Math ∩ Programming

The Boosting Margin, or Why Boosting Doesn't Overfit

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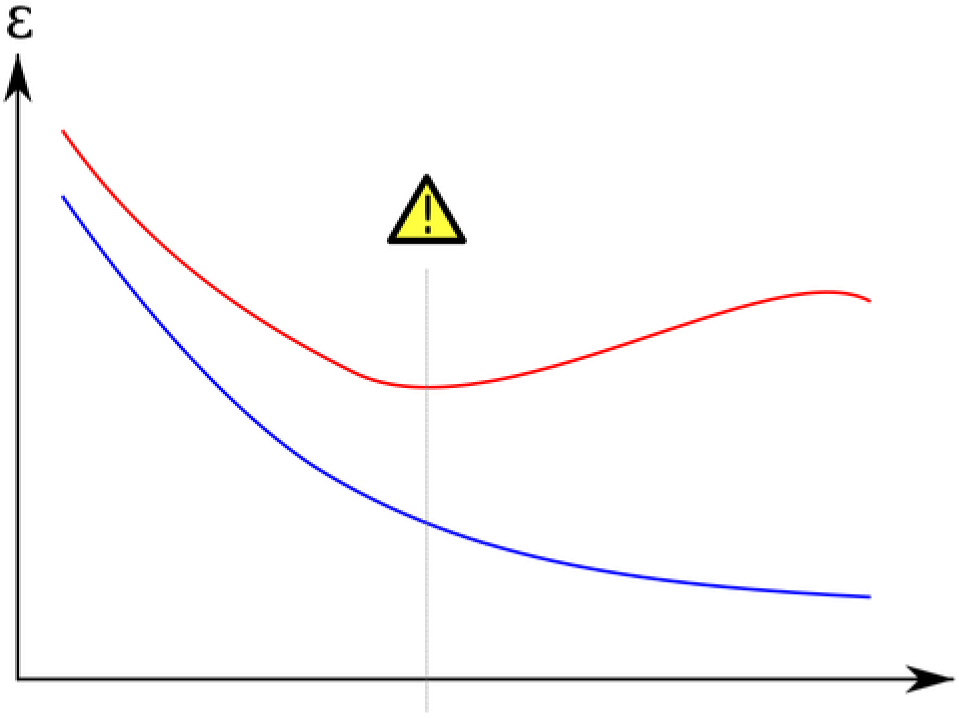
There's a well-understood phenomenon in machine learning called *overfitting*. The idea is best shown by a graph:



(https://jeremykun.files.wordpress.com/2015/06/overfitting.png)

Let me explain. The vertical axis represents the error of a hypothesis. The horizontal axis represents the complexity of the hypothesis. The blue curve represents the error of a machine learning algorithm's output on its training data, and the red curve represents the *generalization* of that hypothesis to the real world. The overfitting phenomenon is marker in the middle of the graph, before which the training error and generalization error both go down, but after which the training error continues to fall while the generalization error rises.

The explanation is a sort of numerical version of Occam's Razor (https://en.wikipedia.org/wiki/Occam%27s_razor) that says more complex hypotheses can model a *fixed* data set better and better, but at some point a simpler hypothesis better models the underlying phenomenon that generates the data. To optimize a particular learning algorithm, one wants to set parameters of their model to hit the minimum of the red curve.

This is where things get juicy. Boosting, which we covered in gruesome detail previously (https://jeremykun.com/2015/05/18/boosting-census/), has a natural measure of complexity represented by the number of rounds you run the algorithm for. Each round adds one additional "weak learner" weighted vote. So running for a thousand rounds gives a vote of a thousand weak learners. Despite this, boosting **doesn't overfit** on many datasets. In fact, and this is a shocking fact, researchers observed that Boosting would hit **zero training error,** they kept running it for more rounds, and the generalization error kept going down! It seemed like the complexity could grow arbitrarily without penalty.

Schapire, Freund, Bartlett, and Lee (http://www.cc.gatech.edu/~isbell/tutorials/boostingmargins.pdf) proposed a theoretical explanation for this based on the notion of a margin, and the goal of this post is to go through the details of their theorem and proof. Remember that the standard AdaBoost algorithm (https://jeremykun.com/2015/05/18/boosting-census/) produces a set of *weak hypotheses* $h_i(x)$ and a corresponding weight $\alpha_i \in [-1, 1]$ for each round $i = 1, \dots, T$. The classifier at the end is a weighted majority vote of all the weak learners (roughly: weak learners with high error on "hard" data points get less weight).

