Boosting

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Outline

- Model Averaging
  - Bagging
  - Boosting
- History of Boosting
- Stagewise Additive Modeling
- Boosting and Logistic Regression
- MART
- Boosting and Overfitting
- Summary of Boosting, and its place in the toolbox.

Methods for improving the performance of weak learners. Classification trees are adaptive and robust, but do not generalize well. The techniques discussed here enhance their performance considerably.

Reference: Chapter 10.
Data \((X, Y) \in R^p \times \{0, 1\}\).

\(X\) is predictor, feature; \(Y\) is class label, response. 
\((X, Y)\) have joint probability distribution \(\mathcal{D}\).

Goal: Based on \(N\) training pairs \((X_i, Y_i)\) drawn from \(\mathcal{D}\) produce a classifier \(\hat{C}(X) \in \{0, 1\}\)

Goal: choose \(\hat{C}\) to have low generalization error

\[
R(\hat{C}) = P_{\mathcal{D}}(\hat{C}(X) \neq Y) = E_{\mathcal{D}}[1(\hat{C}(X) \neq Y)]
\]
$X \in \mathbb{R}^p$ has distribution $\mathcal{D}$.

$C(X)$ is \textbf{deterministic function} $\in$ \textbf{concept class}.

Goal: Based on $N$ training pairs $(X_i, Y_i = C(X_i))$ drawn from $\mathcal{D}$ produce a classifier $\hat{C}(X) \in \{0, 1\}$

Goal: choose $\hat{C}$ to have low \textbf{generalization error}

$$R(\hat{C}) = P_{\mathcal{D}}(\hat{C}(X) \neq C(X))$$
$$= E_{\mathcal{D}}[1_{(\hat{C}(X) \neq C(X))}]$$
Classification Tree

Sample of size 200
When the \textit{nested spheres} are in $\mathbb{R}^{10}$, CART produces a rather noisy and inaccurate rule $\hat{G}(X)$, with error rates around 30%.
Model Averaging

Classification trees can be simple, but often produce noisy (bushy) or weak (stunted) classifiers.

- Bagging (Breiman, 1996): Fit many large trees to bootstrap-resampled versions of the training data, and classify by majority vote.

- Boosting (Freund & Shapire, 1996): Fit many large or small trees to reweighted versions of the training data. Classify by weighted majority vote.

In general Boosting $\succ$ Bagging $\succ$ Single Tree.

“AdaBoost · · · best off-the-shelf classifier in the world” — Leo Breiman, NIPS workshop, 1996.
Bagging or bootstrap aggregation averages a given procedure over many samples, to reduce its variance — a poor man’s Bayes. See pp 246. Suppose $G(X, x)$ is a classifier, such as a tree, producing a predicted class label at input point $x$. To bag $G$, we draw bootstrap samples $X^*^1, \ldots X^*^B$ each of size $N$ with replacement from the training data. Then

$$\hat{G}_{bag}(x) = \text{Majority Vote } \{G(X^*_b, x)\}_{b=1}^B.$$ 

Bagging can dramatically reduce the variance of unstable procedures (like trees), leading to improved prediction. However any simple structure in $G$ (e.g a tree) is lost.
Bagging averages many trees, and produces smoother decision boundaries.
**Boosting**

**Final Classifier**

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

- \( G_1(x) \)
- \( G_2(x) \)
- \( G_3(x) \)
- \( G_M(x) \)

Weighted Sample

Training Sample
Bagging and Boosting

2000 points from Nested Spheres in $R^{10}$; Bayes error rate is 0%.

Trees are grown Best First without pruning.

Leftmost iteration is a single tree.
AdaBoost (Freund & Schapire, 1996)

1. Initialize the observation weights
   \[ w_i = 1/N, \ i = 1, 2, \ldots, N. \]

2. For \( m = 1 \) to \( M \) repeat steps (a)–(d):
   (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) Update weights for \( i = 1, \ldots, N \):
      \[ w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))] \]
      and renormalize to \( w_i \) to sum to 1.

