Contents

Introduction

Programme of the course

Arguments treated:

1. **Motivation**: components of the learning problem and applications of Machine Learning. Supervised and unsupervised learning.
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3. **Probabilistic models and assumptions on the data**: the regression function. Regression and classification.
4. **When is a model good?**: model complexity, bias variance tradeoff/generalization (VC dimension, generalization error).
5. **Models for regression**: linear regression (scalar and multivariate), subset selection, linear-in-the-parameters models, regularization.
6. **Simple models for classification**: logistic regression, perceptron, naïve bayes classifier.
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8. **Neural Networks**.
9. **Deep Learning**: Convolutional Neural Networks.
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Chapter 1

Machine Learning framework

1.1 A formal model

We begin with the description of a formal model in order to capture what could be the learning tasks. The fundamental points are:

- **The learner's input**:
  - A domain set $\mathcal{X}$, whose points are the istances we want to label.
  - A label set $\mathcal{Y}$.
  - The training dataset $S = \mathcal{X} \times \mathcal{Y}$. It is a finite sequence of label domain points.
- **The learner's output**:
  - A prediction rule $h : \mathcal{X} \to \mathcal{Y}$ (also called predictor or hyothesis or classifier). It is used to predict the label of new domain points. Therefore $A(S)$ is the hypothesis, where A represents the algorithm.
  - **Simple data-generation model**:
    Assume that the training data are generated by a probability distribution $\mathbb{D}$ (over $\mathcal{X}$). Moreover, suppose that the learner doesn't know anything about the distribution and that there exists some "correct" labeling function $f \ : \ \mathcal{X} \to \mathcal{Y}$ such that $y_i = f(x_i) \ \forall i$ (and it is unknown to the learner as well). So, in summary each S is generated by first sampling a point x_i according to $\mathcal{D}$ and then labeling it with the function f.
- **Measures of success**:
  A definition of "**Error of the classifier**" sohuld be introduced: it is the probability to draw a random instance x, according to D, such that $h(x) \neq f(x)$. Formally: $A \subset \mathcal{X} \implies \mathcal{D}(A)$ determines how likely it is to observe a $x \in A$, where:

  $$A = \{x \in \mathcal{X} \ : \ \pi(x) = 1\} \quad \text{with} \quad \pi \ : \ \mathcal{X} \to \{0, 1\}$$

  We refer to A as an event and therefore:

  $$\mathcal{D}(A) \equiv \mathbb{P}_{x \sim \mathcal{D}}[\pi(x)]$$

  The error of $h \ : \ \mathcal{X} \to \mathcal{Y}$ is finally:

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

  Note that $(\mathcal{D}, f)$ means that the error is computed with respect to the probability distribution $\mathcal{D}$ and the correct labeling function f. Moreover, remind that the learner is blind to the $\mathcal{D}$ and f.

1.2 Empirical Risk Minimization (ERM)

As mentioned before, a learning algorithm receives as input a training set S, sampled from an unknown distriibution D and labeled by some target function f, and should output a predictor $h_S : \mathcal{X} \to \mathcal{Y}$. The goal of the algorithm is to find h_S that minimizes the error with respect to the unknown D and f. Since the learner doesn't know what D and f are, the true error is not directly available to the learner. However, we can define the useful notion of **training error**, i.e. the error the classifier incurs over the training sample:

$$L_S(h) := \frac{|\{i \in [m] \ : \ h(x_i) \neq y_i\}|}{m} \tag{1.1}$$

where $[m] = \{1, \dots, m\}$. Note that the terms *empirical error* and *empirical risk* are often used with the same meaning to indicate Eq. 1.1.

1.2.1 Something may go wrong: Overfitting

This approach can fail miserably if naively used and lead to this phenomenon. Our aim is to find some conditions that guarantee the absence of overfitting.
Intuitively, overfitting occurs when our hypotesis fits the training data "too well" and so our algorithm won't have good performances on a new never-seen dataset.

