Understanding Machine Learning: Part I

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Slides adapted from Mirzadeh'21

Understanding Machine Learning

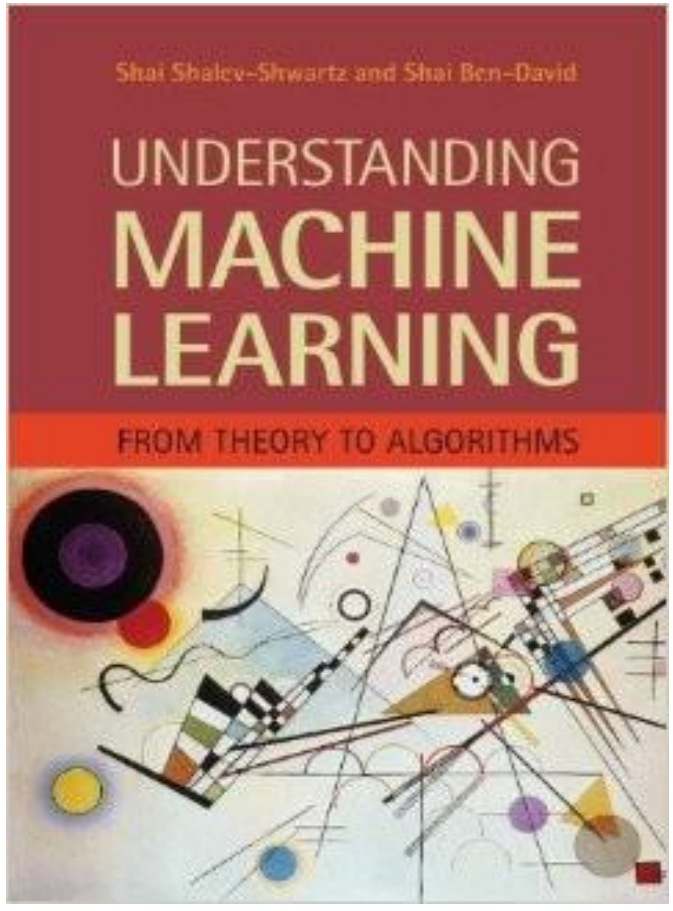

Figure: from
https://www.cs.huji.ac.il/~shais/UnderstandingMachineLearning/

Outline

Introduction

- Statistical Learning Framework
- Measure of Success

Empirical Risk Minimization (ERM)

- Overfitting
- Inductive Bias
- Finite Hypothesis Class

Mathematical Analysis of ERM with Inductive Bias

- ERM with Finite Hypothesis Class

PAC Learning

- Relaxed Assumptions
- Agnostic PAC Learnability for General Loss Functions

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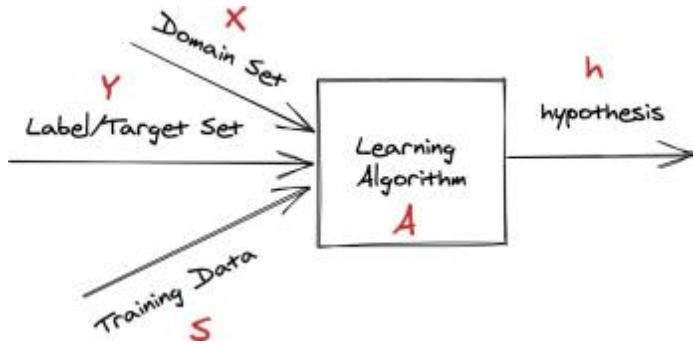
Statistical Learning Framework

Learner's Input:

- **Domain Set** (Input Space): Set of all possible examples/instances we wish to label, shown by $\mathcal{X}$.
- **Label Set** (Target Space): Set of all possible labels, shown by $\mathcal{Y}$. For simplicity, we only consider binary classification, *i.e.* $\mathcal{Y} = \{0,1\}$
- **Sample** (Training Data): A finite sequence of pairs in $\mathcal{X} \times \mathcal{Y}$ shown by $S = ((x_1, y_1), \cdots, (x_m, y_m))$.



Lerner's Output:

- **Hypothesis**: The learner outputs a mapping function $h : \mathcal{X} \to \mathcal{Y}$ 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 $h_S : \mathcal{X} \to \mathcal{Y}$.

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2. The labels are generated using a target function $f : \mathcal{X} \rightarrow \mathcal{Y}$, that is $f(x_i) = y_i, \ \forall x_i \in S$
3. The learner doesn't know anything about $\mathcal{D}$ and only observes sample S.

Measures of Success

Measures of Success

Definition (True Risk/Error, or Generalization Error)

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

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

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Definition (Empirical Risk/Error, or Training Error)

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

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

Note that the the learner doesn't have access to $\mathcal{D}$ and can only see sample S.

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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*.

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

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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Overfitting

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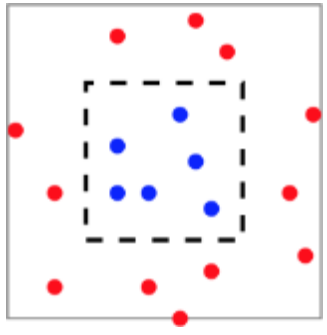
i.i.d. samples $\sim \mathcal{D}$ such that the instances are distributed uniformly within the gray square below.

