Boosting - AdaBoost

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Boosting - AdaBoost

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 - Algorithm
 - Additive structure
 - Different view of AdaBoost
 - Investigate the loss function
 - Margin theory

Boosting

- Motivation: "Can a set of weak learners create a single strong learner?"
 - Kearns & Valiant (1988, 1989)
 - Weak learner: a ML algorithm with performance slightly better than random guessing.

Yes!

Brief history

- 1990 First simple boosting procedure (Schapire)
 - Showed that a weak learner could always improve its performance
 - Initial classifier + two classifiers trained on misidentified/disagreed data by previous classifier
- 1993 Idea of "Boost by majority" (Freund)
- ---- Border between theoretical and practical ----
- 1995 AdaBoost (Freund & Schapire)
 - Significant improvement, combines many weighted weak learners, adjusted training weight

AdaBoost

Use binary classification as an example

FINAL CLASSIFIER

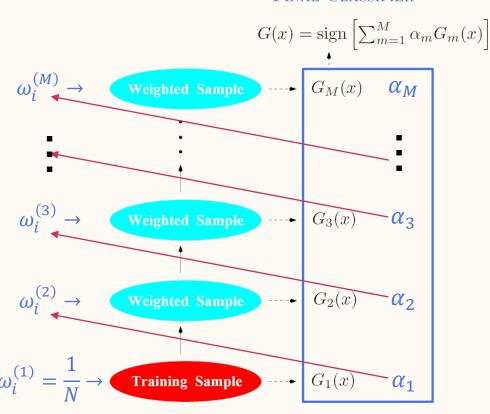


FIGURE 10.1. Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.

Algorithm 10.1 AdaBoost.M1.

- 1. Initialize the observation weights $w_i = 1/N$, i = 1, 2, ..., N.
- 2. For m=1 to M:
 - (a) Fit a classifier $G_m(x)$ to the training data using weights w_i .
 - (b) Compute

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

- (c) Compute $\alpha_m = \log((1 \operatorname{err}_m)/\operatorname{err}_m)$.
- (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))], i = 1, 2, \dots, N.$
- 3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

Points

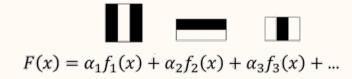
- It's a sequential process
 - Updated weights on training sample, focusing on mistakes made by previous classifiers
- It's a family of ensemble technique
 - Weighted combination of classifiers at different stage, good classifier's decision is more important

Details

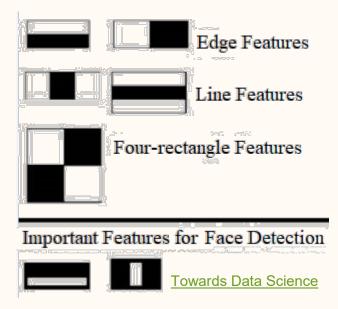
- Base classifier G is not specified
 - Decision tree is an ideal choice

Why AdaBoost has big impact

- It's simple yet effective
 - The idea behind can be applied to different fields
 - Computer vision: Viola-Jones detector
 - Base classifiers are the haar-like feature with examples given on the right side
 - On average only 8 features need to be evaluated



- Guaranteed by the theory to be valid
 - Train err decrease exponentially
 - "Never" overtrained in practice





AdaBoost: additive structure

The structure of AdaBoost is indicated in the expression of final prediction

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

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

More generally, basis function expansions takes the form

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

- β_m , $m=1,2,\cdots,M$ are the expansion coefficients
- $b(x; \gamma_m) \in \mathbb{R}$ are usually simple functions
 - Taking multivariate input x
 - Defined by parameter set γ

Use of additive expansions

- Additive expansions are at the heart of many of the learning techniques
 - Neural network with single hidden layer
 - $b(x; \gamma) = \sigma(\gamma^T x)$, σ is the activation function, γ are the linear combination weights for input x
 - Multivariate adaptive regression splines (MARS)
 - b is from truncated-power spline basis functions, γ is the choice of x_{ij} , $i=1,2,\cdots,N$, $j=1,2,\cdots,p$
 - Tree methods
 - b is simple tree, γ defines splits and prediction at leaf nodes

