## CIS 625: Introduction to Computational Learning Theory Lecture Notes

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#### 1. A Theoretical Model for Classification

We define X,  $\mathcal{D}$ ,  $\mathcal{C}$ ,  $c_t$ , and EX here:

- an input space X (e.g.  $X = \mathbb{R}^n$ ,  $X = \{0, 1\}^n$ )
- unknown and arbitrary distribution  $\mathcal{D}$  over X
- known class C of binary functions
  - examples:  $c \in C$ ,  $c: X \to \{1, -1\}$  or  $c: X \to \{0, 1\}$
- unknown target function  $c_t \in \mathcal{C}$
- access to procedure (oracle)  $\mathrm{EX}(c_t,\mathcal{D})$  that returns  $\langle x,c_t(x)\rangle$  pairs where  $X\sim D$ 
  - This oracle essentially gives you training data.
- The goal is not to fit the training data from the oracle well but to learn a function  $h \in \mathcal{C}$  that generalizes well. In other words, we'd like to learn a function h that is close to the target function  $c_t \in \mathcal{C}$ . Notice that in this model, the function we learn and the target function are both in the same class of binary functions.
- The learning algorithm is constrained by "sample efficiency" and "computational efficiency." These are formalized below.

# 1.1 Probably Approximately Correct (PAC) Learning Definition

A class C is PAC-learnable if:

 $\exists$  an algorithm L such that

 $\forall c_t \in \mathcal{C}, \forall \mathcal{D} \text{ over } X, \forall \epsilon, \delta > 0,$ 

given  $\epsilon$ ,  $\delta$ , and  $\mathrm{EX}(c_t, D)$ , L outputs  $h \in \mathcal{C}$  with probability  $1 - \delta$  ("Probably") and the following conditions hold:

1. Learning Condition ("Approximately Correct"):

$$\Pr_{X \sim \mathcal{D}}[h(x) \neq c_t(x)] \le \epsilon$$

2. Sample Efficiency:

number of calls to 
$$\mathrm{EX}(c_t,\mathcal{D})$$
 is poly  $\left(\frac{1}{\epsilon},\frac{1}{\delta},n\right)$ 

3. Computational Efficiency:

running time of 
$$L$$
 is poly  $\left(\frac{1}{\epsilon}, \frac{1}{\delta}, n\right)$ 

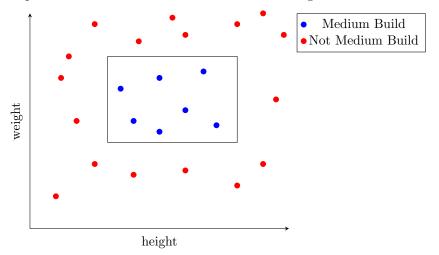
Note that with the model of computation where EX takes constant time, this  $3^{\rm rd}$  condition implies the  $2^{\rm nd}$  condition.

#### 1.2 Rectangle Example

Consider the problem of classifying people of medium build. It might make sense to classify a person as having medium build if they're inside some rectangle. Similarly, all people outside the rectangle would be classified as not having medium build.

- Input Space:  $X = \mathbb{R}^2$
- Known Class of Binary Functions: C = all axis-aligned (edges parallel to coordinate axes) rectangles in  $\mathbb{R}^2$

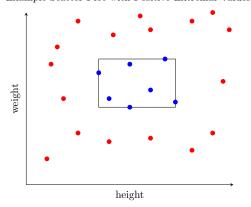
Example Scatter Plot with some Classification Rectangle:

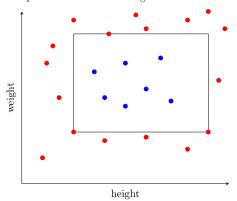


Because the rectangle (h) above correctly classifies all the data points, we say h is consistent. More formally,  $c \in \mathcal{C}$  is consistent with S if for all  $1 \leq i \leq m$ ,  $c(x_i) = b_i$  where  $S = \{\langle x_1, b_1 \rangle, \dots, \langle x_m, b_m \rangle\}$  is the training data obtained from the oracle. There are many different consistent  $c \in C$ . For example, there is one on the next page that draws the rectangle according to the extremal values of the *positive* examples (left) and the other draws the rectangle according to the extremal values of the negative examples (right).

Example Scatter Plot with Positive Extremal Values:

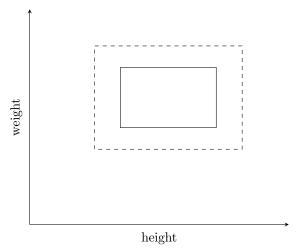
Example Scatter Plot with Negative Extremal Values:





Although these two rectangles are consistent, they might not generalize as well to data not in S because they tightly fit either the positive training examples (left) or the negative training examples (right).

Let's consider the rectangle on the left, the one that is drawn tightly around the extremal values of the positive training examples. Let that rectangle be the function we have learned so far: h. It is the solid rectangle in the graph below. The dotted rectangle is the target function  $c_t$ .



We want to bound the probability that h differs from  $c_t$ . To do this, first consider just the topmost strip between the edge of h and the edge of  $c_t$ . We'll call this region T.



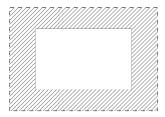
We can bound the size of T. Let the probability mass that's in T be  $\frac{\epsilon}{4}$ . This choice will make sense soon. This means that when sampling a single example  $x_i$  from EX, we know the following:

$$\Pr_{X \sim \mathcal{D}}[x_i \text{ not in } T] = 1 - \frac{\epsilon}{4}$$

Assuming independence, for m examples from EX, we know:

$$\Pr_{X \sim \mathcal{D}}[\text{all of } x_1 \dots x_m \text{ are not in } T] = \left(1 - \frac{\epsilon}{4}\right)^m$$

This is important because the probability of not expanding h is exponentially small in our number of training examples. Now that we've examined a single strip, let's look at the whole portion of area that is outside of h and inside of  $c_t$ . Let this region be B.



If we let each of the strips have roughly the same probability mass, we can bound the probability of not getting a single example in B using the union bound:

$$\Pr_{X \sim \mathcal{D}}[\text{all of } x_1 \dots x_m \text{ are not in } B] \le 4 \left(1 - \frac{\epsilon}{4}\right)^m$$

What we've been doing is working on making that shaded rectangular border B as small as necessary to make h close to  $c_t$ . This is the learning condition or the "Approximately Correct" (AC) part of PAC learning. To get the "Probably" (P) part of PAC learning, we need to bound this probability:

$$4\left(1 - \frac{\epsilon}{4}\right)^m \le \delta$$

Using  $(1-x) \approx e^{-x}$  (for small x), we have:

$$4e^{-\frac{\epsilon}{4}m}\approx 4\left(1-\frac{\epsilon}{4}\right)^m\leq \delta$$

$$4e^{-\frac{\epsilon}{4}m} \le \delta$$
$$-\frac{\epsilon}{4}m \le \ln\frac{\delta}{4}$$
$$m \ge \frac{4}{\epsilon}\ln\frac{4}{\delta}$$

Because m is polynomial in  $\frac{1}{\epsilon}$  and logarithmic in  $\frac{1}{\delta}$ , we have satisfied the Sample Efficiency condition. Although we did this analysis for 2D, the number of "strips" grows linearly with the number of dimensions, so that's not a problem. Also, the analysis doesn't use the distribution  $\mathcal{D}$  at all. It only uses independence of training examples.

## 2. PAC Learning Model

Let's first review the definition of a PAC-learnable class of functions:

Given the instance space  $\mathcal{X}$ , we say that a **concept** c is a subset  $c \subseteq \mathcal{X}$ . A concept may be considered a set of all positive instances that satisfy a particular rule. Therefore, we can write  $c: \mathcal{X} \to \{0,1\}$ . A **concept class** is a collection of concepts over  $\mathcal{X}$ .

Given a model's hypothesis h(x) and the target concept c(x), we define the **general error** or **true error** of the model as follows:

$$err_D(h) = P_{x \sim D}(h(x) \neq c(x))$$

The true error describes the probability of that the hypothesis misclassifies an arbitrary data point from  $\mathcal{X}$ . That is, it characterizes how well our hypothesis performs well on test data, not just the training set.