Definition: The *signed confidence* of a labeled example (x, y) is the weighted sum:

$$\textup{conf}(x) = \sum_{i=1}^T \alpha_i h_i(x)$$

The *margin* of (x, y) is the quantity $\textup{margin}(x, y) = y \textup{conf}(x)$. The notation implicitly depends on the outputs of the AdaBoost algorithm via "conf."

We use the product of the label and the confidence for the observation that $y \cdot \textup{conf}(x) \leq 0$ if and only if the classifier is incorrect. The theorem we'll prove in this post is

Theorem: With high probability over a random choice of training data, for any $0 < \theta < 1$ generalization error of boosting is bounded from above by

$$\Pr_{\textup{train}} [\textup{margin}(x) \leq \theta] + O \left (\frac{1}{\theta} (\textup{typical error terms}) \right)$$

In words, the generalization error of the boosting hypothesis is bounded by the distribution of margins observed *on the training data*. To state and prove the theorem more generally we have to return to the details of PAC-learning. Here and in the rest of this post, $\Pr_D$ denotes $\Pr_{x \sim D}$, the probability over a random example drawn from the distribution D, and $\Pr_S$ denotes the probability over a random (training) set of examples drawn from D.

Theorem: Let S be a set of m random examples chosen from the distribution D generating the data. Assume the weak learner corresponds to a finite hypothesis space H of size $|H|$, and let $\delta > 0$. Then with probability at least $1 - \delta$ (over the choice of S), **every** weighted-majority vote function f satisfies the following generalization bound for every $\theta > 0$.

$$\Pr_D[yf(x) \leq 0] \leq \Pr_S[yf(x) \leq \theta] + O \left (\frac{1}{\sqrt{m}} \sqrt{\frac{\log m \log |H|}{\theta^2} + \log(1/\delta)} \right)$$

In other words, this phenomenon is a fact about voting schemes, not boosting in particular. From now on, a "majority vote" function $f(x)$ will mean to take the sign of a sum of the form $\sum_{i=1}^N a_i h_i(x)$, where $a_i \geq 0$ and $\sum_i a_i = 1$. This is the "convex hull" of the set of weak learners H. If H is infinite (in our proof it will be finite, but we'll state a generalization afterward), then only finitely many of the a_i in the sum may be nonzero.

To prove the theorem, we'll start by defining a class of functions corresponding to "unweighted majority votes with duplicates:"

Definition: Let C_N be the set of functions $f(x)$ of the form $\frac{1}{N} \sum_{i=1}^N h_i(x)$ where $h_i \in H$ and the h_i may contain duplicates (some of the h_i may be equal to some other of the h_j).

Now every majority vote function f can be written as a weighted sum of h_i with weights a_i (I'm using a instead of α to distinguish arbitrary weights from those weights arising from Boosting). So any such $f(x)$ defines a natural distribution over H where you draw function h_i with probability a_i. I'll call this distribution A_f. If we draw from this distribution N times and take an unweighted sum, we'll get a function $g(x) \in C_N$. Call the random process (distribution) generating functions in this way Q_f. In diagram form, the logic goes

$f \to$ weights $a_i \to$ distribution over $H \to$ function in C_N by drawing N times according to H.

The main fact about the relationship between f and Q_f is that each is completely determined by the other. Obviously Q_f is determined by f because we defined it that way, but f is also completely determined by Q_f as follows:

$$f(x) = \mathbb{E}_{g \sim Q_f}[g(x)]$$

Proving the equality is an exercise for the reader.

Proof of Theorem. First we'll split the probability $\Pr_D[yf(x) \leq 0]$ into two pieces, and then bound each piece.

First a probability reminder. If we have two events A and B (in what's below, this will be $yg(x) \leq \theta/2$ and $yf(x) \leq 0$, we can split up $\Pr[A]$ into $\Pr[A \textup{ and } B] + \Pr[A \textup{ and } \overline{B}]$ (where $\overline{B}$ is the opposite of B). This is called the law of total probability. Moreover, because $\Pr[A \textup{ and } B] = \Pr[A | B] \Pr[B]$ and because these quantities are all at most 1, it's true that $\Pr[A \textup{ and } B] \leq \Pr[A \mid B]$ (the conditional probability) and that $\Pr[A \textup{ and } B] \leq \Pr[B]$.

