

Statistical Learning Theory: Models, Concepts, and Results

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1 Introduction

Statistical learning theory provides the theoretical basis for many of today’s machine learning algorithms and is arguably one of the most beautifully developed branches of artificial intelligence in general. It originated in Russia in the 1960s and gained wide popularity in the 1990s following the development of the so-called *Support Vector Machine (SVM)*, which has become a standard tool for pattern recognition in a variety of domains ranging from computer vision to computational biology. Providing the basis of new learning algorithms, however, was not the only motivation for developing statistical learning theory. It was just as much a philosophical one, attempting to answer the question of what it is that allows us to draw valid conclusions from empirical data.

In this article we attempt to give a gentle, non-technical overview over the key ideas and insights of statistical learning theory. We do not assume that the reader has a deep background in mathematics, statistics, or computer science. Given the nature of the subject matter, however, some familiarity with mathematical concepts and notations and some intuitive understanding of basic probability is required. There exist many excellent references to more technical surveys of the mathematics of statistical learning theory: the monographs by one of the founders of statistical learning theory (Vapnik, 1995, Vapnik, 1998), a brief overview over statistical learning theory in Section 5 of Schölkopf and Smola (2002), more technical overview papers such as Bousquet et al. (2003), Mendelson (2003), Boucheron et al. (2005), Herbrich and Williamson (2002), and the monograph Devroye et al. (1996).

2 The standard framework of statistical learning theory

2.1 Background

In our context, learning refers to the process of inferring general rules by observing examples. Many living organisms show some ability to learn. For instance, children can learn what “a car” is, just by being shown examples of objects that are cars and objects that are not cars. They do not need to be told any rules about what is it that makes an object a car, they can simply learn the concept “car” by observing examples.

The field of machine learning does not study the process of learning in living organisms, but instead studies the process of learning in the abstract. The question is how a machine, a computer, can “learn” specific tasks by following specified learning algorithms. To this end, the machine is shown particular examples of a specific task. Its goal is then to infer a general rule which can both explain the examples it has seen already and which can generalize to previously unseen, new examples.

Machine learning has roots in artificial intelligence, statistics, and computer science, but by now has established itself as a scientific discipline in its own right. As opposed to artificial intelligence, it does not try to explain or generate “intelligent behavior”, its goal is more modest: it just wants to discover mechanisms by which very specific tasks can be “learned” by a computer. Once put into a formal framework, many of the problems studied in machine learning sound familiar from statistics or physics: regression, classification, clustering, and so on. However, machine learning looks at those problems with a different focus: the one of inductive inference and generalization ability.

The most well-studied problem in machine learning is the problem of classification. Here we deal with two kind of spaces: the input space \mathcal{X} (also called space of instances) and the output space (label space) \mathcal{Y} . For example, if the task is to classify certain objects into a given, finite set of categories such as “car”, “chair”, “cow”, then \mathcal{X} consists of the space of all possible objects (instances) in a certain, fixed representation, while \mathcal{Y} is the space of all available categories. In order to learn, an algorithm is given some training examples $(X_1, Y_1), \dots, (X_n, Y_n)$, that is pairs of objects with the corresponding category label. The goal is then to find a mapping $f : \mathcal{X} \rightarrow \mathcal{Y}$ which makes “as few errors as possible”. That is, among all the elements in \mathcal{X} , the number of objects which are assigned to the wrong category is as small as possible. The mapping $f : \mathcal{X} \rightarrow \mathcal{Y}$ is called a classifier.

In general, we distinguish between two types of learning problems: supervised ones and unsupervised ones. Classification is an example of a supervised learning problem: the training examples consist both of instances X_i and of the correct labels Y_i on those instances. The goal is to find a functional relationship between instances and outputs. This setting is called supervised because at least on the training examples, the learner can evaluate whether an answer is correct, that is the learner is being supervised. Contrary to this, the training data in the unsupervised setting only consists of instances X_i , without any further information about what kind of output is expected on those instances. In this setting, the question of learning is more about discovering some “structure” on the underlying space of instances. A standard example of such a setting is clustering. Given some input points X_1, \dots, X_n , the learner is requested to construct “meaningful groups” among the instances. For example, an online retailer might want to cluster his customers based on shopping profiles. He collects all kinds of potentially meaningful information about his customers (this will lead to the input X_i for each customer) and then wants to discover groups of customers with similar behavior. As opposed to classification, however, it is not specified beforehand which customer should belong to which group – it is the task of the clustering algorithm to work that out.

Statistical learning theory (SLT) is a theoretical branch of machine learning and attempts to lay the mathematical foundations for the field. The questions asked by SLT are fundamental:

- Which learning tasks can be performed by computers in general (positive and negative results)?
- What kind of assumptions do we have to make such that machine learning can be successful?
- What are the key properties a learning algorithm needs to satisfy in order to be successful?
- Which performance guarantees can we give on the results of certain learning algorithms?

To answer those questions, SLT builds on a certain mathematical framework, which we are now going to introduce. In the following, we will focus on the case of supervised learning, more particular on the case of binary classification. We made this choice because the theory for supervised learning, in particular classification, is rather mature, while the theory for many branches of unsupervised learning is still in its infancy.

2.2 The formal setup

In supervised learning, we deal with an *input space (space of instances, space of objects)* \mathcal{X} and an *output space (label space)* \mathcal{Y} . In the case of binary classification, we identify the label space with the set $\{-1, +1\}$. That is, each object can belong to one out of two classes, and by convention we denote those classes by -1 and 1 . The question of learning is reduced to the question of

estimating a functional relationship of the form $f : \mathcal{X} \rightarrow \mathcal{Y}$, that is a relationship between input and output. Such a mapping f is called a *classifier*. In order to do this, we get access to some *training points (training examples, training data)* $(X_1, Y_1), \dots, (X_n, Y_n) \in \mathcal{X} \times \mathcal{Y}$. A *classification algorithm (classification rule)* is a procedure that takes the training data as input and outputs a classifier f . We do not make specific assumptions on the spaces \mathcal{X} or \mathcal{Y} , but we do make an assumption on the mechanism which generates those training points. Namely, we assume that there exists a *joint probability distribution* P on $\mathcal{X} \times \mathcal{Y}$, and the training examples (X_i, Y_i) are sampled independently from this distribution P . This type of sampling is often denoted as iid sampling (independent and identically distributed). There are a few important facts to note here.

1. *No assumptions on P .* In the standard setting of SLT we do not make any assumption on the probability distribution P : it can be any distribution on $\mathcal{X} \times \mathcal{Y}$. In this sense, statistical learning theory works in an agnostic setting which is different from standard statistics, where one usually assumes that the probability distribution belongs to a certain family of distributions and the goal is to estimate the parameters of this distribution.
2. *Non-deterministic labels due to label noise or overlapping classes.* Note that P is a probability distribution not only over the instances \mathcal{X} , but also over the labels \mathcal{Y} . As a consequence, labels Y_i in the data are not necessarily just a deterministic function of the objects X_i , but can be random themselves. There are two main reasons why this can be the case. The first reason is that the data generating process can be subject to label noise. That is, it can happen that label Y_i we get as a training label in the learning process is actually wrong. This is an important and realistic assumption. For example, to generate training data for email spam detection, humans are required to label emails by hand into classes “spam” and “not spam”. All humans make mistakes from time to time. So it will happen that some emails accidentally get labeled as “spam” even though they are not spam, or vice versa. Of course, the hope is that such wrong labels only occur with a relatively small probability. The second major reason which can lead to non-deterministic labels is the case of overlapping classes. As an example, consider the task of predicting the gender of a person based on their height. It is clear that a person of height 1.80 meters, say, could in principle be male or female, thus we cannot assign a unique label Y to the input $X = 1.80$.

For the purpose of learning, we will see that in the end it does not matter which of the reasons is the one leading to non-deterministic labels. It will turn out that the important quantity which covers both cases is the conditional likelihood of the labels, namely the probability that the label Y is 1, under the condition that the data point under consideration is the point x :

$$\eta(x) := P(Y = 1 \mid X = x). \tag{1}$$

Note that we only consider the case $Y = 1$ as the case $Y = -1$ can simply be computed by $P(Y = -1 \mid X = x) = 1 - \eta(x)$. In the case of small label noise, the conditional probability $\eta(x)$ is either close to 1 or close to 0 (depending on whether the true label is +1 or -1). For large label noise, on the other hand, the probability $\eta(x)$ gets closer to 0.5 and learning becomes more difficult. Similar reasoning applies to the case of overlapping classes. In the example of predicting the gender of a person based on height, the classes overlap quite strongly. For example, the probability $P(Y = \text{“male”} \mid X = 1.70)$ might only be 0.6. That is, if we want to predict the gender of a person of height 1.70 we will, on average, make an error of at least 40%. Both in cases of label noise and of overlapping classes, learning becomes more difficult the closer the function $\eta(x)$ comes to 0.5, and it becomes unavoidable that a classifier makes a relatively large number of errors.

3. *Independent sampling.* It is an important assumption of SLT that data points are sampled independently. This is a rather strong assumption, which is justified in many applications, but not in all of them. For example, consider the example of pattern recognition for hand written digits. Given some images of hand written digits, the task is to train a machine to automatically recognize new hand written digits. For this task, the training set usually consists of a large collection of digits written by many different people. Here it is safe to assume that those digits form an independent sample from the whole “population” of all hand written digits. As an example where the independence assumption is heavily violated, consider the

case of drug discovery. This is a field in pharmacy where people try to identify chemical compounds which might be helpful for designing new drugs. Machine learning is being used for this purpose: the training examples consist of chemical compounds X_i with a label Y_i which indicates whether this compound is useful for drug design or not. It is expensive to find out whether a chemical compound possesses certain properties that render it a suitable drug because this would require running extensive lab experiments. As a result, only rather few compounds X_i have known labels Y_i , and those compounds have been carefully selected in the first place. Here, we cannot assume that the X_i are a representative sample drawn independently from some distribution of chemical compounds, as the labeled compounds are hand-selected according to some non-random process.

Note that in some areas of machine learning, researchers try to relax the independence assumption. For example in active learning one deals with the situation where users can actively select the points they want to get labeled. Another case is time series prediction, where training instances are often generated from overlapping (and thus dependent) windows of a temporal sequence. We are not going to discuss those areas in this paper.

4. *The distribution P is fixed.* In the standard setting of SLT, we do not have any “time” parameter. In particular, we do not assume any particular ordering of the training examples, and the underlying probability distribution does not change over time. This assumption would not be true if we wanted to argue about time series, for example. Another situation that has recently attracted attention is the case where training and test distributions differ in certain aspects (e.g., under the heading of “covariate shift”).
5. *The distribution P is unknown at the time of learning.* It is important to recall that at the time of training the underlying distribution is not known. We will see below that if we knew P , then learning would be trivial as we could simply write down the best classifier by a given formula. Instead, we only have access to P indirectly, by observing training examples. Intuitively this means that if we get enough training examples, we can “estimate” all important properties of P pretty accurately, but we are still prone to errors. It is one of the big achievements of statistical learning theory to provide a framework to make theoretical statements about this error.

As already mentioned above, the goal of supervised learning is to learn a function $f : \mathcal{X} \rightarrow \mathcal{Y}$. In order to achieve this, we need to have some measure of “how good” a function f is when used as a classifier. To this end, we introduce a *loss function*. This is a function ℓ which tells us the “cost” of classifying instance $X \in \mathcal{X}$ as $Y \in \mathcal{Y}$. For example, the simplest loss function in classification is the 0-1-loss or misclassification error: the loss of classifying X by label $f(X)$ is 0 if $f(X)$ is the correct label for X , and 1 otherwise:

$$\ell(X, Y, f(X)) = \begin{cases} 1 & \text{if } f(X) \neq Y \\ 0 & \text{otherwise.} \end{cases}$$

In regression, where the output variables Y take values that are real numbers rather than class labels, a well-known loss function is the squared error loss function $\ell(X, Y, f(X)) = (Y - f(X))^2$. The general convention is that a loss of 0 denotes perfect classification, and higher loss values represent worse classification performance.

While the loss function measures the error of a function on some individual data point, the *risk* of a function is the average loss over data points generated according to the underlying distribution P ,

$$R(f) := E(\ell(X, Y, f(X))).$$

That is, the risk of a classifier f is the expected loss of the function f at all points $X \in \mathcal{X}$. Intuitively, this risk “counts” how many elements of the instance space \mathcal{X} are misclassified by the function f . Of course, a function f is a better classifier than another function g if its risk is smaller, that is if $R(f) < R(g)$. To find a good classifier f we need to find one for which $R(f)$ is as small

as possible. The best classifier is the one with the smallest risk value $R(f)$.

One aspect we have left open so far is what kind of functions f to consider. To formalize this, we consider some underlying *space \mathcal{F} of functions* which map \mathcal{X} to \mathcal{Y} . This is the space of functions from which we want to choose our solution. At first glance, the most natural way would be to allow all possible functions from \mathcal{X} to \mathcal{Y} as classifier, that is to choose $\mathcal{F}_{all} = \{f : \mathcal{X} \rightarrow \mathcal{Y}\}$. (We ignore issues about measurability at this point; for readers familiar with measure theory, note that one usually defines the space \mathcal{F}_{all} to be the space of measurable functions between \mathcal{X} and \mathcal{Y} .) In this case, one can formally write down what the optimal classifier should be. Given the underlying probability distribution P , this classifier is defined as follows:

$$f_{Bayes}(x) := \begin{cases} 1 & \text{if } P(Y = 1 \mid X = x) \geq 0.5 \\ -1 & \text{otherwise.} \end{cases} \quad (2)$$

This is the so-called “*Bayes classifier*”. Intuitively, what it does is as follows. For each point in the space \mathcal{X} , it looks at the function $\eta(x) := P(Y = 1 \mid X = x)$ introduced in Eq. (1). If we assume that $P(Y = 1 \mid X = x) = 1$, this means that the true label Y of the point $X = x$ satisfies $Y = 1$ with certainty (probability 1). Hence, an optimal classifier should also take this value, that is it should choose $f(x) = 1$. Now assume that the classes slightly overlap, for example $P(Y = 1 \mid X = x) = 0.9$. This still means that in an overwhelming number of cases (in 90 % of them), the label of object x is +1, thus this is what the classifier f should choose. The same holds as long as the overlap is so small that $\eta(x) \geq 0.5$. By choosing $f(x) = 1$, the classifier f will be correct in the majority of all cases. Only when $\eta(x)$ goes below 0.5, the situation flips and the optimal choice is to choose $f = -1$. We will come back to this example in Section 3.

In practice, it is impossible to directly compute the Bayes classifier. The reason is that, as we explained above, the underlying probability distribution is unknown to the learner. Hence, the Bayes classifier cannot be computed, as we would need to evaluate the conditional probabilities $P(Y = 1 \mid X = x)$. With all those definitions in mind, we can formulate the standard problem of binary classification as follows:

Given some training points $(X_1, Y_1), \dots, (X_n, Y_n)$ which have been drawn independently from some unknown probability distribution P , and given some loss function ℓ , how can we construct a function $f : \mathcal{X} \rightarrow \mathcal{Y}$ which has risk $R(f)$ as close as possible to the risk of the Bayes classifier?

At this point, note that not only is it impossible to compute the Bayes error, but also the risk of a function f cannot be computed without knowledge of P . All in all, it looks like a pretty desperate situation: we have defined the goal of binary classification (to minimize the risk of the classifier), and can even formally write down its solution (the Bayes classifier). But at the time of training, we do not have access to the important quantities to compute either of them. This is where SLT comes in. It provides a framework to analyze this situation, to come up with solutions, and to provide guarantees on the goodness of these solutions.