3. Output \( G(x) = \text{sign} \left[ \sum_{m=1}^{M} \alpha_m G_m(x) \right] \).
History of Boosting

- **L.G. Valiant (1984)**
- **R.E Schapire (1990)**
- **Y. Freund (1995)**
- **Schapire & Freund (1995,1997)**
- **Freund & Schapire (1996)**
- **R. Quinlan (1996)**
- **Breiman(1996, 1997)**
- **Schapire, Freund, P. Bartlett, Lee (1997)**
- **Schapire, Y. Singer (1998)**
- **Schapire, Singer, Freund, Iyer (1998)**
- **Friedman, Hastie, Tibshirani (1998)**

### Genesis of
**PAC Learning Model**

### Concept of
**Boosting appears**

### Adaboost
**is born**

### Experiments
**with Adaboost**

### Attempts to
**explain why Adaboost works**

**Improvements**
Definition: Consider a concept class $C$ defined over a set $X$ of length $N$. $L$ is a learner (algorithm) using hypothesis space $H$. $C$ is PAC learn-able by $L$ using $H$ if for all $C \in C$, all distributions $D$ over $X$ and all $\epsilon, \delta \in (0, \frac{1}{2})$, learner $L$ will, with $Pr \geq (1 - \delta)$, output an $h \in H$ s.t. $\text{error}_D(h) \leq \epsilon$ in time polynomial in $1/\epsilon, 1/\delta, N$ and $\text{size}(C)$.

Such an $L$ is called a strong Learner.
Boosting a Weak Learner

Weak learner $L$ produces an $h$ with error rate $\beta = (\frac{1}{2} - \varepsilon) < \frac{1}{2}$, with $Pr \geq (1 - \delta)$ for any $\mathcal{D}$. $L$ has access to continuous stream of training data and a class oracle.

1. $L$ learns $h_1$ on first $N$ training points.

2. $L$ randomly filters the next batch of training points, extracting $N/2$ points correctly classified by $h_1$, $N/2$ incorrectly classified, and produces $h_2$.

3. $L$ builds a third training set of $N$ points for which $h_1$ and $h_2$ disagree, and produces $h_3$.

4. $L$ outputs $h = \text{Majority Vote}(h_1, h_2, h_3)$

**THEOREM (Schapire, 1990): “The Strength of Weak Learnability”**

$$\text{error}_D(h) \leq 3\beta^2 - 2\beta^3 < \beta$$
A stump is a two-node tree, after a single split. Boosting stumps works remarkably well on the nested-spheres problem.
Boosting & Training Error

Nested spheres in $R^{10}$ — Bayes error is 0%.

**Stumps**

Boosting drives the training error to zero. Further iterations continue to improve test error in many examples.
Boosting Noisy Problems

Nested Gaussians in $\mathbb{R}^{10}$ — Bayes error is 25%.

**Stumps**

![Graph showing train and test error with Bayes error as a horizontal line]

Here the test error does increase, but quite slowly.
Stagewise Additive Modeling

Boosting builds an additive model

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

Here \( b(x, \gamma_m) \) is a tree, and \( \gamma_m \) parametrizes the splits.

We do things like that in statistics all the time!

- **GAMs:** \( f(x) = \sum_j f_j(x_j) \)

- **Basis expansions:** \( f(x) = \sum_{m=1}^{M} \theta_m h_m(x) \)

Traditionally the parameters \( f_m, \theta_m \) are fit jointly (i.e. least squares, maximum likelihood).

With boosting, the parameters \((\beta_m, \gamma_m)\) are fit in a stagewise fashion. This slows the process down, and tends to overfit less quickly.
Suppose we have available a basis family $b(x; \gamma)$ parametrized by $\gamma$. For example, a simple family is $b(x; \gamma_j) = x_j$.