Back to the proof. Notice that for any $g(x) \in C_N$ and any $\theta > 0$, we can write $\Pr_D[yf(x) \leq 0]$ as a sum:

$$\begin{aligned} &\Pr_D[yf(x) \leq 0] = \\ &\Pr_D[yg(x) \leq \theta/2 \textup{ and } yf(x) \leq 0] + \Pr_D[yg(x) > \theta/2 \textup{ and } yf(x) \leq 0] \end{aligned}$$

Now I'll loosen the first term by removing the second event (that only makes the whole probability bigger) and loosen the second term by relaxing it to a conditional:

$$\Pr_D[yf(x) \leq 0] \leq \Pr_D[yg(x) \leq \theta/2] + \Pr_D[yg(x) > \theta/2 \mid yf(x) \leq 0]$$

Now because the inequality is true for every $g(x) \in C_N$, it's also true if we take an expectation of the RHS over any distribution we choose. We'll choose the distribution Q_f to get

$$\Pr_D[yf(x) \leq 0] \leq T_1 + T_2$$

And T_1 (term 1) is

$$T_1 = \Pr_{x \sim D, g \sim Q_f}[yg(x) \leq \theta/2] = \mathbb{E}_{g \sim Q_f}[\Pr_D[yg(x) \leq \theta/2]]$$

And T_2 is

$$\Pr_{x \sim D, g \sim Q_f}[yg(x) > \theta/2 \mid yf(x) \leq 0] = \mathbb{E}_D[\Pr_{g \sim Q_f}[yg(x) > \theta/2 \mid yf(x) \leq 0]]$$

We can rewrite the probabilities using expectations because (1) the variables being drawn in the distributions are independent, and (2) the probability of an event is the expectation of the indicator function of the event.

Now we'll bound the terms T_1, T_2 separately. We'll start with T_2.

Fix (x, y) and look at the quantity inside the expectation of T_2.

$$\Pr_{g \sim Q_f}[yg(x) > \theta/2 \mid yf(x) \leq 0]$$

This should intuitively be very small for the following reason. We're sampling g according to a distribution whose expectation is f, and we *know* that $yf(x) \leq 0$. Of course $yg(x)$ is unlikely to be large.

Mathematically we can prove this by transforming the thing inside the probability to a form suitable for the Chernoff bound (https://jeremykun.com/2013/04/15/probabilistic-bounds-a-primer/). Saying $yg(x) > \theta/2$ is the same as saying $|yg(x) - \mathbb{E}[yg(x)]| > \theta/2$, i.e. that some random variable which is a sum of independent random variables (the h_i) deviates from its expectation by at least $\theta/2$. Since the y's are all ± 1 and constant inside the expectation, they can be removed from the absolute value to get

$$\leq \Pr_{g \sim Q_f}[g(x) - \mathbb{E}[g(x)] > \theta/2]$$

The Chernoff bound (https://jeremykun.com/2013/04/15/probabilistic-bounds-a-primer/) allows us to bound this by an exponential in the number of random variables in the sum, i.e. N. It turns out the bound is $e^{-N\theta^2/8}$.

Now recall T_1

$$T_1 = \Pr_{x \sim D, g \sim Q_f}[yg(x) \leq \theta/2] = \mathbb{E}_{g \sim Q_f}[\Pr_D[yg(x) \leq \theta/2]]$$

For T_1, we don't want to bound it absolutely like we did for T_2, because there is nothing stopping the classifier f from being a bad classifier and having lots of error. Rather, we want to bound it in terms of the probability that $yf(x) \leq \theta$. We'll do this in two steps. In step 1, we'll go from $\Pr_D$ of the g's to $\Pr_S$ of the g's.

