}$**'s**



Current strong classifier

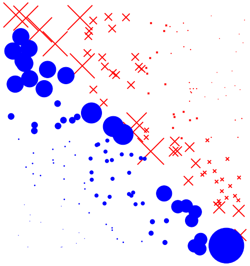
$G(\mathbf{x})$

Round 7



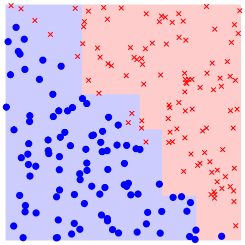
Chosen weak classifier

$\epsilon_7 = 0.2680$, $\alpha_7 = 1.0049$



Re-weight training points

$w_i^{(8)}$**'s**

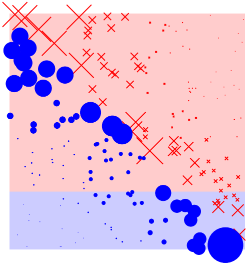


Current strong classifier

$G(\mathbf{x})$

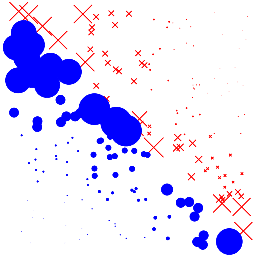
Example

Round 8



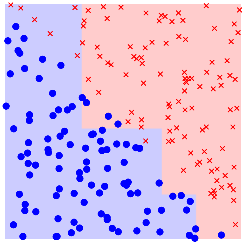
Chosen weak classifier

$\epsilon_8 = 0.3282$, $\alpha_8 = 0.7165$



Re-weight training points

$w_i^{(9)}$**'s**

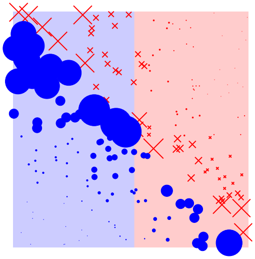


Current strong classifier

$G(\mathbf{x})$

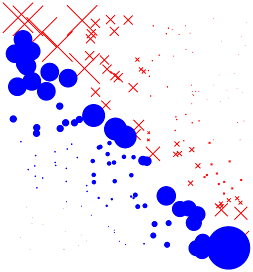
Example

Round 9



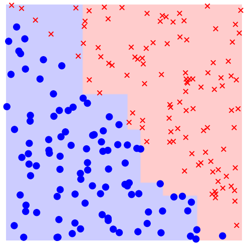
Chosen weak classifier

$\epsilon_9 = 0.3048$, $\alpha_9 = 0.8246$



Re-weight training points

$w_i^{(10)}$**'s**

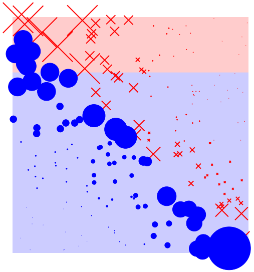


Current strong classifier

$G(\mathbf{x})$

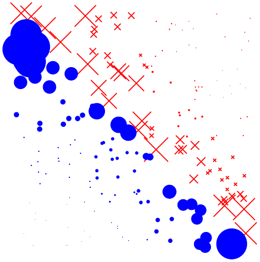
Example

Round 10



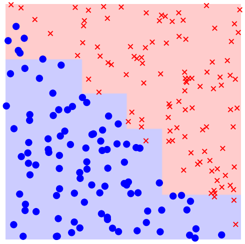
Chosen weak classifier

$\epsilon_{10} = 0.2943$, $\alpha_{10} = 0.8744$



Re-weight training points

$w_i^{(11)}$**'s**

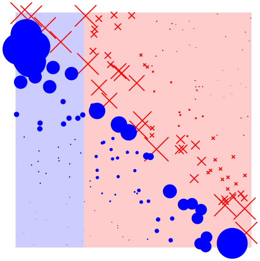


Current strong classifier

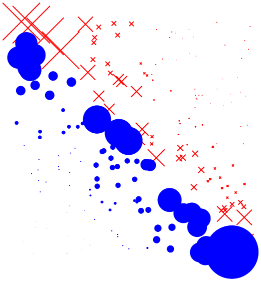
$G(\mathbf{x})$

Example

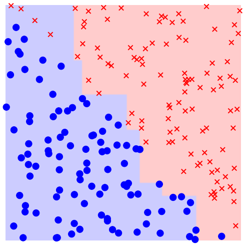
Round 11


Chosen weak classifier

$\epsilon_{11} = 0.2876$, $\alpha_{11} = 0.9071$


Re-weight training points

$w_i^{(12)}$**'s**

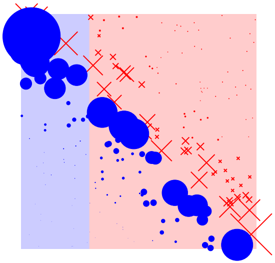

Current strong classifier

$G(\mathbf{x})$

Example

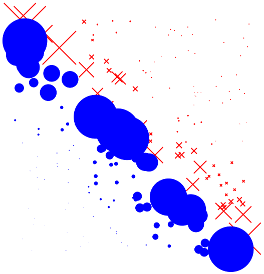
Example

Round 21



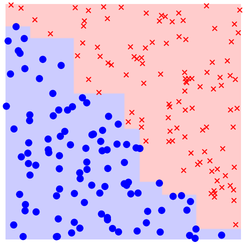
Chosen weak classifier

$\epsilon_{21} = 0.3491$, $\alpha_{21} = 0.6232$



Re-weight training points

$w_i^{(22)}$**'s**



Current strong classifier

$G(\mathbf{x})$

AdaBoost performance

AdaBoost can dramatically increases the performance of very weak classifier.

In this chapter authors

- Show AdaBoost fits an additive model in a base learner, optimizing a novel exponential loss function
- Show the population minimizer of the exponential loss function is the log-odds of the class probabilities
- Present loss functions that are more robust than squared error or exponential loss
- Argue decision trees are an ideal base learner for data mining applications of boosting.
- Develop class of gradient boosted models (GBMs), for boosting trees with any loss function.
- Emphasize the importance of "*slow learning*".