2.3 Generalization and consistency

There are a few more important notions we need to explain at this point. The most important one is “generalization”. Assume we are given some training set $(X_1, Y_1), \dots, (X_n, Y_n)$, and by some algorithm come up with a classifier f_n . Even though we cannot compute the true underlying risk $R(f_n)$ of this classifier, what we can do is to “count” the number of mistakes on the training points. The resulting quantity also has a name, it is called the *empirical risk* or the *training error*. Formally, for any function f it is defined as

$$R_{\text{emp}}(f) := \frac{1}{n} \sum_{i=1}^n \ell(X_i, Y_i, f(X_i)).$$

Usually, for a classifier f_n learned on a particular training set, the empirical risk $R_{\text{emp}}(f_n)$ is relatively small – otherwise, the learning algorithm does not even seem to be able to explain the training data. However, it is not clear whether a function f_n which makes few errors on the training set also makes few errors on the rest of the space \mathcal{X} , that is whether it has a small overall risk $R(f_n)$. We say that a classifier f_n *generalizes* well if the difference $|R(f_n) - R_{\text{emp}}(f_n)|$ is small. Note that with this definition, good generalization performance does not necessarily mean that a classifier has a small overall error R_{emp} . It just means that the empirical error $R_{\text{emp}}(f_n)$ is a good estimate of the true error $R(f_n)$. Particularly bad in practice is the situation where $R_{\text{emp}}(f_n)$ is much smaller than $R(f_n)$. In this case, using the empirical risk as an estimator of the true risk would lead us to be overly optimistic about the quality of our classifier.

Consider the following regression example. We are given empirical observations, $(x_1, y_1), \dots, (x_m, y_m) \in \mathcal{X} \times \mathcal{Y}$ where for simplicity we take $\mathcal{X} = \mathcal{Y} = \mathbb{R}$. For example, the data could have been collected in a physical experiment where X denotes the weight of an object, and Y the force we need to pull this object over a rough surface. Figure 1 shows a plot of such a dataset (indicated by the round points), along with two possible functional dependencies that could underlie the data. The dashed line f_{dashed} represents a fairly complex model, and fits the training data perfectly, that is it has a training error of 0. The straight line f_{straight} , on the other hand, does not completely “explain” the training data, in the sense that there are some residual errors, leading to a small positive training error (for example, measured by the squared loss function). But what about the true risks $R(f_{\text{dashed}})$ and $R(f_{\text{straight}})$? The problem is that we cannot compute this risk from the training data. Moreover, the functions f_{dashed} and f_{straight} have very different behavior. For example, if the straight line was the true underlying function, then the dashed function f_{dashed} would have a high true risk, as the “distance” between the true and the estimated function is very large. The same also holds the other way around. In both cases the true risk would be much higher than the empirical risk.

This example points out an important choice we have to make. Do we prefer to fit the training data with a relatively “complex” function, leading to a very small training error, or do we prefer to fit it with a “simple” function at the cost of a slightly higher training error? In the example above, a physicist measuring these data points would argue that it cannot be by chance that the measurements lie almost on a straight line and would much prefer to attribute the residuals to measurement error than to an erroneous model. But is it possible to *characterize* the way in which the straight line is simpler, and why this should imply that it is, in some sense, closer to an underlying true dependency? What is the “amount of increase in training error” we should be willing to tolerate for fitting a simpler model?

In one form or another, this issue has long occupied the minds of researchers studying the problem of learning. In classical statistics, it has been studied as the *bias-variance dilemma*. If we computed a linear fit for every data set that we ever encountered, then every functional dependency we would ever “discover” would be linear. But this would not come from the data; it would be a *bias* imposed by us. If, on the other hand, we fitted a polynomial of sufficiently high degree to any given data set, we would always be able to fit the data perfectly, but the exact model we came up with would be subject to large fluctuations, depending on how accurate our measurements were in the first place — the model would suffer from a large *variance*. A related dichotomy is the one between *estimation error* and *approximation error*. If we use a small class of functions, then even the best possible solution will poorly approximate the “true” dependency, while a large class of functions will lead to a large statistical estimation error. We will discuss these dichotomies in more detail in Section 2.4. In the terminology of applied machine learning, the complex explanation shows *overfitting*, while an overly simple explanation imposed by the learning machine design would lead to *underfitting*.

A concept which is closely related to generalization is the one of *consistency*. However, as opposed to the notion of generalization discussed above, consistency is not a property of an individual function, but a property of a set of functions. As in classical statistics, the notion of consistency aims to make a statement about what happens in the limit of infinitely many sample points. Intuitively, it seems reasonable to request that a learning algorithm, when presented more and more training examples, should eventually “converge” to an optimal solution.

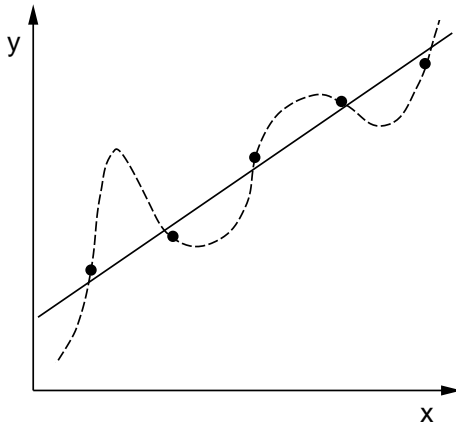


Figure 1: Suppose we want to estimate a functional dependence from a set of examples (black dots). Which model is preferable? The complex model perfectly fits all data points, whereas the solid line exhibits residual errors. Statistical learning theory formalizes the role of the capacity of the model class, and gives probabilistic guarantees for the validity of the inferred model (from Schölkopf and Smola (2002)).

There exist two different types of consistency in the literature, depending on the taste of the authors, and both of them are usually just called “consistency” without any distinction. To introduce these concepts, let us make the following notation. Given any particular classification algorithm, by f_n we will denote its outcome on a sample of n training points. It is not important how exactly the algorithm chooses this function. But note that any algorithm chooses its functions from some particular function space \mathcal{F} . For some algorithms this space is given explicitly, for others it only exists implicitly via the mechanism of the algorithm. No matter how this space \mathcal{F} is defined, the algorithm attempts to choose the function $f_n \in \mathcal{F}$ which it considers as the best classifier in \mathcal{F} , based on the given training points. On the other hand, in theory we know precisely what the best classifier in \mathcal{F} is: it is the one that has the smallest risk. For simplicity, we assume that it is unique and denote it as $f_{\mathcal{F}}$, that is

$$f_{\mathcal{F}} = \operatorname{argmin}_{f \in \mathcal{F}} R(f). \quad (3)$$

The third classifier we will talk about is the Bayes classifier f_{Bayes} introduced in Equation (2) above. This is the best classifier which exists at all. In the notation above we could also denote it by $f_{\mathcal{F}_{\text{all}}}$ (recall the notation \mathcal{F}_{all} for the space of all functions). But as it is unknown to the learner, it might not be contained in the function space \mathcal{F} under consideration, so it is very possible that $R(f_{\mathcal{F}}) > R(f_{\text{Bayes}})$. With the notation for these three classifiers f_n , $f_{\mathcal{F}}$, and f_{Bayes} we can now define different types of convergence:

Definition 1 Let $(X_i, Y_i)_{i \in \mathbb{N}}$ be an infinite sequence of training points which have been drawn independently from some probability distribution P . Let ℓ be a loss function. For each $n \in \mathbb{N}$, let f_n be a classifier constructed by some learning algorithm on the basis of the first n training points.

1. The learning algorithm is called consistent with respect to \mathcal{F} and P if the risk $R(f_n)$ converges in probability to the risk $R(f_{\mathcal{F}})$ of the best classifier in \mathcal{F} , that is for all $\varepsilon > 0$,

$$P(R(f_n) - R(f_{\mathcal{F}}) > \varepsilon) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

2. The learning algorithm is called Bayes-consistent with respect to P if the risk $R(f_n)$ converges to the risk $R(f_{\text{Bayes}})$ of the Bayes classifier, that is for all $\varepsilon > 0$,

$$P(R(f_n) - R(f_{\text{Bayes}}) > \varepsilon) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

3. The learning algorithm is called universally consistent with respect to \mathcal{F} (resp. universally Bayes-consistent) if it is consistent with respect to \mathcal{F} (resp. Bayes-consistent) for all probability distributions P .

Note that for simplicity in the following we often say “the classifier f_n is consistent”, meaning that “the classification algorithm which, based on n samples, chooses f_n as classifier is consistent”. Let us try to rephrase the meaning of those definitions in words. We start with Part 1 of the definition. The statement requests that the larger the sample size n gets, the closer the risk of the classifier f_n should get to the risk of the best classifier $f_{\mathcal{F}}$ in the space \mathcal{F} . This should happen “with high probability”: Note that the risk $R(f_n)$ is a random quantity, as it depends on the underlying sample. In rare circumstances (with probability $< \delta$, where δ is supposed to be a small, positive number), it might be the case that we get mainly misleading sample points (for example, lots of points with “wrong” labels due to label noise). In those circumstances, it might happen that our classifier is not very good. However, in the vast majority of all cases (with probability $\geq 1 - \delta$), our training points will not be misleading, at least if we have many of them ($n \rightarrow \infty$). Then the classifier f_n picked by the algorithm will be close to the best classifier the algorithm could have picked at all, the classifier $f_{\mathcal{F}}$, that is $R(f_n) - R(f_{\mathcal{F}}) > \varepsilon$ only with small probability δ , where δ will converge to 0 as $n \rightarrow \infty$.

Part 2 of the definition is similar to Part 1, except that we now compare to the overall best classifier f_{Bayes} . The difference between those statements is obvious: Part 1 deals with the best the algorithm can do under the given circumstances (namely, in the function space \mathcal{F}). Part 2 compares this to the overall best possible result. Traditionally, statistical learning theory often focuses on Part 1, but ultimately we will be more interested in Part 2. Both parts will be treated in the following sections.

To understand Part 3, note the following. In the first two parts, consistency is defined for a fixed probability distribution P . This means that if the true underlying distribution is P , then the sequence of classifiers f_n will converge to the correct result. However, the whole point of machine learning is that we do not know what the underlying distribution P is. So it would make little sense if a learning algorithm is consistent for a certain distribution P , but inconsistent for some other distribution P' . Hence, we define a stronger notion of consistency, termed universal consistency. It states that no matter what the underlying distribution might be, we will always have consistency.

A mathematical detail we would like to skim over is the exact type of convergence. For readers familiar with probability theory: consistency as stated above is called weak consistency, as it is a statement about convergence in probability; the analogous statement for convergence almost surely would be called strong consistency. For exact details see Section 6 in Devroye et al. (1996).

There is one further important fact to note about these definitions: they never mention the empirical risk $R_{\text{emp}}(f_n)$ of a classifier, but are only concerned with the true risk $R(f_n)$. On the one hand, it is clear why this is the case: our measure of quality of a classifier is the true risk, and we want the true risk to become as good as possible. On the other hand, the empirical risk is our first and most important estimator of the true risk of a classifier. So it seems natural that in addition to the convergence of the true risk such as $R(f_n) \rightarrow R(f_{Bayes})$, we also request convergence of the empirical risk: $R_{\text{emp}}(f_n) \rightarrow R(f_{Bayes})$. We will see below that such statements about the empirical risk are the most important steps to prove consistency in the standard approach to statistical learning theory. So even though we did not explicitly require convergence of the empirical risk, it usually comes out as a side result of consistency.

2.4 The bias-variance and estimation-approximation trade-off

The example illustrated in Figure 1 above already pointed out the problem of model complexity in an intuitive way: when is a model “simpler” than another one? Is it good that a model is simple? How simple? We have already stated above that the goal of classification is to get a risk as good as the Bayes classifier. Could we just choose \mathcal{F} as the space \mathcal{F}_{all} of all functions, define the classifier $f_n := \operatorname{argmin}_{f \in \mathcal{F}_{all}} R_{\text{emp}}(f)$, and obtain consistency? Unfortunately, the answer is no. In the sections below we will see that if we optimize over too large function classes \mathcal{F} , and in particular if we make \mathcal{F} so large that it contains all the Bayes classifiers for all different probability distributions P , this will lead to inconsistency. So if we want to learn successfully, we need to work with a smaller function class \mathcal{F} . To investigate the competing properties of model complexity and generalization, we want to introduce a few notions which will be helpful later on.

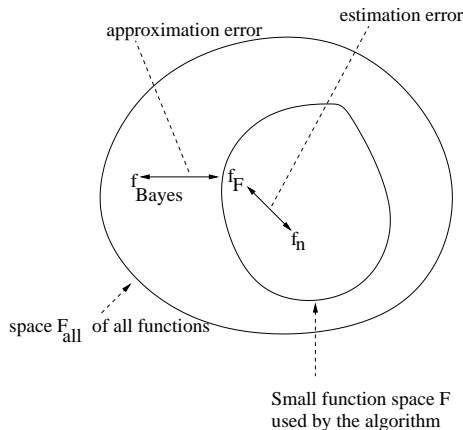


Figure 2: *Illustration of estimation and approximation error.*

Recall the definitions f_n , $f_{\mathcal{F}}$ and f_{Bayes} introduced above. We have seen that Bayes-consistency deals with the convergence of the term $R(f_n) - R(f_{Bayes})$. Note that we can decompose this quantity in the following way:

$$R(f_n) - R(f_{Bayes}) = \underbrace{\left(R(f_n) - R(f_{\mathcal{F}}) \right)}_{\text{estimation error}} + \underbrace{\left(R(f_{\mathcal{F}}) - R(f_{Bayes}) \right)}_{\text{approximation error}} \quad (4)$$

The two terms on the right hand side have particular names: the first one is called the *estimation error* and the second one the *approximation error*; see also Figure 2 for an illustration. The reasons for these names are as follows. The first term deals with the uncertainty introduced by the random sampling process. That is, given the finite sample, we need to estimate the best function in \mathcal{F} . Of course, in this process we will make some (hopefully small) error. This error is called the *estimation error*. The second term is not influenced by any random quantities. It deals with the error we make by looking for the best function in a (small) function space \mathcal{F} , rather than looking for the best function in the entire space \mathcal{F}_{all} of all functions. The fundamental question in this context is how well functions in \mathcal{F} can be used to approximate functions \mathcal{F}_{all} in the space of all functions. Hence the name *approximation error*.

In statistics, estimation error is also called the *variance*, and the approximation error is called the *bias* of an estimator. Originally, these terms were coined for the special situation of regression with squared error loss, but by now people use them in more general settings, like the one outlined above. The intuitive meaning is the same: the first term measures the variation of the risk of the function f_n estimated on the sample, the second one measures the “bias” introduced in the model by choosing too small a function class.

At this point, we would already like to point out that the space \mathcal{F} is the means to balance the trade-off between estimation and approximation error; see Figure 3 for an illustration and Sections 4 and 5 for an in-depth discussion. If we choose a very large space \mathcal{F} , then the approximation term will become small (the Bayes classifier might even be contained in \mathcal{F} or can be approximated closely by some element in \mathcal{F}). The estimation error, however, will be rather large in this case: the space \mathcal{F} will contain complex functions which will lead to overfitting. The opposite effect will happen if the function class \mathcal{F} is very small.

In the following, we will deal with the estimation error and approximation error separately. We will see that they have rather different behavior and that different methods are needed to control both. Traditionally, SLT has a strong focus on the estimation error, which we will discuss in greater depth in Sections 4 and 5. The approximation error will be treated in Section 7.