- After $m - 1$ steps, suppose we have the model $f_{m-1}(x) = \sum_{j=1}^{m-1} \beta_j b(x; \gamma_j)$.
- At the $m$th step we solve
  $$\min_{\beta, \gamma} \sum_{i=1}^{N} (y_i - f_{m-1}(x_i) - \beta b(x_i; \gamma))^2$$

- Denoting the residuals at the $m$th stage by $r_{im} = y_i - f_{m-1}(x_i)$, the previous step amounts to
  $$\min_{\beta, \gamma} (r_{im} - \beta b(x_i; \gamma))^2,$$

- Thus the term $\beta_m b(x; \gamma_m)$ that best fits the current residuals is added to the expansion at each step.
Adaboost: Stagewise Modeling

- AdaBoost builds an additive logistic regression model

\[
f(x) = \log \frac{\Pr(Y = 1|x)}{\Pr(Y = -1|x)} = \sum_{m=1}^{M} \alpha_m G_m(x)
\]

by stagewise fitting using the loss function

\[
L(y, f(x)) = \exp(-y f(x)).
\]

- Given the current \(f_{M-1}(x)\), our solution for \((\beta_m, G_m)\) is

\[
\arg \min_{\beta, G} \sum_{i=1}^{N} \exp[-y_i (f_{m-1}(x_i) + \beta G(x))]
\]

where \(G_m(x) \in \{-1, 1\}\) is a tree classifier and \(\beta_m\) is a coefficient.
With $w_i^{(m)} = \exp(-y_i f_{m-1}(x_i))$, this can be re-expressed as

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

We can show that this leads to the Adaboost algorithm; See pp 305.
Why Exponential Loss?

- $e^{-yF(x)}$ is a monotone, smooth upper bound on misclassification loss at $x$.
- Leads to simple reweighting scheme.
- Has logit transform as population minimizer

$$f^*(x) = \frac{1}{2} \log \frac{\Pr(Y = 1|x)}{\Pr(Y = -1|x)}$$

- Other more robust loss functions, like binomial deviance.
**General Stagewise Algorithm**

We can do the same for more general loss functions, not only least squares.

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

Sometimes we replace step (b) in item 2 by

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

Here $\nu$ is a shrinkage factor, and often $\nu < 0.1$.

See pp 326. Shrinkage slows the stagewise model-building even more, and typically leads to better performance.
• General boosting algorithm that works with a variety of different loss functions. Models include regression, outlier-resistant regression, K-class classification and risk modeling.

• MART uses gradient boosting to build additive tree models, for example, for representing the logits in logistic regression.

• Tree size is a parameter that determines the order of interaction (next slide).

• MART inherits all the good features of trees (variable selection, missing data, mixed predictors), and improves on the weak features, such as prediction performance.

• MART is described in detail in [book], section 10.10.
MART in detail

Model

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

where \( T(x; \Theta) \) is a tree:

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

with parameters \( \Theta = \{R_j, \gamma_j\}_{J}^{1} \)

Fitting Criterion

Given \( \hat{\Theta}_j, j = 1, \ldots, m - 1 \), we obtain \( \hat{\Theta}_m \) via stagewise optimization:

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

For general loss functions this is a very difficult optimization problem. Gradient boosting is an approximate gradient descent method.
Gradient Boosting

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

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

3. Output $\hat{f}(x) = f_M(x)$. 
Tree Size

The tree size $J$ determines the interaction order of the model:

$$
\eta(X) = \sum_j \eta_j(X_j) + \sum_{jk} \eta_{jk}(X_j, X_k) + \sum_{jkl} \eta_{jkl}(X_j, X_k, X_l) + \cdots
$$
Stumps win!

Since the true decision boundary is the surface of a sphere, the function that describes it has the form

\[ f(X) = X_1^2 + X_2^2 + \ldots + X_p^2 - c = 0. \]

Boosted stumps via MART returns reasonable approximations to these quadratic functions.
Example: Predicting e-mail spam

- data from 4601 email messages
- goal: predict whether an email message is spam (junk email) or good.
- input features: relative frequencies in a message of 57 of the most commonly occurring words and punctuation marks in all the training the email messages.
- for this problem not all errors are equal; we want to avoid filtering out good email, while letting spam get through is not desirable but less serious in its consequences.
- we coded spam as 1 and email as 0.
- A system like this would be trained for each user separately (e.g. their word lists would be different)
Predictors

- 48 quantitative predictors—the percentage of words in the email that match a given word. Examples include business, address, internet, free, and george. The idea was that these could be customized for individual users.