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:

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

i.e., I memorize everything that I have seen and output the same label as in my memory, otherwise, I will output 0.

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$$L_{D,f}(h_S) = \mathcal{D}[\{x: h_S(x) \neq f(x)\}]$$

$$= \mathcal{D}[\{x: h_S(x) = 0, f(x) = 1\}]$$

$$= \frac{\text{Area of Inner Square}}{\text{Total Area}} = \frac{1}{2}$$

Inductive Bias

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- We should look for conditions that guarantees ERM doesn't overfit!
- A common way, is to **restrict** the learner choose in advance (before seeing the data) a set of predictors. This set of predictors called a *hypothesis class* and denoted by $\mathcal{H}$.

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- Each hypothesis $h \in \mathcal{H}$ is a function of form $h: \mathcal{X} \to \mathcal{Y}$. Then for a given class $\mathcal{H}$, and a training sample S we define:

$$\boxed{\mathrm{ERM}_{\mathcal{H}} \in \mathrm{argmin}_{h \in \mathcal{H}} L_S(\mathcal{H})} \qquad (4)$$

- By restricting the learner to choosing a predictor from $\mathcal{H}$, we *bias* it toward a particular set of predictors. Such restrictions are often called an *inductive bias*.

Finite Hypothesis Class

- The simplest type of restriction on a class is imposing an upper bound on its size (i.e, the number of predictors $h \in \mathcal{H}$). Such a class called a *finite hypothesis class*.
- The finite class restriction seems to be a strong assumption. But in practice it's not. Why?

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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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Mathematical Setup: Assumptions

Before we start, we need to have two assumptions for our anlysis:

Definition (The Realizability Assumption)

We assume that there exists a hypothesis $h^* \in \mathcal{H}$ such that $L_{D,f}(h^*) = 0$.

Implication: For every ERM hypothesis we have that $L_S(h_S) = 0$.

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Definition (The i.i.d Assumption)

The examples in the training set (Sample S) are independently and identically distributed (i.i.d.) according to the distribution $\mathcal{D}$. (notation: $S \sim \mathcal{D}^m$)

i.e., every $x_i \sim S$ 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, $L_{D,f}(h_S)$is also a random variable!

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- Example, if by chance, our sample S is biased and don't represent $\mathcal{D}$ well, we might get high error. We can't guarantee this won't happen. So we have to account for this.

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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.

Wrap-Up (Review)

So many definitions and notations:

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1. **Risks**: $L_S(h)$ is the *empirical risk*, and $L_{\mathcal{D}}(h)$ is the *true risk*.
2. Our **sample**: S with size m, sampled i.i.d from the distribution $\mathcal{D}$.
3. **ERM hypothesis** $h_s \in \operatorname{argmin}_{h \in \mathcal{H}}$ where $\mathcal{H}$ is our hypothesis class and we assume it has *finite* size.
4. **Confidence Parameter** $(1-\delta)$: The probability of not getting a bad sample $S \sim \mathcal{D}^m$.
5. **Accuracy Parameter** (ϵ): Our failure/success threshold. A learner is successful if $L_{\mathcal{D},f}(h_S) \leq \epsilon$.
6. **Realizability Assumption**: $\exists h \in \mathcal{H}, L_{\mathcal{D},f}(h) = 0, L_S(h) = 0$.

Mathematical Analysis

- What do we want to show?

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- We want to show given our setup, the probability of ERM failing to learn a good hypothesis is bounded.
- i.e., we want to upper bound: $\mathcal{D}^m[\{S: L_{\mathcal{D},f}(h_S) > \epsilon\}]$
- Another notation is: $\mathbb{P}_{S\sim D^m}[L_{\mathcal{D},f}(h_S) > \epsilon]$

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- Also, let's separate "misleading" or (non-representative) samples:
  $M = \{S: \exists h \in \mathcal{H}_B, L_S(h) = 0\}$
- 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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- Now recall the **realizability assumption**:

  $\exists h \in \mathcal{H}: L_{\mathcal{D},f}(h) = 0, L_S(h) = 0$
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- By this assumption know that $L_S(h) = 0$
- Hence, the event $L_{\mathcal{D},f}(h) > \epsilon$ 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.
- Hence, $\{S: L_{\mathcal{D},f}(h_S) > \epsilon\} \subseteq M$

Mathematical Analysis (3)

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- $\mathcal{D}^m[\{S: L_{\mathcal{D},f}(h_S) > \epsilon\}] \leq D^m(M) = D^m[\cup_{h \in \mathcal{H}_B} \{S: L_S(h) = 0\}]$

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

Mathematical Analysis (4)

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- Union bound trick: $P(A \cup B) \leq P(A) + P(B)$

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- $$D^m\left[\cup_{h\in\mathcal{H}_B}\{S: L_S(h) = 0\}\right] \leq \sum_{h\in\mathcal{H}_B} D^m[L_S(h) = 0]$$

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

Mathematical Analysis (∞)

