# 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**:

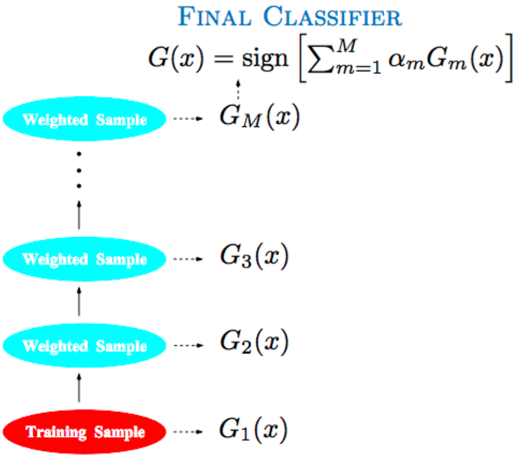
$$\hat{R}_n^w(f) = \frac{1}{W} \sum_{i=1}^{n} w_i \ell\{f(x_i), y_i\} \quad \text{where } W = \sum_{i=1}^{n} w_i$$

- 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 $\alpha_m$'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

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

- Notice: $\mathrm{err}_m \in [0,1]$.
- 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 $\mathrm{err}_m < 0.5$.

# 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

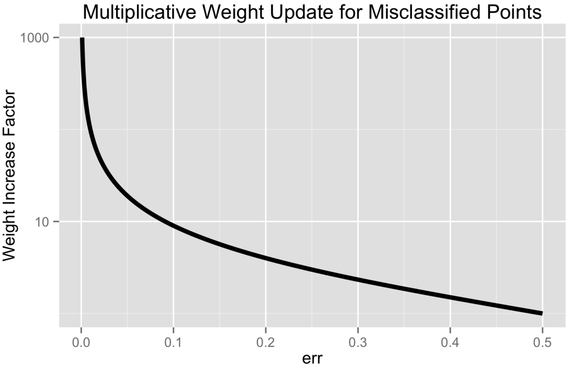
- We train $G_m$ to minimize weighted error, and it achieves $\text{err}_m$.
- Then $\alpha_m = \ln\left(\frac{1-\text{err}_m}{\text{err}_m}\right)$ is the weight of $G_m$ in final ensemble.
- Suppose $w_i$ is weight of example $i$ before training:
  - If $G_m$ classfiies $x_i$ correctly, then $w_i$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

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




- The smaller $\text{err}_m$, 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:

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

    3. Compute $\alpha_m = \ln \left( \frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \right)$.
    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:

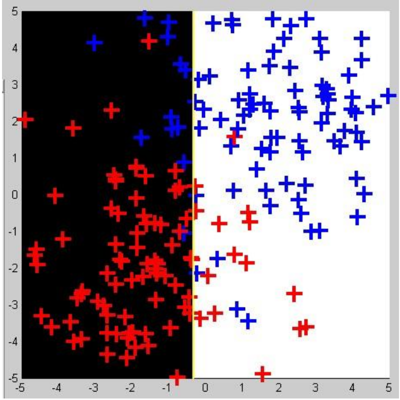



Figure: Plus size represents weight. Blackness represents score for red class.

KPM Figure 16.10

# AdaBoost with Decision Stumps

- After 3 rounds:

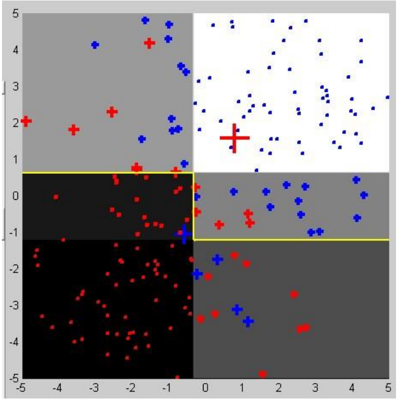



Figure: Plus size represents weight. Blackness represents score for red class.