1.2.2 Empirical Risk Minimization with inductive bias

The ERM rule might lead to overfitting, so we have to find a way to rectify it. In other words, we have to find some conditions that guarantee no overfitting. It means that if the algorithm has good performances with respect to the training data, it is also highly likely to perform well over the underlying data distribution.
A common solution is to apply the ERM learning rule over a restricted search space. Formally, the learner should choose a set of predictors $\mathcal{H}$ before seeing the data. This is a **hypotesis class**. Then, given a training sample S, the $\text{ERM}_{\mathcal{H}}$ learner uses the ERM rule to choose a predictor $h \in \mathcal{H}$ with the lowest possible error over S, which means mathematically:

$$\text{ERM}_{\mathcal{H}}(S) \in \underset{h \in \mathcal{H}}{\text{argmin}} \ L_S(h) \tag{1.2}$$

Such restrictions are often denoted as **inductive bias**.

Finite hypotesis classes

Now we consider a finite hypothesis class $\mathcal{H}$ and denote with h_S the result obtained applying $\text{ERM}_{\mathcal{H}}$ to S, namely Eq. 1.2. We also make the following simplifying assumption:

Definition 1.2.1 (The realizability assumption)**.** There exists $h^* \in \mathcal{H}$ such that $L_{(\mathcal{D},f)}(h^*) = 0$.

Note that this assumption implies that with probability 1 over random samples S we have $L_S(h^*) = 0$, where the istances of S are sampled according to $\mathcal{D}$ and are labeled by f.
Another assumption has to be done, presented in the following definition.

Definition 1.2.2 (Independently and identically distributed)**.** The examples in the training set are independently and identically distributed (i.i.d.) according to the distribution $\mathcal{D}$ if every x_i in S is freshly sampled according to $\mathcal{D}$ and then labeled

according to the labeling function f. We denote this assumption by $S \sim \mathcal{D}^m$, where m is the size of S and $\mathcal{D}^m$ denotes the probability over m-tuples induced by applying $\mathcal{D}$ to pick each element of the tuple independently of the other members of the tuple.

We want to give an upper bound of the probability to sample a m-tuple of istances that will lead to the failure of the learner. Therefore we consider the probability δ of getting a non representative sample S of the distribution. Through δ we define the **confidence parameter** $1-\delta$. We also introduce an **accuracy parameter** ε, with this meaning:

- $L_{(\mathcal{D},f)}(h_S) > \varepsilon \implies$ failure of the learner;
- $L_{(\mathcal{D},f)}(h_S) \leq \varepsilon \implies$ success of the learner.

So we would like to upper bound:

$$\mathcal{D}^m(\{S|_x \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\}) \tag{1.3}$$

For this reason we consider the set of "bad" hypotheses $\mathcal{H}_B$:

$$\mathcal{H} = \{h \in \mathcal{H} \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\} \tag{1.4}$$

In addition, we consider the set of misleading samples:

$$M = \{S|_x \ : \ \exists h \in \mathcal{H}_B, \ L_S(h) = 0\} \tag{1.5}$$

namely, $\forall S|_x \in M \ \exists h \in \mathcal{H}_B$ that looks like a "good" hypothesis on $S|_x$, which means:

$$\{S|_x \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\} \subseteq M \implies M = \bigcup_{h \in \mathcal{H}_B} \{S|_x \ : \ L_S(h) = 0\} \tag{1.6}$$

Hence:

$$\mathcal{D}^m(\{S_x \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\}) \leq \mathcal{D}^m(M) = \mathcal{D}^m\left(\bigcup_{h \in \mathcal{H}_B} \{S|_x \ : \ L_S(h) = 0\}\right) \tag{1.7}$$

Next, we upper bound the right-hand side of Eq. 1.7 using the following lemma, derived from basic properties of probability.

Lemma 1.2.1 (Union Bound)**.** *For any two sets A, B and a distribution $\mathcal{D}$ we have:*

$$\mathcal{D}(A \cup B) \leq \mathcal{D}(A) + \mathcal{D}(B) \tag{1.8}$$

Applying Lemma 1.2.1 to the right-hand side of Eq. 1.7 yields:

$$\mathcal{D}^m(\{S_x \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\}) \leq \sum_{h \in \mathcal{H}_B} \mathcal{D}^m(\{S|_x \ : \ L_S(h) = 0\}) \tag{1.9}$$

