Understanding Machine Learning Theory: Part I

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- Also obviously, please stop me if you don't understand an explanation. This is a rather long presentation. The ambiguity is only going build up! So you might suffer from boredom if you don't ask your questions and ask for clarification!

Understanding Machine Learning Theory

So, I decided to learn more about ML Theory. In my opinion, this book [at least so far!] explains the basics of theory very well.

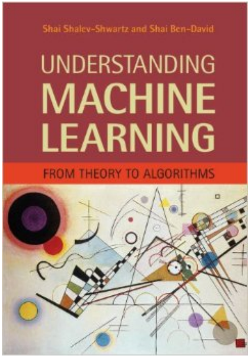
Shai Shalev-Shwartz and Shai Ben-David
UNDERSTANDING
MACHINE
LEARNING
FROM THEORY TO ALGORITHMS

Figure: from
`https://www.cs.huji.ac.il/~shais/UnderstandingMachineLearning/`

Outline

Introduction

- Statistical Learning Framework
- Measures of Success

Empirical Risk Minimization (ERM)

- Overfitting
- Inductive Bias
- Finite Hypothesis Class

Mathematical Analysis of ERM with Inductive Bias

- Mathematical Setup
- ERM with Finite Class Hypothesis

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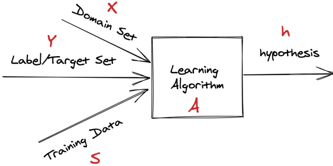
Statistical Learning Framework

Learner's Input:

- **Domain Set** (Input Space): Set of all possible examples/instances we wish to label, shown by X.
- **Label Set** (Target Space): Set of all possible labels, shown by Y.
- **Sample** (Training Data): A finite sequence of pairs in $X \times Y$ shown by $S = ((x_1, y_1), \cdots, (x_m, y_m))$.

Lerner's Output:

- **Hypothesis**: The learner outputs a mapping function $h : X \to Y$ that can assign a value to all $x \in X$. Another notation for the hypothesis can be $A(S)$ which means the output of the learning algorithm A, upon receiving the training sequence S. Also, we might show the hypothesis learned on training data S by $h_S : X \to Y$.



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3. The learner doesn't know anything about $\mathcal{D}$ and only observes sample S.

Measures of Success

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Definition (True Risk/Error, or Generalization Error)

The probability to draw a random instance $x \sim \mathcal{D}$, such that $h(x) \neq f(x)$:

$$\boxed{L_{\mathcal{D},f}(h) = \mathbb{P}_{x \sim \mathcal{D}}[h(x) \neq f(x)] = \mathcal{D}[\{x : h(x) \neq f(x)\}]} \qquad (1)$$

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A measure for the risk/error of the learner's hypothesis on the sample S.

$$\boxed{L_S(h) = \frac{|i \in [m] : h(x_i) \neq y_i|}{m}} \tag{2}$$

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Empirical Risk Minimization (ERM)

Definition

Since the training sample is the snapshot of the world that is available to the learner, it makes sense to search for a solution that works well on that data.
This learning paradigm – coming up with a hypothesis h that minimizes $L_S(h)$ – is called *Empirical Risk Minimization*.

Papayas Example

This is a running example throughout the first few chapters:

Example

Imagine you have just arrived in some small Pacific island. You soon become familiar with a new fruit that you have never tasted before, called *Papaya*! You have to learn how to predict whether a papaya you see in the market is tasty or not

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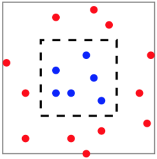
Now, assume that the samples are coming from distribution $\mathcal{D}$ such that the instances are distributed uniformly within the gray square below.

Also, assume the true labeling function f is such that it assigns 1 if an instance is within the inner dashed square, and 0 otherwise. We assume the area of the inner circle equals 1 and the area of the gray square is 2.



Overfitting(2)

Now, let's say we are feeling too smart and come up with this hypothesis:

$$h_S(x) = \begin{cases} y_i & \text{if } \exists i \in [m] : x_i = x \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

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$$\begin{aligned} L_{\mathcal{D},f}(h_S) &= \mathcal{D}[\{x : h_S(x) \neq f(x)\}] \\ &= \mathcal{D}[\{x : h_S(x) = 0, f(x) = 1\}] \\ &= \frac{\text{Area of inner circle}}{\text{Total area}} = \frac{1}{2} \end{aligned}$$

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- The finite class restriction seems to be a strong assumption. But in practice it's not. Why?
- If we assume that we are using a computer to implement our algorithm, then each parameter/variable will have finite bits.

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i.e., every $x_i \in S$ is freshly sampled according to $\mathcal{D}$ and then labeled according to the labeling function, f.