Forward stagewise additive modeling

The additive models discussed in previous page are typically fit by minimizing a loss function averaged over the training data

$$\min_{\{\beta_m,\gamma_m\}_i^M} \sum_{i=1}^N L(y_i, \sum_{m=1}^M \beta_m b(x_i; \gamma_m))$$

■ The loss function *L* could be the squared-error or a likelihood-based loss function

❖ It requires computationally intensive numerical optimization techniques to optimize with all M basis functions considered simultaneously, a simple alternative often can be found when it is feasible to rapidly solve the subproblem of fitting just a single basis function

$$\min_{\{\beta,\gamma\}} \sum_{i=1}^{N} L(y_i, \beta b(x_i; \gamma))$$

Forward stagewise additive modeling (Algorithm)

Algorithm 10.2 Forward Stagewise Additive Modeling.

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

At each stage m only update β_m and γ_m

- by fitting the partial residual $y f_{m-1}(x)$
- without adjusting those have been already fixed in previous stage $1,2,\cdots,m-1$
- we show next that AdaBoost is doing the same equivalently
 - even though we didn't use any loss function in the AdaBoost algorithm described earlier

AdaBoost as a FSAM

AdaBoost is equivalent to forward stagewise additive modeling (FSAM) using the loss function

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

- The reason to use exponential form discussed later
- Note that we have $f(x) \in \{-1,1\} \rightarrow y f(x) = \begin{cases} 1, y = f(x) \\ -1, y \neq f(x) \end{cases}$
- \diamond At stage m, the optimization is done by solving

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

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

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

- w_i^m is fixed in previous stages and can be regarded as a weight applied to observations
- Note $G_m(x)$ also have $G_m(x) \in \{-1, 1\} \to yG_m(x) = \begin{cases} 1, y = G_m(x) \\ -1, y \neq G_m(x) \end{cases}$

Get (β_m, G_m)

 $\boldsymbol{\phi}_m$ is a positive constant even thought it's unknown yet, we consider it as fixed and solve the G_m

$$G_m = \arg\min_{G} \sum_{i=1}^{N} w_i^{(m)} I(y_i \neq G(x_i))$$

• we only consider $y_i \neq G(x_i)$ situation here, because the $y_i = G(x_i)$ situation is the other side of the coin

$$I(y_i = G(x_i)) = 1 - I(y_i \neq G(x_i))$$

• With known G_m the loss function $L_m(\beta)$ will be

$$L_m(\beta) = \sum_{i=1}^{N} w_i^{(m)} \exp(-\beta y_i G_m(x_i)) = e^{-\beta} \sum_{y_i = G(x_i)} w_i^{(m)} + e^{\beta} \sum_{y_i \neq G(x_i)} w_i^{(m)}$$

• Get optimal β to minimize $L_m(\beta)$

$$\beta_m = \frac{1}{2} \ln \left(\frac{1 - err_m}{err_m} \right), err_m = \frac{\sum_{i=1}^{N} w_i^{(m)} I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i^{(m)}}$$

- Note that β_m could be negative if $err_m < 0.5$, in which case it automatically reverse the polarity.
 - Move the "-1" in β_m to G_m : $\beta_m \to -\beta_m > 0$, $G_m(x) \to -G_m(x)$, $err_m \to 1 err_m > 0.5$

