Lecture 2: Probably Approximately Correct Learning

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Contents

1	PAC Lea	arning for Realizable Case	2				
	1.1 Defi	nitions	4				
	1.2 PAC	C-Learnable Guarantees for Finite Hypothesis Sets	,				
	1.3 PAC	C-Learnable Examples for Infinite Hypothesis Sets	,				
2	Agnostic PAC-Learning						
	2.1 Defi	nition and Uniform Deviation Bound					
	2.2 Unif	form Convergence	į				
	2.3 Non	-Realizable Case	1				
3	PAC Lea	arning vs. Universal Consistency	1				

1 PAC Learning for Realizable Case

1.1 Definitions

• Remark (Settings)

In deterministic scenario, denote a collection of n independent identically distributed (i.i.d.) random samples generated by P_X as $X = (X_1, \ldots, X_n)$, and label is generated from a concept $c \in \mathcal{C}$ as $Y_i = c(X_i)$. Denote the sample as

$$\mathcal{D} \equiv \mathcal{D}_n = ((X_1, Y_1), \dots, (X_n, Y_n)) \equiv ((X_1, c(X_1)), \dots, (X_n, c(X_n))).$$

Thus, $\mathcal{D}_n|_X \sim \mathcal{P}_X^n$ is a random sequence of n i.i.d. samples.

A <u>learner</u> \mathcal{A} considers a <u>fixed</u> subset of concepts $\mathcal{H} \subset \mathcal{C}$, which is referred as a <u>hypothesis</u> class, and provides a <u>hypothesis</u> or a <u>classifier</u> or a <u>decision function</u> $h \in \mathcal{H}$. The task of <u>supervised learning</u> is to minimize the generalization error:

$$L(h) \equiv L_{\mathcal{P},c}(h) = \mathcal{P}_X \{ h(X) \neq c(X) \} \equiv \mathbb{E}_{\mathcal{P}} \left[\mathbb{1}_{h(X) \neq c(X)} \right]$$

where $\mathbb{1}_{\omega}$ is the indicator function of the event ω .

In particular, a learning algorithm (such as ERM) A takes sample \mathcal{D}_n as input and output

$$\mathcal{A}(\mathcal{D}_n) = h_n = h_{\mathcal{D}_n}^*(x) \equiv h(x|((X_1, Y_1), \dots, (X_n, Y_n))).$$

Given that \mathcal{D}_n are random samples, $h_n \equiv h_{\mathcal{D}_n}$ are random as well. Thus the generalization error of h_n is a random variable:

$$L_n \equiv L_{\mathcal{P},c}(h_n) := \mathbb{E} \left[\mathbb{1} \left\{ h_{\mathcal{D}_n}(X) \neq c(X) \right\} | \mathcal{D}_n \right] = \mathcal{P} \left\{ h_{\mathcal{D}_n}(X) \neq c(X) | \mathcal{D}_n \right\}.$$

- Remark We denote by $\mathcal{O}(d)$ an upper bound on the cost of the computational representation of any element $x \in \mathcal{X} \subset \mathbb{R}^d$ and by $\operatorname{size}(c)$ the maximal cost of the computational representation of $c \in \mathcal{C}$. For example, x may be a vector in \mathbb{R}^d , for which the cost of an array-based representation would be in $\mathcal{O}(n)$.
- $\bullet \ \mathbf{Remark} \ (\textit{Realizability Assumption})$

There exists a hypothesis $h \in \mathcal{H}$ such that the generalization error is zero.

$$\exists h \in \mathcal{H}, \quad L_{\mathcal{P},c}(h) = 0$$

Every ERM hypothesis has zero training error. In the definition of Probably Approximately Correct (PAC) Learning, we assume the realizability assumption holds.

• Definition (Probably Approximately Correct (PAC) Learning, Realizable Case) Assume that the realizability assumption holds. A hypothesis class \mathcal{H} is said to be <u>Probably Approximately Correct-learnable</u> i.e. <u>PAC-learable</u>, if there exists an algorithm \mathcal{A} and a polynomial function poly $(\cdot, \cdot, \cdot, \cdot)$ such that for any $\epsilon > 0$ and $\delta > 0$, for all distributions \mathcal{P} on \mathcal{X} and for any target concept $c \in \mathcal{C}$, the following holds when the sample size $n \geq \text{poly}(1/\epsilon, 1/\delta, d, \text{size}(c))$:

$$\mathcal{P}\left\{L_{\mathcal{P},c}(\mathcal{A}(\mathcal{D}_n)) \le \epsilon\right\} \ge 1 - \delta. \tag{1}$$

If \mathcal{A} further runs in poly $(1/\epsilon, 1/\delta, d, \text{size}(c))$, then \mathcal{H} is said to be <u>efficiently PAC-learnable</u>. When such an algorithm \mathcal{A} exists, it is called a **PAC-learning algorithm** for \mathcal{H} .