Mathematical Setup: Analysis Parameters

- S is sampled randomly from $\mathcal{D}$. So, when the ERM tries to minimize the error on S, its output h_S is also a random variable. Since h_S is a random variable, $L_{\mathcal{D},f}(h_S)$ is also a random variable!

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Definition (Confidence parameter $(1-\delta)$)

The probability of getting a non-representative sample $S \sim \mathcal{D}^m$ is denoted by δ, and $1-\delta$ is called the *confidence parameter*.

Mathematical Setup: Analysis Parameters

- Not all hypotheses $h \in \mathcal{H}$ is good and we can't guarantee perfect label prediction.

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Any questions on the notations/definitions?

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- Hence, the event $L_{\mathcal{D},f}(h_S) > \epsilon$ can happen if for some $h \in \mathcal{H}_B$ we have $L_S(h) = 0$. i.e., the output of ERM will have 0 empirical loss.

Mathematical Analysis (2)

- We want to upper bound: $\boxed{\mathcal{D}^m[\{S : L_{\mathcal{D},f}(h_S) > \epsilon\}]}$
- Let's separate the set of "bad" hypotheses in $\mathcal{H}$:
  $\boxed{\mathcal{H}_B = \{h \in \mathcal{H} : L_{\mathcal{D},f}(h) > \epsilon\}}$
- Also, let's separate "misleading" or (non-representative) samples:
  $\boxed{M = \{S : \exists h \in \mathcal{H}_B, L_S(h) = 0\}}$
- i.e., For every "misleading" sample $S \in M$, there exist a "bad" hypothesis $h \in \mathcal{H}_B$ such that looks "good" as far as h is concerned (since $L_S(h) = 0$.
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- Hence, $\boxed{\{S : L_{\mathcal{D},f}(h_S) > \epsilon\} \subseteq M}$

Mathematical Analysis (3)

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- So the R.H.S is an upper bound for what we wanted. Can we make it simpler?

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$$\begin{aligned} D^m[S : L_S(h) = 0] &= \mathcal{D}^m[\{S : \forall i : h(x_i) = f(x_i)\}] \\ &= \prod_{i=1}^{m} \mathcal{D}[\{x_i : h(x_i) = f(x_i)\}] \quad \text{i.i.d assumption} \\ &= \prod_{i=1}^{m} 1 - L_{\mathcal{D},f}(h) \leq \prod_{i=1}^{m} 1 - \epsilon \\ &= (1 - \epsilon)^m \leq e^{-\epsilon m} \end{aligned}$$

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- We are done! $\boxed{\mathcal{D}^m[\{S : L_{\mathcal{D},f}(h_S) > \epsilon\}] \leq |\mathcal{H}_B| e^{-\epsilon m} \leq |\mathcal{H}| e^{-\epsilon m}}$

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Corollary

Let $\mathcal{H}$ be a finite hypothesis class. Let $\delta \in (0,1)$ and $\epsilon > 0$ and let m be an integer that satisfies: $m \geq \frac{\ln(|H|/\delta)}{\epsilon}$.
Then for **any labeling function** f, and for **any distribution** $\mathcal{D}$, for which the realizability assumption holds, with probability of at least $1 - \delta$, over the choices of an i.i.d sample S of size m, **every ERM hypothesis** h_S satisfies $L_{\mathcal{D},f}(h_S) \leq \epsilon$

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- Statistical Learning Framework
- Measures of Success

Empirical Risk Minimization (ERM)

- Overfitting
- Inductive Bias
- Finite Hypothesis Class

Mathematical Analysis of ERM with Inductive Bias

- Mathematical Setup
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A Prelude to PAC Learning

Conclusion

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Definition (PAC Learning)

A hypothesis class $\mathcal{H}$ is *PAC learnable* if there exists a function $m_{\mathcal{H}} : (0,1)^2 \mapsto \mathbb{N}$, and a leraning algorithm A with the the following property: For every, $\epsilon, \delta \in (0,1)$, for every distribution $\mathcal{D}$ over X, and for every labeling function $f : X \mapsto \{0,1\}$, if the realizability assumption holds with respect to $\mathcal{H}, \mathcal{D}, f$, then when running algorithm on $m \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d samples generated by $\mathcal{D}$ and labeled by f, the algorithm returns a hypothesis h such that with probability at least $1-\delta$ over the choice of examples, $L_{(\mathcal{D},f)}(h) \leq \epsilon$

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2. Empirical Risk Minimization
3. Mathematical Analysis of Learnability

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Future Lecture

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3. What if our problem is not binary classification?
4. We'll extend the PAC Learning definition by introducing the generalized loss functions into our risk definitions.

Thank you!

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