Boosting Fits an Additive Model

Additive Models

- Boosting fits an additive expansion in a set of elementary *basis functions*.

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

- The basis functions are the weak classifiers $G_m(x) \in \{-1, 1\}$.

- More generally, basis function expansions take the form

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

where β_m's are the expansion coefficients and $b(x; \gamma) \in \mathbb{R}$ are simple functions of the input x parameterized by γ.

Examples of additive models

- **Single-hidden-layer neural networks** where

$$b(x;\gamma) = \frac{1}{1 + \exp(-\gamma_0 - \gamma_1^t x)}$$

- **Multivariate adaptive regression splines (MARS)**
  Use truncated-power spline basis functions where γ parameterizes the variables and values for the knots.

- **Trees**
  γ parameterizes the split variables and split points at the internal nodes, and the predictions at the terminal nodes.

Fitting these additive models

- Typically fit model by minimizing a loss function averaged over the training data:

$$\min_{\beta_1,\gamma_1,\ldots,\beta_M,\gamma_M} \sum_{i=1}^{n} L\left(y_i, \sum_{m=1}^{M} \beta_m \, b(x_i;\gamma_m)\right)$$

- For many loss functions $L(x, f(x))$ and/or basis functions $b(x;\gamma)$ this is too hard....

Forward Stagewise Additive Modeling

Approximate the global solution to fitting additive model

- More simply can greedily add one basis function at a time in the following fashion.
- Set $f_0(x) = 0$
- for $m = 1, \ldots, M$
  - ⋆ Compute

$$(\hat{\beta}_m, \hat{\gamma}_m) = \arg\min_{\beta_m, \gamma_m} \sum_{i=1}^{n} L\left(y_i, \sum_{m=1}^{M} f_{m-1}(x_i) + \beta_m\, b(x_i; \gamma_m)\right)$$

  - ⋆ Set

$$f_m(x) = f_{m-1}(x) + \hat{\beta}_m\, b(x; \hat{\gamma}_m)$$

  - ⋆ **Note**: Previously added terms are not modified.

Exponential Loss and AdaBoost

Interpretation of the Adaboost algorithm

- **Interpretation of AdaBoost.M1**

AdaBoost.M1 $\equiv$ **forward stagewise additive modelling** with an **exponential loss function**.

- Definition of exponential loss

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

- Will now go through the derivation of this result....

Interpretation of the Adaboost algorithm

- **Interpretation of AdaBoost.M1**

AdaBoost.M1 $\equiv$ **forward stagewise additive modelling** with an **exponential loss function**.

- Definition of exponential loss

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

- Will now go through the derivation of this result....

