

# Machine Learning and Computational Statistics

## Homework 6: Ensemble Methods [DRAFT - More Problems Coming]

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**Due: TBD in week after test, at 10pm (Submit via Gradescope)**

**Instructions:** Your answers to the questions below, including plots and mathematical work, should be submitted as a single PDF file. It's preferred that you write your answers using software that typesets mathematics (e.g.  $\text{\LaTeX}$ ,  $\text{\LyX}$ , or MathJax via iPython), though if you need to you may scan handwritten work. You may find the [minted](#) package convenient for including source code in your  $\text{\LaTeX}$  document. If you are using  $\text{\LyX}$ , then the [listings](#) package tends to work better.

### 1 Gradient Boosting Machines

Recall the general gradient boosting algorithm<sup>1</sup>, for a given loss function  $\ell$  and a hypothesis space  $\mathcal{F}$  of regression functions (i.e. functions mapping from the input space to  $\mathbf{R}$ ):

1. Initialize  $f_0(x) = 0$ .

2. For  $m = 1$  to  $M$ :

(a) Compute:

$$\mathbf{g}_m = \left( \left. \frac{\partial}{\partial f(x_j)} \sum_{i=1}^n \ell(y_i, f(x_i)) \right|_{f(x_i)=f_{m-1}(x_i), i=1, \dots, n} \right)_{j=1}^n$$

(b) Fit regression model to  $-\mathbf{g}_m$ :

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

(c) Choose fixed step size  $\nu_m = \nu \in (0, 1]$ , or take

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

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<sup>1</sup>Besides the lecture slides, you can find an accessible discussion of this approach in <http://www.saedsayad.com/docs/gbm2.pdf>, in one of the original references <http://statweb.stanford.edu/~jhf/ftp/trebst.pdf>, and in this review paper <http://web.stanford.edu/~hastie/Papers/buehlmann.pdf>.

(d) Take the step:

$$f_m(x) = f_{m-1}(x) + \nu_m h_m(x)$$

3. Return  $f_M$ .

In this problem we'll derive two special cases of the general gradient boosting framework:  $L_2$ -Boosting and BinomialBoost.

1. Consider the regression framework, where  $\mathcal{Y} = \mathbf{R}$ . Suppose our loss function is given by

$$\ell(\hat{y}, y) = \frac{1}{2} (\hat{y} - y)^2,$$

and at the beginning of the  $m$ 'th round of gradient boosting, we have the function  $f_{m-1}(x)$ . Show that the  $h_m$  chosen as the next basis function is given by

$$h_m = \arg \min_{h \in \mathcal{F}} \sum_{i=1}^n [(y_i - f_{m-1}(x_i)) - h(x_i)]^2.$$

In other words, at each stage we find the weak prediction function  $h_m \in \mathcal{F}$  that is the best fit to the residuals from the previous stage. [Hint: Once you understand what's going on, this is a pretty easy problem.]

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**Answer:**

The negative gradient direction of  $\ell$  can be calculated by:

$$-\frac{\partial \ell(\hat{y}, y)}{\partial \hat{y}} = -(\hat{y} - y) = y - \hat{y} = y - f(x)$$

$h_m$  is chosen to minimize the square error with  $-\frac{\partial \ell(\hat{y}, y)}{\partial \hat{y}}$ , therefore:

$$h_m = \arg \min_{h \in \mathcal{F}} \sum_{i=1}^n [(y_i - f_{m-1}(x_i)) - h(x_i)]^2.$$

2. Now let's consider the classification framework, where  $\mathcal{Y} = \{-1, 1\}$ . In lecture, we noted that AdaBoost corresponds to forward stagewise additive modeling with the exponential loss, and that the exponential loss is not very robust to outliers (i.e. outliers can have a large effect on the final prediction function). Instead, let's consider the logistic loss

$$\ell(m) = \ln(1 + e^{-m}),$$

where  $m = yf(x)$  is the margin. Similar to what we did in the  $L_2$ -Boosting question, write an expression for  $h_m$  as an argmin over  $\mathcal{F}$ .

