Boosting

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Ensembles: Parallel vs Sequential

- Ensemble methods combine multiple models
- **Parallel ensembles**: each model is built independently
    - e.g. bagging and random forests
    - Main Idea: Combine many (high complexity, low bias) models to reduce variance
- **Sequential ensembles**:
    - Models are generated sequentially
    - Try to add new models that do well where previous models lack

The Boosting Question: Weak Learners

- A **weak learner** is a classifier that does slightly better than random guessing.
- Weak learners are like "rules of thumb":
  - If an email has "Viagra" in it, more likely than not it's spam.
  - Email from a friend is probably not spam.
  - A linear decision boundary.
- Can we extract wisdom from a committee of fools?
- Can we **combine** a set of weak classifiers to form single classifier that makes accurate predictions?
  - Posed by Kearns and Valiant (1988,1989):
- Yes! **Boosting** solves this problem. [Rob Schapire (1990).]

AdaBoost: Setting

- Consider $\mathcal{Y} = \{-1, 1\}$ (binary classification).
- Suppose we have a **weak learner**:
  - Hypothesis space $\mathcal{F} = \{f : \mathcal{X} \to \{-1, 1\}\}$.
  - Algorithm for finding $f \in \mathcal{F}$ that's better than random on training data.
- Typical weak learners:
  - **Decision stumps** (tree with a single split)
  - Trees with few terminal nodes
  - Linear decision functions

Weighted Training Set

- Training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Weights $(w_1, \ldots, w_n)$ associated with each example.
- **Weighted empirical risk**:

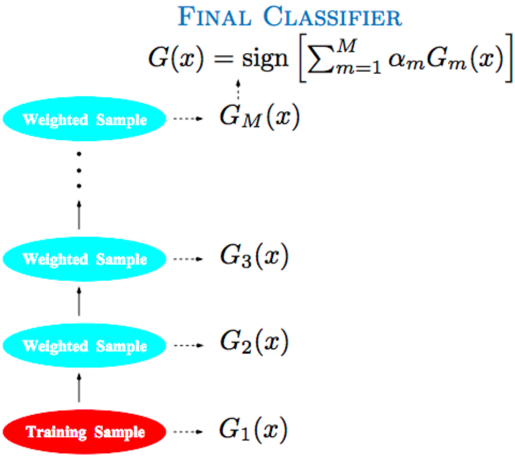
$$\hat{R}_n^w(f) = \frac{1}{W} \sum_{i=1}^{n} w_i \ell\{f(x_i), y_i\} \quad \text{where } W = \sum_{i=1}^{n} w_i$$

- Can train a model to minimize weighted empirical risk.
- What if model cannot conveniently be trained to reweighted data?
- Can sample a new data set from $\mathcal{D}$ with probabilities$(w_1/W, \ldots w_n/W)$.

AdaBoost - Rough Sketch

- Training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Start with equal weight on all training points $w_1 = \cdots = w_n = 1$.
- Repeat for $m = 1, \ldots, M$:
  - Fit weak classifier $G_m(x)$ to weighted training points
  - Increase weight on points $G_m(x)$ misclassifies
- So far, we've generated M classifiers: $G_1(x), \ldots, G_m(x)$.

AdaBoost: Schematic



From ESL Figure 10.1

AdaBoost - Rough Sketch

- Training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- Start with equal weight on all training points $w_1 = \cdots = w_n = 1$.
- Repeat for $m = 1, \ldots, M$:
  - Fit weak classifier $G_m(x)$ to weighted training points
  - Increase weight on points $G_m(x)$ misclassifies
- Final prediction $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
- The α_m's are nonnegative,
  - larger when G_m fits its weighted $\mathcal{D}$ well
  - smaller when G_m fits weighted $\mathcal{D}$ less well

Adaboost: Weighted Classification Error

- In round m, weak learner gets a weighted training set.
  - Returns a classifier $G_m(x)$ that roughly minimizes weighted $0-1$ error.
- The **weighted 0-1 error** of $G_m(x)$ is

$$\text{err}_m = \frac{1}{W} \sum_{i=1}^{n} w_i 1(y_i \neq G_m(x_i)) \quad \text{where } W = \sum_{i=1}^{n} w_i.$$

- Notice: $\text{err}_m \in [0,1]$.
- We treat the weak learner as a black box.
  - It can use any method it wants to find $G_m(x)$. (e.g. SVM, tree, etc.)
  - BUT, for things to work, we need at least $\text{err}_m < 0.5$.

AdaBoost: Classifier Weights

- The weight of classifier $G_m(x)$ is $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$.

- Note that weight $\alpha_m \to 0$ as weighted error $\text{err}_m \to 0.5$ (random guessing).