Specifics of forward stagewise additive modelling (fsam)

- At each iteration of **forward stagewise additive modelling** must solve this optimization problem

$$\begin{aligned}(\beta_m, G_m) &= \arg\min_{\beta, G} \sum_{i=1}^{n} L(y_i, f_{m-1}(x_i) + \beta G(x_i)) \\ &= \arg\min_{\beta, G} \sum_{i=1}^{n} \exp\{-y_i\,(f_{m-1}(x_i) + \beta\, G(x_i))\}\end{aligned}$$

  where we assume an exponential loss and $G(x) \in \{-1, 1\}$.

- Can re-write

$$\begin{aligned}\sum_{i=1}^{n} \exp\{-y_i\,(f_{m-1}(x_i) + \beta\, G(x_i))\} &= \sum_{i=1}^{n} \exp\{-y_i\, f_{m-1}(x_i)\} \exp\{-y_i \beta\, G(x_i)\} \\ &= \sum_{i=1}^{n} w_i^{(m)} \exp\{-y_i \beta\, G(x_i)\,\}\end{aligned}$$

Optimization of the fsam cost function

- The optimization problem becomes

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

- Note

$$y_i\, G(x_i) = \begin{cases} 1 & \text{if } y_i = G(x_i) \\ -1 & \text{if } y_i \neq G(x_i) \end{cases}$$

and this implies $\exp\{-y_i \beta\, G(x_i)\}$ is equal to

$$e^{\beta}\, \mathsf{Ind}(y_i \neq G(x_i)) + e^{-\beta}\ (1 - \mathsf{Ind}(y_i \neq G(x_i)))$$

- The above implies $\sum_{i=1}^{n} w_i^{(m)} \exp\{-y_i \beta\, G(x_i)\}$ can be written as:

$$(e^{\beta} - e^{-\beta}) \sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) + e^{-\beta} \sum_{i=1}^{n} w_i^{(m)}$$

Optimization of the fsam cost function: G_m?

- The optimization problem becomes

$$\begin{aligned}
&\arg\min_G \sum_{i=1}^{n} w_i^{(m)} \exp\{-y_i \beta\, G(x_i)\} \\
&= \arg\min_G \left((e^{\beta} - e^{-\beta}) \sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) + e^{-\beta} \sum_{i=1}^{n} w_i^{(m)} \right) \\
&= \arg\min_G \left(\sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) \right)
\end{aligned}$$

- Therefore

$$G_m = \arg\min_G \left(\sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) \right)$$

G_m **minimizes the weighted error in the AdaBoost algorithm.** (if the $w_i^{(m)}$'s have the same definition....)

Optimization of the fsam cost function: G_m?

- The optimization problem becomes

$$\begin{aligned}
&\arg\min_G \sum_{i=1}^n w_i^{(m)} \exp\{-y_i \beta\, G(x_i)\} \\
&= \arg\min_G \left((e^\beta - e^{-\beta}) \sum_{i=1}^n w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) + e^{-\beta} \sum_{i=1}^n w_i^{(m)} \right) \\
&= \arg\min_G \left(\sum_{i=1}^n w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) \right)
\end{aligned}$$

- Therefore

$$G_m = \arg\min_G \left(\sum_{i=1}^n w_i^{(m)} \mathsf{Ind}(y_i \neq G(x_i)) \right)$$

G_m **minimizes the weighted error in the AdaBoost algorithm.** (if the $w_i^{(m)}$'s have the same definition....)

Optimization of the fsam cost function: β_m?

- Plugging G_m into the original optimization problem

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

and using the previous result, it becomes

$$\arg\min_{\beta} \left((e^{\beta} - e^{-\beta}) \sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G_m(x_i)) + e^{-\beta} \sum_{i=1}^{n} w_i^{(m)} \right)$$

- This quantity is minimized when

$$\beta_m = \frac{1}{2} \log \frac{1 - \mathsf{err}_m}{\mathsf{err}_m}$$

where

$$\mathsf{err}_m = \frac{\sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G_m(x_i))}{\sum_{i=1}^{n} w_i^{(m)}}$$

- **Expression for β_m same (upto a multiplicative constant) as for α_m in AdaBoost.M1** (if the $w_i^{(m)}$'s have same definition....)

Optimization of the fsam cost function: β_m?

- Plugging G_m into the original optimization problem

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

  and using the previous result, it becomes

$$\arg\min_{\beta} \left((e^{\beta} - e^{-\beta}) \sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G_m(x_i)) + e^{-\beta} \sum_{i=1}^{n} w_i^{(m)} \right)$$

- This quantity is minimized when

$$\beta_m = \frac{1}{2} \log \frac{1 - \mathsf{err}_m}{\mathsf{err}_m}$$

  where

$$\mathsf{err}_m = \frac{\sum_{i=1}^{n} w_i^{(m)} \mathsf{Ind}(y_i \neq G_m(x_i))}{\sum_{i=1}^{n} w_i^{(m)}}$$

- **Expression for β_m same (upto a multiplicative constant) as for α_m in AdaBoost.M1** (if the $w_i^{(m)}$'s have same definition....)