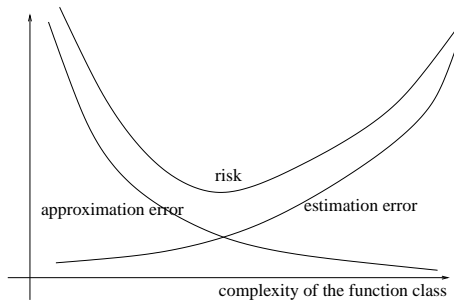


Figure 3: *The trade-off between estimation and approximation error. If the function space \mathcal{F} used by the algorithm has a small complexity, then the estimation error is small, but the approximation error is large (underfitting). If the complexity of \mathcal{F} is large, then the estimation error is large, while the approximation error is small (overfitting). The best overall risk is achieved for “moderate” complexity.*

3 Consistency and generalization for the k -nearest neighbor classifier

For quite some time, until 1977, it was not known whether a universally consistent classifier exists. This question has been solved positively by Stone (1977), who showed by an elegant proof that a particular classifier, the so-called k -nearest neighbor classifier, is universally consistent. As the k -nearest neighbor classifier is one of the simplest classifiers and is still widely used in practice, we would like to spend this section illustrating the notions introduced in the last section such as generalization, overfitting, underfitting, and consistency at the example of the k -nearest neighbor classifier.

Assume we are given a sample of points and labels $(X_1, Y_1), \dots, (X_n, Y_n)$ which live in some metric space. This means that we have some way of computing distances between points in this space. Very generally, the paradigm of learning is to assign “similar output to similar inputs”. That is, we believe that points which are “close” in the input space tend to have the same label in the output space. Note that if such a statement does not hold, learning becomes very difficult or even impossible. For successful learning, there needs to be some way to relate the labels of training points to those of test points, and this always involves some prior assumptions about relations between input points. The easiest such relation is a distance between points, but other ways of measuring similarity, such as “kernels,” exist and indeed form the basis of some of the most popular existing learning algorithms (Schölkopf and Smola, 2002).

So assume that there exists a distance function on the input space, that is a function $d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ which assigns a distance value $d(X, X')$ to each pair of training points X, X' . Given some training points, we now want to predict a good label for a new test point X . A simple idea is to search for the training point X_i which has the smallest distance to X , and then give X the corresponding label Y_i of that point. To define this more formally, denote by $\text{NN}(X)$ the nearest neighbor of X among all training points, that is

$$\text{NN}(X) = \operatorname{argmin} \{X' \in \{X_1, \dots, X_n\} \mid d(X, X') \leq d(X, X'') \text{ for all } X'' \in \{X_1, \dots, X_n\}\}.$$

We can then define the classifier f_n based on the sample of n points by

$$f_n(X) = Y_i \text{ where } X_i = \text{NN}(X).$$

This classifier is also called the 1-nearest neighbor classifier (1NN classifier). A slightly more general version is the k -nearest neighbor classifier (k NN classifier). Instead of just looking at the closest training point, we consider the closest k training points, and then take the average over all their labels. That is, we define the k -nearest neighbors $\text{kNN}(X)$ of X as the set of those k training points which are closest to X . Then we set the k NN classifier

$$f_n(X) = \begin{cases} +1 & \text{if } \sum_{X_i \in \text{kNN}(X)} Y_i > 0 \\ -1 & \text{otherwise.} \end{cases}$$

That is, we decide on the label of X by majority vote among the labels of the training points in the k -nearest neighborhood of X . To avoid ties one usually chooses k as an uneven number.

Let us first consider the simpler case of the 1-nearest neighbor classifier. Is this classifier Bayes-consistent? Unfortunately, the answer is no. To see this, we consider the following counter-example: Assume our data space is the real interval $\mathcal{X} = [0, 1]$. As distribution P we choose the distribution which gives uniform weight to all points $X \in [0, 1]$, and which assigns labels with noise such that $P(Y = 1 \mid X = x) = 0.9$ for all $x \in \mathcal{X}$. That is, the “correct” label (the one assigned by the Bayes classifier) is $+1$ for all points $x \in \mathcal{X}$. We have already mentioned this example when we introduced the Bayes classifier. In this case, the Bayes classifier is simply the function which outputs 1 for all points in \mathcal{X} , and its Bayes risk with respect to the 0-1-loss is 0.1. Now let us investigate the behavior of the 1NN classifier in this case. When we draw some training points $(X_i, Y_i)_{i=1, \dots, n}$ according to the underlying distribution, then they will be roughly “evenly spread” on the interval $[0, 1]$. On average, every 10th point will have training label -1 , all others have training label $+1$. If we now consider the behavior of the 1NN classifier f_n on this example, we can write its risk with respect to the 0-1-loss function as follows:

$$\begin{aligned} R(f_n) &= P(Y \neq f_n(X)) = P(Y = 1 \mid f_n(X) = 0) + P(Y = 0 \mid f_n(X) = 1) \\ &\approx 0.1 \cdot 0.9 + 0.9 \cdot 0.1 = 2 \cdot 0.1 \cdot 0.9 = 0.18 \end{aligned}$$

The approximation sign \approx is used because in this argument we suppress the variations introduced by the random sampling process to keep things simple. We can see that the risk $R(f_n)$ of the classifier f_n is approximately 0.18, independently of the sample size n , while the Bayes risk would be 0.1. Hence, the 1NN classifier is not consistent as $R(f_n) \not\rightarrow R(f_{\text{Bayes}})$. On the other hand, note that if we consider the 100-nearest neighbor classifier instead of the 1-nearest neighbor classifier in this example, we would make much fewer mistakes: it is just very unlikely to have a neighborhood of 100 points in which the majority vote of training points is -1 . Thus, the 100-nearest neighbor classifier, while still not being consistent, makes a smaller error than the 1-nearest neighbor classifier.

The trick to achieve consistency is related to this observation. Essentially, one has to allow that the size k of the neighborhood under consideration grows with the sample size n . Formally, one can prove the following theorem:

Theorem 2 (Stone, 1977) *Let f_n be the k -nearest neighbor classifier constructed on n sample points. If $n \rightarrow \infty$ and $k \rightarrow \infty$ such that $k/n \rightarrow 0$, then $R(f_n) \rightarrow R(f_{\text{Bayes}})$ for all probability distributions P . That is, the k -nearest neighbor classification rule universally Bayes-consistent.*

Essentially, this theorem tells us that if we choose the neighborhood parameter k such that it grows “slowly” with n , for example $k \approx \log(n)$, then the k NN classification rule is universally Bayes-consistent.

In the last sections we mentioned that the function class \mathcal{F} from which the classifier is chosen is an important ingredient for statistical learning theory. In the case of the k NN classifier, this is not as obvious as it will be for the classifiers we are going to study in later sections. Intuitively, one can say that for a fixed parameter k , the function class \mathcal{F}_k is a space of piecewise constant functions. The larger k is, the larger the k -neighborhoods become and thus the larger the pieces of functions which have to be constant. This means that for very large k , the function class \mathcal{F}_k is rather “small” (the functions cannot “wobble” so much). In the extreme case of $k = n$, the k -neighborhood simply includes all training points, so the k NN classifier cannot change its sign at all — it has to be constant on the whole input space \mathcal{X} . In this case, the function class \mathcal{F}_k contains only two elements: the function which is constantly $+1$ and the function which is constantly -1 . On the other hand, if k is small then \mathcal{F}_k becomes rather large (the functions can change their

labels very often and abruptly). In the terms explained in the last sections, one can say that if we choose k too small, then the function class overfits: for example, this happens in the extreme case of the 1NN classifier. On the other hand, if k is too large, then the function class underfits — it simply does not contain functions which are able to model the training data.

In this section we merely touched on the very basics of the kNN classifier and did not elaborate on any proof techniques. For a very thorough treatment of theoretical aspects of kNN classifiers we recommend the monograph Devroye et al. (1996).

4 Empirical risk minimization

In the previous section we encountered our first simple classifier: the kNN classifier. In this section we now want to turn to a more powerful way of classifying data, the so called empirical risk minimization principle. Recall the assumption that the data are generated iid (independent and identically distributed) from an unknown underlying distribution $P(X, Y)$. As we have already seen, the learning problem consists in minimizing the *risk* (or *expected loss* on the test data),

$$R(f) = E(\ell(X, Y, f(X))) \quad (5)$$

where f is a function mapping the input space \mathcal{X} into the label space \mathcal{Y} , and ℓ is the loss function. The difficulty of this task stems from the fact that we are trying to minimize a quantity that we cannot actually evaluate: since we do not know the underlying probability distribution P , we cannot compute the risk $R(f)$. What we *do* know, however, are the training data sampled from P . We can thus try to infer a function f from the training sample whose risk is *close* to the best possible risk. To this end, we need what is called an *induction principle*.

Maybe the most straightforward way to proceed is to approximate the true risk by the empirical risk computed on the training data. Instead of looking for a function which minimizes the true risk $R(f)$, we try to find the one which minimizes the empirical risk

$$R_{\text{emp}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(X_i, Y_i, f(X_i)). \quad (6)$$

That is, given some training data $(X_1, Y_1), \dots, (X_n, Y_n)$, a function space \mathcal{F} to work with, and a loss function ℓ , we define the classifier f_n as the function

$$f_n := \underset{f \in \mathcal{F}}{\operatorname{argmin}} R_{\text{emp}}(f).$$

This approach is called the *empirical risk minimization induction principle*, abbreviated by ERM. The motivation for this principle is given by the law of large numbers, as we will now explain.

4.1 The law of large numbers

The law of large numbers is one of the most important theorems in statistics. In its simplest form it states that under mild conditions, the mean of random variables ξ_i which have been drawn iid from some probability distribution P converges to the mean of the underlying distribution itself when the sample size goes to infinity:

$$\frac{1}{n} \sum_{i=1}^n \xi_i \rightarrow E(\xi) \quad \text{for } n \rightarrow \infty.$$

Here the notation assumes that the sequence ξ_1, ξ_2, \dots has been sampled iid from P and that ξ is also distributed according to P . This theorem can be applied to the case of the empirical and the true risk. In order to see this, note that the empirical risk is defined as the mean of the loss $\ell(X_i, Y_i, f(X_i))$ on individual sample points, and the true risk is the mean of this loss over the

whole distribution. That is, from the law of large numbers we can conclude that for a fixed function f , the empirical risk converges to the true risk as the sample size goes to infinity:

$$R_{\text{emp}}(f) = \frac{1}{n} \sum_{i=1}^n \ell(X_i, Y_i, f(X_i)) \rightarrow E(\ell(X, Y, f(X))) \quad \text{for } n \rightarrow \infty.$$

Here the loss function $\ell(X, Y, f(X))$ plays the role of the random variable ξ above. For a given, finite sample this means that we can approximate the true risk (the one we are interested in) very well by the empirical risk (the one we can compute on the sample). A famous inequality due to Chernoff (1952), later generalized by Hoeffding (1963), characterizes how well the empirical mean approximates the expected value. Namely, if ξ_i are random variables which only take values in the interval $[0, 1]$, then

$$P\left(\left|\frac{1}{n} \sum_{i=1}^n \xi_i - E(\xi)\right| \geq \epsilon\right) \leq 2 \exp(-2n\epsilon^2). \quad (7)$$

This theorem states that the probability that the sample mean deviates by more than ϵ from the expected value of the distribution is bounded by a very small quantity, namely by $2 \exp(-2n\epsilon^2)$. Note that the higher n is, the smaller this quantity becomes, that is the probability for large deviations decreases very fast with n . Again, we can apply this theorem to the setting of empirical and true risk. This leads to a bound which states how likely it is that for a given function f the empirical risk is close to the actual risk:

$$P(|R_{\text{emp}}(f) - R(f)| \geq \epsilon) \leq 2 \exp(-2n\epsilon^2). \quad (8)$$

For any fixed function (and sufficiently large n), it is thus highly probable that the training error provides a good estimate of the test error.

There are a few important facts concerning the Chernoff bound (8). First, a crucial property of the Chernoff bound is that it is probabilistic in nature. It states that the probability of a large deviation between the test error and the training error of f is small; the larger the sample size n , the smaller the probability. Hence, it does not rule out the presence of cases where the deviation is large, it just says that for a fixed function f , this is very unlikely to happen. The reason why this has to be the case is the random generation of training points. It could be that in a few unlucky cases, our training data is so misleading that it is impossible to construct a good classifier based on it. However, as the sample size gets larger, such unlucky cases become very rare. In this sense, any consistency guarantee can only be of the form “the empirical risk is close to the true risk, with high probability”.

At first sight, it seems that the Chernoff bound (8) is enough to prove consistency of empirical risk minimization. However, there is an important caveat: the Chernoff bound only holds for a fixed function f which *does not depend on the training data*. However, the classifier f_n of course does depend on the training data (we used the training data to select f_n). While this seems like a subtle mathematical difference, this is where empirical risk minimization can go completely wrong. We will now discuss this problem in detail, and will then discuss how to adapt the strong law of large numbers to be able to deal with data-dependent functions.

4.2 Why empirical risk minimization can be inconsistent

Assume our underlying data space is $\mathcal{X} = [0, 1]$. Choose the uniform distribution on \mathcal{X} as probability distribution and define the label Y for an input point X deterministically as follows:

$$Y = \begin{cases} -1 & \text{if } X < 0.5 \\ 1 & \text{if } X \geq 0.5. \end{cases} \quad (9)$$

Now assume we are given a set of training points $(X_i, Y_i)_{i=1, \dots, n}$, and consider the following classifier:

$$f_n(X) = \begin{cases} Y_i & \text{if } X = X_i \text{ for some } i = 1, \dots, n \\ 1 & \text{otherwise.} \end{cases} \quad (10)$$

This classifier f_n perfectly classifies all training points. That is it has empirical risk $R_{\text{emp}}(f_n) = 0$. Consequently, as the empirical risk cannot become negative, f_n is a minimizer of the empirical

risk. However, f_n clearly has not learned anything, the classifier just memorizes the training labels and otherwise simply predicts the label 1. Formally, this means that the classifier f_n will not be consistent. To see this, suppose we are given a test point (X, Y) drawn from the underlying distribution. Usually, this test point will not be identical to any of the training points, and in this case the classifier simply predicts the label 1. If X happened to be larger than 0.5, this is the correct label, but if $X < 0.5$, it is the wrong label. Thus the classifier f_n will err on half of all test points, that is it has test error $R(f_n) = 1/2$. This is the same error one would make by random guessing! In fact, this is a nice example of overfitting: the classifier f_n fits perfectly to the training data, but does not learn anything about new test data. It is easy to see that the classifier f_n is inconsistent. Just note that as the labels are a deterministic function of the input points, the Bayes classifier has risk 0. Hence we have $1/2 = R(f_n) \not\rightarrow R(f_{\text{Bayes}}) = 0$.

We have constructed an example where empirical risk minimization fails miserably. Is there any way we can rescue the ERM principle? Luckily, the answer is yes. The main object we have to look at is the function class \mathcal{F} from which we draw our classifier. If we allow our function class to contain functions which just memorize the training data, then the ERM principle cannot work. In particular, if we choose the empirical risk minimizer from the space \mathcal{F}_{all} of all functions between \mathcal{X} and \mathcal{Y} , then the values of the function f_n at the training points X_1, \dots, X_n do not necessarily carry any information about the values at other points. Thus, unless we make restrictions on the space of functions from which we choose our estimate f , we cannot hope to learn anything. Consequently, machine learning research has studied various ways to implement such restrictions. In statistical learning theory, these restrictions are enforced by taking into account the *capacity* of the space of functions that the learning machine can implement.