- Remark A hypothesis class \mathcal{H} is thus **PAC-learnable** if the hypothesis returned by the algorithm after observing a number of points **polynomial** in $1/\epsilon$ and $1/\delta$ is
 - 1. approximately correct (error at most ϵ)
 - 2. with high probability (at least 1δ),

which justifies the PAC terminology.

- 1. $\delta > 0$ is used to define **the confidence** 1δ
- 2. and $\epsilon > 0$ the accuracy 1ϵ .

Note that if the running time of the algorithm is **polynomial** in $1/\epsilon$ and $1/\delta$, then **the sample size** n must also be polynomial if the full sample is received by the algorithm.

- Remark (Confidence and Accuracy)
 - 1. For a fixed classifer h, the accuracy of that classifer is measured by $1 L_{\mathcal{P},c}(h)$.
 - 2. The confidence of learning algorithm is measured by the probability of failure for hypothesis returned by the learning algorithm. A failure happens when the learned classifier h has low accuracy, i.e. $L_{\mathcal{P},c}(h) > \epsilon$. Since classifier $h_{\mathcal{D}}$ is function of data \mathcal{D}_n , the confidence is measured by the probability of encountering bad samples \mathcal{D}_n such that $\widehat{L}_{\mathcal{D}}(h_{\mathcal{D}}) = 0$ but $L_{\mathcal{P},c}(h_{\mathcal{D}}) > \epsilon$.

 \mathcal{H} is PAC-learnable when a learning algorithm has $high\ confidence$ to obtain a classifier $h \in \mathcal{H}$ with $high\ accuracy\ regardless$ of the underlying $data\ distribution$ and $labeling\ logic$.

- Remark Several key points of the PAC definition are worth emphasizing.
 - 1. First, the PAC framework is a **distribution-free**: no particular assumption is made about the distribution \mathcal{P} from which examples are drawn.
 - 2. Second, the training sample and the test examples used to define the error are drawn according to the same distribution \mathcal{P} . This is a necessary assumption for generalization to be possible in most cases.
 - 3. Third, the PAC framework is non-asymptotic in which it provides a concentration inequality that holds for all n.
 - 4. Finally, the PAC framework deals with the question of learnability for a hypothesis class \mathcal{H} and not a particular hypothesis h. Note that the concept class \mathcal{C} is known to the algorithm, but of course target concept $c \in \mathcal{C}$ is unknown.

We may omit the polynomial dependency on n and size(c) in the PAC definition and focus only on the sample complexity.

1.2 PAC-Learnable Guarantees for Finite Hypothesis Sets

• Remark (Finite Hypothesis Sets)

We will see if the size of hypothesis class \mathcal{H} is finite, i.e. $|\mathcal{H}| < \infty$, we can achieve PAC learnability under the realizability assumption:

• Proposition 1.1 (Learning bounds, Finite \mathcal{H} , Realizable Case) [Mohri et al., 2018] Let \mathcal{H} be a finite set of functions mapping from \mathcal{X} to \mathcal{Y} . Let \mathcal{A} be an algorithm that for any target concept $c \in \mathcal{H}$ and i.i.d. sample \mathcal{D}_n returns a consistent hypothesis h_n , i.e. the training error of h_n is zero: $\widehat{L}(h_n) = 0$. Then, for any $\epsilon, \delta > 0$, the inequality

$$\mathcal{P}^n \left\{ L_{\mathcal{P},c}(h_n) \le \epsilon \right\} \ge 1 - \delta$$

holds if

$$n \ge \frac{1}{\epsilon} \log \left(\frac{|\mathcal{H}|}{\delta} \right) \tag{2}$$

This sample complexity result admits the following equivalent statement as a generalization bound: for any $\epsilon, \delta > 0$, with **probability** at least $1 - \delta$,

$$L_n \equiv L_{\mathcal{P},c}(h_n) \le \frac{1}{n} \log \left(\frac{|\mathcal{H}|}{\delta} \right).$$
 (3)

Proof: We want to upper bound the probability of event

$$M := \left\{ \mathcal{D}_n \sim \mathcal{P}^n : \exists h \in \mathcal{H}, \ L_{\mathcal{P},c}(h) > \epsilon \wedge \widehat{L}(h) = 0 \right\}.$$