Optimization of the fsam cost function: $w_i^{(m)}$?

Update of the weights: Expression for $w_i^{(m+1)}$

- Need the following result

$$\begin{aligned} -y_i\, G_m(x_i) &= -\text{Ind}(y_i = G(x_i)) + \text{Ind}(y_i \neq G(x_i)) \\ &= -(1 - \text{Ind}(y_i \neq G(x_i))) + \text{Ind}(y_i \neq G(x_i)) \\ &= -1 + 2\,\text{Ind}(y_i \neq G(x_i)) \end{aligned}$$

- The updated weights can then be written as

$$\begin{aligned} w_i^{(m+1)} = e^{-y_i f_m(x_i)} &= e^{-y_i (f_{m-1}(x) + \beta_m\, G_m(x))} \\ &= w_i^{(m)}\, e^{-y_i \beta_m G_m(x))} \\ &= w_i^{(m)}\, e^{2\beta_m\, \text{Ind}(y_i \neq G_m(x))}\, e^{-\beta_m} \end{aligned}$$

- As factor $e^{-\beta_m}$ is the same for all weights it has no effect.

- **Expression for weight update for each example is the same as for AdaBoost.M1 as $\alpha_m = 2\beta_m$.**

Optimization of the fsam cost function: $w_i^{(m)}$?

Update of the weights: Expression for $w_i^{(m+1)}$

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- **Expression for weight update for each example is the same as for AdaBoost.M1 as $\alpha_m = 2\beta_m$.**

Adaboost minimizes the exponential loss

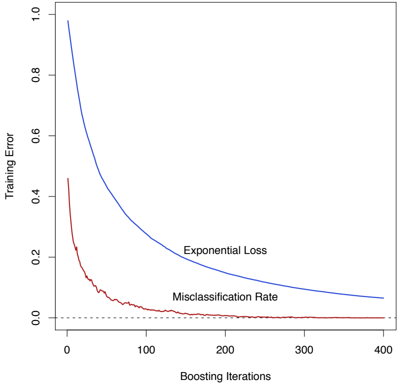
- Hence can view **AdaBoost.M1** as a method that approximates minimizing

$$\arg \min_{\beta_1, G_1, \ldots \beta_M, G_M} \sum_{i=1}^{n} \exp(\, -y_i \sum_{m=1}^{M} \beta_m G_m(x_i) \,)$$

  via a **forward-stagewise additive modeling approach**.

Adaboost minimizes the exponential loss

For a simulated problem the training-set mis-classification error and average exponential loss:



While the mis-classification error decreases to zero ≈ 250 iterations, the exponential loss keeps decreasing.

Loss Functions and Robustness

Loss functions for classification

- **Exponential Loss**

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

- **Binomial deviance loss**

$$L(y, f(x)) = -\log\left(1 + \exp\{-2yf(x)\}\right)$$

where

$$p(x) = P(Y = 1 \mid x) = \frac{1}{1 + \exp\{-2f(x)\}}$$

- **Misclassification loss**

$$L(y, f(x)) = \mathsf{Ind}(y\, f(x) < 0)$$

The margin

- These loss functions are functions of the "*margin*": $y\,f(x)$
- Classification rule

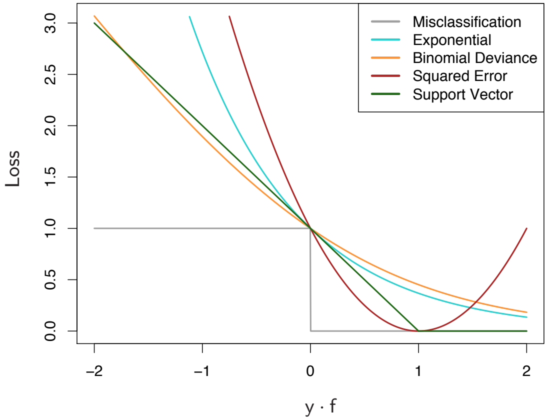
$$G(x) = \text{sign}\{f(x)\}$$

$\Longrightarrow$ training examples with

- positive margin $y_i\,f(x_i) > 0$ are correctly classified and
- negative margin $y_i\,f(x_i) < 0$ are misclassified

- Decision boundary defined by $f(x) = 0$
- Classification algorithms attempt to produce positive margins for each training data point.
- Loss criterion for classification should penalize negative margins more heavily than positive margins.