4.3 Uniform convergence

It turns out the conditions required to render empirical risk minimization consistent involve *restricting the set of admissible functions*. The main insight of VC (Vapnik-Chervonenkis) theory is that the consistency of empirical risk minimization is determined by the *worst case* behavior over all functions $f \in \mathcal{F}$ that the learning machine could choose. We will see that instead of the standard law of large numbers introduced above, this worst case corresponds to a version of the law of large numbers which is *uniform* over all functions in \mathcal{F} . Figure 4 gives a simplified depiction of the uniform law of large numbers and the question of consistency. Both the empirical risk and the actual risk are plotted as functions of f . For simplicity, we have summarized all possible functions f by a single axis of the plot. Empirical risk minimization consists in picking the f that yields the minimal value of R_{emp} . It is consistent if the minimum of R_{emp} converges to that of R as the sample size increases. One way to ensure the convergence of the minimum of all functions in \mathcal{F} is uniform convergence over \mathcal{F} : we require that for *all* functions $f \in \mathcal{F}$, the difference between $R(f)$ and $R_{\text{emp}}(f)$ should become small *simultaneously*. That is, we require that there exists some large n such that for sample size at least n , we know *for all functions* $f \in \mathcal{F}$ that $|R(f) - R_{\text{emp}}(f)|$ is smaller than a given value ε . In the figure, this means that the two plots of R and R_{emp} become so close that their distance is never larger than ε . Mathematically, the statement “ $|R(f) - R_{\text{emp}}(f)| \leq \varepsilon$ for all $f \in \mathcal{F}$ ” can be expressed using a supremum (readers not familiar with the notion of “supremum” should think of a maximum instead):

$$\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \leq \varepsilon.$$

Intuitively it is clear that if we know that for all functions $f \in \mathcal{F}$ the difference $|R(f) - R_{\text{emp}}(f)|$ is small, then this holds in particular for any function f_n we might have chosen based on the given training data. That is, for any function $f \in \mathcal{F}$ we have

$$|R(f) - R_{\text{emp}}(f)| \leq \sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)|.$$

In particular, this also holds for a function f_n which has been chosen based on a finite sample of training points. From this we can draw the following conclusion:

$$P(|R(f_n) - R_{\text{emp}}(f_n)| \geq \varepsilon) \leq P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \geq \varepsilon). \quad (11)$$

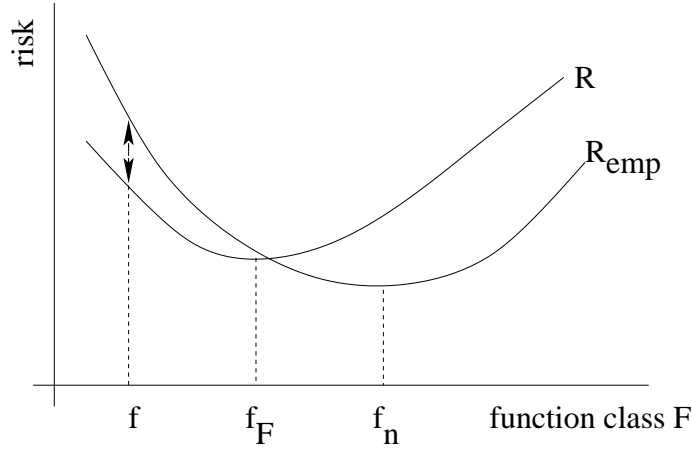


Figure 4: *Simplified depiction of the convergence of empirical risk to actual risk. The x-axis gives a one-dimensional representation of the function class \mathcal{F} (denoted F in the figure); the y axis denotes the risk. For each fixed function f , the law of large numbers tells us that as the sample size goes to infinity, the empirical risk $R_{\text{emp}}(f)$ converges towards the true risk $R(f)$ (indicated by the arrow). This does not imply, however, that in the limit of infinite sample sizes, the minimizer of the empirical risk, f_n , will lead to a value of the risk that is as good as the risk of the best function $f_{\mathcal{F}}$ in the function class (denoted f_F in the figure). For the latter to be true, we require the convergence of $R_{\text{emp}}(f)$ towards $R(f)$ to be uniform over all functions in \mathcal{F} (from Schölkopf and Smola, 2002).*

The quantity on the right hand side is now what the uniform law of large numbers deals with. We say that the law of large numbers holds uniformly over a function class \mathcal{F} if for all $\varepsilon > 0$,

$$P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \geq \varepsilon) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

One can now use (11) to show that if the uniform law of large numbers holds for some function class \mathcal{F} , then empirical risk minimization is consistent with respect to \mathcal{F} . To see this, consider the following derivation:

$$\begin{aligned} & |R(f_n) - R(f_{\mathcal{F}})| \\ & \quad (\text{by definition of } f_{\mathcal{F}} \text{ we know that } R(f_n) - R(f_{\mathcal{F}}) \geq 0) \\ & = R(f_n) - R(f_{\mathcal{F}}) \\ & = R(f_n) - R_{\text{emp}}(f_n) + R_{\text{emp}}(f_n) - R_{\text{emp}}(f_{\mathcal{F}}) + R_{\text{emp}}(f_{\mathcal{F}}) - R(f_{\mathcal{F}}) \\ & \quad (\text{note that } R_{\text{emp}}(f_n) - R_{\text{emp}}(f_{\mathcal{F}}) \leq 0 \text{ by def. of } f_n) \\ & \leq R(f_n) - R_{\text{emp}}(f_n) + R_{\text{emp}}(f_{\mathcal{F}}) - R(f_{\mathcal{F}}) \\ & \leq 2 \sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \end{aligned}$$

So we can conclude:

$$P(|R(f_n) - R(f_{\mathcal{F}})| \geq \varepsilon) \leq P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \geq \varepsilon/2).$$

Under the uniform law of large numbers, the right hand side tends to 0, which then leads to consistency of ERM with respect to the underlying function class \mathcal{F} . In other words, uniform convergence over \mathcal{F} is a sufficient condition for consistency of the empirical risk minimization over \mathcal{F} .

What about the other way round? Is uniform convergence also a *necessary* condition? Part of the elegance of VC theory lies in the fact that this is the case (see for example Vapnik and Chervonenkis, 1971, Mendelson, 2003, Devroye et al., 1996):

Theorem 3 (Vapnik and Chervonenkis) *Uniform convergence*

$$P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon) \rightarrow 0 \text{ as } n \rightarrow \infty, \quad (12)$$

for all $\epsilon > 0$, is a necessary and sufficient condition for consistency of empirical risk minimization with respect to \mathcal{F} .

In Section 4.2 we gave an example where we considered the set of all possible functions, and showed that learning was impossible. The dependence of learning on the underlying set of functions has now returned in a different guise: the condition of uniform convergence crucially depends on the set of functions for which it must hold. Intuitively, it seems clear that the larger the function space \mathcal{F} , the larger $\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)|$. Thus, the larger \mathcal{F} , the larger $P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon)$. Thus, the larger \mathcal{F} , the more difficult it is to satisfy the uniform law of large numbers. That is, for larger function spaces \mathcal{F} consistency is “harder” to achieve than for “smaller” function spaces.

This abstract characterization of consistency as a uniform convergence property, whilst theoretically intriguing, is not all that useful in practice. The reason is that it seems hard to find out whether the uniform law of large numbers holds for a particular function class \mathcal{F} . Therefore, we next address whether there are properties of function spaces which *ensure* uniform convergence of risks.

5 Capacity concepts and generalization bounds

So far, we have argued which property of the function space determines whether the principle of empirical risk minimization is consistent, i.e., whether it will work “in the limit.” This property was referred to as uniform convergence. To make statements about what happens after seeing only finitely many data points — which in reality will always be the case — we need to take a closer look at this convergence. It will turn out that this will provide us with bounds on the risk, and it will also provide insight into which properties of function classes determine whether uniform convergence can take place. To this end, let us take a closer look at the subject of Theorem 3: the probability

$$P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon). \quad (13)$$

Two tricks are needed along the way: the *union bound* and the method of *symmetrization by a ghost sample*.

5.1 The union bound

The union bound is a simple but convenient tool to transform the standard law of large numbers of individual functions into a uniform law of large numbers over a set of finitely many functions. Suppose the set \mathcal{F} consists just of finitely many functions, that is $\mathcal{F} = \{f_1, f_2, \dots, f_m\}$. Each of the functions $f_i \in \mathcal{F}$ satisfies the standard law of large numbers in form of the Chernoff bound, that is

$$P(|R(f_i) - R_{\text{emp}}(f_i)| \geq \epsilon) \leq 2 \exp(-2n\epsilon^2). \quad (14)$$

Now we want to transform these statements about the individual functions f_i into a uniform law of large numbers. To this end, note that we can rewrite:

$$\begin{aligned} & P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| \geq \epsilon) \\ &= P\left(|R(f_1) - R_{\text{emp}}(f_1)| \geq \epsilon \text{ or } |R(f_2) - R_{\text{emp}}(f_2)| \geq \epsilon \text{ or } \dots \text{ or } |R(f_m) - R_{\text{emp}}(f_m)| \geq \epsilon\right) \\ &\leq \sum_{i=1}^m P(|R(f_i) - R_{\text{emp}}(f_i)| \geq \epsilon) \\ &\leq 2m \exp(-2n\epsilon^2) \end{aligned} \quad (15)$$

Let us go through these calculations step by step. The first equality comes from the way the supremum is defined. Namely, the supremum over certain expressions is larger than ϵ if at least

one of the expressions is larger than ε , which leads to the statements with the “or” combinations. The next step uses a standard tool from probability theory, the union bound. The union bound states that the probability of a union of events (that is, events coupled with “or”) is smaller or equal to the sum of the individual probabilities. Finally, the last step is a simple application of the Chernoff bound of Eq. (14) to each of the terms in the sum.

From left to right, the statements in Eq. (15) show us how to convert the Chernoff bound for individual functions f_i into a bound which is uniform over a finite number m of functions. As we can see, the difference between the Chernoff bound for the individual functions and the right hand side of (15) is just a factor m . If the function space \mathcal{F} is fixed, this factor can be regarded as a constant, and the term $2m \exp(-2n\varepsilon^2)$ still converges to 0 as $n \rightarrow \infty$. Hence, the empirical risk converges to 0 uniformly over \mathcal{F} as $n \rightarrow \infty$. That is, we have proved that empirical risk minimization over a *finite* set \mathcal{F} of functions is consistent with respect to \mathcal{F} .

We next describe a trick used by Vapnik and Chervonenkis to reduce the case of an infinite function class to the case of a finite one. It consists of introducing what is sometimes called a ghost sample. It will enable us to replace the factor m in (15) by more general *capacity measures* that can be computed for infinite function classes.

5.2 Symmetrization

Symmetrization is an important technical step towards using capacity measures of function classes. Its main purpose is to replace the event $\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)|$ by an alternative event which can be solely computed on a given sample. Assume we are given a sample $(X_i, Y_i)_{i=1, \dots, n}$. We now introduce a new sample called the *ghost sample*. This ghost sample is just another sample $(X'_i, Y'_i)_{i=1, \dots, n}$ which is also drawn iid from the underlying distribution and which is independent of the first sample. It is called ghost sample because we do not need to physically draw this sample in practice. It is just a mathematical tool, that is we play “as if we had a second sample”. Of course, given the ghost sample we can also compute the empirical risk of a function with respect to this ghost sample, and we will denote this risk by $R'_{\text{emp}}(f)$. With the help of the ghost sample, one can now prove the following simple statement:

Lemma 4 (Vapnik and Chervonenkis) *For $m\varepsilon^2 \geq 2$, we have*

$$P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \varepsilon) \leq 2P(\sup_{f \in \mathcal{F}} |R_{\text{emp}}(f) - R'_{\text{emp}}(f)| > \varepsilon/2). \quad (16)$$

Here, the first P refers to the distribution of an iid sample of size n , while the second one refers to the distribution of two samples of size n (the original sample and the ghost sample), that is the distribution of iid samples of size $2n$. In the latter case, R_{emp} measures the empirical loss on the first half of the sample, and R'_{emp} on the second half.

Although we do not prove this lemma, it should be fairly plausible: if the empirical risks on two independent n -samples are close to each other, then they should also be close to the true risk.

This lemma is called the symmetrization lemma. Its name refers to the fact that we now look at an event which depends in a symmetric way on a sample, now of size $2n$. The main purpose of this lemma is that the quantity $R(f)$, which cannot be computed on a finite sample, has been replaced by the quantity $R'_{\text{emp}}(f)$, which can be computed on a finite sample.

Now let us explain what the symmetrization lemma is used for. In the last section we have seen how to bound the probability of uniform convergence (13) in terms of a probability of an event referring to a *finite* function class. The crucial observation is now that even if \mathcal{F} contains infinitely many functions, the different ways it can classify a training set of n sample points is finite. Namely, for any given training point in the training sample, a function can only take the values -1 or $+1$. On a sample of n points X_1, \dots, X_n , a function can act in at most 2^n different ways: it can choose each Y_i as -1 or $+1$. This has a very important consequence. Even if a function class \mathcal{F} contains infinitely many functions, there are at most 2^n different ways those functions can classify the points

of a finite sample of n points. This means that if we consider the term

$$\sup_{f \in \mathcal{F}} |R_{\text{emp}}(f) - R'_{\text{emp}}(f)|$$

then the supremum effectively only runs over a finite function class. To understand this, note that two functions $f, g \in \mathcal{F}$ which take the same values on the given sample have the same empirical risk, that is $R_{\text{emp}}(f) = R_{\text{emp}}(g)$. The analogous statement holds for the ghost sample and R'_{emp} . Hence, all functions f, g which coincide both on the sample and the ghost sample will lead to the same term $|R_{\text{emp}}(f) - R'_{\text{emp}}(f)|$. Thus, the only functions we need to consider to compute the supremum are the 2^{2n} functions we can obtain on sample and ghost sample together. Hence, we can replace the supremum over $f \in \mathcal{F}$ by the supremum over a finite function class with at most 2^{2n} functions.

Note that this step is only possible due to the symmetrization lemma. If we had considered the term $\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)|$, the argument from above would not hold, as the value of $R(f)$ not only depends on the values of f on the sample.

In the following we now want to show how the insights gained in the symmetrization step can be used to derive a first capacity measure of a function class.

5.3 The shattering coefficient

For the purpose of bounding (13), Lemma 4 implies that the function class \mathcal{F} is effectively finite: restricted to the $2n$ points appearing on the right hand side of (16), it has *at most* 2^{2n} elements. This is because only the values of the functions *on the sample points and the ghost sample points* count. The number of effectively different functions can be smaller than 2^{2n} , however. For example, it could be the case that \mathcal{F} does not contain a single function which takes value $+1$ on the first training point. We now want to formalize this. Let $Z_n := ((X_1, Y_1), \dots, (X_n, Y_n))$ be a given sample of size n . Denote by $|\mathcal{F}_{Z_n}|$ be the cardinality of \mathcal{F} when restricted to $\{X_1, \dots, X_n\}$, that is, the number of functions from \mathcal{F} that can be distinguished from their values on $\{X_1, \dots, X_n\}$. Let us, moreover, denote the maximum number of functions that can be distinguished in this way as $\mathcal{N}(\mathcal{F}, n)$, where the maximum runs over all possible choices of samples, that is

$$\mathcal{N}(\mathcal{F}, n) = \max\{|\mathcal{F}_{Z_n}| \mid X_1, \dots, X_n \in \mathcal{X}\}.$$

The quantity $\mathcal{N}(\mathcal{F}, n)$ is referred to as the *shattering coefficient of the function class \mathcal{F} with respect to sample size n* . It has a particularly simple interpretation: it is the number of different outputs (Y_1, \dots, Y_n) that the functions in \mathcal{F} can achieve on samples of a given size n . In other words, it measures the *number of ways that the function space can separate the patterns into two classes*. Whenever $\mathcal{N}(\mathcal{F}, n) = 2^n$, this means that there exists a sample of size n on which all possible separations can be achieved by functions of the class \mathcal{F} . If this is the case, the function space is said to *shatter n points*. Note that because of the maximum in the definition of $\mathcal{N}(\mathcal{F}, n)$, shattering means that there *exists* a sample of n patterns which can be separated in all possible ways — it does not mean that this applies to *all* possible samples of n patterns.