Stage updates

 \bullet In each stage m, the prediction function is updated as

$$f_m(x) = f_{m-1}(x) + \beta_m G_m(x)$$

• where β_m and G_m are estimated as illustrated in the previous page

- \bullet In next stage m+1
 - the weight $w_i^{(m)}$ in loss function is updated to $w_i^{(m+1)}$ by

$$w_i^{(m+1)} = w_i^{(m)} \cdot e^{-\beta_m y_i G_m(x_i)}$$

• then β_{m+1} and G_{m+1} are updated following the same procedures

AdaBoost as a Newton-like method

Again, start from the exponential loss $L(y, f(x)) = \exp(-yf(x))$. Suppose we seek an improvement

$$f(x) + cg(x)$$

- here c is a constant to be determined and $g(x) \in \{-1,1\}$ giving a binary prediction
- We can expand L at g(x) = 0

$$L(y, f(x) + cg(x)) = \exp(-yf(x)) \exp(-ycg(x))$$

$$\approx \exp(-yf(x)) \left[1 - cyg(x) + \frac{c^2}{2}\right] \stackrel{\text{def}}{=} L'$$

- notice the derivation of $\frac{c^2}{2}$ use the fact that $y^2 = 1$ and $g(x)^2 = 1$
- $= \exp(-yf(x))$ is determined by previous process and can be view as weight w

Get g(x)

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igh

$$g(x) = \begin{cases} 1, & p(y=1) > p(y=-1) \\ -1, & otherwise \end{cases}$$

• Again, use the fact that $y^2 = 1$ and $g(x)^2 = 1$

$$yg(x) = -\frac{[y - g(x)]^2}{2} + 1$$

 \diamond Then minimizing L' is equivalent to minimizing the least-square loss

$$\frac{[y-g(x)]^2}{2}-1$$

Get c

❖ With solved $g(x) \in \{-1,1\}$, we can get c again by optimizing L. The essential component is

$$\exp(-ycg(x)) = \sum_{y_i = g(x_i)} e^{-c} + \sum_{y_i \neq g(x_i)} e^{c} = n_T e^{-c} + n_F e^{c} \stackrel{\text{def}}{=} l(c)$$

- where n_T is the number of correct classification and n_F is the number of incorrect classification
- Minimizing the equation above

$$\frac{\partial l(c)}{\partial c} = -n_T e^{-c} + n_F e^c = 0 \rightarrow c = \frac{1}{2} \ln \frac{n_T}{n_F} = \frac{1}{2} \ln \frac{1 - err}{err}$$

• where $err = \frac{n_T}{n_T + n_F} = \frac{n_T}{n}$

Stage updates

We get the exactly same form of coefficient and update function as what we got when we consider AdaBoost as FSAM

And we can now construct a Newton-like method's update in each stage

$$f(x) \to f(x) + \frac{1}{2} \ln \frac{1 - err}{err} g(x)$$

In next round, the weight w is updated by

$$w \rightarrow w \cdot e^{-cyg(x)} = w \cdot e^{-c(1-2I(y\neq g(x)))}$$

What does exponential loss estimate?

 \bullet Investigating the population minimizer of $\exp(-yf(x))$

$$f^*(x) = \arg\min_{f(x)} E_{y|x}(e^{-yf(x)})$$

• Get derivative $E_{y|x}(e^{-yf(x)})$ w.r.t f(x) and set to zero

$$\frac{\partial E_{y|x}(e^{-yf(x)})}{\partial f(x)} = E_{y|x}(-ye^{-yf(x)}) = E_{y=1|x}(-ye^{-yf(x)}) + E_{y=-1|x}(-ye^{-yf(x)})$$
$$= -\Pr(y=1|x) e^{-f(x)} + \Pr(y=-1|x) e^{f(x)} = 0$$

Solve the equation

$$f^*(x) = \frac{1}{2} \ln \left(\frac{\Pr(y = 1|x)}{\Pr(y = -1|x)} \right) \text{ or } \Pr(y = 1|x) = \frac{1}{1 + e^{-2f^*(x)}}$$

- \bullet It is estimating the log-odds of Pr(y = 1|x)
 - This provides an inspect to justify that we use the sign of the model prediction as classification $\{-1,1\}$, where we have $G(x) = \underset{m=1}{sign}(\sum_{m=1}^{M} \alpha_m G_m(x))$.
 - if we have higher probability to predict y = 1, $f^*(x)$ will be "+"
 - if we have higher probability to predict y = -1, $f^*(x)$ will be "-",