Loss functions for classification



Loss functions for classification

- *Exponential* and *deviance* loss continuous approx. to *mis-classification* loss.
- They increasingly penalize negative margin values more heavily than they reward positive ones.
- Binomial deviance penalty increases linearly with negative margin.
- Exponential loss penalty increases exponentially with negative margin.
- $\Longrightarrow$ in training the exponential criterion concentrates more of its efforts on large negative margin examples than the binomial criterion.
- Thus binomial criterion is far more robust than the exponential criterion in noisy settings - mislabels, overlapping classes.

Robust loss functions for regression

- **Squared error loss**

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

  Population optimum for this loss function: $f(x) = E[Y \mid x]$

- **Absolute loss**

$$L(y, f(x)) = |y - f(x)|$$

  Population optimum for this loss function: $f(x) = \text{median}(Y \mid x)$

- On finite samples **squared error loss** puts far more emphasis on observations with large $|y_i - f(x_i)|$ than **absolute loss**.

- Thus **squared error loss** is less robust and performance degrades for long-tailed error distributions and mis-labellings.

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- Thus **squared error loss** is less robust and performance degrades for long-tailed error distributions and mis-labellings.

Robust loss functions for regression

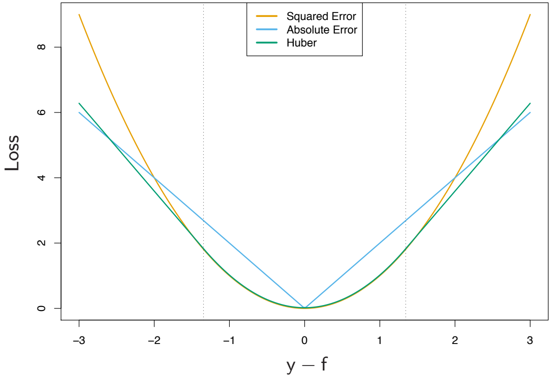
- **Huber loss**

$$L(y, f(x)) = \begin{cases} (y - f(x))^2 & \text{for } |y - f(x)| \leq \delta \\ 2\delta|y - f(x)| - \delta^2 & \text{otherwise} \end{cases}$$

  - strong resistance to gross outliers while
  - being nearly as efficient as least squares for Gaussian errors

- Combines the good properties of squared-error loss near zero and absolute error loss when $|y - f|$ is large.

Robust loss functions for regression



Have a problem

- When robustness is an issue
  - **squared-error loss** for regression and
  - **exponential loss** for classification

  are **not** the best criterion to be optimizing.
- But, both these loss functions lead to elegant modular boosting algorithms in the context of *forward stagewise additive modelling*.
- For classification: perform a weighted fit of the base learner to the outputs y_i with weights $w_i = \exp\{-y_i f(x_i)\}$
- More robust criteria in their place do not give rise to such simple feasible boosting algorithms
- Later derive simple boosting algorithms based on any differentiable loss criterion.

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“Off-the-Shelf” Procedures for Data Mining

TABLE 10.1. *Some characteristics of different learning methods. Key:* ▲ *= good,* ◆ *=fair, and* ▼ *=poor.*

Characteristic	Neural Nets	SVM	Trees	MARS	k-NN, Kernels
Natural handling of data of "mixed" type	▼	▼	▲	▲	▼
Handling of missing values	▼	▼	▲	▲	▲
Robustness to outliers in input space	▼	▼	▲	▼	▲
Insensitive to monotone transformations of inputs	▼	▼	▲	▼	▼
Computational scalability (large N)	▼	▼	▲	▲	▼
Ability to deal with irrelevant inputs	▼	▼	▲	▲	▼
Ability to extract linear combinations of features	▲	▲	▼	▼	◆
Interpretability	▼	▼	◆	▲	▼
Predictive power	▲	▲	▼	◆	▲

Book's conclusion

- Trees are great except....
  - they are inaccurate at making predictions.
- Boosting decision trees improve their accuracy but at the cost of
  - speed
  - interpretability and
  - for AdaBoost, robustness against overlapping class distributions and especially mislabeling of the training data.
- A gradient boosted model (GBM) is a generalization of tree boosting that attempts to mitigate these problems.
- It aims to produce an accurate and effective off-the-shelf procedure for data mining.