The shattering coefficient is a capacity measure of a function class, that is it measures the “size” of a function class in some particular way. Note that if a function class \mathcal{F} contains very many functions, then the shattering coefficient tends to be larger than for a function class which only contains very few functions. However, the shattering coefficient is more subtle than simply counting the number of functions in a class. It only counts the number of functions in relation to the samples we are interested in. The following section will now finally show how to use the shattering coefficient to derive a generalization bound for empirical risk minimization on infinite function classes \mathcal{F} .

5.4 Uniform convergence bounds

Given an arbitrary, possibly infinite function class, we now want to take a look at the right hand side of (16). We now consider a sample of $2n$ points, that is a set Z_{2n} , where we interpret the first

n points as the original sample and the second n points as the ghost sample. The idea is now to replace the supremum over \mathcal{F} by the supremum over the set $\mathcal{F}_{Z_{2n}}$, use that the set $\mathcal{F}_{Z_{2n}}$ contains at most $\mathcal{N}(\mathcal{F}, n) \leq 2^{2n}$ different functions, then apply the union bound on this finite function set and then the Chernoff bound. This leads to a bound like (15), with $\mathcal{N}(\mathcal{F}, 2n)$ playing the role of m . Essentially, those steps can be written down as follows:

$$\begin{aligned}
& P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon) \\
& \quad (\text{due to symmetrization}) \\
& \leq 2P(\sup_{f \in \mathcal{F}} |R_{\text{emp}}(f) - R'_{\text{emp}}(f)| > \epsilon/2) \\
& \quad (\text{only functions in } \mathcal{F}_{Z_{2n}} \text{ are important}) \\
& = 2P(\sup_{f \in \mathcal{F}_{Z_{2n}}} |R_{\text{emp}}(f) - R'_{\text{emp}}(f)| > \epsilon/2) \\
& \quad (\mathcal{F}_{Z_{2n}} \text{ contains at most } \mathcal{N}(\mathcal{F}, 2n) \text{ functions, independently of } Z_{2n}) \\
& \quad (\text{use union bound argument and Chernoff}) \\
& \leq 2\mathcal{N}(\mathcal{F}, 2n) \exp(-n\epsilon^2/4)
\end{aligned}$$

So all in all we see that

$$P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon) \leq 2\mathcal{N}(\mathcal{F}, 2n) \exp(-n\epsilon^2/4). \quad (17)$$

Now we can use this expression to draw conclusions about consistency of empirical risk minimization. Namely, ERM is consistent for function class \mathcal{F} if the right hand side of this expression converges to 0 as $n \rightarrow \infty$. Let us look at a few examples.

First of all, consider a case where the shattering coefficient $\mathcal{N}(\mathcal{F}, 2n)$ is considerably smaller than 2^{2n} , say $\mathcal{N}(\mathcal{F}, 2n) \leq (2n)^k$ for some constant k (this means that the shattering coefficient grows polynomially in n). Plugging this in the right hand side of (17), we get

$$2\mathcal{N}(\mathcal{F}, 2n) \exp(-n\epsilon^2/4) = 2 \cdot (2n)^k \cdot \exp(-n\epsilon^2/4) = 2 \exp(k \cdot \log(2n) - n\epsilon^2/4).$$

Here we can see that for all ϵ , if n is large enough the whole expression converges to 0 for $n \rightarrow \infty$. From this we can conclude that whenever the shattering coefficient $\mathcal{N}(\mathcal{F}, 2n)$ only grows polynomially with n , then empirical risk minimization is consistent with respect to \mathcal{F} .

On the other hand, consider the case where we use the function class \mathcal{F}_{all} . It is clear that this class can classify each sample in every possible way, that is $\mathcal{N}(\mathcal{F}, 2n) = 2^{2n}$ for all values of n . Plugging this in the right hand side of (17), we get

$$2\mathcal{N}(\mathcal{F}, 2n) \exp(-n\epsilon^2/4) = 2 \cdot 2^{2n} \exp(-n\epsilon^2/4) = 2 \exp(n(2 \log(2) - \epsilon^2/4)).$$

We can immediately see that this expression does not tend to 0 when $n \rightarrow \infty$, that is we cannot conclude consistency for \mathcal{F}_{all} . Note that we cannot directly conclude that ERM using \mathcal{F}_{all} is inconsistent, either. The reason is that (17) only gives an upper bound on $P(\sup_{f \in \mathcal{F}} |R(f) - R_{\text{emp}}(f)| > \epsilon)$, that is it only provides a sufficient condition for consistency, not a necessary one. However, with more effort one can also prove necessary statements. For example, a necessary and sufficient condition for consistency of ERM is that

$$\log \mathcal{N}(\mathcal{F}, n)/n \rightarrow 0$$

(cf. Mendelson, 2003, for related theorems also see Vapnik and Chervonenkis, 1971, 1981, or Section 12.4. of Devroye et al., 1996). The proof that this condition is necessary is more technical, and we omit it. In case of the examples above, this condition immediately gives the desired results: if $\mathcal{N}(\mathcal{F}, n)$ is polynomial, then $\log \mathcal{N}(\mathcal{F}, n)/n \rightarrow 0$. On the other hand, for \mathcal{F}_{all} we always have $\mathcal{N}(\mathcal{F}, n) = 2^n$, thus $\log \mathcal{N}(\mathcal{F}, n)/n = n/n = 1$, which does not converge to 0. Thus, ERM using \mathcal{F}_{all} is not consistent.

5.5 Generalization bounds

It is sometimes useful to rewrite (17) “the other way round”. That is, instead of fixing ε and then computing the probability that the empirical risk deviates from the true risk by more than ε , we specify the probability with which we want the bound to hold, and then get a statement which tells us how close we can expect the risk to be to the empirical risk. This can be achieved by setting the right hand side of (17) equal to some $\delta > 0$, and then solving for ε . As a result, we get the statement that with a probability at least $1 - \delta$, any function $f \in \mathcal{F}$ satisfies

$$R(f) \leq R_{\text{emp}}(f) + \sqrt{\frac{4}{n}(\log(2\mathcal{N}(\mathcal{F}, n)) - \log(\delta))}. \quad (18)$$

In the same way as above, we can use this bound to derive consistency statements. For example, it is now obvious that empirical risk minimization is consistent for function class \mathcal{F} if the term $\sqrt{\log(2\mathcal{N}(\mathcal{F}, 2n))/n}$ converges to 0 as $n \rightarrow \infty$. Again, this is for example the case if $\mathcal{N}(\mathcal{F}, 2n)$ only grows polynomially with n .

Note that the bound (18) holds for all functions $f \in \mathcal{F}$. On the one side, this is a strength of the bound, as it holds in particular for the function f_n minimizing the empirical risk, which is what we wanted. Moreover, many learning machines do not truly minimize the empirical risk, and the bound thus holds for them, too. However, one can also interpret it as a weakness, since by taking into account more information about the function we are interested in, one could hope to get more accurate bounds.

Let us try to get an intuitive understanding of this bound. It tells us that if both $R_{\text{emp}}(f)$ and the square root term are small simultaneously, then we can guarantee that with high probability, the risk (i.e., the error on future points that we have not seen yet) will be small. This sounds like a surprising statement, however, it does not claim anything impossible. If we use a function class with relatively small $\mathcal{N}(\mathcal{F}, n)$, i.e., a function class which cannot “explain” many possible functions, and then notice that using a function of this class we can nevertheless explain data sampled from the problem at hand, then it is likely that this is not a coincidence, and we can have captured some essential aspects of the problem. If, on the other hand, the problem is too hard to learn from the given amount of data then we will find that in order to explain the data (i.e., to achieve a small $R_{\text{emp}}(f)$), we need a function class which is so large that it can basically explain anything, and thus the square root term would be large. Note, finally, that whether a problem is hard to learn is entirely determined by whether we can come up with a suitable function class, and thus by our prior knowledge of it. Even if the optimal function is subjectively very complex, if our function class contains that function, and few or no other functions, we are in an excellent position to learn. There exists a large number of bounds similar to (17) and its alternative form (18). Differences occur in the constants, both in front of the exponential and in its exponent. The bounds also differ in the exponent of ε (see Devroye et al., 1996, Vapnik, 1998 and references therein) and in the way they measure capacity. We will not elaborate on those issues.

5.6 The VC dimension

Above we have formulated the generalization bounds in terms of the shattering coefficient $\mathcal{N}(\mathcal{F}, n)$. The downside is that they are usually difficult to evaluate. However, there exists a large number of different capacity concepts, with different advantages and disadvantages. We now want to introduce the most well known one, the so-called VC dimension (named after Vapnik and Chervonenkis). Its main purpose is to characterize the growth behavior of the shattering coefficient using a single number.

We say that a sample Z_n of size n is *shattered by function class* \mathcal{F} if the function class can realize any labeling on the given sample, that is $|\mathcal{F}_{Z_n}| = 2^n$. The *VC dimension of* \mathcal{F} , denoted by $\text{VC}(\mathcal{F})$, is now defined as the largest number n such that there exists a sample of size n which is shattered by \mathcal{F} . Formally,

$$\text{VC}(\mathcal{F}) = \max\{n \in \mathbb{N} \mid |\mathcal{F}_{Z_n}| = 2^n \text{ for some } Z_n\}.$$

If the maximum does not exist, the VC dimension is defined to be infinity. For many examples of function classes and their VC dimensions see for example Kearns and Vazirani (1994) or Anthony and Biggs (1992).

A beautiful combinatorial result proved simultaneously by several people (Sauer, 1972, Shelah, 1972, Vapnik and Chervonenkis, 1971) characterizes the growth behavior of the shattering coefficient and relates it to the VC dimension:

Lemma 5 (Vapnik, Chervonenkis, Sauer, Shelah) *Let \mathcal{F} be a function class with finite VC dimension d . Then*

$$N(\mathcal{F}, n) \leq \sum_{i=0}^d \binom{n}{i}$$

for all $n \in \mathbb{N}$. In particular, for all $n \geq d$ we have

$$N(\mathcal{F}, n) \leq \left(\frac{en}{d}\right)^d.$$

The importance of this statement lies in the last fact. If $n \geq d$, the shattering coefficient behaves like a polynomial function of the sample size n . This is a very remarkable result: once we know the VC-dimension of a function class \mathcal{F} is finite, we already know that the shattering coefficients grow polynomially with n . By the results of the last section this implies the consistency of ERM. Note that we also have a statement in the other direction. If the VC-dimension is infinite, this means that for each n there exists some sample which can be shattered by \mathcal{F} , that is $N(\mathcal{F}, n) = 2^n$. For this case we have already seen above that ERM is not consistent. Together, we achieve the following important characterization:

Theorem 6 *Empirical risk minimization is consistent with respect to \mathcal{F} if and only if $VC(\mathcal{F})$ is finite.*

One important property to note both about the shattering coefficient and the VC dimension is that they do not depend on the underlying distribution P , they only depend on the function class \mathcal{F} . On the one hand, this is an advantage, as all generalization bounds derived from those concepts apply to all possible probability distributions. On the other hand, one can also consider this as disadvantage, as the capacity concepts do not take into account particular properties of the distribution at hand. In this sense, those capacity concepts often lead to rather loose bounds.

5.7 Rademacher complexity

A different concept to measure the capacity of a function space is the Rademacher complexity. Compared to the shattering coefficient and the VC dimension, it does depend on the underlying probability distribution, and usually leads to much sharper bounds than both of them. The Rademacher complexity is defined as follows. Let $\sigma_1, \sigma_2, \dots$ independent random variables which attain the two values $+1$ and -1 with probability 0.5 each (such random variables are sometimes called Rademacher variables, therefore the name “Rademacher complexity”). For example, they could be the results of repeatedly tossing a fair coin. We formally define the Rademacher complexity $\mathcal{R}(\mathcal{F})$ of a function space \mathcal{F} as

$$\mathcal{R}(\mathcal{F}) := E \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \sigma_i f(X_i). \quad (19)$$

This expression looks complicated, but it has a nice interpretation. For the moment, consider the values σ_i as fixed, and interpret label σ_i as a label of the point X_i . As both σ_i and $f(X_i)$ only take the values $+1$ or -1 , the product $\sigma_i f(X_i)$ takes the value $+1$ if $\sigma_i = f(X_i)$, and -1 if $\sigma_i \neq f(X_i)$. As a consequence, the sum on the right hand side of Equation (19) will be large if the labels $f(X_i)$ coincide with the labels σ_i on many data points. This means that the function f “fits well” to the labels σ_i : if the labels σ_i were the correct labels, f would have a small training

error R_{emp} . Now taking into account the supremum, we not only look at one function f , but at all functions $f \in \mathcal{F}$. We can see that $\sup_{f \in \mathcal{F}} \sum_{i=1}^n \sigma_i f(X_i)$ is large if there exists a function in \mathcal{F} which fits well to the given sequence σ_i of labels. Finally, recall that the labels σ_i are supposed to be random variables. We can consider them as random labels on the data points X_i . As we take the expectation over both the data points and the random labels, the overall Rademacher complexity is high if the function space \mathcal{F} is able to “fit well” to random labels. This intuition makes sense: a function space has to be pretty large to be able to fit to all kinds of random labels on all kinds of data sets. In this sense, the Rademacher complexity measures how “complex” the function space is: the higher $\mathcal{R}(\mathcal{F})$, the larger the complexity of \mathcal{F} .

From a mathematical point of view, the Rademacher complexity is convenient to work with. One can prove generalization bounds of the following form: with probability at least $1 - \delta$,

$$R(f) \leq R_{\text{emp}}(f) + 2\mathcal{R}(\mathcal{F}) + \sqrt{\frac{\log(1/\delta)}{2n}}$$

Rademacher complexities have some advantages over the classical capacity concepts such as the VC dimension. Most notably, the bounds obtained by Rademacher complexities tend to be much sharper than the ones obtained by the classical tools. The proof techniques are different from the ones explained above, but we do not want to go into details here. For literature on Rademacher complexity bounds, see for example Mendelson (2003), Bousquet et al. (2003) or Boucheron et al. (2005) and references therein.

5.8 Large margin bounds

Finally, we would like to introduce another type of capacity measure of function classes which is more specialized than the general combinatorial quantities introduced above. Consider the special case where the data space consists of points in the two-dimensional space \mathbb{R}^2 , and where we want to separate classes by a straight line. Given a set of training points and a classifier f_n which can perfectly separate them, we define the *margin of the classifier* f_n as the smallest distance of any training point to the separating line f_n (cf. Figure 5). Similarly, a margin can be defined for general linear classifiers in the space \mathbb{R}^d of arbitrary dimension d . It can be proved that the VC dimension of a class \mathcal{F}_ρ of linear functions with all have margin at least ρ can essentially be bounded by the ratio of the radius R of the smallest sphere enclosing the data points with the margin ρ , that is

$$\text{VC}(\mathcal{F}_\rho) \leq \min \left\{ d, \frac{4R^2}{\rho^2} \right\} + 1$$

(cf. Theorem 5.1. in Vapnik, 1995). That is, the larger the margin ρ of the functions in the class \mathcal{F}_ρ , the smaller is its VC dimension. Thus, one can use the margin of classifiers as a capacity concept. One of the most well-known classifiers, the support vector machine (SVM) builds on this result. See Schölkopf and Smola (2002) for a comprehensive treatment. An example of a generalization bound involving the large margin is as follows (for a more precise statement see for example Theorem 7.3. in Schölkopf and Smola, 2002):

Theorem 7 (Large margin bound) *Assume the data space lies inside a ball of radius R in \mathbb{R}^d . Consider the set \mathcal{F}_ρ of linear classifiers with margin at least ρ . Assume we are given n training examples. By $\nu(f)$ denote the fraction of training examples which have margin smaller than ρ or which are wrongly classified by some classifier $f \in \mathcal{F}_\rho$. Then, with probability at least $1 - \delta$, the true error of any $f \in \mathcal{F}_\rho$ can be bounded by*

$$R(f) \leq \nu(f) + \sqrt{\frac{c}{n} \left(\frac{R^2}{\rho^2} \log(n)^2 + \log(1/\delta) \right)}$$

where c is some universal constant.