Binomial deviance could be another candidate

* We now show that binomial deviance (cross-entry) leads to same solution at the population level. Using $y' = \frac{y+1}{2}$ to map $\{-1,1\}$ to $\{0,1\}$, we have the binomial deviance loss

$$l(y, p(x)) = y' \log p(x) + (1 - y') \log(1 - p(x))$$

 \Leftrightarrow Get derivative $E_{y|x}(l(y,p(x)))$ w.r.t p(x) and set to zero

$$\frac{\partial E_{y|x}l(y,p(x))}{\partial p(x)} = E_{y=1|x} \left(\frac{1}{p(x)}\right) + E_{y=-1|x} \left(-\frac{1}{1-p(x)}\right)$$
$$= \frac{\Pr(y=1|x)}{p(x)} - \frac{\Pr(y=-1|x)}{1-p(x)} = 0$$

Solve the equation we get

$$p(x) = \Pr(y = 1|x) = \frac{1}{1 + e^{-2f(x)}}$$

 \diamond Once p(x) is determined, f(x) is also determined via a logit relation

Continue

 \bullet Use f(x) to replace p(x)

$$l(y, p(x)) = y' \log p(x) + (1 - y') \log(1 - p(x)) = \log \frac{e^{(y-1)f(x)}}{1 + e^{-2f(x)}}$$

• Notice that $y \in \{-1,1\}$

$$l(y, p(x)) = \begin{cases} \log \frac{1}{1 + e^{-2f(x)}}, y = 1\\ \log \frac{e^{-2f(x)}}{1 + e^{-2f(x)}}, y = -1 \end{cases} = -\log(1 + e^{-2yf(x)})$$

■ Expand $e^{-yf(x)}$ and -l(y, p(x)) to Taylor series, we have

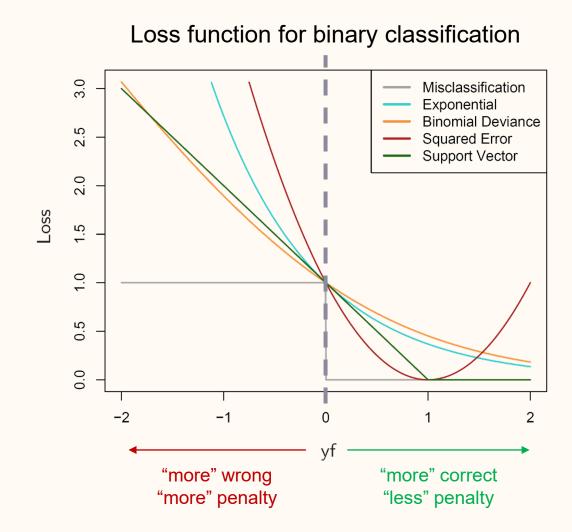
$$-l(y, p(x)) = \log(2) - yf(x) + \frac{y^2}{2}f^2(x) + \cdots$$
$$e^{-yf(x)} = 1 - yf(x) + \frac{y^2}{2}f^2(x) + \cdots$$

Binomial deviance loss and exponential loss are equivalent to second order

$$-l(y,p(x)) \approx e^{-yf(x)} + \log(2) - 1$$

Compare different loss for classification

- ❖ In the right plot, "yf" serves as a margin which plays a role analogous to the residuals y − f(x)
- Investigate positive yf
 - Squared Error will penalize correct predictions
 - All other loss decrease monotonically
- Investigate negative yf
 - All the loss penalize incorrect predictions but with different degree
 - Exponential loss will penalize much more on incorrect predictions so it's less robust
 - If inputs have mislabeled entries, the performance of AdaBoost will degrade dramatically (empirical observation)