Boosting Trees

Regression Tree Recap

- Tree partitions the input space into $\mathcal{R}_j, j = 1, \ldots, J$.
- Terminal/leaf nodes of tree represent the regions $\mathcal{R}_j$
- Constant γ_j assigned to each leaf.
- The predictive rule is

$$x \in \mathcal{R}_j \implies f(x) = \gamma_j$$

- A tree with parameters $\Theta = \{\mathcal{R}_j, \gamma_j\}_{j=1}^J$ is expressed as

$$\boxed{T(x; \Theta) = \sum_{j=1}^{J} \gamma_j \, \mathsf{Ind}(x \in \mathcal{R}_j)}$$

(J is usually treated as a meta-parameter)

Learning a Regression Tree

- Ideally parameters found by minimizing the empirical risk

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

- Very hard optimization problem, instead settle for approximate suboptimal solutions

- Typical approach: Divide optimization into two parts

  - **Find γ_j given $\mathcal{R}_j$**

    Typically trivial - $\hat{\gamma}_j$ the mean of the training y's falling in $\mathcal{R}_j$.

  - **Find $\mathcal{R}_j$**

    Difficult part! Approximate solutions found. One strategy is to use a greedy, top-down recursive partitioning algorithm.

The boosted tree model

- A boosted tree is a sum of regression/classification trees

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

learned in a forward stagewise manner.

- At each step solve

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

for the parameters $\Theta_m = \{\mathcal{R}_{jm}, \gamma_{jm}\}_{j=1}^{J_m}$ of the next tree.

- How do we solve this optimization problem?

Learning a boosted tree model

- **Find γ_{jm} given $\mathcal{R}_{jm}$** - easy

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

- **Find $\mathcal{R}_{jm}$'s** - not so easy....

A few exceptions

- **Squared-error loss**

  At each stage fit a regression tree to residuals $y_i - f_{m-1}(x_i)$

- **Two-class classification and exponential loss**

  Gives rise to an AdaBoost method for boosting classification trees...

Adaboost for boosting classification trees

- If the trees are restricted to type where

$$\beta_m T(x_i; \Theta_m) \quad \text{and each} \quad \gamma_{jm} \in \{-1, 1\}$$

- The solution to

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

  is the tree that minimizes the

$$\sum_{i=1}^{N} w_i^{(m)} \, \mathsf{Ind}(y_i \neq T(x_i; \Theta_m))$$

  with weights

$$w_i^{(m)} = \exp\{-y_i \, f_{m-1}(x_i)\}$$

- Straightforward to implement a greedy recursive-partitioning algorithm with this loss as a splitting criterion.

Adaboost for boosting classification trees

- If the there is no restriction on the type of tree then the solution to

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

is the tree that minimizes the

$$\sum_{i=1}^{N} w_i^{(m)} \exp\{-y_i T(x_i; \Theta_m)\}$$

with weights

$$w_i^{(m)} = \exp\{-y_i \, f_{m-1}(x_i)\}$$

Numerical Optimization via Gradient Boosting

Numerical Optimization

- If the loss, $L(\cdot, \cdot)$, is differentiable, can

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

  be approximately solved with numerical optimization.

- Consider this...

- The loss associated with using any $f(x)$ to predict y is

$$L(f) = \sum_{i=1}^{N} L(y_i, f(x_i))$$

- Goal: Find f which minimizes $L(f)$.

- Re-interpret this optimization problem as find

$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

  where $\mathbf{f} = \{f(x_1), \ldots, f(x_N)\}$.

Numerical Optimization

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$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

where $\mathbf{f} = \{f(x_1), \ldots, f(x_N)\}$.

Numerical Optimization

- Numerical optimization approximates

$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

as a sum of vectors

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

where $\mathbf{f}_0 = \mathbf{h}_0$ is an initial guess and each $\mathbf{f}_m$ is estimated from $\mathbf{f}_{m-1}$.

Steepest Descent

- Steepest descent chooses

$$\mathbf{h}_m = -\rho_m \, \mathbf{g}_m$$

  where

  - ρ_m is a scalar and
  - $\mathbf{g}_m \in \mathbb{R}^N$ is the gradient of $L(\mathbf{f})$ evaluated at $\mathbf{f} = \mathbf{f}_{m-1}$.