Step 1: For any fixed g, θ, if we take a sample S of size m, then consider the event in which the sample probability deviates from the true distribution by some value ε_N, i.e. the event

$$\Pr_D[yg(x) \leq \theta/2] > \Pr_{S, x \sim S}[yg(x) \leq \theta/2] + \varepsilon_N$$

The claim is this happens with probability at most $e^{-2m\varepsilon_N^2}$. This is again the Chernoff bound in disguise, because the expected value of $\Pr_S$ is $\Pr_D$, and the probability over S is an average of random variables (it's a slightly different form of the Chernoff bound; see this post (https://jeremykun.com/2013/04/15/probabilistic-bounds-a-primer/) for more). From now on we'll drop the $x \sim S$ when writing $\Pr_S$.

The bound above holds true for any fixed g, θ, but we want a bound over all g and θ. To do that we use the union bound. Note that there are only $(N+1)$ possible choices for a nonnegative θ because $g(x)$ is a sum of N values each of which is either ± 1. And there are only $|C_N| \leq |H|^N$ possibilities for $g(x)$. So the union bound says the above event will occur with probability at most $(N+1)|H|^N e^{-2m\varepsilon_N^2}$.

If we want the event to occur with probability at most δ_N, we can judiciously pick

$$\varepsilon_N = \sqrt{(1/2m)\log((N+1)|H|^N/\delta_N)}$$

And since the bound holds in general, we can take expectation with respect to Q_f and nothing changes. This means that for any δ_N, our chosen ε_N ensures that the following is true with probability at least $1 - \delta_N$:

$$\Pr_{D, g \sim Q_f}[yg(x) \leq \theta/2] \leq \Pr_{S, g \sim Q_f}[yg(x) \leq \theta/2] + \varepsilon_N$$

Now for step 2, we bound the probability that $yg(x) \leq \theta/2$ on a sample to the probability that $yf(x) \leq \theta$ on a sample.

Step 2: The first claim is that

$$\Pr_{S, g \sim Q_f}[yg(x) \leq \theta/2] \leq \Pr_S[yf(x) \leq \theta] + \mathbb{E}_S[\Pr_{g \sim Q_f}[yg(x) \leq \theta/2 \mid yf(x) \geq \theta]]$$

What we did was break up the LHS into two "and"s, when $yf(x) > \theta$ and $yf(x) \leq \theta$ (this was still an equality). Then we loosened the first term to $\Pr_S[yf(x) \leq \theta]$ since that is only more likely than both $yg(x) \leq \theta/2$ and $yf(x) \leq \theta$. Then we loosened the second term again using the fact that a probability of an "and" is bounded by the conditional probability.

Now we have the probability of $yg(x) \leq \theta/2$ bounded by the probability that $yf(x) \leq 0$ plus some stuff. We just need to bound the "plus some stuff" absolutely and then we'll be done. The argument is the same as our previous use of the Chernoff bound: we assume $yf(x) \geq \theta$, and yet $yg(x) \leq \theta/2$. So the deviation of $yg(x)$ from its expectation is large, and the probability that happens is exponentially small in the amount of deviation. The bound you get is

$$\Pr_{g \sim Q}[yg(x) \leq \theta/2 \mid yf(x) > \theta] \leq e^{-N\theta^2/8}.$$

And again we use the union bound to ensure the failure of this bound for any N will be very small. Specifically, if we want the total failure probability to be at most δ, then we need to pick some δ_j's so that $\delta = \sum_{j=0}^{\infty} \delta_j$. Choosing $\delta_N = \frac{\delta}{N(N+1)}$ works.

Putting everything together, we get that with probability at least $1 - \delta$ for every θ and every N, this bound on the failure probability of $f(x)$:

$$\Pr_{x \sim D}[yf(x) \leq 0] \leq \Pr_{S, x \sim S}[yf(x) \leq \theta] + 2e^{-N\theta^2/8} + \sqrt{\frac{1}{2m}\log\left(\frac{N(N+1)^2|H|^N}{\delta}\right)}.$$

This claim is true for *every* N, so we can pick N that minimizes it. Doing a little bit of behind-the-scenes calculus that is left as an exercise to the reader, a tight choice of N is $(4/\theta)^2 \log(m/\log|H|)$. And this gives the statement of the theorem.