In other word, for each sample $\mathcal{D}_n \in M$, there are bad hypothesis that seems good in the training data \mathcal{D}_n . Under the realizablity assumption, all samples that makes $L_{\mathcal{P},c}(h_n) > \epsilon$ lies in M. Moreover, M can be rewritten as

$$M = \bigcup_{h \in \mathcal{H}_B} \left\{ \mathcal{D}_n \sim \mathcal{P}^n : \widehat{L}(h) = 0 \right\}$$

where $\mathcal{H}_B := \{h \in \mathcal{H} : L_{\mathcal{P},c}(h) > \epsilon\}$. Then by union bound,

$$\mathcal{P}^{n}\left\{L_{\mathcal{P},c}(h_{\mathcal{D}_{n}}) > \epsilon\right\} \leq \mathcal{P}^{n}\left\{\bigcup_{h \in \mathcal{H}_{B}} \left\{\mathcal{D}_{n} : \widehat{L}(h) = 0\right\}\right\}$$

$$\leq \sum_{h \in \mathcal{H}_{B}} \mathcal{P}^{n}\left\{\mathcal{D}_{n} : \widehat{L}(h) = 0\right\}$$

$$(4)$$

Note that

$$\mathcal{P}^n \left\{ \mathcal{D}_n : \widehat{L}(h) = 0 \right\} = \mathcal{P}^n \left\{ h(X_i) = c(X_i), i = 1, \dots, n \right\}$$
$$= \prod_{i=1}^n \mathcal{P} \left\{ h(X_i) = c(X_i) \right\}$$

For each individual sampling of an element of the training set we have

$$\mathcal{P}\left\{h(X_i) = c(X_i)\right\} = 1 - L_{\mathcal{P},c}(h) \le 1 - \epsilon$$

where the last inequality follows from the fact that $h \in \mathcal{H}_B$. Thus, for all $h \in \mathcal{H}_B$,

$$\mathcal{P}^n \left\{ \mathcal{D}_n : \widehat{L}(h) = 0 \right\} \le (1 - \epsilon)^n \le \exp(-n\epsilon)$$

where the last inequality comes from $1 - x \le e^{-x}$. Combining this equation with (4) we conclude that

$$\mathcal{P}^{n}\left\{L_{\mathcal{P},c}(h_{\mathcal{D}_{n}}) > \epsilon\right\} \leq |\mathcal{H}_{B}| \exp\left(-n\epsilon\right) \leq |\mathcal{H}| \exp\left(-n\epsilon\right).$$

Setting the right-hand side to be equal to δ and solving for ϵ concludes the proof.

0	1	-	0	1	Ι	+
0	Ι	1	Τ	1	Ι	+
0	0	1	1	0	1	-
0	Τ	Τ	Τ	1	Ι	+
1	0	0	1	1	0	-
0	T	0	0	Ι	Ι	+
0	I	?	?	T	T	

Figure 1: Algorithm to find concept behind the conjunction of boolean literals under realizability assumption [Mohri et al., 2018]

• Example (Conjunction of Boolean Literals) [Mohri et al., 2018] Consider learning the concept class C_n of conjunctions of at most n Boolean literals x_1, \ldots, x_n . A Boolean literal is either a variable $x_i, i \in [1, n]$, or its negation $\neg x_i$. For n = 4, an example is the conjunction: $x_1 \land \neg x_2 \land x_4$, where $\neg x_2$ denotes the negation of the Boolean literal x_2 . (1,0,0,1) is a positive example for this concept $(1 \land \neg 0 \land 1 = 1)$ while (1,0,0,0) is a negative example $(1 \land \neg 0 \land 0 = 0)$.

Algorithm For each **positive example** (b_1, \ldots, b_n) and $i \in [1, n]$, if $b_i = 1$ then $\neg x_i$ is **ruled out** as a possible literal in the concept class and if $b_i = 0$ then x_i is ruled out. The conjunction of all the literals **not ruled out** is thus a hypothesis **consistent with the target**.

Figure 1 shows an example when n=6. Each of the first six rows of the table represents a training example with its label, + or -, indicated in the last column. The last row contains 0 (respectively 1) in column $i \in [1,6]$ if the i-th entry is 0 (respectively 1) for all the positive examples. It contains "?" if both 0 and 1 appear as an i-th entry for some positive example. Thus, for this training sample, the hypothesis returned by the consistent algorithm described in the text is $\neg x_1 \land x_2 \land x_5 \land x_6$.