*PAC-learnability.* A concept class  $\mathcal{C}$  is PAC-learnable if  $\exists$  a learning algorithm  $\mathcal{L}$  such that  $\forall c_t \in \mathcal{C}$ ,  $\forall$  distributions  $\mathcal{D}$  over  $\mathcal{X}$ , and  $\forall \epsilon, \delta > 0$ , and given some  $\epsilon$ ,  $\delta$ , and an oracle  $EX(c_t, \mathcal{D})$ ,  $\mathcal{L}$  outputs an  $h \in \mathcal{C}$  such that with probability at least  $1 - \delta$  it satisfies the following conditions:

- 1. (Learning Condition)  $err_D(h) \leq \epsilon$ . That is, the probability of a misclassification is bounded by a constant.
- 2. (Sample Efficiency) The number of calls to EX(c,D) is polynomial with respect to  $\frac{1}{\epsilon}$ ,  $\frac{1}{\delta}$ , and n.
- 3. (Computational Efficiency) The running time is polynomial with respect to  $\frac{1}{\epsilon}$ ,  $\frac{1}{\delta}$ , and n.

Consistency. Given labeled samples  $S = \{ \langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle, ..., \langle x_m, y_m \rangle | y_i = c(x_i) \ \forall 1 \leq i \leq m \}$ , then we say some  $h \in \mathcal{C}$  is **consistent** with S if  $\forall 1 \leq i \leq m, h(x_i) = y_i$ . That is, a function  $h \in \mathcal{C}$  is consistent with our sample data if it correctly classifies every sample in our sample data S.

## 3. Generalizing the Sample Bound

Suppose then, that we have a learning algorithm  $\mathcal{L}$  that always finds a hypothesis  $h \in \mathcal{C}$  that is consistent over a sample S, where  $\mathcal{C}$  is a finite concept class. We can upper bound the probability that the general error of h will never exceed some  $\epsilon$  and use this to compute a prudent choice of m = |S|. We can then say that the learning algorithm  $\mathcal{L}$  satisfies the learning-condition from our PAC model.

 $\epsilon$ -badness. We say that some hypothesis  $h \in \mathcal{C}$  is  $\epsilon$ -bad if  $err_D(h) > \epsilon$ . Inversely, h is  $\epsilon$ -good if  $err_D(h) \leq \epsilon$ .

This means that for an  $\epsilon$ -bad hypothesis h and a sample S of m points drawn from the distribution  $\mathcal{D}$ , the probability that h is consistent over S is

$$P_{S \sim \mathcal{D}, c}(\epsilon\text{-bad } h \text{ consistent with } S) \leq (1 - \epsilon)^m$$

What if we wanted to find the same probability, except for some  $h \in \mathcal{C}$ ? That is, what if we wanted to find the probability that some  $h \in \mathcal{C}$  is consistent with S and  $\epsilon$ -bad? We could assume that the probability that each h is consistent with S is independent for the purpose of defining an upper bound. Thus we can say that

$$P_{S \sim D,c}(\exists \epsilon \text{-bad } h \text{ that is consistent with } S) \leq |\mathcal{C}|(1-\epsilon)^m$$

by using a union bound.

Now we want to show that this probability is less than some  $\delta$  so that we can meet the guarantee that with probability at least  $1-\delta$  our algorithm doesn't output an  $\epsilon$ -bad function.

$$\begin{aligned} |\mathcal{C}|(1-\epsilon)^m &\leq \delta \\ &\leq |\mathcal{C}|e^{-\epsilon m} \leq \delta \\ &\implies m \geq \frac{c_0}{\epsilon} \ln(\frac{|\mathcal{C}|}{\delta}) \end{aligned}$$

where  $c_0$  is some constant. Thus, we have shown that if we have  $m \geq \frac{c_0}{\epsilon} \ln(\frac{|\mathcal{C}|}{\delta})$  samples, the learning algorithm  $\mathcal{L}$  satisfies the learning condition.

Then, given a number of m examples, the error we expect is, with probability at least  $1 - \delta$ ,

$$err_D(h) \le \frac{c_0}{m} \ln(\frac{|\mathcal{C}|}{\delta})$$

We can formalize this as a theorem:

**Theorem 1.** Let C be a finite concept class defined on the domain X. Let  $\mathcal{L}$  be an algorithm such that for any m and for any  $c \in C$ , if S is a labeled training set  $\{\langle x_i, c(x_i) \rangle\}_{i=1}^m$ , then the hypothesis h generated by  $\mathcal{L}(S)$  is consistent with S. Then, with sample complexity  $m \geq \frac{c_0}{\epsilon} \ln(\frac{|C|}{\delta})$ ,  $\mathcal{L}$  satisfies the learning condition with probability  $1 - \delta$ .

## 4. Application 1: Learning Boolean Conjunctions

We can define the problem of learning boolean conjunctions. Here, our instance space is  $X = \{0,1\}^n$ , and our class of functions  $\mathcal{C}$  are the conjunctions over  $x_1, x_2, ..., x_n$ . For example, one such  $c \in \mathcal{C}$  could be  $x_3 \land \neg x_5 \land x_6 \land \neg x_{10}$ . We can see that  $\mathcal{C}$  is finite, with  $|C| = 3^n$ , since for each  $x_i$  we can either include it, include its negation, or not include it.

One simple algorithm to solve this problem is shown below.

```
h \leftarrow x_1 \wedge \neg x_1 \wedge x_2 \wedge \neg x_2 \dots x_n \wedge \neg x_n
for \langle x_i, y \rangle \in S do
  if y is false then
   ignore
  else
  if x_i = 1 then
   delete \neg x_i from h
  else
  delete x_i from h
```

Simple learning algorithm for boolean conjunctions.

While there could be more specific algorithms that, for example, use the false samples, we can see that this one is consistent with our samples and thus, by the theorem above, will satisfy the learning condition given enough samples.

Some things to note about this algorithm:

- This algorithm works even if all samples are negative, because it always returns no (since it never modifies its original value of h, which is guaranteed to return false), which makes it consistent with the samples. This still satisfies the learning condition because it means the probability of a sample evaluating to true is extremely low.
- If this was an online learning algorithm, it would make at most 2n mistakes, since it would delete at least 1 contradicting literal each time it gets

## 5. Application 2: Learning Decision Lists

Like before, we have  $X = \{0,1\}^n$ , except this time  $\mathcal{C}$  is the set of all decision lists over  $x_1, ... x_n$ . A decision list is like a "chain" version of a decision tree: at each rule, if the result is yes, the decision list breaks and returns a specified output. If the comparison returns no, then the decision list moves on to the next comparison. We can see that |C| is large, but still finite (and its log is still polynomial in n).

Unlike the last algorithm, where we started with a "full" conjunction, for this one we'll start with an empty decision list and slowly build it up. So how do we find the first rule in our decision list? One approach would be to do something similar to a greedy algorithm. We could find a subset of the x's such that they all have the same  $x_i$  and they all evaluate to the same thing (either True or False), remove those samples from our set, and then turn the value of  $x_i$  and the corresponding output into a new rule in our decision list. We can keep repeating this until no samples are left. To formalize this:

```
B \leftarrow \{f(x) | \langle x, f(x) \rangle \in S\}

while |B| > 1 do

Let x_i be a component with no rule in the decision list

Let j be 0 or 1

Q \leftarrow \{f(x) | \langle x, f(x) \rangle \in S \text{ and } x_i = j\}

if |Q| = 1 then

Make new rule: If x_i = j then f(x) = Q

S \leftarrow S \setminus \{\langle x, f(x) \rangle | x_i = j\}

B \leftarrow \{f(x) | \langle x, f(x) \rangle \in S\}

Output final return value to be B
```

Simple learning algorithm for decision lists.

## 6. Intractability of Learning 3-Term DNF

We now return to the concept class of boolean conjunctions and instead consider a slight generalization: the class of disjunctions of three boolean conjunctions (3-term disjunctive normal form formulae). We will show that this concept class is *not* efficiently PAC-learnable unless every problem in NP can be solved efficiently in a worst-case sense by a randomized algorithm!