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**Answer:** The negative gradient direction is calculated by:

$$-\frac{\partial \ell(y, f(x))}{\partial f(x)} = \frac{ye^{-yf(x)}}{1 + e^{-yf(x)}}$$

$h_m$  is chosen by:

$$\arg \min_{h \in \mathcal{F}} \sum_{i=1}^n \left[ \frac{ye^{-yf(x)}}{1 + e^{-yf(x)}} - h(x_i) \right]^2$$

## 2 From Margins to Conditional Probabilities<sup>2</sup>

Let's consider the classification setting, in which  $(x_1, y_1), \dots, (x_n, y_n) \in \mathcal{X} \times \{-1, 1\}$  are sampled i.i.d. from some unknown distribution. For a prediction function  $f : \mathcal{X} \rightarrow \mathbf{R}$ , we define the **margin** on an example  $(x, y)$  to be  $m = yf(x)$ . Since our class predictions are given by  $\text{sign}(f(x))$ , we see that a prediction is correct iff  $m(x) > 0$ . We have said we can interpret the magnitude of the margin  $|m(x)|$  as a measure of confidence. However, it is not clear what the “units” of the margin are, so it is hard to interpret the magnitudes beyond saying one prediction is more or less confident than another. In this problem, we investigate how we can translate the margin into a conditional probability, which is much easier to interpret. In other words, we are looking for a mapping  $m(x) \mapsto p(y = 1 | x)$ .

In this problem we will consider margin-based losses. A loss function is a **margin-based loss** if it can be written in terms of the margin  $m = yf(x)$ . We are interested in how we can go from an empirical risk minimizer of a margin loss,  $\hat{f} = \arg \min_{f \in \mathcal{F}} \sum_{i=1}^n \ell(y_i f(x_i))$ , to a conditional probability estimator  $\hat{\pi}(x) \approx p(y = 1 | x)$ . Our approach will be to try to find a way to use the Bayes prediction function<sup>3</sup>  $f^* = \arg \min_f \mathbb{E}_{x,y} [\ell(yf(x))]$  to get the true conditional probability  $p(y = 1 | x)$ , and then apply the same mapping to the empirical risk minimizer. While there is plenty that can go wrong with this “plug-in” approach (primarily, the empirical risk minimizer from a hypothesis space  $\mathcal{F}$  may be a poor estimate for the Bayes prediction function), it is at least well-motivated, and it can work well in practice. And **please note** that we can do better than just hoping for success: if you have enough validation data, you can directly assess how well “calibrated” the predicted probabilities are. This blog post has some discussion of calibration plots: <https://jmetzen.github.io/2015-04-14/calibration.html>.

It turns out it is straightforward to find the Bayes prediction function  $f^*$  for margin losses, at least in terms of the data-generating distribution: For any given  $x \in \mathcal{X}$ , we'll find the best possible prediction  $\hat{y}$ . This will be the  $\hat{y}$  that minimizes

$$\mathbb{E}_y [\ell(y\hat{y}) | x].$$

If we can calculate this  $\hat{y}$  for all  $x \in \mathcal{X}$ , then we will have determined  $f^*(x)$ . We will simply take

$$f^*(x) = \arg \min_{\hat{y}} \mathbb{E}_y [\ell(y\hat{y}) | x].$$

Below we'll calculate  $f^*$  for several loss functions. It will be convenient to let  $\pi(x) = \mathbb{P}(y = 1 | x)$  in the work below.

1. Write  $\mathbb{E}_y [\ell(yf(x)) | x]$  in terms of  $\pi(x)$  and  $\ell(f(x))$ . [Hint: Use the fact that  $y \in \{-1, 1\}$ .]