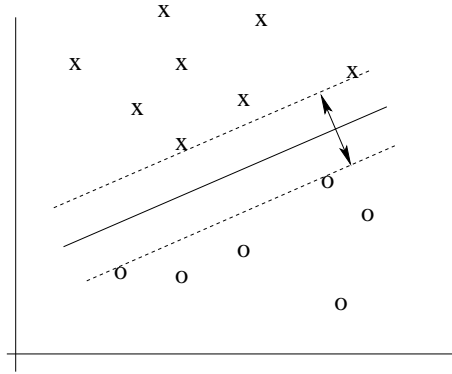


Figure 5: *Margin of a linear classifier: the crosses depict training points with label +1, the circles training points with label -1. The straight line is the linear classifier f_n , and the dashed line shows the margin. The width ρ of the margin is depicted by the arrow.*

5.9 Other generalization bounds and capacity concepts

Above we have introduced a few capacity concepts for function classes such as the shattering coefficient, the VC dimension, or the Rademacher complexity. In the literature, there exist many more capacity concepts, and introducing all of them will be beyond the scope of this overview. However, we would like to point out the general form which most generalization bounds take. Usually, those bounds are composed of three different terms and have a form like: with probability at least $1 - \delta$,

$$R(f) \leq R_{\text{emp}}(f) + \text{capacity}(\mathcal{F}) + \text{confidence}(\delta).$$

That is, one can bound the true risk of a classifier by its empirical risk, some capacity term which in the simplest case only depends on the underlying function class, and a confidence term which depends on the probability with which the bound should hold. Note that by nature, all bounds of this form are worst case bounds: as the bound holds for all functions in the class \mathcal{F} , the behavior of the bound is governed by the “worst” or “most badly behaved” function in the class. This point is often used to criticize this approach to statistical learning theory, as natural classifiers do not tend to pick the worst function in a class.

6 Incorporating knowledge into the bounds

In the previous section we presented the standard approach to derive risk bounds using uniform laws of large numbers. The bounds are agnostic in the sense that they do not make any prior assumptions on the underlying distribution P .

In many cases, however, it is desirable to be able to take into account some prior knowledge we might have about our problem. There are several good reasons for doing so. First, the bounds we considered above are worst case bounds over all possible distributions. That is, their behavior might be governed by completely unnatural distributions which would never occur in practice (such as distributions on Cantor sets, for example). In this sense, the bounds are overly pessimistic. As we often believe that “real” distributions have certain regularity aspects, we might improve the results obtained above by making use of this regularity. A more fundamental reason for incorporating prior knowledge is the no free lunch theorem, which will be discussed in Section 8. In a nutshell, the no free lunch theorem states that learning is impossible unless we make assumptions on the underlying distribution. Thus it seems a good idea to work out ways to state prior assumptions on distributions, and to build them into our learning framework. In this section we want to point out a few ways of doing so.

6.1 How to encode prior knowledge in the classical approach

Let us step back and try to figure out where prior knowledge enters a learning problem:

1. Via the formalization of the data space \mathcal{X} , for example its topology. For example, we might construct a distance function or a similarity function which tells us how “similar” different input values in \mathcal{X} are. A learning algorithm then tries to assign similar output labels to similar input labels. The topology of \mathcal{X} is one of the most important places to encode prior knowledge, not only for theory but in particular for practical applications.
2. Via the elements of \mathcal{F} . Here we encode our assumptions on how a useful classifier might look. While in theory this is an important way to encode prior assumptions, it does not play such a big role in practice. The reason is that it is not so easy to formulate any prior assumptions in terms of the function space. In applications, people thus often use one out of a handful of standard function spaces, and do not consider this as the main place to encode prior assumptions. An exception are Bayesian approaches, see below.
3. Via the loss function ℓ . This function encodes what the “goal” of learning should be. While the loss functions we mentioned above are pretty straightforward, there are many ways to come up with more elaborate loss functions. For example, we can weight errors on individual data points more heavily than those on other data points. Or we can weight different kinds of errors differently. For example, in many problems the “false positives” and “false negatives” have different costs associated to them. In the example of spam filtering, the cost of accidentally labeling a spam email as “not spam” is not so high (the user can simply delete this mail). However, the cost of labeling a “non-spam” email as “spam” can be very high (the mail might have contained important information for the user, but got deleted without his knowledge).
4. Via assumptions on the underlying probability distributions. So far, the classical approach presented above was agnostic in the sense that it did not make any assumptions on the underlying probability distribution. That is, no matter what probability distribution P generated our data, the generalization bounds from above apply. Due to this property they are often called “worst case bounds”, as they even hold for the worst and most unlikely distribution one can imagine.

This worst case approach has often been criticized as being overly pessimistic. The accusation is that the behavior of the results is governed by artificial, pathological probability distributions which would never occur in practice, and thus the results do not have much meaning for the “real world”. To circumvent this, one could make assumptions on the underlying probability distributions. For example, one could assume that the distribution is “nice” and “smooth”, that the labels are not overly noisy, and so on. Such assumptions can lead to a dramatic improvement of the learning guarantees, as is discussed in Section 7.4 in connection with the fast learning rates. On the other hand, making assumptions on the distributions contradicts the agnostic approach towards learning we wanted to make in the beginning. It is often perceived problematic to make such assumptions, because after all one does not know whether those assumptions hold for “real world” data, and guarantees proved under those assumptions could be misleading in cases where the assumptions are violated.

In some sense, all those quantities mentioned above do enter the classical generalization bounds: The loss function is directly evaluated in the empirical risk of the bound. The topology of \mathcal{X} and the choice of \mathcal{F} are both taken into account when computing the capacity measure of \mathcal{F} (for example the margin of functions).

However, the capacity measures are often perceived as a rather cumbersome and crude way to incorporate such assumptions, and the question is whether there are any other ways to deal with knowledge. In this section we now want to focus on a few advanced techniques, all of which try to improve the framework above from different points of view. The focus of the attention is on how to incorporate more “knowledge” in the bounds than just counting functions in \mathcal{F} : either knowledge we have a priori, or knowledge we can obtain a posteriori.

6.2 PAC Bayesian bounds

The classical SLT approach has two features which are important to point out. The capacity term in the generalization bound always involves some quantity which measures the “size” of the function space \mathcal{F} . However, this quantity usually does not directly depend on the complexity of the individual functions in \mathcal{F} , it rather counts how many functions there are in \mathcal{F} . Moreover, the bounds do not contain any quantity which measures the complexity of an individual function f itself. In this sense, all functions in the function space \mathcal{F} are treated the same: as long as they have the same training error, their bound on the generalization error is identical. No function is singled out in any special way.

This can be seen as an advantage or a disadvantage. If we believe that all functions in \mathcal{F} are similarly well suited to fit a certain problem, then it would not be helpful to introduce any “ordering” between them. However, often this is not the case. We already have some “prior knowledge” which we accumulated in the past. This knowledge might tell us that some functions $f \in \mathcal{F}$ are much more likely to be a good classifier than others. The Bayesian approach is one way to try to incorporate such prior knowledge into statistical inference. The general idea is to introduce some prior distribution π on the function space \mathcal{F} . This prior distribution expresses our belief about how likely a certain function is to be a good classifier. The larger the value $\pi(f)$ is, the more confident we are that f might be a good function. The important point is that this prior will be chosen before we get access to the data. It should be selected only based on background information or prior experience.

It turns out that this approach can be effectively combined with the classic SLT framework. For example, one can prove that for a finite function space \mathcal{F} , with probability at least $1 - \delta$,

$$R(f) \leq R_{\text{emp}}(f) + \sqrt{\frac{\log(1/\pi(f)) + \log(1/\delta)}{2n}}$$

where $\pi(f)$ denotes the value of the prior on f . This is the simplest PAC-Bayesian bound. The name comes from the fact that it combines the classical bounds (sometimes called PAC bounds where “PAC” stands for “probably approximately correct”) and the Bayesian framework. Note that the right hand side does not involve a capacity term for \mathcal{F} , but instead “punishes” individual functions f according to their prior likelihood $\pi(f)$. The more unlikely we believed f to be, the smaller $\pi(f)$, and the larger the bound. This mechanism shows that among two functions with the same empirical risk on the training data, one prefers the one with the higher prior value $\pi(f)$. For background reading on PAC-Bayesian bounds, see for example Section 6 of Boucheron et al. (2005) and references therein.

6.3 Luckiness approach

There is one important aspect of the bounds obtained in the classical approach (and in the PAC-Bayesian approach as well): all quantities in the capacity term of the bound have to be evaluated *before* getting access to the data. The mathematical reason for this is that capacity measures are not treated as random quantities, they are considered to be deterministic functions of a fixed function class. For example, the large margin bound in Section 5.8 has to be parsed as follows: “if we knew that the linear classifier we are going to construct has margin ρ , then the generalization bound of Theorem 7 would hold”. From this statement, it becomes apparent that there is a problem: in practice, we do not know in advance whether a given classifier will have a certain margin, this will strongly depend on the data at hand. At first glance, this problem sounds superficial, and many people in the machine learning community are not even aware of it. It is closely related to the question what prior assumptions we want to encode in the learning problems before seeing actual data, and which properties of a problem should only be evaluated a posteriori, that is after seeing the data. While the PAC-Bayesian framework deals with a priori knowledge, we still need a framework to deal with “a posteriori” knowledge.

This problem is tackled in the “luckiness framework”, first introduced in Shawe-Taylor et al. (1998) and then considerably extended in Herbrich and Williamson (2002). On a high level, the idea is as follows. Instead of proving bounds where the capacity term just depends on the underlying function class, one would like to allow this capacity to depend on the actual data at hand. Some samples are considered to be very “lucky”, while others are “unlucky”. The rationale is that for

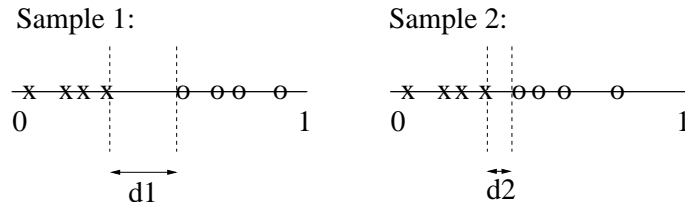


Figure 6: *Luckiness approach*

some samples it is easy to decide on a good function from the given function class, while the same is difficult for some other samples. As a result, one can prove generalization bounds which do depend on the underlying sample in terms of their “luckiness value”.

We would like to illustrate the basic idea with a small toy example. Suppose our data space \mathcal{X} is just the interval $[0, 1]$, and define the functions f_a as

$$f_a(x) = \begin{cases} -1 & \text{if } x \leq a \\ +1 & \text{if } x > a \end{cases}$$

As function space we use the space $\mathcal{F} := \{f_a \mid a \in [0, 1]\}$. Moreover, assume that the true underlying distribution can be classified by a function in \mathcal{F} with 0 error, that is we do not have any label noise. Now consider two particular samples, see Figure 6 for illustration. In the first sample, the two data points which are closest to the decision boundary have distance d_1 , which is fairly large compared to the corresponding distance d_2 in the second sample. It is clear that the true decision boundary has to lie somewhere in the interval d_1 (d_2 , respectively). The uncertainty about the position of the decision boundary is directly related to the lengths d_1 and d_2 , respectively: we can be confident that the error on Sample 2 will be much smaller than the error on Sample 1. In this sense, Sample 2 is more “lucky” than Sample 1. Now consider two classifiers f_1 and f_2 constructed using Sample 1 and Sample 2, and which have 0 training error. Classic generalization bounds such as the ones in Section 5 give exactly the same risk value to both classifiers: they have the same training error and use the same function space \mathcal{F} . This is where the luckiness approach comes in. It assigns a “luckiness value” to all samples, and then derives a generalization bound which not only depends on the training error and the capacity of the underlying function class, but also on the luckiness value of the sample at hand. The technical details are fairly complicated, and we refrain from introducing them here. Let us just remark that in the example above, the luckiness approach would attribute a smaller risk to Sample 2 than to Sample 1. For more material on how this works exactly see Shawe-Taylor et al. (1998) and Herbrich and Williamson (2002). Also note that similar approaches have been developed in classical statistics under the name “conditional confidence sets”, see Kiefer (1977).

7 The approximation error and Bayes consistency

In the previous sections we have investigated the standard approach to bound the estimation error of a classifier. This is enough to achieve consistency with respect to a given function class \mathcal{F} . In this section, we now want to look at the missing piece towards Bayes-consistency: the approximation error.

Recall that the estimation error was defined as $R(f_n) - R(f_{\mathcal{F}})$ and the approximation error as $R(f_{\mathcal{F}}) - R(f_{Bayes})$, cf. Section 2.4. In order to achieve Bayes-consistency, both terms have to vanish when $n \rightarrow \infty$. We have seen above that for the estimation error to converge to 0 we have to make sure that the function space \mathcal{F} has a reasonably small capacity. But this now poses a problem for the approximation error: if the function space \mathcal{F} has a small capacity, this means in particular that the space \mathcal{F} is considerably smaller than the space \mathcal{F}_{all} of all functions. Thus, if we fix the function class \mathcal{F} and the Bayes classifier f_{Bayes} is not contained in \mathcal{F} , then the approximation error might not be 0.

There are only two ways to solve this problem. The first one is to make assumptions on the functional form of the Bayes classifier. If $f_{Bayes} \in \mathcal{F}$ for some known function space \mathcal{F} with small capacity, we know that the approximation error is 0. In this case, Bayes-consistency reduces to consistency with respect to \mathcal{F} , which can be achieved by the methods discussed in the last section. However, if we do not want to make assumptions on the Bayes classifier, then we have to choose a different construction.

7.1 Working with nested function spaces

In this construction, we will not only consider one function class \mathcal{F} , but a sequence $\mathcal{F}_1, \mathcal{F}_2, \dots$ of function spaces. When constructing a classifier on n data points, we will do this based on function space \mathcal{F}_n . The trick is now that the space \mathcal{F}_n should become more complex the larger the sample size n is. The standard construction is to choose the spaces \mathcal{F}_n such that they form an increasing sequence of nested function spaces, that is $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \mathcal{F}_3 \subset \dots$. The intuition is that we start with a simple function space and then slowly add more and more complex functions to the space. If we are now given a sample of n data points, we are going to pick our classifier from the space \mathcal{F}_n . If we want this classifier to be Bayes-consistent, there are two things we need to ensure:

1. The estimation error has to converge to 0 as $n \rightarrow \infty$. To this end, note that for each fixed n we can bound the estimation error by one of the methods of Section 5. This bound is decreasing as the sample size increases, but it is increasing as the complexity term increases. We now have to make sure that the overall estimation error is still decreasing, that is the complexity term must not dominate the sample size term. To ensure this, we have to make sure that the complexity of \mathcal{F}_n does not grow too fast as the sample size increases.
2. The approximation error has to converge to 0 as $n \rightarrow \infty$. To this end, we need to ensure that eventually for some large n , each function of \mathcal{F}_{all} is either contained in \mathcal{F}_n , or that it can be approximated by a function from \mathcal{F}_n . We are going to discuss below how this can be achieved.