**3-Term DNF Formulae.** The representation class  $C_n$  of 3-term DNF formulae is the set of all disjunctions  $T_1 \vee T_2 \vee T_3$ , where each  $T_i$  is a conjunction of literals over the boolean variables  $x_1, \ldots, x_n$ . We define the maximum size of an instance of the 3-term DNF formula to be  $size(c) \leq 6n$ , as there can be at most 2n literals in each of the three terms. An efficient learning algorithm for this problem therefore must run in time polynomial in n,  $1/\epsilon$ , and  $1/\delta$ .

**Theorem 2.** If  $RP \neq NP$ , the representation class of 3-term DNF formulae is not efficiently PAC learnable when restricting the output hypothesis to the class of 3-term DNF formulae.

*Proof.* The core of this proof is to reduce an NP-complete language A to the problem of PAC learning 3-term DNF formulae. To be precise, suppose we have any string  $\alpha$  for which we want to determine whether  $\alpha \in A$ . We will find a mapping from  $\alpha$  to some set  $S_{\alpha}$  of labeled examples, where  $|S_{\alpha}|$  is polynomially bounded by  $|\alpha|$ . We will show that given a PAC learning algorithm  $\mathcal{L}$  for 3-term DNF formula, we can run  $\mathcal{L}$  on  $S_{\alpha}$  to determine with high probability whether  $\alpha \in A$ .

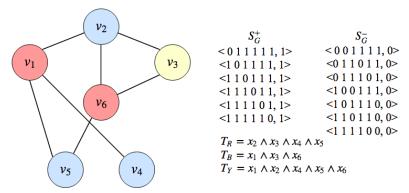
The mapping we want to find will demonstrate the key property:  $\alpha \in A$  iff  $S_{\alpha}$  is **consistent** with some concept  $c \in \mathcal{C}$ .

Determining Existence of a Concept Consistent with  $S_{\alpha}$ . Let us assume that we have found our desired mapping such that  $\alpha \in A$  iff  $S_{\alpha}$  is consistent with some  $c \in \mathcal{C}$ . We then demonstrate how a PAC learning algorithm  $\mathcal{L}$  may be used to determine whether there exists a concept  $c \in \mathcal{C}$  consistent with  $S_{\alpha}$  (and thus whether  $\alpha \in A$ ) with high probability.

Set  $\epsilon = \frac{1}{2|S_{\alpha}|}$ . When running  $\mathcal{L}$  on  $S_{\alpha}$ , whenever  $\mathcal{L}$  requests a new sample, select a pair  $\langle x_i, b_i \rangle$  uniformly at random from  $S_{\alpha}$ . If there does in fact exist a concept  $c \in \mathcal{C}$ , then this process simulates the oracle  $EX(c, \mathcal{D})$ , where  $\mathcal{D}$  is uniform over the instances appearing in  $S_{\alpha}$ .

Given the choice of  $\epsilon$ , we can guarantee that any hypothesis h with error less than  $\epsilon$  must be consistent with  $S_{\alpha}$ . If h were to incorrectly classify even a single example in  $S_{\alpha}$ , its error with respect to c and  $\mathcal{D}$  is at least  $\frac{1}{|S_{\alpha}|} = 2\epsilon > \epsilon$ . Of course, if there is no concept in  $\mathcal{C}$  consistent with  $S_{\alpha}$ ,  $\mathcal{L}$  can not find one. Therefore, we can simply verify the output of  $\mathcal{L}$  for consistency with  $S_{\alpha}$  to determine with confidence  $1 - \delta$  whether such a consistent concept exists in  $\mathcal{C}$ .

We can therefore use this process combined with the assumed mapping from  $\alpha \to S_{\alpha}$  to determine with probability at least  $1 - \delta$  whether  $\alpha \in A$  by simulating  $\mathcal{L}$  on  $S_{\alpha}$ .



A graph G with a legal 3-coloring, the associated sample, and the terms defined by the coloring.

**The Graph 3-Coloring Problem.** Given an undirected graph G = (V, E) with vertex set  $V = \{1, ..., n\}$  and edge set  $E \subseteq V \times V$  and three different colors  $c_1, c_2, c_3$ , determine whether there is such a mapping  $c : V \to \{c_1, c_2, c_3\}$  such that for every edge  $(i, j) \in E$ ,  $c(i) \neq c(j)$ .

Mapping from Graph 3-Coloring to 3-Term DNF Formulae. We now define the mapping from an instance G=(V,E) of Graph 3-Coloring to a set  $S_G$  of labeled examples. We say  $S_G=S_G^+\cup S_G^-$ , where  $S_G^+$  is the set of positively labeled examples and  $S_G^-$  the set of negatively labeled ones.

For each  $1 \leq i \leq n$ ,  $S_G^+$  contains the labeled example  $\langle v(i), 1 \rangle$ , where  $v(i) \in \{0, 1\}^n$  is the vector of all 1's except with a 0 in the *i*th position.

For each edge  $(i,j) \in E$ , the set  $S_G^-$  contains the labeled example  $\langle e(i,j), 0 \rangle$ , where  $e(i,j) \in \{0,1\}^n$  is the vector of all 1's except with 0's in the *i*th and *j*th positions.

We now show that G is 3-colorable iff  $S_G$  is consistent with some 3-term DNF formula. Let us first consider the necessary condition. Suppose G is 3-colorable and fix a 3-coloring of G. Let G be the set of all red vertices, and let G be the conjunction of all variables in G whose index does not appear in G. Therefore, for each G is G whose index does not appear in G in G can satisfy G can satisfy G and G is and G can't both be colored red, at least G in G in G must be in G whose index does not appear in G in G can't both be colored red, at least G in G in G is a similar fashion, with no negative examples being accepted by any term.

We now show the other direction. Assume that the formula  $T_R \vee T_B \vee T_Y$  is consistent with  $S_G$ . We define a 3-coloring of G: the color of the vertex i is red if v(i) satisfies  $T_R$ , blue if v(i) satisfies  $T_R$ , and yellow if v(i) satisfies  $T_Y$ .

Break ties arbitrarily if v(i) satisfies more than one term. Since the formula is consistent with  $S_G$ , then every v(i) must satisfy some term and every vertex must be assigned a color.

We now prove that this is a valid legal 3-coloring. Assume WLOG that two vertices i and j with  $(i \neq j)$  are given the same color, red. Then, both v(i) and v(j) satisfy  $T_R$ . By the definition of  $v(\cdot)$ , the ith bit of v(i) is 0 and the ith bit of v(j) is 1. Hence, neither  $x_i$  nor  $\neg x_i$  can appear in  $T_R$  - and the ith assignment does not affect the result of  $T_R$ . Since v(j) and e(i,j) differ only in the ith bits, if v(j) satisfies  $T_R$ , then so does e(i,j). This implies that  $e(i,j) \notin S_G^-$  and hence  $(i,j) \notin E$ .

We therefore observe that 3-term DNF formulae are not efficiently PAC learnable under the following assumptions:

- $\bullet$  NP-complete problems cannot be solved with high probability by a probabilistic polynomial time algorithm
- the PAC learning algorithm is restricted to outputting a hypothesis from the same representation class as the target concept.

## 7. Using 3-CNF to Avoid Intractability

If we relax the constraint on learning 3-term DNF formulae by expanding the output hypothesis concept class to one that is more expressive, then the class of 3-term DNF formula is in fact efficiently PAC-learnable.

We first observe that any 3-term DNF formula over the variables  $x_1, \ldots, x_n$  may be expanded to an equivalent 3-term CNF formula via distributivity of  $\vee$  over  $\wedge$ .

$$T_1 \lor T_2 \lor T_3 \equiv \bigwedge_{u \in T_1, v \in T_2, w \in T_3} (u \lor v \lor w)$$

We can reduce the problem of PAC learning 3-CNF formulae to the problem of PAC learning conjunctions, which we saw in section 3. Given an oracle for random examples for some unknown target 3-CNF formula, we can apply a transformation to render each positive/negative example into a corresponding positive/negative example over a larger set of variables. This transformation will render the 3-CNF formula as a simple boolean conjunction which we may efficiently learn.