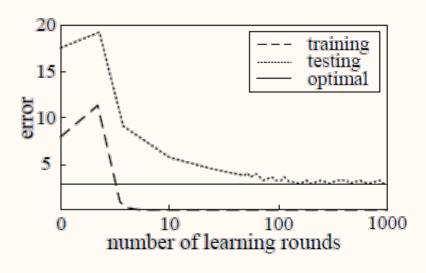
AdaBoost doesn't overfit

- AdaBoost often doesn't overfit in practice
- Freund & Schapire[JCSS97] proved that the generalization error of AdaBoostis bounded by:

$$\epsilon_{\mathrm{D}} \le \epsilon_{D} + \tilde{O}\left(\sqrt{\frac{dM}{n}}\right)$$

- with probability at least 1δ , where d represents the complexity of base learners,n is the number of training instances, M is the number of learning rounds and \tilde{O} hides the logarithmic and constant terms
- It implies that AdaBoost will overfit if M is large
- Is there tighter bound to explain the observation in practice?

A typical performance plot of AdaBoost on real data



Seems contradict with the Occam's Razor

Margin

- We have discussed the statistical view above. However, it did not explain why AdaBoost is resistant to overfitting according to observation in practice.
 - This can be explained by using margin

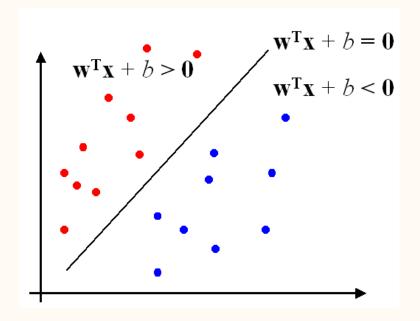
Example

 Binary classification can be viewed as the task of separating classes in a feature space

•
$$f(x) = sign(w^T x + b)$$

- Margin of a single classifier f: yf(x)
- Margin of the additive model F

$$yF(x) = \sum_{m=1}^{M} \alpha_m y f_m(x)$$



The bigger the margin, the higher the predictive confidence

Margin explanation of AdaBoost

* Based on the concept of margin, Schapire et al. [1998] proved that, given any threshold $\theta > 0$ of margin over the training data D, with probability at least $1 - \delta$, the test error of the ensemble $\epsilon_{\mathbb{D}} = P_{x \sim \mathbb{D}}(y \neq F(x))$ is bounded by

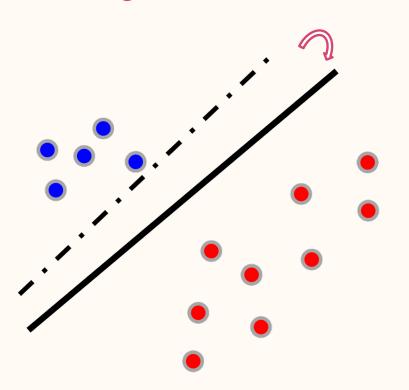
$$\epsilon_{D} \leq P_{x \sim D}(yF(x) \leq \theta) + \tilde{O}\left(\sqrt{\frac{d}{n\theta^{2}} + \ln\frac{1}{\delta}}\right)$$

$$\leq 2^{M} \prod_{m=1}^{M} \sqrt{\epsilon_{m}^{1-\theta} (1 - \epsilon_{m})^{1+\theta}} + \tilde{O}\left(\sqrt{\frac{d}{n\theta^{2}} + \ln\frac{1}{\delta}}\right)$$

This bound implies that, when other variables are fixed, the larger the margin over the training data, the smaller the test error

Margin explanation of AdaBoost (continued)

- Why AdaBoost tends to be resistant to overfitting?
- Margin theory: Because it is able to increase the ensemble margin even after the training error reaches zero



- > This explanation is quite intuitive
- > It receives good support in empirical study