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**Answer:**

$$\pi(x)\ell(f(x)) + (1 - \pi(x))\ell(-f(x))$$

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<sup>2</sup>This problem is based on Section 7.5.3 of Schapire and Freund's book *Boosting: Foundations and Algorithms*.

<sup>3</sup>In this context, the Bayes prediction function is often referred to as the “population minimizer.” In our case, “population” refers to the fact that we are minimizing with respect to the true distribution, rather than a sample. The term “population” arises from the context where we are using a sample to approximate some statistic of an entire population (e.g. a population of people or trees).

2. Show that the Bayes prediction function  $f^*(x)$  for the exponential loss function  $\ell(y, f(x)) = e^{-yf(x)}$  is given by

$$f^*(x) = \frac{1}{2} \ln \left( \frac{\pi(x)}{1 - \pi(x)} \right)$$

and, given the Bayes prediction function  $f^*$ , we can recover the conditional probabilities by

$$\pi(x) = \frac{1}{1 + e^{-2f^*(x)}}.$$

[Hint: Differentiate the expression in the previous problem with respect to  $f(x)$ . To make things a little less confusing, and also to write less, you may find it useful to change variables a bit: Fix an  $x \in \mathcal{X}$ . Then write  $p = \pi(x)$  and  $\hat{y} = f(x)$ . After substituting these into the expression you had for the previous problem, you'll want to find  $\hat{y}$  that minimizes the expression. Use differential calculus. Once you've done it for a single  $x$ , it's easy to write the solution as a function of  $x$ .]

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**Answer:**

Let  $R$  be the Bayes risk:

$$\begin{aligned} R &= \mathbb{E}_y [\ell(yf(x)) \mid x] = \pi(x)e^{-f(x)} + (1 - \pi(x))e^{f(x)} \\ \frac{\partial R}{\partial f(x)} &= -\pi(x)e^{-f(x)} + (1 + \pi(x))e^{f(x)} \end{aligned} \quad (1)$$

The Bayes risk minimizer should have  $\frac{\partial R}{\partial f(x)} = 0$ .

$$\begin{aligned} \frac{\partial R}{\partial f(x)} = 0 &\iff (1 + \pi(x))e^{f^*(x)} = \pi(x)e^{-f^*(x)} \\ \frac{e^{f^*(x)}}{e^{-f^*(x)}} &= \frac{\pi(x)}{1 + \pi(x)} \\ f^*(x) &= \frac{1}{2} \ln \left( \frac{\pi(x)}{1 + \pi(x)} \right) \end{aligned} \quad (2)$$

Rearrange (1) we get:

$$\pi(x) = \frac{1}{1 + e^{-2f^*(x)}}.$$

3. Show that the Bayes prediction function  $f^*(x)$  for the logistic loss function  $\ell(y, f(x)) = \ln(1 + e^{-yf(x)})$  is given by

$$f^*(x) = \ln\left(\frac{\pi(x)}{1 - \pi(x)}\right)$$

and the conditional probabilities are given by

$$\pi(x) = \frac{1}{1 + e^{-f^*(x)}}.$$

Again, we may assume that  $\pi(x) \in (0, 1)$ .

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**Answer:**

Let  $R$  be the Bayes risk:

$$\begin{aligned} R &= \mathbb{E}_y [\ell(yf(x)) \mid x] = \pi(x)(1 + e^{-f(x)}) + (1 - \pi(x))(1 + e^{f(x)}) \\ \frac{\partial R}{\partial f(x)} &= -\pi(x)e^{-f(x)} + (1 - \pi(x))e^{f(x)} \end{aligned} \tag{3}$$

Notice that (3) and (2) are exactly the same thus we have

$$f^*(x) = \ln\left(\frac{\pi(x)}{1 - \pi(x)}\right)$$

Rearrange we get:

$$\pi(x) = \frac{1}{1 + e^{-2f^*(x)}}.$$

So Logistic lost and exponential lost have the exactly same population minimizer.