The transformation is as follows: for every triple of literals u, v, w over the original variable set  $x_1, \ldots, x_n$ , the new variable set contains a variable  $y_{u,v,w} = u \lor v \lor w$ . When u = v = w,  $y_{u,v,w} = u$ . Hence, this expanded variable set fully

contains all of the original variables. The total number of new variables is thus  $(2n)^3 = O(n^3)$ .

Thus, for any assignment  $a \in \{0,1\}^n$  to the original variables  $x_1, \ldots, x_n$ , we can compute the corresponding assignment a' to the new variables  $\{y_{u,v,w}|u,v,w\in\{x_1,\ldots,x_n\}\}$  in  $O(n^3)$  time. It is obvious that any 3-CNF formula over  $x_1,\ldots x_n$  is a simple boolean conjunction over  $y_{u,v,w}$ . We can run the algorithm for learning boolean conjunctions by expanding each assignment to  $x_1,\ldots,x_n$  that is a positive example for the target formula to an assignment for the corresponding  $y_{u,v,w}$  and giving this expanded assignment to the algorithm as a positive example for the unknown conjunction over  $y_{u,v,w}$ . When finished, we can convert the hypothesis conjunction h' back to a 3-CNF h by expanding every variable to its corresponding 3-term conjunction.

To conclude, we must argue that if c and  $\mathcal{D}$  are the target 3-CNF formula and distribution over  $\{0,1\}^n$ , and c' and  $\mathcal{D}'$  are the corresponding conjunction over the  $y_{u,v,w}$  and induced distribution over assignments a' to the  $y_{u,v,w}$ , then if h' has error less than  $\epsilon$  with respect to c' and  $\mathcal{D}'$ , h has error less than  $\epsilon$  with respect to c and  $\mathcal{D}$  as well. This is simple to see when noting that the applied transformation is injective. If  $a_1$  is mapped to  $a'_1$  and  $a_2$  is mapped to  $a'_2$ , then  $a_1 \neq a_2$  implies  $a'_1 \neq a'_2$ . Thus, each assignment a' on which h' differs from c' has a unique pre-image a on which h differs from c, and the weight of a under  $\mathcal{D}$  is exactly that of a' under  $\mathcal{D}'$ . (Do note that the reduction exploits the notion that the conjunctions learning algorithm works for any distribution  $\mathcal{D}$ , as the transformation alters the original distribution).

Therefore, we have proven:

**Theorem 3.** The representation class of 3-CNF formulae is efficiently PAC learnable.

Therefore, we can efficiently PAC-learn 3-term DNF formulae by rendering them as 3-CNF and allowing the hypothesis to be a 3-CNF formula. This does not hold if we restrict the hypothesis class to 3-term DNF! As it turns out, this statement holds for any constant  $k \geq 2$  for k-term DNF formulae and k-CNF formulae.

It is critical to recognize that even with a fixed concept class from which targets are chosen, the choice of *hypothesis representation* can have a huge impact on efficiency and tractability.

## 8. Boosting

In the problem of PAC-learnability, we were trying to find learning algorithms that learned the problem really well - to within some  $\epsilon$  error rate. This is a pretty strong guarantee, so what if we have a problem where we can only find an algorithm that does slightly better than random guessing? To formalize this a little bit, let us define weak PAC-learning. Weak PAC-learning is largely the same as PAC-learning, except we alter the learning condition to be (for a binary classification problem)

$$err_D(h) \leq \frac{1}{2} - \alpha.$$

for some  $0 < \alpha < \frac{1}{2}$ . Clearly, this is a much weaker guarantee than the standard PAC-learning model, so we can call learning algorithms that are successful under this model weak learners and learning algorithms successful under standard PAC-learning strong learners. It is also easy to see that a strong learner is also a weak learner. However, a somewhat counterintuitive claim is that all weak learners are capable of strong learning. How?

In knowledge-based game shows, a common "lifeline" to help out a contestant is to let them ask the audience what they think the answer is and then that contestant can use the most popular answer from the crowd as their answer. This crowdsourcing idea can be quite powerful and we can do something similar with weak learners. If you had a weak learner  $\mathcal{L}$ , we could keep an *ensemble* of separate instances of  $\mathcal{L}$  and take the majority opinion to be your classification. This would almost surely be better than a single weak learner, but considering each ensemble member is still only a weak learner, there is still a significant chance the majority could be wrong. A natural improvement on this algorithm would be to take a weighted majority by weighting the opinion of each member of the ensemble based on its error rate, so that "better" members are weighted more highly.

We can do even better than this though. Using a technique called *adaptive boosting*, or AdaBoost for short, we have a guaranteed method of turning a weak learner into a strong learner. You can read more about the AdaBoost algorithm in Appendix D.

## A. Appendix A: Agnostic Learning

**Unrealizable case.** In the sample-bound analysis presented earlier, we consider the case where the target concept c(x) always exists and  $c \in \mathcal{C}$ . We call this the realizable case. In the *unrealizable* situation, such a c may not exist. Hence, we may not be able to produce a hypothesis that is perfectly consistent with a training set.

Agnostic learnability. A concept class  $\mathcal{C}$  is agnostically learnable if  $\exists$  a learning algorithm  $\mathcal{L}$  such that  $\forall c_t \in \mathcal{C}$ ,  $\forall$  distributions  $\mathcal{D}$  over  $\mathcal{X}$ , and  $\forall \epsilon, \delta > 0$ , and given some  $\epsilon, \delta$ , and an oracle  $EX(c_t, \mathcal{D})$ ,  $\mathcal{L}$  outputs an  $h \in \mathcal{H}$  such that with probability at least  $1 - \delta$  it satisfies along with the efficiency conditions for PAC-learning:

$$err_D(h) \le \min_{h' \in \mathcal{C}} er\hat{r}_D(h') + \epsilon$$

As a note, in various contexts you may see  $min_{h' \in \mathcal{C}} \hat{err}_D(h')$  written as  $Opt(\mathcal{C})$  - the minimal empirical error over all the possible hypotheses in  $\mathcal{C}$ .

The idea is that we want an algorithm that minimizes true error despite that the true errors of the functions in C are unknown.

As before, we want to identify a sufficient sample size m that will let a learning algorithm produce a minimal error hypothesis. First, we'll show that for any particular h, the empirical and true errors converge. Then, we'll show that the errors converge for all  $h \in \mathcal{C}$  - thus, minimizing  $e\hat{r}r_D(h)$  over all  $h \in \mathcal{C}$  will approximately minimize  $err_D(h)$ .

Claim. Let h be a function  $h: \mathcal{X} \to \mathcal{Y} = \{0, 1\}$ . Then,

$$P(|er\hat{r}_D(h) - err_D(h)| \ge \epsilon) \le 2e^{-2\epsilon^2 m}$$

for any probability distribution  $\mathcal{D}$ , any  $\epsilon > 0$ , and any positive integer m.

*Proof.* Consider the indicator function  $f_i(x_i)$ ,

$$f_i(x_i) = \begin{cases} 1 & \text{if } h(x_i) \neq y_i \\ 0 & \text{otherwise} \end{cases}$$

Then, we can define the empirical error - the probability that h misclassifies a point over the examples.

$$e\hat{r}r_D(h) = \frac{1}{m} \sum_{i=1}^m f_i(x_i)$$

Finally, we define true error as:

$$err_D(h) = E_{X \sim D}[f_i(x)]$$

Using the Hoeffding inequality (see Appendix A), we can then write:

$$P(|er\hat{r}_D(h) - err_D(h)| \ge \epsilon) \le 2e^{-2\epsilon^2 m}$$

This concentration inequality tells us that with larger sample size m, the empirical error exponentially rapidly approaches the true error.

The above claim gives a bound on the difference between empirical and true error for a particular hypothesis h. We now bound the difference between the errors for all  $h \in \mathcal{C}$ .