We have $|\mathcal{H}| = |\mathcal{C}_n| = 3^n$, since each literal can be included *positively*, with negation, or not included. Using the result of PAC Learning with realizability assumption, we see that for any $\epsilon > 0, \delta > 0$,

$$n \ge \frac{1}{\epsilon} \log \left(\frac{|\mathcal{H}|}{\delta} \right) = \frac{1}{\epsilon} \left(n \log 3 - \log \delta \right)$$

Thus, the class of conjunctions of at most n Boolean literals is PAC-learnable. Note that the computational complexity is also polynomial, since the training cost per example is in $\mathcal{O}(n)$

• Example (k-term DNF Formulae) [Mohri et al., 2018] A disjunctive normal form (DNF) formula is a formula written as the disjunction of several terms, each term being a conjunction of Boolean literals. A k-term DNF is a DNF formula defined by the disjunction of k terms, each term being a conjunction of at most n Boolean literals. Thus, for k = 2 and n = 3, an example of a k-term DNF is $(x_1 \wedge \neg x_2 \wedge x_3) \vee (x_1 \wedge x_3)$.

The cardinality of the class is 3^{nk} , since each term is a conjunction of at most n variables and there are 3^n such conjunctions, as seen previously.

Is the class C of k-term DNF formulae is PAC-learnable? The hypothesis set \mathcal{H} must contain C for realizability assumption to hold, thus $|\mathcal{H}| \geq 3^{nk}$. The generalization bound gives the sample complexity as

$$n \ge \frac{1}{\epsilon} \left(nk \log 3 - \log \delta \right)$$

which is **polynomial**. **However**, it can be shown that the problem of learning k-term DNF is in \underline{RP} , the complexity class of problems that **admit a** randomized polynomial-time **decision solution**. The problem is therefore **computationally intractable** unless RP = NP, which is commonly conjectured not to be the case. Thus, while the sample size needed for learning k-term DNF formulae is only polynomial, **efficient PAC-learning** of this class is **not possible** unless RP = NP.

• Example (k-CNF Formulae) [Mohri et al., 2018] A conjunctive normal form (CNF) formula is a conjunction of disjunctions. A k- \overline{CNF} formula is an expression of the form $T_1 \wedge \ldots \wedge T_j$ with arbitrary length $j \in \mathbb{N}$ and with each term T_i being a disjunction of at most k Boolean attributes.

The problem of *learning* k-CNF formulae can be reduced to that of *learning conjunctions of Boolean literals*, which, as seen previously, is a PAC-learnable concept class. To do so, it suffices to associate to each term T_i a new variable. Then, this can be done with the following bijection:

$$a_i(x_1) \wedge \ldots \wedge a_i(x_n) \rightarrow Y_{a_i(x_1),\ldots,a_i(x_n)}$$

where $a_i(x_j)$ denotes the assignment to x_j in term T_i . Thus, the **PAC-learnability** of conjunctions of Boolean literals implies that of k-CNF formulae.

This is a surprising result, however, since any k-term DNF formula can be written as a k-CNF formula.

$$\bigvee_{i=1}^k a_i(x_1) \wedge \ldots \wedge a_i(x_n) = \bigwedge_{i_1,\ldots,i_k=1}^n a_i(x_{i_1}) \wedge \ldots \wedge a_k(x_{i_k}).$$

But, as we previously saw, k-term DNF formula are not efficiently PAC-learnable.

What can explain this apparent inconsistency? Observe that the number of new variables needed to write a k-term DNF as a k-CNF formula via the transformation just described is exponential in k, it is in $\mathcal{O}(n^k)$. The discrepancy comes from the size of the representation of a concept. A k-term DNF formula can be an exponentially more compact representation, and efficient PAC-learning is intractable if a time-complexity polynomial in that size is required.

Thus, this apparent paradox deals with key aspects of PAC-learning, which include the cost of the representation of a concept and the choice of the hypothesis set.

1.3 PAC-Learnable Examples for Infinite Hypothesis Sets

- Example (Learning Axis-Aligned Rectangles) [Mohri et al., 2018] Consider the case where the set of instances are points in the plane, $\mathcal{X} = \mathbb{R}^2$, and the concept class \mathcal{C} is the set of all axis-aligned rectangles lying in \mathbb{R}^2 . Thus, each concept c is the set of points inside a particular axis-aligned rectangle. The learning problem consists of determining with small error a target axis-aligned rectangle using the labeled training sample. We will show that the concept class of axis-aligned rectangles is PAC-learnable.
- Example (*Threshold Function Class is Learnable*) [Shalev-Shwartz and Ben-David, 2014, Mohri et al., 2018]

Let \mathcal{H} be the set of threshold functions over the *real line*, namely,

$$\mathcal{H} = \{h_{\alpha} : \alpha \in \mathbb{R}\}, \text{ where } h_{\alpha}(x) = \mathbb{1}_{\{x < \alpha\}}.$$

Clearly, \mathcal{H} is of infinite size.

Nevertheless, the following lemma shows that \mathcal{H} is learnable in the PAC model using the ERM algorithm.