- 6 quantitative predictors—the percentage of characters in the email that match a given character. The characters are ch;, ch[, ch!, ch$, and ch#.

- The average length of uninterrupted sequences of capital letters: CAPAVE.

- The length of the longest uninterrupted sequence of capital letters: CAPMAX.

- The sum of the length of uninterrupted sequences of capital letters: CAPTOT.
Some important features

39% of the training data were spam.

Average percentage of words or characters in an email message equal to the indicated word or character. We have chosen the words and characters showing the largest difference between spam and email.

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<th>george</th>
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<td>0.18</td>
<td>0.42</td>
<td>0.29</td>
<td>0.01</td>
</tr>
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</table>
Spam Example Results

With 3000 training and 1500 test observations, MART fits an additive logistic model

\[ f(x) = \log \frac{\Pr(\text{spam}|x)}{\Pr(\text{email}|x)} \]

using trees with \( J = 6 \) terminal-node trees.

MART achieves a test error of 4%, compared to 5.3% for an additive GAM, 5.5% for MARS, and 8.7% for CART.
Spam: Variable Importance

Relative importance
\[ \bar{f}_S(X_S) = \frac{1}{N} \sum_{i=1}^{N} f(X_S, x_{iC}) \]
Spam: Partial Dependence

\[ \bar{f}_S(X_S) = \frac{1}{N} \sum_{i=1}^{N} f(X_S, x_{iC}) \]
Freund & Schapire (1997): Boosting generalizes because it pushes the training margins well above zero, while keeping the VC dimension under control (also Vapnik, 1996). With $Pr \geq (1 - \delta)$

$$P_{Test}(M(X) \leq 0) \leq P_{Train}(M(X) \leq \theta) + O\left(\frac{1}{\sqrt{N}} \left(\frac{\log N \log |\mathcal{H}|}{\theta^2 + \log 1/\delta}\right)^{\frac{1}{2}}\right)$$

define $\text{margin}(X) = M(X) = 2\hat{P}_{C(X)} - 1$
How does Boosting avoid overfitting?

- As iterations proceed, impact of change is localized.

- Parameters are not jointly optimized — stagewise estimation slows down the learning process.

- Classifiers are hurt less by overfitting (Cover and Hart, 1967).


- Jury is still out!
• $\epsilon$ forward stagewise: (idealized boosting with shrinkage). Given a family of basis functions $h_1(x), \ldots h_M(x)$, and loss function $L$.

• Model at $k$th step is $F_k(x) = \sum_m \beta_m^k h_m(x)$.

• At step $k + 1$, identify coordinate $m$ with largest $|\partial L/\partial \beta_m|$, and update $\beta_m^{k+1} \leftarrow \beta_m^k + \epsilon$.

• Equivalent to the lasso: $\min L(\beta) + \lambda_k \|\beta\|_1$
Summary and Closing Comments

- The introduction of **Boosting** by Schapire, Freund, and colleagues has brought us an exciting and important set of new ideas.

- Boosting fits additive logistic models, where each component (base learner) is simple. The complexity needed for the base learner depends on the target function.

- Little connection between weighted boosting and bagging; boosting is primarily a bias reduction procedure, while the goal of bagging is variance reduction.

- Boosting can of course overfit; stopping early is a good way to regularize boosting.

- Our view of boosting is stagewise and slow optimization of a loss function. For example, gradient boosting approximates the gradient updates by small trees fit to the empirical gradients.
• Modern versions of boosting use different loss functions, and incorporate shrinkage. Can handle a wide variety of regression modeling scenarios.

• Later on we will compare boosting with support vector machines.
**Comparison of Learning Methods**

Some characteristics of different learning methods.
Key: ● = good, ○ = fair, and ◯ = poor.

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<th>Characteristic</th>
<th>Neural Nets</th>
<th>SVM</th>
<th>CART</th>
<th>GAM</th>
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<td>Ability to extract linear combinations of features</td>
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