Claim. 
$$P(\exists h \in \mathcal{C} : |err_D(h) - e\hat{r}r_D(h)| \ge \epsilon) \le 2|\mathcal{C}|e^{-2\epsilon^2 m}$$

*Proof.* The claim immediately follows from the union bound:

$$P(\exists h \in \mathcal{C} : |err_D(h) - e\hat{r}r_D(h)| \ge \epsilon) = P(\bigcup_{h \in \mathcal{C}} \left\{ |err_D(h) - e\hat{r}r_D(h)| \ge \epsilon \right\})$$

$$\le \sum_{h \in \mathcal{C}} P(|err_D(h) - e\hat{r}r_D(h)| \ge \epsilon)$$

$$\le 2|\mathcal{C}|e^{-2\epsilon^2 m}$$

We set  $\delta \geq 2|\mathcal{C}|e^{-2\epsilon^2m}$ . This way, we upper bound the probability of any h's true and empirical errors not converging. Solving for m,

$$\delta \ge 2|\mathcal{C}|e^{-2\epsilon^2 m}$$

$$\ln \delta \ge \ln 2|\mathcal{C}| - 2\epsilon^2 m$$

$$2\epsilon^2 m \ge \ln 2|\mathcal{C}| - \ln \delta$$

$$m \ge \frac{\ln 2|\mathcal{C}| + \ln \frac{1}{\delta}}{2\epsilon^2}$$

Looking at the equation obtained for finding an appropriate m, we observe that the sample size depends on  $\epsilon^2$  as opposed to  $\epsilon$  in the PAC-learning case. Thus, in practice when we cannot find a consistent hypothesis, we need more data to obtain a hypothesis with less true error.

Equivalently, given some number m of examples, the error we expect is, with probability at least  $1-\delta$ ,

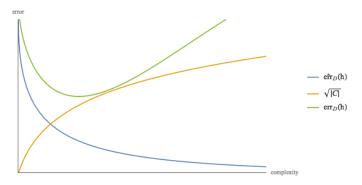
$$err_D(h) \le e\hat{r}r_D(h) + O\left(\sqrt{\frac{\ln(2|\mathcal{C}|) + \ln(\frac{1}{\delta})}{m}}\right)$$

From this, we can derive three core conditions for learning:

•  $large\ amount\ of\ training\ data$  - by increasing m, the second term becomes smaller, decreasing the total error

- low training error the first term in the summation decreasing training error consequently decreases the true error
- *simple hypothesis space* the measure for simplicity here is the size of the hypothesis class. The smaller the hypothesis, the lower the true error

Additionally, there is a trade-off between decreasing training error and maintaining a simple hypothesis. As the complexity of the hypotheses increases, the probability of finding a consistent hypothesis increases and the training error tends to zero. However, the big-Oh term will eventually begin to dominate, and after  $err_D(h)$  reaches a minimum, it will begin to rise again. At this point, we have *overfitting*, and while the hypothesis chosen is consistent on the training data, the variance introduced is too high! Complex hypotheses assume more about the data "from thin air" without actual training data to support the complexity.



empirical error vs. true error

Overfitting is one of the most difficult and most important issues to deal with in practical machine learning. Often times, only the training error  $er\hat{r}_D(h)$  can be observed directly, making it difficult to minimize the other term. Here are a couple of main approaches towards solving the overfitting problem:

- Structural Risk Minimization (SRM): an inductive principle for model selection. Select from a set of models in order of increasing complexity pick one for which the sum of empirical risk and complexity (VC-dimension) is minimal. The goal is to find the exact value of the theoretical bounds to minimize the bound directly.
- Cross-Validation: Separate training data into two parts: a training and a testing set. This lets us estimate the true error and identify the stopping point for the algorithm (i.e. when the true error reaches a minimal point). Variations on this include splitting the data into k parts (k-fold CV), or trying the algorithm on all data points except one and repeating (LOOCV).

As a side note (this is outside the scope of this lecture), this theorem can actu-

ally be generalized to infinite classes. But then wouldn't the number of samples needed just be infinity, you ask? Actually, no! We can use something called the Vapnik-Chervonenkis dimension, which is the largest dimension in which all labels of points can be induced by functions in  $\mathcal{C}$ . Appendix B further explores the notion of VC dimension. Using this concept gives us the following theorem:

**Theorem 4.** If you find an algorithm that is consistent given  $m \geq \frac{VCD(\mathcal{C})}{\epsilon} \ln(\frac{1}{\delta})$  samples, then with probability  $1 - \delta$  it satisfies the learning condition.

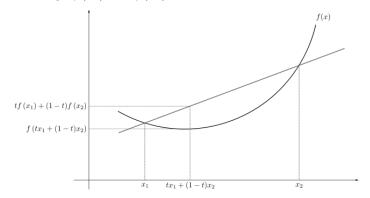
# B. Appendix B: Jensen's and Hoeffding's Inequalities

Jensen's Inequality. Jensen's inequality is arguably one of the most significant inequalities in all of statistics, and we will in fact use it later to prove Hoeffding's lemma. The inequality relates the convex function of an expectation to the expectation of the convex function. We first briefly review important properties of convex functions.

Convex function. Let I be an open subset of  $\mathbb{R}$ . Let  $f: I \to \mathbb{R}$ . We say that g is **convex** if  $\forall x_1, x_2 \in I$  and  $\forall t \in [0, 1]$  we have

$$f(tx_1 + (1-t)x_2) \le tf(x_1) + (1-t)f(x_2)$$

In layman's terms, this means that the value of a convex function evaluated at a value in the range  $[x_1, x_2]$  is always bounded above by a point through the secant line through  $f(x_1)$  and  $f(x_2)$ .



We can also define convex functions in more familiar terms:

**Lemma.** (Sufficient conditions for convexity)

Let I be an open subset of  $\mathbb{R}$ . Let  $f: I \to \mathbb{R}$ . If either

1. f' is nondecreasing and continuous on I, or

2. 
$$f'' \ge 0$$
 on  $I$ 

then f is convex.

Before we prove Jensen's inequality, we will prove the following useful property of convex functions.

**Lemma.** If  $\psi$  is a convex function on the open subset  $I \subset \mathbb{R}$ , then for any  $x_0 \in I$  there exists a support line  $l_0$  such that

$$l_0(x) \le \psi(x) \ \forall x \in I \ and \ l_0(x_0) = \psi(x_0)$$

This means that for any function that is convex on a given interval, the function lies above its tangent lines at any point in the interval.

*Proof.* We first observe two facts:

1. For any h > 0, we have

$$\frac{\psi(x) - \psi(x - h)}{h} \le \frac{\psi(x + h) - \psi(x)}{h}$$

We can obtain this result from the definition of convexity:

$$\psi(t(x-h)+(1-t)(x+h)) \le t\psi(x-h)+(1-t)\psi(x+h)$$
 
$$\psi(x) \le \frac{1}{2}\psi(x-h)+\frac{1}{2}\psi(x+h) \qquad \text{letting } t = \frac{1}{2}$$
 
$$\psi(x)-\psi(x-h) \le \psi(x+h)-\psi(x)$$

Dividing both sides by the constant h gives us the desired result. (1) effectively states that a right derivative will always be larger than a left derivative for a convex function.

2. For any  $h_1 > h_2$ ,

$$\frac{\psi(x) - \psi(x - h_1)}{h_1} \le \frac{\psi(x) - \psi(x - h_2)}{h_2}$$

$$\frac{\psi(x+h_1) - \psi(x)}{h_1} \ge \frac{\psi(x+h_2) - \psi(x)}{h_2}$$

We obtain the first inequality from the definition of convexity where t =

 $\frac{h2}{h1}$ , and the points are  $x - h_1$  and x.

$$\psi(\frac{h_2}{h_1}(x-h_1) + (1-\frac{h_2}{h_1})x) \le \frac{h_2}{h_1}\psi(x-h_1) + (1-\frac{h_2}{h_1})\psi(x)$$
$$\psi(x-h_2) \le \frac{h_2}{h_1}\psi(x-h_1) + \psi(x) - \frac{h_2}{h_1}\psi(x)$$
$$\frac{h_2}{h_1}\psi(x) - \frac{h_2}{h_1}\psi(x-h_1) \le \psi(x) - \psi(x-h_2)$$
$$\frac{\psi(x) - \psi(x-h_1)}{h_1} \le \frac{\psi(x) - \psi(x-h_2)}{h_2}$$

The second inequality may be found in a similar fashion, except using the points  $x + h_1$  and x.