An example how those two points can be stated in a formal way is the following theorem, adapted from Theorem 18.1 of Devroye et al. (1996):

Theorem 8 *Let $\mathcal{F}_1, \mathcal{F}_2, \dots$ be a sequence of function spaces, and consider the classifiers*

$$f_n = \operatorname{argmin}_{f \in \mathcal{F}_n} R_{\text{emp}}(f).$$

Assume that for any distribution P the following two conditions are satisfied:

1. *The VC-dimensions of the spaces \mathcal{F}_n satisfy $VC(\mathcal{F}_n) \cdot \log n/n \rightarrow 0$ as $n \rightarrow \infty$.*
2. *$R(f_{\mathcal{F}_n}) \rightarrow R(f_{Bayes})$ as $n \rightarrow \infty$.*

Then, the sequence of classifiers f_n is Bayes-consistent.

Let us try to understand this theorem. We are given a sequence of increasing function spaces \mathcal{F}_n . For each sample of size n , we pick the function in \mathcal{F}_n which has the lowest empirical risk. This is our classifier f_n . If we want this to be consistent, two conditions have to be satisfied. The first condition says that the complexity of the function classes, as measured by the VC dimension, has to grow slowly. For example, if we choose the function spaces \mathcal{F}_n such that $VC(\mathcal{F}_n) \approx n^\alpha$ for some $\alpha \in]0, 1[$, then the first condition is satisfied because

$$VC(\mathcal{F}_n) \cdot (\log n)/n \approx n^\alpha (\log n)/n = (\log n)/n^{1-\alpha} \rightarrow 0.$$

However, if we choose $VC(\mathcal{F}_n) \approx n$ (that is, $\alpha = 1$ in the above calculation), then this is no longer the case:

$$VC(\mathcal{F}_n) \cdot (\log n)/n \approx \log n \rightarrow \infty.$$

The second condition of the theorem simply states that the approximation error has to converge to 0, but the theorem does not give any insight how to achieve this. But as we discussed above it is clear that the latter can only be achieved for an increasing sequence of function classes.

7.2 Regularization

An implicit way of working with nested function spaces is the principle of regularization. Instead of minimizing the empirical risk $R_{\text{emp}}(f)$ and then expressing the generalization ability of the resulting classifier f_n using some capacity measure of the underlying function class \mathcal{F} , one can pursue a more direct approach: one directly minimizes the so-called regularized risk

$$R_{\text{reg}}(f) = R_{\text{emp}}(f) + \lambda\Omega(f).$$

Here, $\Omega(f)$ is the so-called regularizer. This regularizer is supposed to punish overly complex functions. For example, one often chooses a regularizer which punishes functions with large fluctuations, that is one chooses $\Omega(f)$ such that it is small for functions which vary slowly, and large for functions which fluctuate a lot. Or, as another example, for linear classifiers one can choose $\Omega(f)$ as the inverse of the margin of a function (recall the definition of a margin in Section 5.8).

The λ in the definition of the regularized risk is a trade-off constant. It “negotiates” between the importance of $R_{\text{emp}}(f)$ and of $\Omega(f)$. If λ is very large, we take the punishment induced by $\Omega(f)$ very seriously, and might prefer functions with small $\Omega(f)$ even if they have a high empirical risk. On the other hand, if λ is small, the influence of the punishment decreases, and we merely choose functions based on their empirical risks.

The principle of regularization consists in choosing the classifier f_n that minimizes the regularized risk R_{reg} . Many of the widely-used classifiers can be cast into the framework of regularization, for example the support vector machine (see Schölkopf and Smola, 2002, for details).

To prove Bayes-consistency of regularized classifiers one essentially proceeds as outlined in the subsection above: for some slowly increasing sequence $\omega_1, \omega_2, \dots$ we consider nested function spaces $\mathcal{F}_{\omega_1}, \mathcal{F}_{\omega_2}, \dots$, where each \mathcal{F}_{ω_i} contains all functions f with $\Omega(f) \leq \omega_i$. Eventually, if i is very large, the space \mathcal{F}_{ω_i} will approximate the space \mathcal{F}_{all} of all functions. For consistency, one has to take the constant λ to 0 as $n \rightarrow \infty$. This ensures that eventually, for large n we indeed are allowed to pick functions from a space close to \mathcal{F}_{all} . On the other hand, the constant λ must not converge to 0 too fast, otherwise we will already start overfitting for small values of n (as with a small constant λ , one essentially ignores the regularizer and consequently performs something close to ERM over a very large set of functions). A paper which carefully goes through all those steps for the example of the support vector machine is Steinwart (2005).

Note that there is one important conceptual difference between empirical risk minimization and regularization. In regularization, we have a function Ω which measures the “complexity” of an individual function f . In ERM, on the other side, we never look at complexities of individual functions, but only at the complexity of a function class. The latter, however, is more a measure of capacity, that is a measure of the “number of functions” in \mathcal{F} , and only indirectly a measure of how complex the individual functions in the class are. From an intuitive point of view, the first approach is often easier to grasp, as the complexity of an individual function is a more intuitive concept than the capacity of a function class.

7.3 Achieving zero approximation error

The theorem above shows the general principle how we can achieve Bayes-consistency. However, the theorem simply postulated as its second condition that the approximation error should converge to 0. How can this be achieved in practice? It turns out that there are many situations where this is not so difficult. Essentially we have to make sure that each function of \mathcal{F}_{all} is either contained in \mathcal{F}_n for some large n , or that it can be approximated arbitrarily well by a function from \mathcal{F}_n . The area in mathematics dealing with such kind of problems is called approximation theory, but for learning theory purposes simple approximation results are often enough (for more sophisticated ones see for example Cucker and Zhou (2007)). The only technical problem we have to solve is that we need a statement of the following form: if two functions are “close” to each other, then their corresponding risk values are also “close”.

Such statements are often quite easy to obtain. For example, it is straightforward to see that if f is a binary classification function (i.e., with $f(x) \in \{\pm 1\}$) and g any arbitrary (measurable) function, and the L_1 -distance between f and g is less than δ , then so is their difference in 0-1-risk, i.e., $P(f(x) \neq \text{sgn}(g(x))) < \delta$. This means that in order to prove that the approximation error of a function space \mathcal{F} is smaller than δ , we just have to know that every function in \mathcal{F}_{all} can be approximated up to δ in the L_1 -norm by functions from \mathcal{F} . Results of this kind are abundant in the mathematics literature. For example, if \mathcal{X} is a bounded subset of the real numbers, it is well known that one can approximate any measurable function on this set arbitrarily well by a polynomial. Hence, we could choose the spaces \mathcal{F}_n as spaces of polynomials with degree at most d_n where d_n slowly grows with n . This is enough to guarantee convergence of the approximation error.

7.4 Rates of convergence

We would like to point out one more fundamental difference between estimation and approximation error: the uniform rates of convergence. In a nutshell, a “rate of convergence” gives information about how “fast” a quantity converges. In our case, the rate says something about how large n has to be in order to ensure that an error is smaller than a certain quantity. Such a statement could be: in order to guarantee (with high probability) that the estimation error is smaller than 0.1 we need at least $n = 1000$ sample points. Usually it is the case that rates of convergence depend on many parameters and quantities of the underlying problem. In the learning setting, a particularly important question is whether the rate of convergence also depends on the underlying distribution. And this is where the difference between estimation error and approximation error happens. For the estimation error, there exist rates of convergence which hold independently of the underlying distribution P . This is important, as it tells us that we can give convergence guarantees even though we do not know the underlying distribution. For the approximation error, however, it is not possible to give rates of convergence which hold for all probability distributions P . This means that a statement like “with the nested function classes $(\mathcal{F}_n)_n$ we need at least $n = 1000$ to achieve approximation error smaller than 0.01” could only be made if we knew the underlying probability distribution. One can prove that unless one makes some further assumptions on the true distribution, for any fixed sequence $(\mathcal{F}_n)_n$ of nested function spaces the rate of convergence of the approximation error can be arbitrarily slow. Even though we might know that it eventually converges to 0 and we obtain consistency, there is no way we could specify what “eventually” really means.

It is important to note that statements about rates of convergence strongly depend on the underlying assumptions. For example, above we have already pointed out that even under the assumption of independent sampling, no uniform rate of convergence for the approximation error exists. A similar situation occurs for the estimation error if we weaken the sampling assumptions. If we no longer require that samples X_i have to be independent from each other, then the situation changes fundamentally. While for “nearly independent sampling” (such as stationary α -mixing processes) it might still be possible to recover results similar to the ones presented above, as soon as we leave this regime it can become impossible to achieve such results. (For the specialists: even in the case of stationary ergodicity, we can no longer achieve universal consistency, see Nobel, 1999.) For more discussion see also Steinwart et al. (2006) and references therein.

On the other hand, if we strengthen our sampling assumptions, we can even improve the rates of convergence. If we assume that the data points are sampled independently, and if we make a few assumptions on the underlying distribution (in particular on the label noise), then the uniform rates of convergence of the estimation error can be improved dramatically. There is a whole branch of learning theory which deals with this phenomenon, usually called “fast rates”. For an overview see Section 5.2. of Boucheron et al. (2005).

Finally, note that both consistency and rates of convergence deal with the behavior of an algorithm as the sample size tends to infinity. Intuitively, consistency is a “worst case statement”: it says that ultimately, an algorithm will give a correct solution and does not make systematic errors. Rates of convergence, on the other hand, make statements about how “well behaved” an algorithm can be. Depending on prior assumptions, one can compare different algorithms in terms of their rates

of convergence. This can lead to insights into which learning algorithms might be better suited in which situations, and it might help us to choose a particular algorithm for a certain application on which we have prior knowledge.

8 No free lunch theorem

Up to now, we have reported many positive results in statistical learning theory. We have formalized the learning problem, defined the goal of learning (to minimize the risk), specified which properties a classifier should have (consistency), and devised a framework to investigate these properties in a fundamental way. Moreover, we have seen that there exist different ways to achieve consistent classifiers (k -nearest neighbor, empirical risk minimization), and of course there exist many more consistent ways to achieve consistency. Now it is a natural question to ask which of the consistent classifiers is “the best” classifier.

Let us first try to rephrase our question in a more formal way. Under the assumption of independent sampling from some underlying, but unknown probability distribution, is there a classifier which “on average over all probability distributions” achieves better results than any other classifier? Can we compare classifiers pairwise, that is compare whether a classifier A is better than classifier B, on average over all distributions? The reasons why we consider statements “on average over all distributions” lies in the fact that we do not want to make any assumption on the underlying distribution. Thus it seems natural to study the behavior of classifiers on any possible distribution. Regrettably, those questions have negative answers which are usually stated in the form of the so-called “no free lunch theorem”. A general proof of this theorem appeared in Wolpert and Macready (1997) and Wolpert (2001). A simpler but more accessible version for finite data spaces has been published by Ho and Pevy (2002). For versions with focus on convergence rates, see Section 7 of Devroye et al. (1996).

For the ease of understanding, consider the following simplified situation: assume that our input space \mathcal{X} only consists of a finite set of points, that is $\mathcal{X} = \{x_1, \dots, x_m\}$ for some large number m . Now consider all possible ways to assign labels to those data points, that is we consider all possible probability distributions on \mathcal{X} . Given some small set of training points $(X_i, Y_i)_{i=1, \dots, n}$ we use some fixed classification rule to construct a classifier on those points, say the k NN classifier. Now consider all points of \mathcal{X} which have not been training points and call this set of points the test set. Of course there exists a label assignment P_1 on the test set for which the classifier makes no error at all, namely the assignment which has been chosen by the classifier itself. But there also exists some label assignment P_2 on which the classifier makes the largest possible error, namely the inverse of the assignment constructed by the classifier. In the same way, we can see that essentially for any given error R , we can construct a probability distribution on \mathcal{X} such that the error of f_n on the test set has error R . The same reasoning will apply to any other classifier (for more precise reasoning, cf. Ho and Pevy, 2002). Thus, averaged over all possible probability distributions on \mathcal{X} , all classifiers f_n will achieve the same test error: whenever there is a distribution where the classifier performs well, there is a corresponding “inverse” distribution on the test set, on which the classifier performs poorly. In particular, on average over all probability distributions, no classifier can be better than random guessing on the test set!

This is a very strong result, and it touches the very base of machine learning. Does it in fact say that learning is impossible? Well, the answer is “it all depends on the underlying assumptions”. The crucial argument exploited above is that we take the average over *all* possible probability distributions, and that all probability distributions are considered to be “equally likely” (in the Bayesian language, we choose a uniform prior over the finite set of distributions). Those distributions also include cases where the labels are assigned to points “without any system”. For example, somebody could construct a probability distribution over labels by simply throwing a coin and for each data point, deciding on its true label by the outcome of the random coin tossing. It seems plausible that in such a scenario it does not help to know the labels on the training points — they are completely independent of the labels of all other points in the space. In such a scenario, learning is impossible.

The only chance for learning is to exclude such artificial cases. We need to ensure that there is

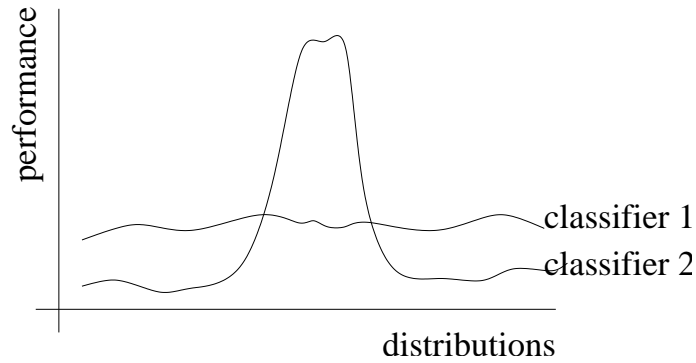


Figure 7: *No free lunch theorem: Classifier 1 depicts a general purpose classifier. It performs moderately on all kinds of distributions. Classifier 2 depicts a more specialized classifier which has been tailored towards particular distributions. It behaves very good on those distributions, but worse on other distributions. According to the no free lunch theorem, the average performance of all classifiers over all distributions, that is the area under the curves, is identical for all classifiers.*

some inherent mechanism by which we can use the training labels to generalize successfully to test labels. Formally, this means that we have to restrict the space of probability distributions under consideration. Once we make such restrictions, the no free lunch theorem breaks down. Restrictions can come in various forms. For example, we could assume that the underlying distribution has a “nice density” and a “nice function η ”. Or we can assume that there is a distance function on the space and the labels depend in some “continuous” way on the distance, that is points which are close to each other tend to have similar labels. If we make such assumptions, it is possible to construct classifiers which exploit those assumptions (for example, the kNN classifier to exploit distance structure). And those classifiers will then perform well on data sets for which the assumptions are satisfied. Of course, the no free lunch theorem still holds, which means that there will be some other data sets where this classifier will fail miserably. However, those will be data sets which come from distributions where the assumptions are grossly violated. And in those cases it makes complete sense that a classifier which relies on those assumptions does not stand a chance any more.

The no free lunch theorem is often depicted by a simple figure, see Figure 7. The figure shows the performance of two different classifiers (where, intuitively, the performance of a classifier is high if it achieves close to the Bayes risk). The x -axis depicts the space of all probability distributions. Classifier 1 represents a general purpose classifier. It performs moderately on all kinds of distributions. Classifier 2 depicts a more specialized classifier which has been tailored towards particular distributions. It behaves very good on those distributions, but worse on other distributions. According to the no free lunch theorem, the average performance, that is the area under the two curves, is the same for both classifiers.