Lemma 1.2 | Shalev-Shwartz and Ben-David, 2014|

Let \mathcal{H} be the class of **thresholds** as defined earlier. Then, \mathcal{H} is **PAC learnable**, using the ERM rule, with **sample complexity** of

$$m_{\mathcal{H}}(\epsilon, \delta) \le \left\lceil \log \left(\frac{2/\delta}{\epsilon} \right) \right\rceil.$$

2 Agnostic PAC-Learning

2.1 Definition and Uniform Deviation Bound

• Definition (Agnostic PAC-Learning)

Let \mathcal{H} be a hypothesis set. \mathcal{A} is an <u>agnostic PAC-learning algorithm</u> if there exists a **polynomial function** poly $(\cdot, \cdot, \cdot, \cdot)$ such that for any $\epsilon > 0$ and $\delta > 0$, for all distributions \mathcal{P} over $\mathcal{X} \times \mathcal{Y}$, the following holds for any sample size $n \geq \text{poly}(1/\epsilon, 1/\delta, d, \text{size}(c))$:

$$\mathcal{P}\left\{L_{\mathcal{P}}(\mathcal{A}(\mathcal{D}_n)) - \inf_{h \in \mathcal{H}} L(h) \le \epsilon\right\} \ge 1 - \delta.$$
 (5)

If \mathcal{A} further runs in $poly(1/\epsilon, 1/\delta, d, size(c))$, then \mathcal{C} is said to be <u>efficiently agnostic</u> PAC-learnable.

• Remark (Bounding Excess Risk via Uniform Deviation)

The difference between the error of a hypothesis $h \in \mathcal{H}$ and the Bayes error can be decomposed as:

$$L(h) - L^* = \underbrace{\left(L(h) - \inf_{h \in \mathcal{H}} L(h)\right)}_{estimation\ error} + \underbrace{\left(\inf_{h \in \mathcal{H}} L(h) - L^*\right)}_{approximation\ error}.$$

where the first term is the *estimation error* and the second term is the *approximation error*.

- When \mathcal{H} and \mathcal{P} are fixed, the approximation error is fixed.
- The definition of agnostic PAC learnability requires that the estimation error would be bounded above uniformly over all distributions.

$$L(h_n) - \inf_{h \in \mathcal{H}} L(h) = L(h_n) - \widehat{L}(h_n) + \widehat{L}(h_n) - L(h^*)$$

$$\leq L(h_n) - \widehat{L}(h_n) + \widehat{L}(h^*) - L(h^*)$$

$$\leq 2 \sup_{h \in \mathcal{H}} \left| L(h) - \widehat{L}(h) \right|$$
(6)

where $h^* = \operatorname{argmin}_{h \in \mathcal{H}} L(h)$ and $\widehat{L}(h)$ is the training error of g. The second last inequality is due to the fac that h_n minimizes the training error. Thus the estimation error can be bounded uniformly by the generalization error bound $|L(h) - \widehat{L}(h)|$ for any $h \in \mathcal{H}$.

• Remark (*Empirical Process*)

From the inequality (6), we see that **the excess risk** (estimation error) is **uniformly bounded** by the deviation of generation error from the training error.

$$\sup_{h \in \mathcal{H}} \left| \widehat{L}(h) - L(h) \right| := \left\| \widehat{\mathcal{P}}_n - \mathcal{P} \right\|_{\mathcal{H}}$$

Definition (*Glivenko-Cantelli Class*) [Wainwright, 2019, Giné and Nickl, 2021] We say that \mathcal{H} is a *Glivenko-Cantelli class* for \mathcal{P} if $\|\widehat{\mathcal{P}}_n - \mathcal{P}\|_{\mathcal{H}}$ converges to zero in probability as $n \to \infty$.

We can define an empirical process X_{f_h} indexed by \mathcal{F} as

$$X_{f_h} := \frac{1}{n} \sum_{i=1}^{n} f_h(X_i) - \mathbb{E}[f_h(X)]$$

where $f_h(x) = \mathbb{1} \{h(x) \neq c(x)\} \in \mathcal{F}$.