4. [Optional] Show that the Bayes prediction function  $f^*(x)$  for the hinge loss function  $\ell(y, f(x)) = \max(0, 1 - yf(x))$  is given by

$$f^*(x) = \text{sign} \left( \pi(x) - \frac{1}{2} \right).$$

Note that it is impossible to recover  $\pi(x)$  from  $f^*(x)$  in this scenario. However, in practice we work with an empirical risk minimizer, from which we may still be able to recover a reasonable estimate for  $\pi(x)$ . An early approach to this problem is known as “Platt scaling”: [https://en.wikipedia.org/wiki/Platt\\_scaling](https://en.wikipedia.org/wiki/Platt_scaling).

### 3 AdaBoost Actually Works [Optional]

#### Introduction

Given training set  $D = \{(x_1, y_1), \dots, (x_n, y_n)\}$ , where  $y_i$ 's are either  $+1$  or  $-1$ , suppose we have a weak learner  $G_t$  at time  $t$  and we will perform  $T$  rounds of AdaBoost. Initialize observation weights uniformly by setting  $W^1 = (w_1^1, \dots, w_n^1)$  with  $w_i^1 = 1/n$  for  $i = 1, 2, \dots, n$ . For  $t = 1, 2, \dots, n$ :

1. Fit the weak learner  $G_t$  at time  $t$  to training set  $D$  with weighting  $W^t$ .
2. Compute the weighted misclassification error:  $\text{err}_t = \sum_D w_i^t 1(G_t(x_i) \neq y_i) / \sum_i w_i^t$
3. Compute the contribution coefficient for the weak learner:  $\alpha_t = \frac{1}{2} \log(\frac{1}{\text{err}_t} - 1)$
4. Update the weights:  $w_i^{t+1} = w_i^t \exp(-\alpha_t y_i G_t(x_i))$

After  $T$  steps, the cumulative contributions of weak learners is  $G(x) = \text{sign}(\sum_{t=1}^T \alpha_t G_t(x))$  as the final output. We will prove that with a reasonable weak learner the error of the output decreases exponentially fast with the number of iterations.

#### Exponential bound on the training loss

More precisely, we will show that the training error  $L(G, D) = \frac{1}{n} \sum_{i=1}^n 1_{\{G(x_i) \neq y_i\}} \leq \exp(-2\gamma^2 T)$  where the error of the weak learner is less than  $1/2 - \gamma$  for some  $\gamma > 0$ . To start, let's denote two cumulative variables: the output at time  $t$  as  $f_t = \sum_{s \leq t} \alpha_s G_s$  and  $Z_t = \frac{1}{n} \sum_{i=1}^n \exp(-y_i f_t(x_i))$ .

1. For any function  $g$ , show that  $1_{\{g(x) \neq y\}} < \exp(-yg(x))$ .
2. Use this to show  $L(G, D) < Z_T$
3. Show that  $w_i^{t+1} = \exp(-y_i f_t(x_i))$
4. Use part 3 to show  $\frac{Z_{t+1}}{Z_t} = 2\sqrt{\text{err}_{t+1}(1 - \text{err}_{t+1})}$  (Hint: use the definition of weight updates and separate the sum on where  $G_t$  is equal to 1 and  $-1$ .)

5. Show that the function  $g(a) = a(1 - a)$  is monotonically increasing on  $[0, 1/2]$ . Show that  $1 - a \leq \exp(-a)$ . And use the assumption on the weak learner to show that  $\frac{Z_{t+1}}{Z_t} \leq \exp(-2\gamma^2)$
6. Conclude the proof!

## 4 AdaBoost is FSAM With Exponential Loss [Optional]

The AdaBoost score function  $G(x) = \sum_{t=1}^T \beta_t G_t(x)$  is a linear combination (actually a conic combination) of functions. (The prediction function is, of course, the sign of the score function.) Forward stagewise additive modeling (FSAM) is another approach to fitting a function of this form.