- $\boxed{\mathcal{D}^m\left[\left\{S: L_{\mathcal{D},f}(h_S) > \epsilon\right\}\right] \leq |\mathcal{H}_B| e^{-\epsilon m} \leq |\mathcal{H}| e^{-\epsilon m}}$
- The above bound holds for **any** ϵ, δ. So, if we want to to make sure that (ϵ, δ), our learner succeeds, how many examples do we need?
- $|\mathcal{H}| e^{-\epsilon m} \leq \delta$, solve for m. We get: $\boxed{m \geq \frac{\ln(|H|/\delta)}{\epsilon}}$

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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A Prelude to PAC Learning

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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 $L_{\mathcal{D},f}(h_S) \leq \epsilon$

Definition (PAC Learning)

A hypothesis class $\mathcal{H}$ is *PAC learnable* if there exists a function $m_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ and a leraning algorithm A with the the following property: For every $\epsilon, \delta \in (0,1)$, for every distribution $\mathcal{D}$ over $\mathcal{X}$, and for every labeling function $f: \mathcal{X} \to \{0,1\}$, 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, $L_{\mathcal{D},f}(h) \leq \epsilon$.

PAC Learning

- A good learner with learn with high probability and close approximation to the target concept given sufficiently large samples.

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- Remark 1: $m_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ determines the sample complexity of learning $\mathcal{H}$: how many examples are required to guarantee a probably approximately correct solution.

- Remark 2: ϵ measures the accuracy of the learning algorithm ("approximately correct") and δ measures how likely the classifier is to meet the accuracy requirement ("probably")

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- Remark 3: $m_{\mathcal{H}}(\epsilon, \delta)$ is the minimal integer that satisfies the requirement

Corollary

Every finite hypothesis class is PAC learnable with sample complexity

$$m_{\mathcal{H}}(\epsilon, \delta) \leq \lceil \frac{\log(|\mathcal{H}/\delta|)}{\epsilon} \rceil$$

Relaxation of Assumptions

Assumption about data generation model:

1. The instances of training data, S, is generated using a probability distribution $\mathcal{D}$ over $\mathcal{X} \times \mathcal{Y}$.
2. ~~The labels are generated using a target function $f : \mathcal{X} \rightarrow \mathcal{Y}$, that is $f(x_i) = y_i, \forall x_i \in S$~~
3. The learner doesn't know anything about $\mathcal{D}$ and only observes sample S.

Revisiting Measures of Success

Definition (True Risk/Error, or Generalization Error)

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

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

Definition (Empirical Risk/Error, or Training Error)

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

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

Note that the the learner doesn't have access to $\mathcal{D}$ and can only see sample S.

Generalized Loss Functions

Definition (True Risk/Error, or Generalization Error)

The expected loss of a classifier $h \in \mathcal{H}$ w.r.t. a probability distribution $\mathcal{D}$ over some domain Z, namely,

$$\boxed{L_D(h) = \mathbb{E}_{z \sim \mathcal{D}}[\ell(h, z)]} \quad (1)$$

Definition (Empirical Risk/Error, or Training Error)

Expected Loss over a given samples $S = (z_1, \ldots, z_m) \in Z^m$, namely

$$\boxed{L_S(h) = \frac{1}{m} \sum_{i=1}^{m} \ell(h, z_i)} \quad (2)$$

Note that the the learner doesn't have access to $\mathcal{D}$ and can only see sample S.

Our Goal

Definition (True Risk/Error, or Generalization Error)

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

$$L_D(h) = \mathbb{P}_{(x,y)\sim\mathcal{D}}[h(x) \neq y] = \mathcal{D}[\{(x, y): h(x) \neq y\}] \quad (1)$$

- Minimize $L_{\mathcal{D}}(h)$
- The Bayes Optimal Predictor

$$f_{\mathcal{D}}(x) = \begin{cases} 1 & \text{if } \mathbb{P}[y = 1|x] \geq 1/2 \\ 0 & \text{otherwise} \end{cases}$$

Agnostic PAC Learnability

Definition (Agnostic PAC Learnability)

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

$$L_D(h) \leq \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') + \epsilon$$

- Remark: This generalizes the definition of PAC learning. A learner can still declare success if its error is not much larger than the best error achievable by a predictor from the class $\mathcal{H}$.

Agnostic PAC Learnability for Generalized Loss Functions

Definition (Agnostic PAC Learnability for G.L.F)

A hypothesis class $\mathcal{H}$ is *agnostic PAC learnable* with respect to a set Z and a loss function $\ell: \mathcal{H} \times Z \to \mathbb{R}_+$, if there exists a function $m_{\mathcal{H}}: (0,1)^2 \to \mathbb{N}$ and a learning algorithm with the the following property: For every $\epsilon, \delta \in (0,1)$, for every distribution $\mathcal{D}$ over Z, when running the learning algorithm on $m \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d samples generated by $\mathcal{D}$, the algorithm returns a hypothesis h such that with probability at least $1 - \delta$ over the choice of examples,

$$L_D(h) \leq \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') + \epsilon$$

where $L_{\mathcal{D}}(h) = \mathbb{E}_{z \sim \mathcal{D}}[\ell(h, z)]$.