- Components of $\mathbf{g}_m$ are

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

- Step length is the solution to

$$\rho_m = \arg\min_{\rho} L(\mathbf{f}_{m-1} - \rho \, \mathbf{g}_m)$$

- Solution is updated: $\mathbf{f}_m = \mathbf{f}_{m-1} - \rho_m \, \mathbf{g}_m$

Forward stagewise Tree Boosting & Gradient Boosting

- Forward stagewise boosting is also a very greedy strategy:

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

- Tree predictions $T(x_i; \Theta_m)$ are analogous to the negative gradients $-g_{1m}, \ldots, -g_{Nm}$.

- But $\mathbf{t}_m = \{T(x_1; \Theta_m), \ldots, T(x_N; \Theta_m)\}$ are constrained to be predictions of a J_m-terminal node decision tree

- Whereas $-\mathbf{g}_m$ is the unconstrained maximal descent direction.

- Also analogous

$\rho_m = \arg\min_{\rho} L(\mathbf{f}_{m-1} - \rho\, \mathbf{g}_m)$ to $\hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in \mathcal{R}_{jm}} L(y_i, f_{m-1}(x_i) + \gamma_{jm})$

but perform a *line search* for each terminal node.

Forward stagewise Tree Boosting & Gradient Boosting

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

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$$\rho_m = \arg\min_{\rho} L(\mathbf{f}_{m-1} - \rho\,\mathbf{g}_m) \quad \text{to} \quad \hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in \mathcal{R}_{jm}} L(y_i, f_{m-1}(x_i) + \gamma_{jm})$$

but perform a *line search* for each terminal node.

Forward stagewise Tree Boosting & Gradient Boosting

- If only goal is minimizing

$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f})$$

  then perform steepest descent.

- However, the ultimate goal is to generalize $f_M(x)$ to new unseen data.

- A possible solution is as follows....

Gradient Tree Boosting

- Fit a tree $T(x;\Theta_m)$ at mth iteration whose predictions $\mathbf{t}_m$ are as close as possible to the negative gradient

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

- From the solution regions $\tilde{\mathcal{R}}_{jm}$ set

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

- The regions $\tilde{\mathcal{R}}_{jm}$ will not be identical to the regions $\mathcal{R}_{jm}$ that solve the original problem, but they are similar enough.

Gradients for 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	$\lvert y_i - f(x_i)\rvert$	$\text{sign}\{y_i - f(x_i)\}$
Regression	Huber	$\begin{cases} y_i - f(x_i) & \text{if } \lvert y_i - f(x_i)\rvert \leq \delta_m \\ \delta_m \, \text{sign}\{y_i - f(x_i)\} & \text{if } \lvert y_i - f(x_i)\rvert > \delta_m \end{cases}$
Classification	Deviance	kth component: $\text{Ind}(y_i = G_k) - p_k(x_i)$

where the K-class deviance loss function is

$$L(y,p(x)) = -\sum_{k=1}^{K} \text{Ind}(y=G_k)\ \log p_k(x) = -\sum_{k=1}^{K} \text{Ind}(y=G_k) + \log\left(\sum_{l=1}^{K} \exp\{f_l(x)\}\right)$$