2.2 Uniform Convergence

• **Definition** (ϵ -Representative Sample). [Shalev-Shwartz and Ben-David, 2014] A training set \mathcal{D} is called $\underline{\epsilon}$ -representative (w.r.t. domain \mathcal{X} , hypothesis class \mathcal{H} , loss function ℓ , and distribution $\overline{\mathcal{P}}$) if

$$\forall h \in \mathcal{H}, \quad \left| \widehat{L}_{\mathcal{D}}(h) - L_{\mathcal{P}}(h) \right| \leq \epsilon.$$

• Our analysis on the uniform deviation bound for excess risk shows the following results:

Lemma 2.1 (ERM Excess Risk given Representative Sample) [Shalev-Shwartz and Ben-David, 2014]

Assume that a training set \mathcal{D} is $(\epsilon/2)$ -representative (w.r.t. domain \mathcal{X} , hypothesis class \mathcal{H} , loss function ℓ , and distribution \mathcal{P}). Then, any output of $ERM_{\mathcal{H}}(\mathcal{D})$, namely, any $h_{\mathcal{D}} \in \operatorname{argmin}_{h \in \mathcal{H}} \widehat{L}_{\mathcal{D}}(h)$, satisfies

$$L_{\mathcal{P}}(h_{\mathcal{D}}) \leq \inf_{h \in \mathcal{H}} L_{\mathcal{P}}(h) + \epsilon.$$

- Remark The preceding lemma implies that to ensure that the *ERM rule is an agnostic PAC learner*, it suffices to show that with probability of at least 1δ over the random choice of a training set, it will be an ϵ -representative training set.
- **Definition** (*Uniform Convergence*). [Shalev-Shwartz and Ben-David, 2014] We say that a hypothesis class \mathcal{H} has <u>the uniform convergence property</u> (w.r.t. a domain \mathcal{D} and a loss function ℓ) if there exists a function $n_{\mathcal{H}}^{UC}:(0,1)^2 \to \mathbb{N}$ such that for every $\epsilon, \delta \in (0,1)$ and **for every probability distribution** \mathcal{P} over \mathcal{X} , if \mathcal{D}_n is a sample of $n \geq n_{\mathcal{H}}^{UC}(\epsilon,\delta)$ examples drawn i.i.d. according to \mathcal{P} , then, with probability of at least $1-\delta$, \mathcal{D}_n is ϵ -representative.
- Remark (Regardless of \mathcal{H} and \mathcal{P})
 The term uniform here refers to having a fixed sample size that works for all members of \mathcal{H} and over all possible probability distributions over the domain.

It means that for all distribution \mathcal{P} , the uniform deviation is bounded with probability at least $1 - \delta$.

$$\mathcal{P}^{n} \left\{ \sup_{h \in \mathcal{H}} \left| L_{\mathcal{P}}(h) - \widehat{L}_{\mathcal{D}_{n}}(h) \right| \leq \phi(n, \delta, \mathcal{H}) \right\} \geq 1 - \delta$$

Corollary 2.2 (ERM is Agnostic PAC Learnable) [Shalev-Shwartz and Ben-David, 2014]
If a class H has the uniform convergence property with a function n_H^{UC} then the class is agnostically PAC learnable with the sample complexity n(ε, δ) ≤ n_H^{UC}(ε/2, δ). Furthermore, in that case, the ERM_H paradigm is a successful agnostic PAC learner for H.

2.3 Non-Realizable Case

• Remark (Realizability Assumption or Not)

Under realizability assumption, the target concept $c \in \mathcal{H}$ is in the hypothesis class. Under this assumption, a learning algorithm knows that there exists a solution that **match all positive** and negative decisions. Moreover, a perfect match in training set is sufficient to guarantee good performance in generalization error.

Thus the task of algorithm under realizability assumption is essentially **detection**: we begin with finite training samples and make sure our choice of solution will not conflict any of them. If we find one, then this one must be the one with zero generalization error as well since we know that there exists one single logic behind both training data and general population.

If we drop the realizability assumption, the task becomes to find a solution that is as close to the best solution in \mathcal{H} as possible. This task is much challenging since it involves an **optimization** over an extremely large space \mathcal{H} .

• To prove the general case, we use a bound from *Hoeffding's inequality*:

Proposition 2.3 Fix $\epsilon > 0$ and let \mathcal{D}_n denote an i.i.d. sample of size n. Then, for any

hypothesis $h: \mathcal{X} \to \{0,1\}$, the following inequalities hold:

$$\mathcal{P}^{n}\left\{\widehat{L}(h) - L(h) \ge \epsilon\right\} \le \exp\left(-2n\epsilon^{2}\right) \tag{7}$$

$$\mathcal{P}^{n}\left\{\widehat{L}(h) - L(h) \le -\epsilon\right\} \le \exp\left(-2n\epsilon^{2}\right) \tag{8}$$

By the union bound, this implies the following two-sided inequality:

$$\mathcal{P}^{n}\left\{ \left| \widehat{L}(h) - L(h) \right| \ge \epsilon \right\} \le 2 \exp\left(-2n\epsilon^{2}\right). \tag{9}$$

Setting the right-hand side of (9) to be equal to δ and solving for ϵ yields immediately the following bound for a single hypothesis

Corollary 2.4 (Generalization bound for Single Hypothesis) [Mohri et al., 2018] Fix a hypothesis $h: \mathcal{X} \to \{0,1\}$. Then, for any $\delta > 0$, the following inequality holds with probability at least $1 - \delta$:

$$L(h) \le \widehat{L}(h) + \sqrt{\frac{\log \frac{2}{\delta}}{2n}} \tag{10}$$

This error bound can be seen as coming from the randomness of coin tossing when approximate the generalization error L(h) by training error. Thus it will always exist for any generalization error bound.