The next step is to bound each summand of the right-hand side of Ineq. 1.9. Let's fix some "bad" hypothesis $h \in \mathcal{H}_B$. The event $L_S(h) = 0$ is equivalent to the event $\forall i, \ h(x_i) = f(x_i)$. Since the examples in the training dataset are sampled i.i.d. we get:

$$\mathcal{D}^m(\{S|_x \ : \ L_S(h) = 0\}) = \mathcal{D}^m(\{S|_x \ : \ \forall i, \ h(x_i) = f(x_i)\}) \tag{1.10}$$

$$= \prod_{i=1}^{m} \mathcal{D}(\{x_i \ : \ h(x_i) = f(x_i)\}) \tag{1.11}$$

Lastly, for each individual sampling of an element of the training set we have:

$$\mathcal{D}(\{x_i \ : \ h(x_i) = y_i\}) = 1 - L_{(\mathcal{D},f)}(h) \leq 1 - \varepsilon \tag{1.12}$$

The last inequality follows from the fact that $h \in \mathcal{H}_B$. So we combine Eq. 1.12 with Eq. and we use the inequality $1 - \varepsilon \leq e^{-\varepsilon}$ to get $\forall h \in \mathcal{H}_B$:

$$\mathcal{D}^m(\{S|_x \ : \ L_S(h) = 0\}) \leq (1 - \varepsilon)^m \leq e^{-\varepsilon m} \tag{1.13}$$

Combining Eq. 1.13 with Eq. 1.9 we conclude that:

$$\mathcal{D}^m(\{S_x \ : \ L_{(\mathcal{D},f)}(h_S) > \varepsilon\}) \leq |\mathcal{H}_B| e^{-\varepsilon m} \leq |\mathcal{H}| e^{-\varepsilon m} \tag{1.14}$$

Finally, we get the following useful corollary.

Corollary 1.2.1.1. *Let $\mathcal{H}$ be a finite hypothesis class. Let $\delta \in (0,1)$ and $\varepsilon > 0$ and let m be an integer that satisfies:*

$$m \geq \frac{\log(|\mathcal{H}|/\delta)}{\varepsilon}$$

Then, for any labeling function, f, and for any distribution, $\mathcal{D}$, for which the realizability assumption holds (for some $h \in \mathcal{H}$, $L_{(\mathcal{H},f)}(h) = 0$), with probability of at least $1 - \delta$ over the choice of an i.i.d. sample S of size m, we have that for every ERM hypothesis, h_S, it holds that:

$$L_{(\mathcal{H},f)}(h_S) \leq \varepsilon$$

The Corollary 1.2.1.1 tells us that for a sufficiently large m, the $\text{ERM}_{\mathcal{H}}$ rule over a finite hypotesis class will be *probably* (with confidence $1-\delta$) *approximately* (up to an error of ε) correct.

Chapter 2

A formal learning model

2.1 Probably Approximated Correct (PAC) learning

Definition 2.1.1 (PAC learnability)**.** A hypothesis class $\mathcal{H}$ is PAC learnable if there exist a function $m_{\mathcal{H}} : (0,1)^2 \to \mathbb{N}$ and a learning algorithm with the following property: $\forall \varepsilon, \delta \in (0,1)$, for every distribution $\mathcal{D}$ over $\mathcal{X}$, and for every labeling function $f : \mathcal{X} \to \{0,1\}$, if the realizable assumption holds with respect to $\mathcal{H}, \mathcal{D}, f$, then when running the learning algorithm on $m \geq m_{\mathcal{H}}(\varepsilon, \delta)$ i.i.d. examples generated by $\mathcal{D}$ and labeled by f, the algorithm returns a hypotesis h such that, with probability of at least $1 - \delta$ (over the choice of the examples), $L_{(\mathcal{D},f)}(h) \leq \varepsilon$.

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

Corollary 2.1.0.1. *Every finite class is PAC learnable with sample complexity:*

$$m_{\mathcal{H}}(\varepsilon, \delta) \leq \left\lceil \frac{1}{\varepsilon} \log\left(\frac{|\mathcal{H}|}{\delta}\right) \right\rceil \tag{2.1}$$

Now we want to generalize by:

- Removing the realizability assumption.
  For practical learning tasks, this assumption may be too strong and it isn't necessarily met.