AdaBoost: Example Reweighting

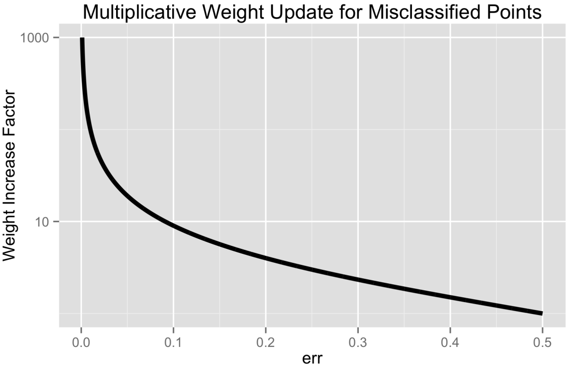
- We train G_m to minimize weighted error, and it achieves err_m.
- Then $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$ is the weight of G_m in final ensemble.
- Suppose w_i is weight of example i before training:
  - If G_m classfiies x_i correctly, then w_i is unchanged.
  - Otherwise, w_i is increased as

$$
\begin{aligned}
w_i &\leftarrow w_i e^{\alpha_m} \\
&= w_i \left(\frac{1-\text{err}_m}{\text{err}_m}\right)
\end{aligned}
$$

  - [Is it clear why this is always increasing the weight?]

Adaboost: Example Reweighting

- Any misclassified point has weight adjusted as $w_i \leftarrow w_i \left(\frac{1-\text{err}_m}{\text{err}_m}\right)$.



- The smaller err_m, the more we increase weight of misclassified points.

AdaBoost: Algorithm

Given training set $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.

1. Initialize observation weights $w_i = 1/n$, $i = 1, 2, \ldots, n$.
2. For $m = 1$ to M:
    1. Fit weak classifier $G_m(x)$ to $\mathcal{D}$ using weights w_i.
    2. Compute weighted empirical 0-1 risk:
    $$\text{err}_m = \frac{1}{W} \sum_{i=1}^{n} w_i 1(y_i \neq G_m(x_i)) \quad \text{where } W = \sum_{i=1}^{n} w_i.$$
    3. Compute $\alpha_m = \ln\left(\frac{1 - \text{err}_m}{\text{err}_m}\right)$.
    4. Set $w_i \leftarrow w_i \cdot \exp\left[\alpha_m 1(y_i \neq G_m(x_i))\right], \quad i = 1, 2, \ldots, N$
3. Ouptut $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

AdaBoost with Decision Stumps

- After 1 round:

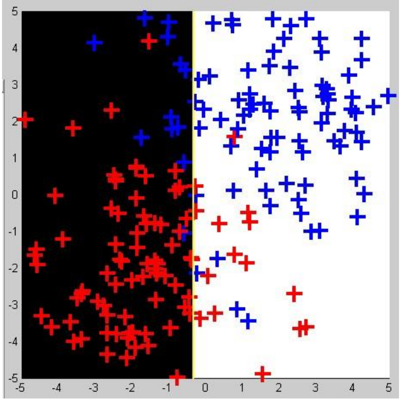


Figure: Plus size represents weight. Blackness represents score for red class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 3 rounds:

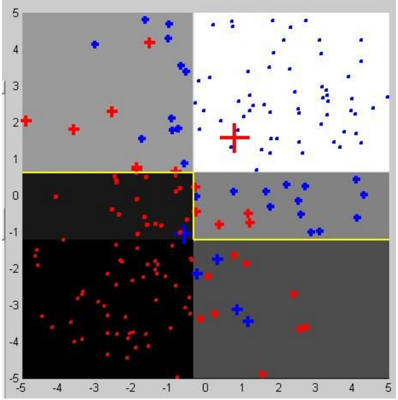


Figure: Plus size represents weight. Blackness represents score for red class.

KPM Figure 16.10

AdaBoost with Decision Stumps

- After 120 rounds:

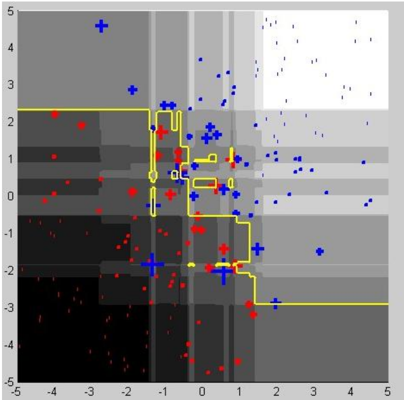


Figure: Plus size represents weight. Blackness represents score for red class.

KPM Figure 16.10

AdaBoost: Does it actually minimize training error?