By (2), we observe that the sequences are monotone. This directly leads from the fact that for a convex function, the derivative is always increasing. Thus, their limits as  $h \to 0^+$  exist by the Monotone Convergence Theorem. We then define:

$$\psi'_{-}(x) = \lim_{h \to 0^{+}} \frac{\psi(x) - \psi(x - h)}{h}$$
 and  $\psi'_{+}(x) = \lim_{h \to 0^{+}} \frac{\psi(x + h) - \psi(x)}{h}$ 

By (1), we have that  $\psi'_{-}(x) \leq \psi'_{+}(x)$  for any x. Then, for fixed z, we can choose some  $m \in [\psi'_{-}(z), \psi'_{+}(z)]$  and define the line  $\ell$ ,

$$\ell_z(x) = \psi(z) + m(x-z)$$

We thus have  $\ell_z(z) = \psi(z)$ . If we consider any x = z + h for some h, it is easy to see that the inequality  $\ell_z(z+h) = \psi(z) + mh \le \psi(z+h)$  holds. (Hint: observe the notion that  $\psi'(x)$  monotonically increases).

We now state Jensen's inequality.

**Theorem 5.** (Jensen's Inequality) Let f be a convex function on I, an open subset of  $\mathbb{R}$ . Let  $x \in I$  with probability 1 and assume X, f(X) have finite expectation. Then

$$f(EX) \le E[f(X)]$$

*Proof.* First, we observe that  $EX \in I$ . Let  $\ell(x) = ax + b$  be the support line for  $f(\cdot)$  at the point EX. Then, by the definition of the support line we have

- 1.  $\ell(EX) = f(EX)$
- 2.  $\ell(x) < f(x) \ \forall x \in I$

Taking expectations in (2), we have:

$$E[f(x)] \geq E[\ell(x)] = E[ax+b] = aE[x] + b = \ell(EX)$$

Then invoking (1), we have  $E[f(x)] \ge f(EX)$  and are done.

**Hoeffding's Inequality.** Hoeffding's inequality is one of the most important inequalities in machine learning literature. It gives an **exponential** bound for sums of random variables whose intervals are bounded. Before introducing and proving Hoeffding's inequality, we first introduce the following lemma.

**Lemma.** Let a, b be constants such that  $a \leq 0, 0 \leq b, a \neq b$ . Let X be any real valued random variable such that EX = 0 and  $a \leq X \leq b$ . For all  $\lambda \in \mathbb{R}$ ,

$$E[e^{\lambda X}] \le \exp(\frac{\lambda^2 (b-a)^2}{8})$$

*Proof.* We first consider the moment generating function  $e^{\lambda X}$ . Since this is a convex function, we may use the fact that  $a \leq X \leq b$  to invoke Jensen's inequality for two points (which is just the definition of a convex function):

$$f(ta + (1-t)b) \le tf(a) + (1-t)f(b)$$

Parameterizing x with respect to  $t \in [0,1]$ , we set x = ta + (1-t)b and have  $t = \frac{b-x}{b-a}$ . Then,

$$e^{\lambda x} \le \frac{b-x}{b-a}e^{\lambda a} + \frac{x-a}{b-a}e^{\lambda b}.$$

Taking expectation with respect to x, we have:

$$E[e^{\lambda x}] \le \frac{b - EX}{b - a} e^{\lambda a} + \frac{EX - a}{b - a} e^{\lambda b}$$
$$= \frac{b}{b - a} e^{\lambda a} - \frac{a}{b - a} e^{\lambda b}$$

Let  $h = \lambda(b-a), p = \frac{-a}{b-a}, L(h) = -hp + \ln(1-p+pe^h).$ 

We then substitute our values.

$$E[e^{\lambda x}] \le (1-p)e^{\lambda a} + pe^{\lambda b}$$

$$\le (1-p)e^{-hp} + pe^{h(1-p)}$$

$$\le (1-p+pe^h)e^{-hp}$$

$$= e^{L(h)}$$

To complete the proof, we will show  $L(h) \leq \frac{1}{8}\lambda^2(b-a)^2$ .

We first compute L'(h) and L''(h). With simple calculus,

$$L'(h) = -p + \frac{1}{1 - p + pe^h} pe^h$$
 
$$L''(h) = \frac{1}{1 - p + pe^h} pe^h - (pe^h)^2 (\frac{1}{1 - p + pe^h})^2$$

Showing the first few terms of the Taylor expansion of  $e^{L(h)}$ ,

$$L(h) \approx L(0) + L'(0)h + \frac{L''(0)}{2!}h^2 + \dots$$

We note that L(0) = L'(0) = 0. We note that since the dominant term in L(h) is of the form  $\ln(1-u)$ , a finite Taylor expansion for L will always be an overestimate. Thus,  $L(h) \leq \frac{L''(0)}{2}h^2$ . We then show that  $L''(0) \leq \frac{1}{4}$ .

Simplifying and evaluating L''(0) is a bit messy.

We first simplify  $1 - p + pe^h = 1 + \frac{a}{b-a} - \frac{a}{b-a}e^h = \frac{b-ae^h}{b-a}$ .

$$L''(h) = \left(\frac{1}{1 - p + pe^h}\right) pe^h - \left(\frac{1}{1 - p + pe^h}\right)^2 (pe^h)^2$$

$$= \frac{pe^h(1 - p + pe^h) - (pe^h)^2}{(1 - p + pe^h)^2}$$

$$= \frac{(b - a)^2 \left[\frac{-a}{b - a}e^h\left(\frac{b - ae^h}{b - a}\right) - e^{2h}\frac{a^2}{(b - a)^2}\right]}{(b - ae^h)^2}$$

$$= \frac{-ae^h(b - ae^h) - e^{2h}a^2}{(b - ae^h)^2}$$

$$= \frac{-bae^h + e^{2h}a^2 - e^{2h}a^2}{(b - ae^h)^2}$$

$$= \frac{-bae^h}{(b - ae^h)^2}$$

Evaluating at h = 0, we have

$$L''(0) = \frac{-ba}{(b-a)^2} \le \frac{1}{4}$$
$$-4ba \le b^2 - 2ab + a^2$$
$$0 \le b^2 + 2ab + a^2 = (b+a)^2$$

This is clearly always true, and we therefore have

$$E[e^{\lambda x}] \le e^{L(h)} = e^{\frac{1}{8}h^2} = e^{\frac{1}{8}\lambda^2(b-a)^2}$$

**Theorem 6.** (Hoeffding's Inequality.) Let  $X_1, \ldots, X_n$  be independent random variables bounded such that  $X_i \in [a_i, b_i]$ .

$$P(\bar{X} - E\bar{X} \ge t) \le \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right)$$

*Proof.* Suppose that  $X_1, \ldots, X_n$  are n independent random variables such that

$$P(X_i \in [a_i, b_i]) = 1$$

for  $1 \le i \le n$ . Let  $S_n = X_1 + \cdots + X_n$ . Then for  $s, t \ge 0$ , we can invoke Markov's inequality:

$$P(S_n - E[S_n] \ge t) = P(e^{s(S_n - E[S_n])} \ge e^{st})$$

$$\le e^{-st} E[e^{s(S_n - E[S_n])}] \qquad \text{Markov's inequality}$$

$$= e^{-st} \prod_{i=1}^n E[e^{s(X_i - E[X_i])}] \qquad \text{Expectation of product of indep. R.V.s}$$

$$\le e^{-st} \prod_{i=1}^n \exp(\frac{1}{8}s^2(b_i - a_i)^2) \qquad \text{Hoeffding's Lemma}$$

$$= \exp(-st + \frac{1}{8}s^2 \sum_{i=1}^n (b_i - a_i)^2)$$

To find the tightest upper bound, we want to minimize the right hand side of the last inequality as a function of s. We define  $g(s) = -st + \frac{s^2}{8} \sum_{i=1}^{n} (b_i - a_i)^2$ .

Since g is a quadratic function of s, we can solve g'(s) = 0 to find the minimum:

$$s = \frac{4t}{\sum_{i=1}^{n} (b_i - a_i)^2}$$

Plugging back in to g(s), we get the tight bound:

$$P(S_n - E[S_n] \ge t) \le \exp\left(-\frac{2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right)$$

If we define some  $\bar{X} = \frac{S_n}{n}$ , we can rewrite the above to get the form shown in the theorem.