• Proposition 2.5 (Learning bounds, Finite H, Non-Realizable Case) [Mohri et al., 2018]

Let \mathcal{H} be a **finite** set of functions mapping from \mathcal{X} to \mathcal{Y} . Then, for any $\delta > 0$ with probability at least $1 - \delta$, the following inequality holds: for all $h \in \mathcal{H}$

$$L(h) \le \widehat{L}(h) + \sqrt{\frac{\log |\mathcal{H}| + \log \frac{2}{\delta}}{2m}}$$
(11)

Thus for a finite hypothesis set \mathcal{H} ,

$$L(h) \le \widehat{L}(h) + O\left(\sqrt{\frac{\log |\mathcal{H}|}{m}}\right)$$
 (12)

Proof: Let $h_1, \ldots, h_{|\mathcal{H}|}$ be the elements of \mathcal{H} . Using the union bound and applying Corollary 2.4 to each hypothesis yield:

$$\mathcal{P}^{n}\left\{\mathcal{D}_{n}: \exists h \in \mathcal{H}, \left| L(h) - \widehat{L}_{\mathcal{D}_{n}}(h) \right| > \epsilon \right\} \leq \sum_{h \in \mathcal{H}} \mathcal{P}^{n}\left\{ \left| L(h) - \widehat{L}_{\mathcal{D}_{n}}(h) \right| > \epsilon \right\}$$
$$\leq 2 |\mathcal{H}| \exp\left(-2n\epsilon^{2}\right)$$

Setting the right-hand side to be equal to δ completes the proof.

• Remark (Sample Efficiency \Leftarrow Representation Efficiency of Hypothesis Class) As already pointed out, $\log |\mathcal{H}|$ can be interpreted as the number of bits needed to represent \mathcal{H} . Several other remarks similar to those made on the generalization bound in the consistent case can be made here:

a larger sample size m guarantees **better generalization**, and the bound **increases** with $|\mathcal{H}|$, but only **logarithmically**.

But, here, the bound is a less favorable function of $\log |\mathcal{H}|/m$; it varies as **the square root** of this term. This is not a minor price to pay: for a fixed $|\mathcal{H}|$, to attain the same guarantee as in the **consistent case**, a **quadratically larger labeled** sample is needed.

3 PAC Learning vs. Universal Consistency

- Remark (*Universal Consistency is Not Enough*) [Shalev-Shwartz and Ben-David, 2014] We compare the *universal consistency* and *PAC learnability* as *performance guarantee* for a classification rule:
 - 1. The universal consistency of a classification rule provides a performance guarantee in terms of <u>asymptotic analysis</u>. It concerns that if the generalization error of classification rule $\{h_n\}$ will reach to infimum within given class \mathcal{H} when the sample size is infinity $n \to \infty$. The universal consistency is a meaningle of correctness, i.e. the classification rule can reach to correct solution eventually regardless of the underlying distribution of data.

On the other hand, it does not anwser how many examples are required to be as good as the best hypothesis in \mathcal{H} . The answer to this question depends on the underlying distribution $\mathcal{P}_{X,Y}$ in consistency statement. The consistency statement is more related to large sample statistical behavior.

2. The PAC learnability of a classification rule provides a performance guarantee in terms of <u>non-asymptotic analysis</u>. It provide a measure of <u>efficiency</u>. An algorithm is efficient if it obtain a solution close to correct solution (within an error rate ϵ) with high probability $(1 - \delta)$ given a finite set of $n \ge n(\epsilon, \delta)$ samples.

The PAC learnability is a measure for the **algorithm** as well as **the statistical nature** of the problem. Its formulation is closer to computer science than to statistics.

Moreover, the definition of PAC learning yields the limitation of learning (via the No-Free-Lunch theorem) and the necessity of prior knowledge. It gives us a crisp way to encode prior knowledge by choosing a hypothesis class, and once this choice is made, we have a generic learning rule - ERM. Compared to PAC learning, the definition of consistency does not yield a natural learning paradigm or a way to encode prior knowledge. In fact, in many cases there is no need for prior knowledge at all since the consistency only cares about the asymptotic behavior.