KPM Figure 16.10

# AdaBoost with Decision Stumps

- After 120 rounds:

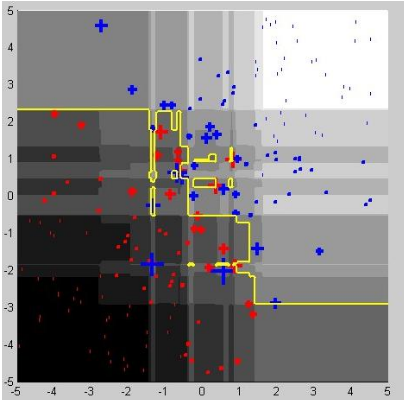



Figure: Plus size represents weight. Blackness represents score for red class.

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:

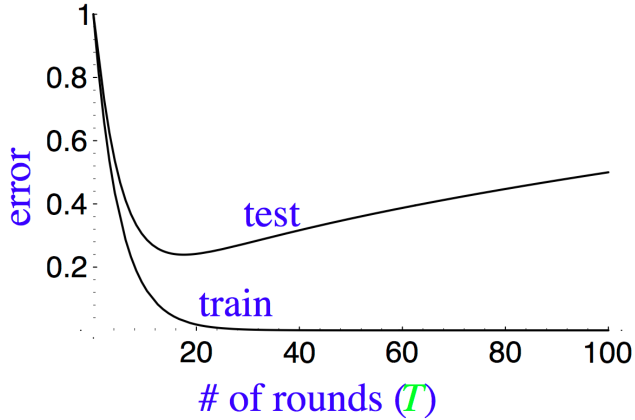
$$\begin{aligned} .98^{100} &\approx .133 \\ .98^{200} &\approx .018 \\ .98^{300} &\approx .002 \end{aligned}$$

- 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

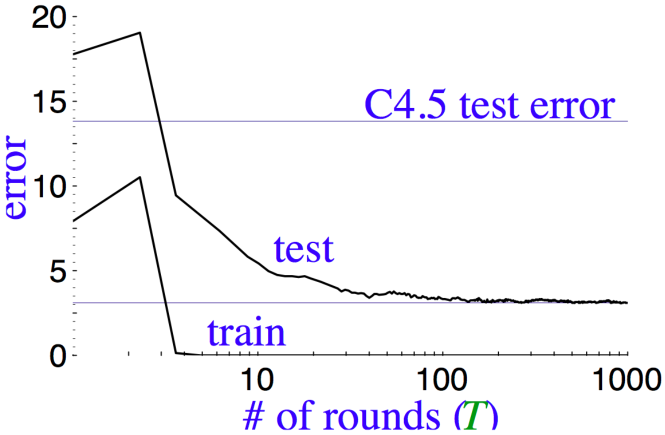
- Might expect too many rounds of boosting to overfit:




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 $\beta_m$ are **expansion coefficients**
  - and $b(x; \gamma_m)$ is a function of $x$, parameterized by $\gamma_m$.
- For example, each $b(x; \gamma_m)$ could be a tree
  - $\gamma_m$ would characterize the splits and the terminal node predictions
- If the $\gamma_m$'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

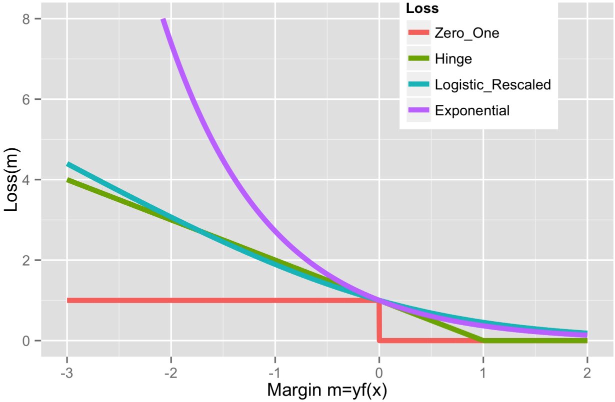
$$\ell(y, f(x)) = \exp(-yf(x)).$$

- 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 $\operatorname{sign}$, we cannot solve for the probabilities.

# Forward Stagewise Modeling and Iterative Optimization

1. We start at $f_0(x) = 0$.
2. In each step, we find
   1. function $b(\cdot;\gamma)$ (like a step direction)
   2. expansion coefficient $\beta$ (like a step size)
   3. $f_m(x) = f_{m-1}(x) + \beta_m b(x;\gamma_m)$.

Just like in gradient descent and SGD, final result is the sum of all of our steps.