In the special case where  $a_i = 0$  and  $b_i = 1$ , we have:

$$P(\bar{X} - E[\bar{X}] \ge t) \le e^{-nt^2}$$

This form is particularly important, as it is applied to the case of i.i.d. Bernoulli random variables often in computer science.

## C. Appendix C: VC-Dimension

In our foray into learning algorithms, we only considered cases where the hypothesis classes chosen were of finite size. However, this is a significant limitation - and often times we will want to consider hypothesis classes of infinite cardinality.

In the inequalities for  $err_D(h)$  obtained in both the PAC-learning and agnostic learning cases, we have terms containing  $\ln(|\mathcal{C}|)$ . If  $\mathcal{C}$  is of infinite cardinality, we effectively have an infinite upper bound on the true error, which is useless! We instead introduce the notion of the Vapnik-Chervonenkis dimension measure - even though  $\mathcal{C}$  may have infinite cardinality, the restriction of the application of concepts in  $\mathcal{C}$  to a finite sample S has a finite outcome.

As before, we assume that  $\mathcal{C}$  is a concept class over the instance space  $\mathcal{X}$ , both of which may be infinite. We define each  $c \in \mathcal{C}$  such that  $c : \mathcal{X} \to \{0,1\}$  (i.e. positive or negative labels). A training sample S of m samples  $x_1, \ldots, x_m$  is drawn i.i.d. according to some fixed but unknown distribution D. We further reserve  $c \in \mathcal{C}$  to denote the target concept and  $h \in \mathcal{C}$  to denote an arbitrary concept.

#### Dichotomies on S.

$$\Pi_{\mathcal{C}}(S) = \{ (h(x_1), \dots, h(x_m) : h \in \mathcal{C} \},\$$

where  $\Pi_{\mathcal{C}} \in \{0,1\}^m$ .

 $\Pi_{\mathcal{C}}(S)$  is a set whose members are m-dimensional boolean vectors induced by concepts in  $\mathcal{C}$ . We refer to these members as dichotomies or behaviors on S induced or realized by  $\mathcal{C}$ . We say that  $\mathcal{C}$  fully realizes S if  $|\Pi_{\mathcal{C}}(S)| = 2^m$  - that is, every possible m-dimensional boolean vector can be obtained by passing S through all concepts  $h \in \mathcal{C}$ .

Equivalently,  $\Pi_{\mathcal{C}}(S)$  can be represented as a collection of subsets of S:

$$\Pi_{\mathcal{C}}(S) = \{ h \cap S : h \in \mathcal{C} \},\$$

where each  $h \in \mathcal{C}$  makes a partition of S into two sets, the positive and negative points. We say that  $h \cap S$  yields a subset of S containing the positive points of S under h. Under this representation,  $\mathcal{C}$  fully realizes S when the total number

of  $h \cap S = 2^m$  for all  $h \in \mathcal{C}$ . We can view this as taking the sum  $\sum_{i=0}^m {m \choose i}$ , the total number of ways of picking any number  $0 \le i \le m$  of the points to be labeled positive.

**Shattering.** If  $|\Pi_{\mathcal{C}}(S)| = 2^m$ , then S is considered shattered by  $\mathcal{C}$ . In other words, S is shattered by  $\mathcal{C}$  if  $\mathcal{C}$  fully realizes S.

*Example*. Consider the finite concept class  $C = \{c_1, \ldots, c_4\}$  applied to three instance vectors  $\mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}$  with the results:

|       | $\mathbf{x_1}$ | $\mathbf{x_2}$ | $\mathbf{x_3}$ |
|-------|----------------|----------------|----------------|
| $c_1$ | 1              | 1              | 1              |
| $c_2$ | 0              | 1              | 1              |
| $c_3$ | 1              | 0              | 0              |
| $c_4$ | 0              | 0              | 0              |

$$\Pi_{\mathcal{C}}(\{\mathbf{x_1}\}) = \{(0), (1)\}$$
 shattered  $\Pi_{\mathcal{C}}(\{\mathbf{x_1}, \mathbf{x_3}\}) = \{(1, 1), (0, 1), (1, 0), (0, 0)\}$  shattered  $\Pi_{\mathcal{C}}(\{\mathbf{x_2}, \mathbf{x_3}\}) = \{(1, 1), (0, 0)\}$  not shattered

In the final case, choosing  $S = \{\mathbf{x_2}, \mathbf{x_3}\}$  only yields 2 of the 4 possible dichotomies of S. We now finally define VC dimension.

**Vapnik-Chervonenkis Dimension**. The VC dimension of the concept class  $\mathcal{C}$ , denoted as  $VCdim(\mathcal{C})$ , is the cardinality of the largest set S shattered by  $\mathcal{C}$ . If all sets S that are arbitrarily large can be shattered by  $\mathcal{C}$ , then  $VCdim(\mathcal{C}) = \infty$ .

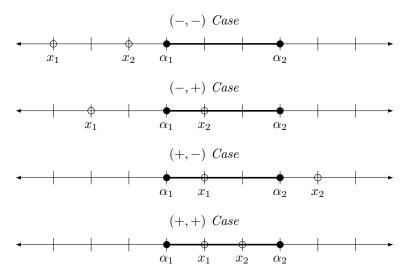
We observe that the VC dimension of a concept class is a combinatorial measure of its complexity. We can interpret the VC dimension as the point d at which all samples S with complexity |S| > d can no longer be shattered by  $\mathcal{C}$ . In other words, for all  $h \in \mathcal{C}$ , it is not possible to obtain all possible results (dichotomies)! Intuitively, this marks the VC dimension as a good metric for complexity, as it tells us at which point a concept class exhausts its capacity to fully realize all results for the input.

As an important note, it is crucial to realize that if the VC dimension is at least d, then this means that there exists some sample |S| = d that is shattered by C. This does not imply that all samples of size d are shattered by C. Conversely, to show that the VC dimension is at most d, one must show that no sample of size d+1 can be shattered by C.

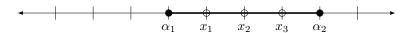
We now look at an example concept-class and its VC dimension.

Intervals on the Reals. The concept class C is governed by two parameters  $\alpha_1, \alpha_2$  in the closed interval [0,1]. A concept from the class will label an in-

put instance 0 < x < 1 as positive if  $\alpha_1 \le x \le \alpha_2$  and negative otherwise. We show that the VC dimension is at least 2. Select any sample of 2 points  $x_1, x_2$  positioned in the open interval (0, 1). It is clear that one can pick values of  $\alpha_1, \alpha_2$  to produce all the possible four dichotomies (+, +), (-, -), (+, -), (-, +).



To show that the VC dimension is at most 2, it suffices to show that any sample  $x_1, x_2, x_3$  on the line (0,1) cannot be shattered by  $\mathcal{C}$ . We note that the dichotomy (+, -, +) can never be realized by any satisfying sample.



We apply labels WLOG such that  $x_1 < x_2 < x_3$ . As shown above, if  $x_1$  and  $x_3$  are both classified as +, i.e. both points are in the range  $[\alpha_1, \alpha_2]$ , then  $x_2$  must also be in the range and therefore classified +. Therefore, it is not possible to obtain the dichotomy (+, -, +) from  $\mathcal{C}$ , and the VC dimension of  $\mathcal{C}$  is 2.

## D. Appendix D: AdaBoost

Using a technique called adaptive boosting, or AdaBoost for short, we have a guaranteed method of turning a weak learner into a strong learner. We can begin by calling our weak-learning algorithm  $\mathcal{L}$  to obtain a hypothesis  $h_1$ . Now we can modify our original distribution  $\mathcal{D}$  to create  $\mathcal{D}_2$ , where we have reweighted the distribution to slightly favor those samples that  $h_1(x)$  classified incorrectly. We can do this again, except use a  $\mathcal{D}_3$  where those samples for which  $h_1$  differs from  $h_2$  have higher weight. After repeating this for T iterations, we have produced T hypotheses to use as our ensemble.