In FSAM, we have a base hypothesis space  $\mathcal{H}$  of real-valued functions  $h : \mathcal{X} \rightarrow \mathbf{R}$  and a loss function  $\ell(y, \hat{y})$ . In FSAM, we attempt to find a linear combination of  $h$ 's in  $\mathcal{H}$  that minimize the empirical risk. The procedure initializes  $f_0(x) = 0$ , and then repeats the following steps for  $t = 1, \dots, T$ :

1.  $(\beta_t, h_t) = \operatorname{argmin}_{\beta \in \mathbf{R}, h \in \mathcal{H}} \sum_{i=1}^n \ell(y_i, f_{t-1}(x_i) + \beta h(x_i))$
2.  $f_t(x) = f_{t-1}(x) + \beta_t h_t(x)$

### Exponential loss and AdaBoost

Consider a generic input space  $\mathcal{X}$ , the classification outcome space  $\mathcal{Y} = \{-1, 1\}$ , the exponential loss function  $\ell(y, f(x)) = \exp(-yf(x))$ , and an arbitrary base hypothesis space  $\mathcal{H}$  consisting of  $\{-1, 1\}$ -valued functions. We will show that FSAM in this setting is equivalent to a version of AdaBoost (Algorithm 1) described below. To get this equivalence, we either need to assume that FSAM chooses nonnegative step sizes, i.e.  $\beta_t \geq 0$ , or we need to assume that  $\mathcal{H}$  is symmetric, in the sense that if  $h \in \mathcal{H}$ , then  $-h \in \mathcal{H}$  as well.

1. Write the first step of FSAM using the exponential loss function. In particular, show that the FSAM optimization problem can be written as a minimization of a weighted exponential loss of the step  $\beta h$ :

$$(\beta_t, h_t) = \operatorname{argmin}_{\beta, h \in \mathcal{H}} \left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t \exp(-y_i \beta h(x_i)),$$

where  $w_i^t = \exp(-y_i f_{t-1}(x_i))$ . (Note that for any  $t$ , if we rescale each of  $w_1^t, \dots, w_n^t$  by the same constant factor, there is no effect on the arg min. Thus the first factor  $(\sum_{i=1}^n w_i^t)^{-1}$  can be dropped. However, we keep it so we can refer to the expression as a **weighted mean**.)

2. Define the weighted 0/1 error of  $h$  at round  $t$  to be

$$\operatorname{err}_t(h) = \left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t 1(y_i \neq h(x_i)).$$



(It's the weights that are specific to round  $t$ .) Show that the weighted exponential loss at round  $t$  can be written in terms of the weighted 0/1 error. Specifically, show that

$$\left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t \exp(-\beta y_i h(x_i)) = e^{-\beta} + (e^{\beta} - e^{-\beta}) \text{err}_t(h).$$

[Hint: Use indicators  $1(h(x_i) \neq y_i)$  and  $1(h(x_i) = y_i)$  to split the summand on the LHS into pieces. Each piece simplifies, since  $y_i, h(x_i) \in \{-1, 1\}$ . Then note that  $1(h(x_i) = y_i) = 1 - 1(h(x_i) \neq y_i)$ .]

3. We now would like to show that for any fixed “step size”  $\beta$ , the optimal “step direction”  $h$ , for which  $\beta h$  minimizes the weighted exponential loss, can be found by minimizing the weighted 0/1 error of  $h$ . But more precisely, show that if  $\beta \geq 0$  then

$$\text{argmin}_{h \in \mathcal{H}} \left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t \exp(-\beta y_i h(x_i)) = \text{argmin}_{h \in \mathcal{H}} \text{err}_t(h).$$

Also show that if  $\beta < 0$  then

$$\text{argmin}_{h \in \mathcal{H}} \left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t \exp(-\beta y_i h(x_i)) = \text{argmin}_{h \in \mathcal{H}} \text{err}_t(-h).$$