The minimal margin bound

- Schapire et al.'s bound depends heavily on the smallest margin
 - If the smallest margin is large, $P_{x\sim D}(yF(x) \le \theta)$ will be small
- Thus, by considering the minimum margin:

$$\varrho = \min_{x \in D} yF(x)$$

* Breiman [Neural Comp. 1999] proved a test error bound $(0(\frac{\log n}{n}))$, which is tighter than Schapire et al.'s bound

$$\epsilon_{\mathbb{D}} \le R \left(\ln(2n) + \ln\left(\frac{1}{R}\right) + 1 \right) + \frac{1}{n} \ln\frac{|\mathcal{H}|}{\delta}$$

The doubt about margin theory

- Breiman [Neural Comp. 1999] designed a variant of AdaBoost, the arc-gv algorithm, which directly maximizes the minimum margin
 - the margin theory would appear to predict that arc-gv should perform better than AdaBoost
- However, experiments show that, comparing with AdaBoost:
 - arc-gv does produce uniformly larger minimum margin
 - the test error increases drastically in almost every case
- Thus, Breiman convincingly concluded that the margin theory was in serious doubt. This almost sentenced the margin theory to death

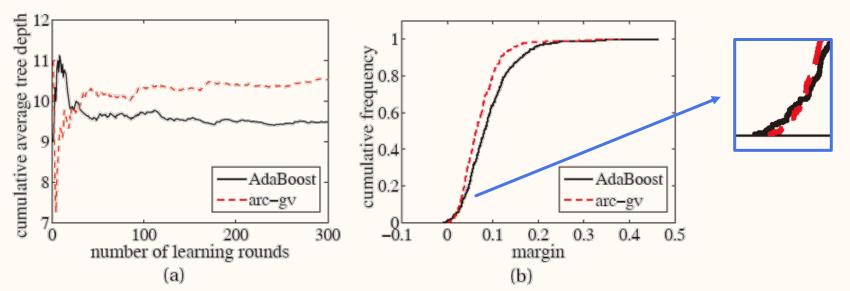
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7 years later

- Reyzin& Schapire [ICML'06 best paper] found that, amazingly, Breiman had not controlled model complexity well in exps
 - Breiman controlled the model complexity by using decision trees with a fixed number of leaves
 - Reyzin & Schapire found that, the trees of arc-gv are generally "deeper" than the trees of AdaBoost
- Reyzin& Schapire repeated Brieman's exps using decision stumps with two leaves: arc-gv is with larger minimum margin, but worse margin distribution

R&S claimed that the minimum margin is not crucial, and the average or median margin is

crucial



Supporting theory

- Equilibrium margin (Emargin) bound
 - Considered factors different from Schapire et al. and Breiman's bounds
 - No intuition to optimize
- The kth margin bound
 - The minimum margin bound and Emargin bound are special cases of the kth margin bound, both are single-margin bound (not margin distribution bound)
- Finally
 - Random choice of sample S with size $n \ge 5$, every voting classifier $f \in C(H)$ satisfies

$$\epsilon_{\text{D}} \le \frac{2}{n} + \inf_{\theta \in (0,1]} \left[\Pr_{S}[yf(x) < \theta] + \frac{7\mu + 3\sqrt{3\mu}}{3\mu} + \sqrt{\frac{3\mu}{n}} \Pr_{S}[yf(x) < \theta] \right]$$

Where

 $O(\log n/n)$

$$\mu = \frac{8}{\theta^2} \ln n \ln(2|H|) + \ln \frac{2|H|}{\delta}.$$

- Uniformly tighter than Breiman's as well as Schapire et al.' bounds
- Considers the same factors as Schapire et al. and Breiman
- thus, defends the margin theory against Breiman'sdoubt

Variance of margin also matters

Related to average margin

We should pay attention to both average margin and margin variance.