- Extending to learning problems beyond the simple binary classification.
  One may wish to predict real valued numbers or a label picked from a finite set of labels. Therefore our analysis can be extended to many othere scenarios by allowing a variety of loss functions.

2.2 Agnostic PAC learning

We introduce a more realistic model for the data-generating distribution. From now on, let $\mathcal{D}$ be a probability distribution over $\mathcal{X} \times \mathcal{Y}$ (the meaning of the notation hasn't changed). $\mathcal{D}$ is a **joint distribution** over domain points and labels and it can be viewed as the composition of two parts:

- A distribution $\mathcal{D}_x$ over unlabeled domain points (also called **marginal distribution**).

- A **conditional probability** $\mathcal{D}((x,y)|x)$ over labels for each domain point.

2.2.1 Empirical and true error revised

One can measure how likely h is to make an error when labeled points are randomly drawn according to $\mathcal{D}$ previously introduced. So we redefine the true error of a prediction rule h:

$$L_{\mathcal{D}}(h) := \underset{(x,y)\sim\mathcal{D}}{\mathbb{P}}[h(x) \neq y] := \mathcal{D}(\{(x,y) \ : \ h(x) \neq y\}) \tag{2.2}$$

We would like to find a predictor h for which the error in Eq. 2.2 will be minimized. However, the learner doesn't know the data generating $\mathcal{D}$, but he has access only to the training set S. Hence the definition of the empirical risk remains the same as before:

$$L_S(h) := \frac{|\{i \in [m] \ : \ h(x_i) \neq y_i\}|}{m} \tag{2.3}$$

The goal is to find some hypotesis $h \ : \ \mathcal{X} \to \mathcal{Y}$ that (probably approximately) minimizes the true risk, $L_{\mathcal{D}}(h)$.

2.2.2 Bayes optimal predictor

Given any probability distribution $\mathcal{D}$ over $\mathcal{X} \times \{0,1\}$, the best label predicting function from $\mathcal{X}$ to $\{0,1\}$ will be:

$$f_{\mathcal{D}}(x) = \begin{cases} 1 & \text{if } \mathbb{P}[y=1|x] \geq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases} \tag{2.4}$$

Proposition 2.2.1. *For every probability distribution $\mathcal{D}$, the Bayes optimal predictor $f_{\mathcal{D}}$ is optimal, in the sense that no other classifier $g \ : \ \mathcal{X} \to \{0,1\}$ has a lower error. Mathematically:*

$$L_{\mathcal{D}}(f_{\mathcal{D}}) \leq L_{\mathcal{D}}(g) \qquad \forall g \tag{2.5}$$

Clearly, we can't hope that the learning algorithm will find a hypotesis whose error is smaller than the minimal possible error of the Bayes predictor. We require that the learning algorithm will find a predictor whose error is not much larger than the best possible error of a predictor in some given benchmark hypotesis class. So, we generalize the definition of PAC learning.

Definition 2.2.1 (Agnostic PAC learnability)**.** A hypotesis class is PAC learnable if there exist a function $m_{\mathcal{H}} \ : \ (0,1)^2 \to \mathbb{N}$ and a learning algorithm with the following property: for every $\varepsilon, \delta \in (0,1)$ and for every distribution $\mathcal{D}$ over $\mathcal{X} \times \mathcal{Y}$, when running the learning algorithm on $m \geq m_{\mathcal{H}}(\varepsilon, \delta)$ i.i.d. examples generated by $\mathcal{D}$, the algorithm returns a hypotesis h such that, with probability of at least $1-\delta$ (over the choice of the m training examples):

$$L_{\mathcal{D}}(h) \leq \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') + \varepsilon \tag{2.6}$$

In the agnostic case, the learner is required to achieve a small error relative to the best error achievable by the hypotesis class and not in absolute terms. In other words, we drop the requirement of finding the best predictor, but we don't want to be too far from it.

2.2.3 Scope of the learning problems

We want to extend our model so that it can be applied to a wide variety of learning tasks, such as:

- **Multiclass Classification**:
  Our classification doesn't have to be binary. The label set can be much more complex, for example it can be a set of real numbers.