Why does this make sense? Well, if we reweight our distribution to favor samples that our hypothesis was wrong on such that the hypothesis is no better than random guessing and then rerun our learning algorithm, we know it has to perform better than random guessing so our algorithm must learn some hypothesis that performs better on the samples the first hypothesis erred on.

This means that we will have a set of hypotheses, each of which perform better on different areas of the sample space. Thus we can output a final output that weights each of these hypotheses:

$$H(x) = sign\left(\sum_{i=1}^{T} \alpha_i h_i(x)\right).$$

The creation of the AdaBoost algorithm, below, specified exactly how to calculate the weights  $\alpha_i$  and generate the new distribution  $D_{t+1}$ .

```
D_1(i) \leftarrow \frac{1}{n} \text{ for } i \leftarrow 1, \dots, n
\text{for } t \leftarrow 1, \dots, T \text{ do}
\text{Produce hypothesis } h_t \text{ from distribution } D_t
\text{Let } \epsilon_t = Pr_{i \sim D_t}[h_t(x_i) \neq y_i]
\text{Let } \alpha_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right)
\text{for } i \leftarrow 1, \dots, n \text{ do}
D_{t+1}(i) = \frac{D_t(i)}{Z_t} e^{-\alpha_t h_t(x_i)y_i}, \text{ where } Z_t \text{ is a normalization constant to enforce } D \text{ to be a distribution.}
\text{Output } H(x) = sign\left( \sum_{t=1}^T \alpha_t h_t(x) \right)
```

The AdaBoost algorithm.

In this current form, however, it can be quite computationally inefficient to perform this algorithm because of all the logarithms and exponentials. With some mathematical manipulations, however, we can make this much more efficient.

We can begin by rewriting  $\alpha_t$ :

$$\alpha_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right) = \ln \left( \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}} \right)$$

Next, we can plug the value of  $\alpha_t$  into the equation for  $D_{t+1}(i)$ :

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} e^{-\ln\left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}}\right) h_t(x_i) y_i}$$

$$= \frac{D_t(i)}{Z_t} * \begin{cases} \sqrt{\frac{\epsilon_t}{1-\epsilon_t}}, & \text{if } h_t(x_i) y_i = 1\\ \sqrt{\frac{1-\epsilon_t}{\epsilon_t}}, & \text{if } h_t(x_i) y_i = -1 \end{cases}$$

Note that  $h_t(x_i)y_i = 1$  iff the hypothesis  $h_t$  is correct for sample  $x_i$  and -1 if it is incorrect.

We can now work on finding an expression for  $Z_t$ . We know that it is the normalizing constant, so therefore:

$$z = \sqrt{\frac{\epsilon_t}{1 - \epsilon_t}} \sum_{\{i | h_t(x_i)y_i = 1\}} D_t(i) + \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}} \sum_{\{i | h_t(x_i)y_i = -1\}} D_t(i)$$

Now, we realize that  $\sum_{\{i|h_t(x_i)y_i=-1\}} D_t(i)$  is in fact  $\epsilon_t$ , making  $\sum_{\{i|h_t(x_i)y_i=1\}} D_t(i)$  equal to  $1-\epsilon_t$ . This means that we can rewrite  $Z_t$  in terms of  $\epsilon_t$ :

$$Z_t = 2\sqrt{\epsilon_t(1 - \epsilon_t)}$$

Combining the above, we get:

$$D_{t+1}(i) = \frac{D_t(i)}{2} * \begin{cases} \frac{1}{1 - \epsilon_t}, & \text{if } h_t(x_i)y_i = 1\\ \frac{1}{\epsilon_t}, & \text{if } h_t(x_i)y_i = -1 \end{cases}$$

We can still do better. Consider

$$\sum_{\{i|h_t(x_i)=y_i\}} D_{t+1}(i) = \frac{1}{2} \frac{1}{1+\epsilon_t} \sum_{\{i|h_t(x_i)=y_i\}} D_t(i)$$

However, we already showed that  $\sum_{\{i|h_t(x_i)=y_i\}} D_t(i) = 1 - \epsilon_t$ , giving us:

$$\sum_{\{i|h_t(x_i)=y_i\}} D_{t+1}(i) = \frac{1}{2}$$

Which also means that:

$$\sum_{\{i|h_t(x_i)\neq y_i\}} D_{t+1}(i) = \frac{1}{2}$$

This means that we evenly reweight all samples we just got correct to collectively appear 1/2 of the time and also reweight those samples we just got wrong to

collectively appear 1/2 of the time, which loops us back around to the original intuition behind AdaBoost.

This seems like a fine and dandy algorithm, but how do we know that it works — that is, how do we know that it reduces the error? Here is a theorem that we will prove that shows that the error decreases exponentially quickly.

**Theorem 7.** If AdaBoost is given a weak learner  $\mathcal{L}$  and is run for t rounds, then if  $\epsilon_t = 1/2 - \gamma_t$ , the training error of the algorithm is at most  $e^{-2\sum_t \gamma_t^2}$ .

To start, let's write  $D_t$  in a recursive form. We know that

$$D_t(i) = \frac{D_{t-1}(i)}{Z_{t-1}} e^{-\alpha_{t-1}h_{t-1}(x_i)y_i}$$

Meaning we can write it as:

$$D_t(i) = D_1(i) \frac{e^{-\alpha_1 h_1(x_i)y_i}}{Z_1} * \dots * \frac{e^{-\alpha_{t-1} h_{t-1}(x_i)y_i}}{Z_{t-1}}$$

This can be simplified (since  $D_1$  is uniformly 1/m):

$$D_t(i) = \frac{1}{m} \frac{e^{\sum_{j=1}^t -\alpha_{j-1}h_{j-1}(x_i)y_i}}{\prod_{j=1}^t z_j}$$

Now we can look at  $D_{T+1}$ :

$$\sum_{i=1}^{m} D_{T+1}(i) = 1 = \frac{1}{m} \left( \frac{\sum_{i=1}^{m} \exp -f(x_i) y_i}{\sum_{t=1}^{T} Z_t} \right)$$

which gives us:

$$\sum_{t=1}^{T} Z_t = \frac{1}{m} \sum_{i=1}^{m} e^{-f(x_i)y_i}$$

Now, let us argue that the training error from the final classifier can be upper bounded by the sum of  $Z_t$ :

$$\frac{1}{m} \sum_{i=1}^{m} I(H(x_i) \neq y_i) \leq \frac{1}{m} \sum_{i=1}^{m} e^{-f(x_i)y_i} = \sum_{t=1}^{T} Z_t$$

This is because if  $I(H(x_i) \neq y_i) = 1$ , that means that  $f(x_i)y_i < 0$ , which means that  $e^{-f(x_i)y_i} \geq I(H(x_i) \neq y_i) = 1$ . If  $I(H(x_i) \neq y_i) = 0$ , then  $f(x_i)y_i > 0$ , which means that  $e^{-f(x_i)y_i} \geq I(H(x_i) \neq y_i) = 0$ .

Now if we let  $\epsilon_t = \frac{1}{2} - \gamma_t$ , we can show that  $Z_t \leq e^{-2\gamma_t^2}$ :

$$\begin{split} Z_t &= 2\sqrt{\epsilon_t(1-\epsilon_t)} \qquad \text{(Using the previously derived expression for } Z_t) \\ &= 2\sqrt{\left(\frac{1}{2}-\gamma_t\right)\left(1-\left(\frac{1}{2}-\gamma_t\right)\right)} \\ &= 2\sqrt{\left(\frac{1}{2}-\gamma_t\right)\left(\gamma_t+\frac{1}{2}\right)} \\ &= 2\sqrt{\frac{1}{4}-\gamma_t^2} \\ &= \sqrt{1-4\gamma_t^2} \\ &= e^{\frac{1}{2}\log(1-4\gamma_t^2)} \\ &\leq e^{\frac{1}{2}(4\gamma_t^2)} \\ &= e^{2\gamma_t^2} \end{split}$$

which means that we can say that

$$\epsilon_{training} \le \prod_t Z_t \le e^{(-2\sum_t \gamma_t^2)}$$

and the proof is complete.