□

We proved this for finite hypothesis classes, and if you know what VC-dimension (https://en.wikipedia.org/wiki/VC_dimension) is, you'll know that it's a central tool for reasoning about the complexity of infinite hypothesis classes. An analogous theorem can be proved in terms of the VC dimension. In that case, calling d the VC-dimension of the weak learner's output hypothesis class, the bound is

$$\Pr_D[yf(x) \leq 0] \leq \Pr_S[yf(x) \leq \theta] + O\left(\frac{1}{\sqrt{m}} \sqrt{\frac{d \log^2(m/d)}{\theta^2} + \log(1/\delta)} \right)$$

How can we interpret these bounds with so many parameters floating around? That's where asymptotic notation comes in handy. If we fix $\theta \leq 1/2$ and $\delta = 0.01$, then the big-O part of the theorem simplifies to $\sqrt{(\log |H| \cdot \log m)/m}$, which is easier to think about since $(\log m)/m$ goes to zero very fast.

Now the theorem we just proved was about any weighted majority function. The question still remains: why is AdaBoost good? That follows from another theorem, which we'll state and leave as an exercise (it essentially follows by unwrapping the definition of the AdaBoost algorithm from last time (https://jeremykun.com/2015/05/18/boosting-census/)).

Theorem: Suppose that during AdaBoost the weak learners produce hypotheses with training errors $\varepsilon_1, \dots , \varepsilon_T$. Then for any θ,

$$\Pr_{(x,y) \sim S} [yf(x) \leq \theta] \leq 2^T \prod_{t=1}^T \sqrt{\varepsilon_t^{(1-\theta)} (1-\varepsilon_t)^{(1+\theta)}}$$

Let's interpret this for some concrete numbers. Say that $\theta = 0$ and ε_t is any fixed value less than $1/2$. In this case the term inside product becomes $\sqrt{\varepsilon (1-\varepsilon)} < 1/2$ and the whole bound tends exponentially quickly to zero in the number of rounds T. On the other hand, if we raise θ to about 1/3, then in order to maintain the LHS tending to zero we would need $\varepsilon < \frac{1}{4} (3 - \sqrt{5})$ which is about 20% error.

If you're interested in learning more about Boosting, there is an excellent book by Freund and Schapire (the inventors of boosting) called Boosting: Foundations and Algorithms (http://www.amazon.com/gp/product/0262526034/ref=as_li_tl?ie=UTF8&camp=1789&creative=9325&creativeASIN=0262526034&linkCode=as2&tag=mathinterpr00-20&linkId=SZ2UCYBU7WCKMWJ2). There they include a tighter analysis based on the idea of Rademacher complexity (https://en.wikipedia.org/wiki/Rademacher_complexity). The bound I presented in this post is nice because the proof doesn't require any machinery past basic probability, but if you want to reach the cutting edge of knowledge about boosting you need to invest in the technical stuff.

Until next time!

This entry was posted in Algorithms, Computing Theory, Learning Theory, Probability Theory and tagged boosting, chernoff bound, classficiation, conditional probability, machine learning, margins, mathematics, occam's razor, overfitting, vc-dimension. Bookmark the permalink.

5 thoughts on "The Boosting Margin, or Why Boosting Doesn't Overfit"

1. **Daniel**

   September 27, 2015 at 6:56 am • Reply

   IMHO this article has too many formulas, the exposition could be more paced with some ideas or insight to make it more interesting for beginners. Just my two cents.

2. **Mathusuthan Kannan**

   September 30, 2015 at 9:50 am • Reply

   Thank you … Super interesting

3. **Daniel**

   October 3, 2015 at 5:25 am • Reply

   I wonder if bagging is going in the nearest neighbor direction, that is like human lungs in which you take more oxygen by growing small alveoli. There could be a king of fractal, since a leaf can become a tree. One kind of "learning algorithm fractal dimension" could define a way in which a fractal derivation of a learning algorithm increase its performance in the test. There could be a "fractal learning dimension" related to principal dimensions but generalizing the algorithms and its properties with a fractal objects, in this case averaging or bagging. Looking forward to your next post.

   As there is nothing new under the sun says, it could happen that the bagging as a fractal device hypothesis or insight has been previously explored, in that case any link could be appreciated.

4. **Mads Lindskou**

   August 15, 2017 at 9:31 am • Reply

   Someone mentioned, that the article has too many formulas. I must disagree; it is VERY useful and add details to the original proof which is more vague. Thank you.

   - **j2kun**

     August 15, 2017 at 5:32 pm • Reply

     Thanks, yes, maybe 20% of the technical posts I write intend to do just that, writing down the details I struggled to work out.