4. Show that if  $\mathcal{H}$  is symmetric, in the sense that  $h \in \mathcal{H}$  implies  $-h \in \mathcal{H}$ , then there is always an optimal FSAM step  $(\beta_t, h_t)$  with  $\beta_t \geq 0$ . Thus if we assume that either  $\mathcal{H}$  is symmetric or FSAM chooses nonnegative step sizes, then we can conclude that

$$h_t = \text{argmin}_{h \in \mathcal{H}} \text{err}_t(h)$$

is a solution to  $h_t$  in the minimization problem in the first part, and thus is the FSAM step direction in round  $t$ .

5. Now that we've found  $h_t$ , show that the corresponding optimal step size is given by  $\beta_t = \frac{1}{2} \log \left( \frac{1 - \text{err}_t}{\text{err}_t} \right)$ , where we let  $\text{err}_t = \text{err}_t(h_t)$  as a shorthand. [Hint: You'll need to use some differential calculus. Show that what you've found is a minimum by showing that the function you're differentiating is convex.]
6. Show that

$$w_i^{t+1} = \begin{cases} e^{-\beta_t} w_i^t & \text{if } y_i = h_t(x_i) \\ e^{-\beta_t} w_i^t e^{2\beta_t} & \text{otherwise,} \end{cases}$$

This is the weight update equation from AdaBoost. [Hint: First show that  $w_i^{t+1} = w_i^t \exp(-\beta_t y_i h_t(x_i))$ . Then write  $y_i h_t(x_i)$  in terms of the indicator function  $y_i \neq h_t(x_i)$ .]

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**Algorithm 1:** Exact AdaBoost

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input: Training set  $\mathcal{D} = ((x_1, y_1), \dots, (x_n, y_n)) \in \mathcal{X} \times \{-1, 1\}$ 
 $w_i^1 = 1$  for  $i = 1, \dots, n$  #Initialize weights
for  $t = 1, \dots, T$ :
     $h_t = \arg \min_{h \in \mathcal{H}} \sum_{i=1}^n w_i^t 1(y_i \neq h(x_i))$ 
     $\text{err}_t = \text{err}_t(h_t) = \left( \frac{1}{\sum_{i=1}^n w_i^t} \right) \sum_{i=1}^n w_i^t 1(y_i \neq h(x_i))$ 
     $\alpha_t = \ln \left( \frac{1 - \text{err}_t}{\text{err}_t} \right)$ 
     $w_i^{t+1} = \begin{cases} w_i^t & \text{if } y_i = h_t(x_i) \\ w_i^t e^{\alpha_t} & \text{otherwise,} \end{cases} \quad \text{for } i = 1, \dots, n$ 
return  $f = \sum_{t=1}^T \alpha_t h_t$  #Returns the score function.
(Predictions are  $x \mapsto \text{sign}(f(x))$ ) .
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7. Let's introduce a specific instance of AdaBoost we'll call "Exact AdaBoost", given in Algorithm 1. The only difference between Exact AdaBoost and AdaBoost is that in Exact AdaBoost, we require that the base classifier return the best possible  $h \in \mathcal{H}$ , while in AdaBoost we only vaguely stated that the "base learner fits the weighted training data", but there was no requirement that the result be the best possible. Indeed, since a typical base classifier is decision trees, and it's computationally prohibitive to find the best possible tree, Exact AdaBoost is not usually an implementable algorithm. Show that the score functions returned by Exact Adaboost and by FSAM (in our setting) differ only by a constant factor, and of course the hard classifications will be exactly the same.
8. Suppose our ultimate goal is to find the score function returned by FSAM after  $T$  rounds in the context described above. Suppose we only have access to an implementation of Exact AdaBoost described in Algorithm 1, and it returns the score function  $f(x)$ . What would be the score function returned by FSAM?