- Methods we've seen so far come in two categories:
    - Convex optimization problems (L1/L2 regression, SVM, kernelized versions)
        - No issue minimizing objective function over hypothesis space
    - Trees
        - Can always fit data perfectly with big enough treehall
- AdaBoost is something new - at this point, it's just an algorithm.
- Will $G(x)$ even minimize training error?
- "Yes", if our weak classifiers have an "edge" over random.

AdaBoost: Does it actually minimize training error?

- As a weak classifier, $G_m(x)$ should have $\text{err}_m < \frac{1}{2}$.
- Define the **edge** of classifier $G_m(x)$ at round m to be

$$\gamma_m = \frac{1}{2} - \text{err}_m.$$

- Measures how much better than random G_m performs.

AdaBoost: Does it actually minimize training error?

Theorem

The empirical 0-1 risk of the AdaBoost classifier $G(x)$ is bounded as

$$\frac{1}{n}\sum_{i=1}^{n} 1(y_i \neq G(x)) \leqslant \prod_{m=1}^{M} \sqrt{1-4\gamma_m^2}.$$

For more details, see the book *Boosting: Foundations and Algorithms* by Schapire and Freund.

AdaBoost: Does it actually minimize training error?

Example

Suppose $\text{err}_m \leqslant 0.4$ for all m.

- Then $\gamma_m = .5 - .4 = .1$, and

$$\frac{1}{n}\sum_{i=1}^{n} 1(y_i \neq G(x)) \leqslant \prod_{m=1}^{M} \sqrt{1-4(.1)^2} \approx (.98)^M$$

- Bound decreases exponentially:

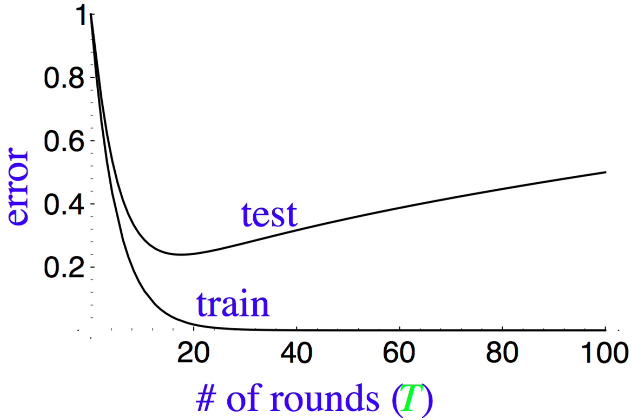
$$\begin{aligned} .98^{100} &\approx .133 \\ .98^{200} &\approx .018 \\ .98^{300} &\approx .002 \end{aligned}$$

- With a consistent edge, training error decreases very quickly to 0.

For more details, see the book *Boosting: Foundations and Algorithms* by Schapire and Freund.

Typical Train / Test Learning Curves

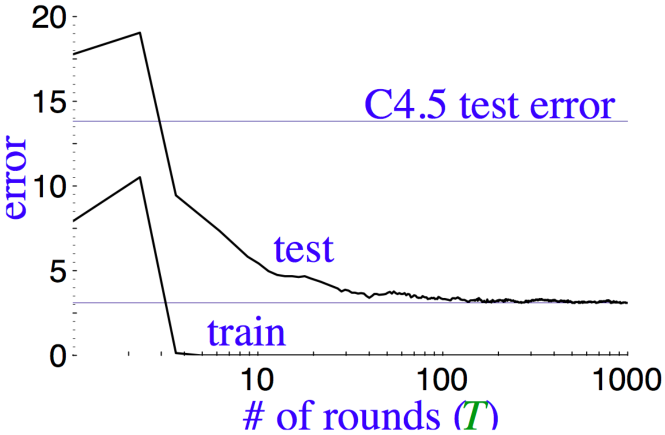
- Might expect too many rounds of boosting to overfit:



From Rob Schapire's NIPS 2007 Boosting tutorial.

Learning Curves for AdaBoost

- In typical performance, AdaBoost is surprisingly resistant to overfitting.
- Test continues to improve even after training error is zero!



From Rob Schapire's NIPS 2007 Boosting tutorial.

Adaptive Basis Function Model

- AdaBoost produces a classification score function of the form

$$\sum_{m=1}^{M} \alpha_m G_m(x)$$

- View this as an **adaptive basis function** model:
    - Linear in the basis functions.
    - But basis functions are learned from the data.