if $p_k(x) = \exp\{f_k(x)\} / \sum_{l=1}^{K} \exp\{f_l(x)\}$

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 $\hat{f}(x) = f_M(x)$.
```

Right-Sized Trees for Boosting

Size of trees in a boosted tree

- Learning a large pruned tree at each round performs poorly.
- Better if
  - Restrict all trees to be same size $J_m = J \; \forall m$
  - Perform cross-validation to choose an optimal J
- Interaction level of tree-based approximations is limited by J:
  - if $J = 2$ then $f_M(x)$ can only be of the form

$$\sum_k \eta_k(X_k)$$

  - if $J = 3$ then $f_M(x)$ can be of the form

$$\sum_k \eta_k(X_k) + \sum_{jk} \eta_{jk}(X_j, X_k)$$

  - if $J = 4$ then $f_M(x)$ can be of the form

$$\sum_k \eta_k(X_k) + \sum_{jk} \eta_{jk}(X_j, X_k) + \sum_{jkl} \eta_{jk}(X_j, X_k, X_l)$$

  - etc...

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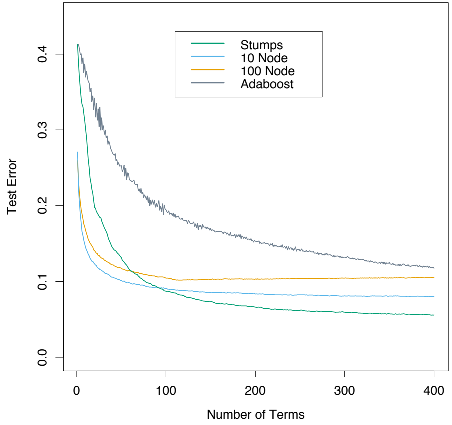
  $$\sum_k \eta_k(X_k) + \sum_{jk} \eta_{jk}(X_j, X_k) + \sum_{jkl} \eta_{jk}(X_j, X_k, X_l)$$
  - etc...

Size of trees in a boosted tree

- For many practical problems low-order interactions dominate.
- Therefore models that produce strong higher-order interaction effects suffer in accuracy.
- Authors claim that $4 \leq J \leq 8$ works well in the context of boosting.

Boosting with different sized trees



$$Y = \begin{cases} 1 & \text{if } \sum_{j=1}^{10} X_j^2 > \chi^2_{10}(.5) \\ -1 & \text{otherwise} \end{cases}$$

where $X_1, \ldots, X_{10}$ are standard indpt Gaussian and $\chi^2_{10}(.5) = 9.34$.

Regularization

Shrinkage & Subsampling

Options for regularization

- Control number of boosting rounds
  - Too large $M \implies$ danger of over-fitting

    $\therefore$ There is a M^* that minimizes future risk

- Shrinkage
  - Scale the contribution of each tree by factor $0 < \nu < 1$

$$f_m(x) = f_{m-1}(x) + \nu \cdot \sum_{j=1}^{J} \gamma_{jm} \, \text{Ind}(x \in \mathcal{R}_{jm})$$

  - Smaller $\nu \implies$ larger M to obtain low training error
  - Empirical finding: small $\nu < .1$ and sufficiently large M $\implies$ better result than no shrinkage. Especially for regression problems

Shrinkage & Subsampling

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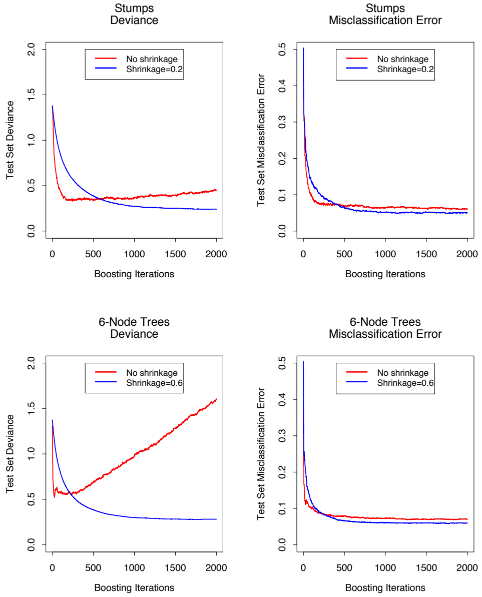
Shrinkage example



$$Y = \begin{cases} 1 & \text{if } \sum_{j=1}^{10} X_j^2 > \chi_{10}^2(.5) \\ -1 & \text{otherwise} \end{cases}$$

where $X_1, \ldots, X_{10}$ are standard indpt Gaussian and $\chi_{10}^2(.5) = 9.34$.

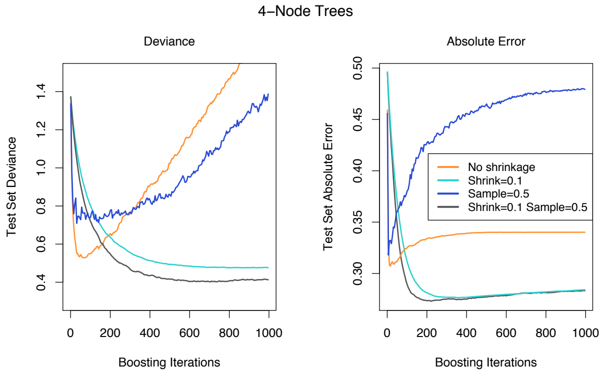
Deviance: $-2 \log \hat{p}_G(X)$

Shrinkage & Subsampling

Options for regularization

- Subsampling
  - Stochastic gradient boosting - each iteration sample a fraction η of the training observations (without replacement).
  - A typical value is $\eta = .5$
  - Empirically subsampling without shrinkage works poorly
  - But subsampling with shrinkage works well
  - Now have 4 parameters to estimate J, M, ν, and η

Subsample example



$$Y = \begin{cases} 1 & \text{if } \sum_{j=1}^{10} X_j^2 > \chi^2_{10}(.5) \\ -1 & \text{otherwise} \end{cases}$$

where $X_1, \ldots, X_{10}$ are standard indpt Gaussian and $\chi^2_{10}(.5) = 9.34$.