Can we look at $b(\cdot;\gamma)$ as a gradient?

Maybe as a projected gradient.

# Functional Gradient Descent

- We want to minimize
$$\sum_{i=1}^{n} \ell\{y_i, f(x_i)\}.$$
- Can do a "functional" gradient descent with respect to $f$?
- Take functional gradient w.r.t. $f$.
- Take a step in the gradient direction (in function space).
- What about the constraint $f \in \mathcal{F}$, to prevent overfitting?
- We can use a projection to keep us in $\mathcal{F}$

# Functional Gradient Descent: Unconstrained Objective

- Note that
$$\sum_{i=1}^{n} \ell\{y_i, f(x_i)\}$$
only depends on $f$ at the training points.
- Define
$$\mathbf{f} = (f(x_1), \ldots, f(x_n))^T$$
and write
$$\min_{\mathbf{f} \in \mathbf{R}^n} \sum_{i=1}^{n} \ell(y_{i,} \mathbf{f}_i).$$
- Corresponds to an unconstrained minimization over $f$ (i.e. over all possible functions).

# Functional Gradient Descent: Unconstrained Step Direction

- Suppose we're at $f_{m-1}(x)$, and we're ready for our next step.
- Write the objective function as

$$J(\mathbf{f}) = \sum_{i=1}^{n} \ell\left(y_i, \mathbf{f}_i\right).$$

- So the negative gradient step direction for step $m$ is

$$-\mathbf{g}_m = -\nabla_{\boldsymbol{f}} J(\mathbf{f}_{m-1}),$$

  which we can easily calculate.
- This is just about how to adjust the values of $f$ at the training data.
- How to keep $f \in \mathcal{F}$?
- Solve both of these problems by projecting $-\mathbf{g}_m$ into $\mathcal{F}$.

# Functional Gradient Descent: Projection Step

- Unconstrained step direction is

$$-\mathbf{g}_m = -\nabla_{\boldsymbol{f}} J(\mathbf{f}_{m-1}).$$

- Suppose $\mathcal{F}$ is our weak hypothesis space.
- Find $h_m \in \mathcal{F}$ that is closest to $-\mathbf{g}_m$ at the training points, in the $\ell^2$ sense:

$$h_m = \underset{h \in \mathcal{F}}{\arg\min} \sum_{i=1}^{n} \left( (-\mathbf{g}_m)_i - h(x_i) \right)^2.$$

- This is a least squares regression problem.
- So $h_m$ is our step direction.

# Functional Gradient Descent: Step Size

- Finally, we choose a stepsize.
- Option 1:

$$\nu_m = \operatorname*{arg\,min}_{\nu > 0} \sum_{i=1}^{n} \ell\{y_i, f_{m-1}(x_i) + \nu h_m(x_i)\}.$$

- Option 2: Use a fixed stepsize, such as $\nu = 0.1$, and treat it as a hyperparameter. (More typical)

# The Gradient Boosting Machine

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to $M$:
    1. Compute:
    $$\mathbf{g}_m = \left( \frac{\partial}{\partial f(x_i)} \left[ \sum_{i=1}^{n} \ell\{y_i, f(x_i)\} \right] \right)_{i=1}^{n}$$
    2. Fit regression model to $-\mathbf{g}_m$:
    $$h_m = \underset{h \in \mathcal{F}}{\arg\min} \sum_{i=1}^{n} \left( (-\mathbf{g}_m)_i - h(x_i) \right)^2.$$
    3. Choose step size:
    $$\nu_m = \underset{\nu > 0}{\arg\min} \sum_{i=1}^{n} \ell\{y_i, f_{m-1}(x_i) + \nu h_m(x_i)\}.$$
    4. Take the step:
    $$f_m(x) = f_{m-1}(x) + \nu_m h_m(x)$$

# Gradient Tree Boosting

- Most common form of gradient boosting machine takes

$$\mathcal{F} = \{\text{regression trees of size } J\},$$

  where $J$ is the number of terminal nodes.
- $J = 2$ gives decision stumps
- HTF recommends $4 \leqslant J \leqslant 8$.
- Software packages:
  - Gradient tree boosting is implemented by the **gbm package** for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in **sklearn**