- **Regression**:11 In this task, one wishes to find some simple pattern in the data, i.e. a functional relationship between the $\mathcal{X}$ and $\mathcal{Y}$ components of the data. For example, one wishes to find a linear function that describes the correlation between a sample of $\mathcal{X}$ and the corresponding value inside $\mathcal{Y}$. However, for this type of tasks, the measure of success has to be changed. We may evaluate the quality of a hypotesis function, $h : \mathcal{X} \to \mathcal{Y}$, by the *expected square difference* between the true labels and their predicted values, namely:

$$L_{\mathcal{D}}(h) := \underset{(x,y)\sim\mathcal{D}}{\mathbb{E}}[h(x) - y]^2 \tag{2.7}$$

To extend the reach of machine learning techniques we must generalize our formalism of the measure of success.

2.2.4 Generalized loss functions and common examples

Given any set $\mathcal{H}$ (our hypotheses or models) and some domain Z, let ℓ be any function from $\mathcal{H} \times Z$ to the set of non-negative real numbers, ℓ, namely $\mathcal{H} \times z \to \mathbb{R}_+$. We call such functions **loss functions**.
We now define the **risk function** to be the expected loss of a classifier $h \in \mathcal{H}$ with respect to a probability distribution $\mathcal{D}$ over Z, namely:

$$L_{\mathcal{D}}(h) := \underset{z\sim\mathcal{D}}{\mathbb{E}}[\ell(h, z)] \tag{2.8}$$

In other words, we consider the expectation of the loss of h over objects z picked randomly according to $\mathcal{D}$. Similarly, we define the **empirical risk** to be the expected loss over a given sample $S = (z_1, \ldots, z_m) \in Z^m$, namely:

$$L_S(h) := \frac{1}{m}\sum_{i=1}^{m} l(h, z_i) \tag{2.9}$$

Some of the most common examples of losses are given below:

- **0-1 loss**:
  Our random variable z ranges over the set of pairs $\mathcal{X} \times \mathcal{Y}$ and the loss function is:

$$\ell_{0-1}(h, (x, y)) := \begin{cases} 0 & \text{if } h(x) = y \\ 1 & \text{if } h(x) \neq y \end{cases} \tag{2.10}$$

  It is used in binary and multiclass classification.

- **Square loss (L2)**:
  Our loss function is:

$$\ell_{\text{sq}}(h, (x, y)) := [h(x) - y]^2 \tag{2.11}$$

  This loss is used in regression problems to penalize few large errors.

- **Absolute value loss (L1)**:
  Just like before, but with modulus and not the square:

$$\ell_{\text{abs}}(h,(x,y)) := |h(x) - y| \tag{2.12}$$

  It is used in regression tasks to penalize many small errors.

To summarize, we formally define agnostic PAC learnability for general loss functions.

Definition 2.2.2 (Agnostic PAC learnability for general loss functions)**.** A hypotesis class $\mathcal{H}$ is PAC learnable with respect to a set Z and a loss function $\ell : \mathcal{H} \times Z \to \mathbb{R}_+$, if there exist a function $m_{\mathcal{H}} : (0,1)^2 \to \mathbb{N}$ and a learning algorithm with the following property: for every $\varepsilon, \delta \in (0,1)$ and for every distribution $\mathcal{D}$ over Z, when running the learning algorithm on $m \geq m_{\mathcal{H}}(\varepsilon, \delta)$ i.i.d. examples generated by $\mathcal{D}$, the algorithm returns $h \in \mathcal{H}$ such that, with probability of at least $1 - \delta$ (over the choice of the m training examples):

$$l_{\mathcal{D}}(h) \leq \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') + \varepsilon \tag{2.13}$$

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

Remark 1. We can consider $\ell(h, \bullet) : Z \to \mathbb{R}_+$ a random variable. Hence $L_{\mathcal{D}}(h)$ is the expected value of this random variable.

Chapter 3

Learning via uniform convergence

In this Chapter we will develop a more general tool, namely the *uniform convergence*, and apply it to show that any finite class is learnable in the agnostic PAC model with general loss functions, as long as the range loss function is bounded.

3.1 Uniform convergence is sufficient for learnability

Bibliography