Consider the classification prediction algorithm Memorize defined as follows. The algorithm memorizes the training examples, and, given a test point x, it predicts the majority label among all labeled instances of x that exist in the training sample (and some fixed default label if no instance of x appears in the training set). It is possible to show (see Exercise below) that the Memorize algorithm is universally consistent for every countable domain \mathcal{X} and a finite label set \mathcal{Y} (w.r.t. the zero-one loss).

Intuitively, it is *not obvious* that the *Memorize* algorithm should be viewed as a *learner*, since it *lacks* the aspect of *generalization*, namely, of using observed data to *predict* the

labels of unseen examples. The fact that *Memorize* is a *consistent algorithm* for the class of all functions over any countable domain set therefore raises doubt about **the usefulness** of consistency guarantees. Furthermore, the sharp-eyed reader may notice that the "bad learner" we introduced in Chapter 2, which led to overfitting, is in fact the *Memorize* algorithm.

• Exercise 3.1 (Memorize Algorithm)

In this example we wish to show that the algorithm Memorize is a consistent learner for every class of (binary-valued) functions over any countable domain.

Let \mathcal{X} be a **countable** domain and let \mathcal{P} be a probability distribution over \mathcal{X} .

1. Let $\{x_i : i \in \mathbb{N}\}\$ be an enumeration of the elements of \mathcal{X} so that for all $i \leq j$, $\mathcal{P}(\{x_i\}) \leq \mathcal{P}(x_j)$. Prove that

$$\lim_{n \to \infty} \sum_{i > n} \mathcal{P}(\{x_i\}) = 0.$$

Note that $\sum_{i=0}^{\infty} \mathcal{P}(\{x_i\}) = 1$ by definition of probability measure.

2. Given any $\epsilon > 0$, prove that there exists $\epsilon_{\mathcal{P}} > 0$ such that

$$\mathcal{P}\left\{x \in \mathcal{X} : \mathcal{P}(\left\{x\right\}) < \epsilon_{\mathcal{P}}\right\} < \epsilon.$$

3. Prove that for every $\eta > 0$, if n is such that $\mathcal{P}(\{x_i\}) < \eta$ for all i > n, then for every $m \in \mathbb{N}$, let \mathcal{D}_n be the sample of size m generated according to \mathcal{P}

$$\mathcal{P}_{\mathcal{D}_m} \{ \exists x_i : \mathcal{P}(\{x_i\}) > \eta \text{ and } x_i \notin \mathcal{D}_m \} \leq ne^{-\eta m}.$$

4. Conclude that if \mathcal{X} is **countable** then for **every probability distribution** \mathcal{P} over \mathcal{X} there exists a function $m_{\mathcal{P}}: (0,1) \times (0,1) \to \mathbb{N}$ such that for every $\epsilon, \delta > 0$ if $m > m_{\mathcal{P}}(\epsilon, \delta)$ then

$$\mathcal{P}_{\mathcal{D}_m} \left\{ \mathcal{P}(\left\{ x : x \notin \mathcal{D}_m \right\}) > \epsilon \right\} < \delta.$$

- 5. Prove that **Memorize** is a consistent learner for every class of (binary-valued) functions over any countable domain.
- Remark (*Universal Consistency May Not be Good Preference*) [Shalev-Shwartz and Ben-David, 2014]

One may argue that even though consistency is a weak requirement, it is desirable that a learning algorithm will be consistent with respect to the set of all functions from \mathcal{X} to \mathcal{Y} , which gives us a guarantee that for enough training examples, we will always be as good as the Bayes optimal predictor. Therefore, if we have two algorithms, where one is consistent and the other one is not consistent, we should prefer the consistent algorithm. **However**, this argument is **problematic** for two reasons.

1. First, maybe it is the case that for most "natural" distributions we will observe in practice that the sample complexity of the consistent algorithm will be so large so that in every practical situation we will not obtain enough examples to enjoy this guarantee.

2. Second, it is not very hard to make any PAC or nonuniform learner consistent with respect to the class of all functions from \mathcal{X} to \mathcal{Y} .

Concretely, consider a countable domain, \mathcal{X} , a finite label set \mathcal{Y} , and a hypothesis class, \mathcal{H} , of functions from \mathcal{X} to \mathcal{Y} . We can make any nonuniform learner for H be consistent with respect to the class of all classifiers from \mathcal{X} to \mathcal{Y} using the following simple trick: Upon receiving a training set, we will first run the nonuniform learner over the training set, and then we will obtain a *bound* on the true risk of the learned predictor. If this bound is *small enough* we are done. Otherwise, we revert to the *Memorize* algorithm. This simple modification makes the algorithm consistent with respect to all functions from \mathcal{X} to \mathcal{Y} .

Since it is easy to make any algorithm consistent, it may not be wise to prefer one algorithm over the other just because of consistency considerations.

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