Adaptive Basis Function Model

- Can write adaptive basis function expansion as

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

  - where β_m are **expansion coefficients**
  - and $b(x;\gamma_m)$ is a function of x, parameterized by γ_m.
- For example, each $b(x;\gamma_m)$ could be a tree
  - γ_m would characterize the splits and the terminal node predictions
- If the γ_m's were known, this would just be a linear model.
- This type of model is also called an **additive** model.

Fitting Adaptive Basis Function Model

- Would be nice directly minimize the empirical risk:

$$\min_{\{\beta_m,\gamma_m\}_{m=1}^M} \sum_{i=1}^n \ell\left(y_i, \sum_{m=1}^M \beta_m b(x_i;\gamma_m)\right).$$

- Prediction function more general than what we've seen before.
- Difficult to solve, in general.
- We'll discuss an approximate "greedy" solution, known as
    - **forward stagewise additive modeling**

Forward Stagewise Additive Modeling

Sequentially add basis functions to the expansion, without adjusting the parameters or coefficients of the functions that have already been added.

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
    1. Compute:
    $$(\beta_m, \gamma_m) = \underset{\beta,\gamma}{\arg\min} \sum_{i=1}^{n} \ell\{y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)\}.$$
    2. Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.
3. Return: $f_M(x)$.

- Note: Actually implementing this minimization is difficult in general. More on this later.

Exponential Loss and AdaBoost

- Take loss function to be

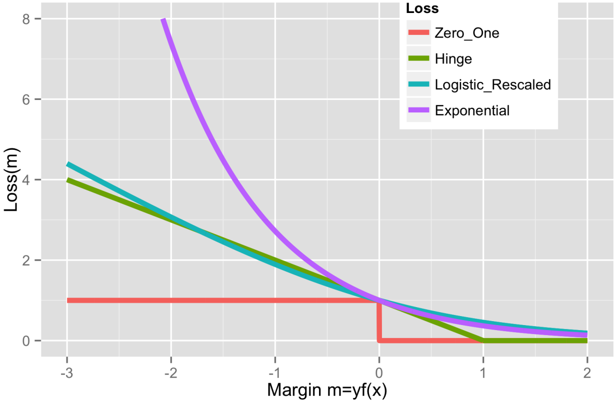
$$\ell(y, f(x)) = \exp\left(-yf(x)\right).$$

- Let $\mathcal{F} = \{b(x;\gamma) \mid \gamma \in \Gamma\}$ be a hypothesis space of weak classifiers.
- Then Forward Stagewise Additive Modeling (FSAM) reduces to AdaBoost!
  - (See HTF Section 10.4 for proof.)
- Only difference:
  - AdaBoost is loose about each G_m "fitting the weighted training data"
  - For FSAM we're explicitly looking for

$$G_m = \underset{G \in \mathcal{F}}{\arg\min} \sum_{i=1}^{N} w_i^{(m)} 1(y_i \neq G(x_i))$$

Exponential Loss

- Note that exponential loss puts a very large weight on bad misclassifications.



AdaBoost / Exponential Loss: Robustness Issues

- When Bayes error rate is high (e.g. $\mathbb{P}(f^*(X) \neq Y) = 0.25$)
  - Training examples with same input, but different classifications.
  - Best we can do is predict the most likely class for each X.
- Some training predictions **should be wrong** (because example doesn't have majority class)
  - AdaBoost / exponential loss puts a lot of focus on geting those right
- Empirically, AdaBoost has degraded performance in situations with
  - high Bayes error rate, or when there's
  - high "**label noise**"
- Logistic loss performs better with high Bayes error

Population Minimizers

- In traditional statistics, the **population** refers to
  - the full population of a group, rather than a sample.
- In machine learning, the **population case** is the hypothetical case of
  - an infinite training sample from $P_{\mathcal{X}\times\mathcal{Y}}$.
- A **population minimizer** for a loss function is another name for the risk minimizer.
- For the exponential loss $\ell(m) = e^{-m}$, the population minimizer is given by

$$f^*(x) = \frac{1}{2}\ln\frac{\mathbb{P}(Y = 1 \mid X = x)}{\mathbb{P}(Y = -1 \mid X = x)}$$

- (Short proof in KPM 16.4.1)
- By solving for $\mathbb{P}(Y = 1 \mid X = x)$, we can give probabilistic predictions from AdaBoost as well.

Population Minimizers

- AdaBoost has the robustness issue because of the exponential loss.
- Logistic loss $\ell(m) = \ln(1 + e^{-m})$ has the same population minimizer.
  - But works better with high lable noise or high Bayes error rate
- Population minimizer of SVM hinge loss is

$$f^*(x) = \operatorname{sign}\left[\mathbb{P}(Y = 1 \mid X = x) - \frac{1}{2}\right].$$

- Because of the sign, we cannot solve for the probabilities.