$$\epsilon_{\mathcal{D}} \leq \frac{1}{n^{50}} + \inf_{\theta \in (0,1]} \left[\Pr_{S}[yf(x) < 0] + n^{-\frac{2}{1 - E_{S}^{2}[yf(x)]} + \frac{\theta}{9}} + \frac{3\sqrt{\mu}}{n^{\frac{3}{2}}} + \frac{7\mu}{3n} + \sqrt{\frac{3\mu}{n}} \widehat{\mathfrak{T}}(\theta) \right]$$

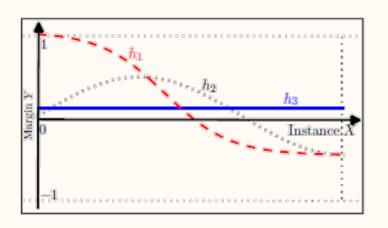
Where

$$\mu = 144 \ln m \ln(2|H|)/\theta^2 + \ln(2|H|/\delta)$$

$$\widehat{\mathfrak{T}}(\theta) = \Pr_{\mathcal{S}}[yf(x) < \theta] \Pr_{\mathcal{S}}[yf(x) \ge \frac{2\theta}{3}]$$

Related to margin variance

Experimental results



Margin variance really important

Figure from [Gao & Zhou, AIJ 2013]

Figure 1: Each curve represents a voting classifier. The X-axis and Y-axis denote example and margin, respectively, and uniform distribution is assumed on the example space. The voting classifiers h_1 , h_2 and h_3 have the same average margin but with different generalization error rates: 1/2, 1/3 and 0.

[Shivaswamy& Jebara, NIPS 2011] tried to design new boosting algorithms by maximizing average margin and minimizing margin variance simultaneously, and the results are encouraging

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Summary

- AdaBoost is an effective ensemble strategy to combines multiple weak models into a strong one
 - Additive structure + focusing on mistakes
 - It's usually easy to find a bunch of weak models but hard to find one single strong model
 - The idea behind the algorithm is more important than the algorithm itself

- We can view the AdaBoost from different perspectives
 - It use a set up of forward stagewise additive modeling
 - It can be considered as a Newton method
 - The concept of margin explains why AdaBoost seems never overtrained

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Homework

For a K-class classification problem, we can recode the class label c with a K-dimensional vector \mathbf{y} with all entries equal to $-\frac{1}{K-1}$ except a 1 in position k if c=k, i.e.,

$$y_k = \begin{cases} 1, & \text{if } c = k, \\ -\frac{1}{K-1}, & \text{if } c \neq k. \end{cases}$$

Let $\mathbf{f} = (f_1(\mathbf{x}), \dots, f_K(\mathbf{x}))^T$ with $\sum_{k=1}^K f_k(\mathbf{x}) = 0$, and define

$$L(\mathbf{y}, \mathbf{f}(\mathbf{x})) = \exp(-\frac{1}{K}\mathbf{y}^T\mathbf{f}(\mathbf{x})).$$

- (a) Using Lagrange multipliers, derive the population minimizer \mathbf{f}^* of $\mathbb{E}_{\mathbf{y}|\mathbf{x}}[L(\mathbf{y}, \mathbf{f}(\mathbf{x}))]$, subject to $\sum_{k=1}^K f_k(\mathbf{x}) = 0$, and relate these to the class probabilities.
- (b) Derive a multiclass boosting algorithm using this loss function and verify that it covers the Adaboost algorithm as a special case (K = 2).
- (c) Implement your derived algorithm, where you are allowed to call package of trees. Compare your implementation with the existing standard gradient boosting package on a multiclass classification problem. Make some discussion about what you observed. (Hint: there are two key differences: First, unlike adaboost which uses classification trees, gradient boosting uses regression trees. Second, gradient boosting has a shrinkage parameter (λ), a smaller learning rate ($\lambda = 0.01$) often dramatically improves the performance compared with $\lambda = 1$).

Backups

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Reference

- ❖ ISL, ESL
- ❖ Boosting 25年 (2014 周志华) Bilibili
- * The Annals of Statistics 2000, Vol. 28, No. 2, 337-407

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