A question which often comes up in the context of no free lunch theorems is how those theorems fit together with the consistency theorems proved above. For example, we have seen in Section 3 that the k -nearest neighbor classifier is *universally* consistent, that is it is consistent for *any* underlying probability distribution P . Is there a contradiction between the no free lunch theorem and the consistency statements? The solution to this apparent paradox lies in the fact that the consistency statements only treat the limit case of $n \rightarrow \infty$. In the example with the finite data space above, note that as soon as the sample size is so large that we essentially have sampled each point of the space at least once, then a classifier which memorizes the training data will not make any mistake any more. Similar statements (but a bit more involved) also hold for cases of infinite data spaces. Thus, no free lunch theorems make statements about some finite sample size n , whereas consistency considers the limit of $n \rightarrow \infty$. In the finite example above, note that unless we know the number m of points in the data space, there is no way we could give any finite sample guarantee on a classifier. If we have already seen half of the data points, then the classifier will perform better than if we have only seen 1/100 of all points. But of course, there is no way we can tell this from a finite sample. A formal way of stating this is as follows:

Theorem 9 (Arbitrarily close to random guessing) Fix some $\varepsilon > 0$. For every $n \in \mathbb{N}$ and every classifier f_n there exists a distribution P with Bayes risk 0 such that the expected risk of f_n is larger than $1/2 - \varepsilon$.

This theorem formally states what we have already hinted above: we can always construct a distribution such that based on a finite sample with fixed size, a given classification rule is not better than random guessing. This and several other versions of the no free lunch theorem can be found in Section 7 of Devroye et al. (1996).

The no free lunch theorem is one of the most important theorems in statistical learning. It simply tells us that in order to be able to learn successfully with guarantees on the behavior of the classifier, we need to make assumptions on the underlying distribution under consideration. This fits very nicely to the insights we gained in Section 5. There we have seen that in order to construct consistent classifiers, we need to make assumptions on the underlying space \mathcal{F} of function one uses. In practice, it makes sense to combine those statements: first restrict the space of probability distributions under consideration, and then use a small function class which is able to model the distributions in this class.

9 Model based approaches to learning

Above we have introduced the standard framework of statistical learning theory. It has been established as one of the main building blocks for analyzing machine learning problems and algorithms, but of course it is not the only approach to do this. In this section we would like to mention a few other ways to view machine learning problems and to analyze them. In particular, we will focus on methods which deviate from the model-free approach of not making any assumption on the underlying distribution.

9.1 The principle of minimum description length

The classical SLT looks at learning very much from the point of view of underlying function classes. The basic idea is that good learning guarantees can be obtained if one uses simple function classes. The simplicity of a function space can be measured by one out of many capacity measures such as covering numbers, VC dimension, Rademacher complexity, and so on.

The minimum description length (MDL) approach is based on a different notion of "simplicity". The concept of simplicity used in MDL is closely related to the literal meaning of simple: an object is called "simple" if it can be described by a "short description", that is if one only needs a small number of bits to describe the object. In the context of MDL, objects can be a sequence of data, or a function, or a class of functions. As an example, consider the following function: "The function $f : [0, 1] \rightarrow \{-1, +1\}$ takes the value -1 on the interval $[0, 0.3]$ and +1 on $]0.3, 1]$." For a function of the class $f : [0, 1] \rightarrow \{-1, +1\}$, this is a rather compact description. On the other hand, consider a function $g : [0, 1] \rightarrow \{-1, +1\}$ which takes the values +1 and -1 at random positions on $[0, 1]$. In order to describe this functions, the best we can do is to compile a table with input and output values:

X	0.01	0.02	0.03	0.04	...
g(X)	1	-1	-1	1	...

It is obvious that compared to the code for f , the code for g will be extremely long (even if we ignore the issue that a function on $[0, 1]$ cannot simply be described in a table with countably many entries).

The question is now how we can formulate such a concept of simplicity in mathematical terms. A good candidate in this respect is the theory of data coding and data compression. A naive way to encode a function (on a finite domain) is to simply provide a table of input and output values. This can be done with any function, and is considered to be our baseline code. Now, given a function f , we try to encode it more efficiently. In order to be able to do this, we need to discover certain "regularities" in the function values. Such a regularity might be that 100 consecutive entries in the function table have the same value $g(X)$, say +1. Then, instead of writing +1 in 100 entries

of the table, we can say something like: “the following 100 entries have value +1”. This is much shorter than the naive approach.

The MDL framework tries to make use of such insights for learning purposes. The general intuition is that learning can be interpreted as finding regularities in the data. If we have to choose between two functions f and g which have a similar training error, then we should always prefer the function which can be described by a shorter code. This is an explicit way to follow Occam’s razor, which in machine learning is usually interpreted as “models should not be more complex than is necessary to explain the data”.

Omitting all technical details, we would just like to point out one possible way to turn the MDL idea in a concrete algorithm for learning. Assume we are given a function space \mathcal{F} , and some training points. One can now try to pick the function $f \in \mathcal{F}$ which minimizes the following expression:

$$L(f) + L(\text{Training Data} \mid f)$$

Let us explain those two terms. $L(f)$ stands for the length of the code to encode the function f in the given function class \mathcal{F} . This is some absolute length which is only influenced by the function itself, and not by the data at hand. We do not go into details how such a code can be obtained, but the general idea is as described above: the shorter the code, the simpler the function. One has to note that in constructing this code, the function space \mathcal{F} might also play a role. For example, one could just encode f by saying “take the 23rd function in space \mathcal{F} ”. In this code, the length $L(f)$ would just depend on the ordering of the functions in \mathcal{F} . If the function we are looking for occurs early in this ordering, it has a short code (“function 23”), but if the function occurs late in this ordering, it has a longer code (“function 4341134”).

The term $L(\text{Training Data} \mid f)$ denotes the length of the code to express the given training data with help of function f . The idea here is simple: if f fits the training data well, it is trivial to describe the training data. We can simply use the function f to compute all the labels of the training points. In this case, the length of the code is very short: it just contains the instruction “apply f to the input to obtain the correct output”. On the other hand, if the function f does not fit the data so well, it will make some misclassifications on the training points. To recover the label of the misclassified training points, we thus need to add some further information to the code. If, say, training points X_2 , X_7 , and X_{14} are misclassified by f , the code for the data might now look as follows: “apply f to all input points to compute the labels. Then flip the labels of training points X_2 , X_7 , and X_{14} ”. It is clear that the more errors f makes on the given training points, the longer this code will get.

Intuitively, the two terms $L(f)$ and $L(\text{Training Data} \mid f)$ play similar roles as some of the quantities in classical SLT. The term $L(\text{Training Data} \mid f)$ corresponds to the training error the function f makes on the data. The term $L(f)$ measures the complexity of the function f . In this sense, the sum of both looks familiar: we sum the training error and some complexity term. One difference to the classical SLT approach is that the complexity term is not only computed based on the underlying function class \mathcal{F} , but can depend on the individual function f .

The approach outline above has often been criticized to be rather arbitrary: a function that has a short description (small $L(f)$) under one encoding method may have a long description (large $L(f)$) under another. How should we decide what description method to use? There are various answers to this questions. The most common one is the idea of *universal coding*. Here codes are associated with classes of models rather than individual classifiers. There exist several ways to build universal codes. One of them is as follows. We decompose the function class \mathcal{F} into subsets $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \dots$. Then we encode the elements of each subset with a fixed-length code which assigns each member of \mathcal{F}_i the same code length. For example, if \mathcal{F}_i is finite and has N elements, one may encode each member $f \in \mathcal{F}_i$ using $\log N$ bits. Or, if the function class \mathcal{F}_i is infinite one can go over to concepts like the VC dimension to encode the functions in the class. As in the finite case, each element $f \in \mathcal{F}_i$ will be encoded with the same length, and this length turns out to be related to the VC dimension of \mathcal{F}_i . Many other ways might be possible. In general, we define the “coding complexity of \mathcal{F}_i ” as the smallest uniform code length one can achieve for encoding the functions

$f \in \mathcal{F}_i$. It is uniquely defined and is “universal” in the sense that it does not rely on any particular coding scheme.

Given a function $f \in \mathcal{F}_i$, we can now go ahead and encode our data in several steps: we first encode the index i of the function class, then use the uniform code described above to encode which element of \mathcal{F}_i the function f is, and finally code the data with the help of f . The code length then becomes

$$L(i) + L(f \mid f \in \mathcal{F}_i) + L(\text{Training Data} \mid f).$$

Note that for the first term $L(i)$ one usually chooses some uniform code for the integers, which is possible as long as we are dealing with finitely many function classes \mathcal{F}_i . Then this term is constant and does not play any role any more. The middle term $L(f \mid f \in \mathcal{F}_i)$ is identical for all $f \in \mathcal{F}_i$. Hence, it does not distinguish between different functions within the class \mathcal{F}_i , but only between functions which come from different classes \mathcal{F}_i . Finally, the last term explains how well the given function f can explain the given training data. The goal of this approach is now to choose the hypothesis f which minimizes this code.

In this formulation one can see that the MDL approach is not that far from standard statistical learning theory approaches. For example, if we are just given one fixed function class \mathcal{F} (and do not split it further into smaller sets \mathcal{F}_i), the code length essentially depends on some complexity measure of \mathcal{F} plus a term explaining how well f fits the given data. In this setting, one can prove learning bounds which show that MDL learns about as fast as the classical methods. One can also see that the approach can be closely related to classical statistical learning approaches based on compression coefficients (Vapnik, 1995). Moreover, in more advanced MDL approaches one may want to assign different code lengths to different elements of \mathcal{F} . This approach is then closely related to the PAC-Bayesian approach (cf. Section 6.2). Finally, it is worth mentioning is that under certain assumptions, MDL can be performed in a consistent way. That is, in the limit of infinitely many data points, the approach can find the correct model for the data.

Of course there are many details to take care of in the MDL approach, but this goes beyond the scope of the current paper. We refer to the monographs Grünwald (2007) and Rissanen (2007) for a comprehensive treatment of the MDL approach and related concepts.

9.2 Bayesian methods

The two traditional schools in statistics are the frequentist and the Bayesian one. Here we would like to briefly recall their approaches to inference and discuss their applications to machine learning. Before we do this, let us introduce the basic setting and some notation. Traditionally, statistical inference is performed in a model-based framework. As opposed to the agnostic approach taken in SLT, we assume that the underlying probability distribution comes from some particular class of probability distributions \mathcal{P} . This class is usually indexed by one (or several) parameters, that is it has the form $\mathcal{P} = \{P_\alpha \mid \alpha \in A\}$. Here, A is a set of parameter values, and P_α a distribution. For example, one could consider the class of normal distributions, indexed by their means and variances.

The standard frequentist approach to statistics. Here, the main goal is to infer, from some given sample of points, the correct parameters of the underlying distribution. Once the parameter is known, it is easy to perform tasks such as classification (for example by using the Bayes classifier corresponding to the estimated distribution). The most important quantity used in the frequentist approach to statistics is the *likelihood of the parameter* α , denoted by $P(\text{data} \mid \alpha)$. This term tells us the probability that, under the assumption that α is the correct parameter of the distribution, the given sample is generated. It is used as an indicator of how good the parameter α “fits” the data: if it is unlikely that the data occurs based on the underlying distribution P_{α_1} , but more likely for P_{α_2} , then one would tend to prefer parameter α_2 over α_1 . This already hints the way parameters are inferred from the data in the frequentist setting: the maximum likelihood (ML)

approach. Here we choose the “best” parameter $\hat{\alpha}$ by maximizing the data likelihood, that is

$$\hat{\alpha}(data) = \operatorname{argmax}_{\alpha \in A} P(data \mid \alpha),$$

where we have used the notation $\hat{\alpha}(data)$ to indicate that $\hat{\alpha}$ depends on the data. It is important to note that the likelihood *does not* make any statement about the “probability that a parameter α is correct”. All inference about α happens indirectly, by estimating the probability of the data given a parameter. The same is also true if we want to make confidence statements. It is impossible to make a statement like “the probability that α is correct is larger than something”. First of all, it is a mathematical problem that we cannot make such a statement: we simply do not have a probability distribution over parameters. If we want to make confidence statements in the traditional approach, this has to be done in a somewhat peculiar way. A confidence statement looks as follows: let $I(data) \in A$ be some interval (or more generally, subset) of parameters which has been constructed from the data. For example, I could be a symmetric interval of a certain width around an estimated parameter value $\hat{\alpha}(data)$, say $I = [\hat{\alpha}(data) - c, \hat{\alpha}(data) + c]$ for some constant c . The set I is called a 95% confidence interval if $P_{\alpha}(\alpha \in I) \geq 95\%$, which is a shorthand for

$$P_{\alpha}(data \mid \alpha \in [\hat{\alpha}(data) - c, \hat{\alpha}(data) + c]) \geq 95\%.$$

Again, it is important to point out that the random quantity in this statement is I , not α . The statement only says that if α happened to be the true parameter, and I is the confidence set we come up with when looking at the data, then in 95% of all samples the true parameter α will lie in I . It does not say that with 95% probability, α is the correct parameter!

This is one of the reasons why the frequentist approach is sometimes perceived as unsatisfactory. It only provides a rather indirect way to perform inference, and confidence statements are hard to grasp.

The Bayesian approach to statistics. The Bayesian framework is an elegant way to circumvent some of the problems of the frequentist one, in particular the indirect mechanism of inference provided by the ML framework. From a technical point of view, the main difference between the Bayesian and the frequentist approach is that the Bayesian approach introduces some “prior” distribution on the parameter space. That is, we define some distribution $P(\alpha)$ which for each parameter α encodes how likely we find it that this is a good parameter to describe our problem. The important point is that this prior distribution is defined *before* we get to see the data points from which we would like to learn. It should just encode our past experiences or any other kind of prior knowledge we might have. Now assume we are given some data points. As in the frequentist approach, one can compute the likelihood term $P(data \mid \alpha)$. Combining it with the prior distribution $P(\alpha)$, we can compute the so-called posterior distribution $P(\alpha \mid data)$. Up to a normalizing constant independent of α , the posterior is given by the product of the prior and the likelihood term, that is

$$P(\alpha \mid data) \propto P(\alpha)P(data \mid \alpha). \tag{20}$$

One can say that the posterior distribution arises by “updating” the prior belief using the data we actually have at hand. As opposed to the frequentist approach, this posterior is now indeed interpreted as the probability that α is the correct parameter, given that we have observed the data, and the prior distribution is “correct”.

Given the posterior distribution, there are two main principles to do inference based on it. The first one is to use the maximum a posteriori (MAP) estimator:

$$\hat{\alpha} = \operatorname{argmax}_{\alpha \in A} P(\alpha \mid data) \tag{21}$$

Here we come up with one fixed value of α , and can now use it to do the inference we are interested in, in a similar way as we can use the ML estimator in the frequentist approach. The second, fully

Bayesian way, is to do the inference based on *any* parameter α , but then weight the result by the posterior probability that α is correct.

What are advantages and disadvantages of the Bayesian approach? One advantage is the fact that the Bayesian approach leads to simple, intuitive statements about the results of a learning algorithm. As opposed to making complicated confidence statements like the ones in the standard SLT approach or the traditional frequentist approach to statistics, in the end one has statements like “with probability 95% we selected the correct parameter α ”. This comes at a price, though. The most vehement objection to the Bayesian approach is often the introduction of the prior itself. The prior does influence our results, and by selecting different priors one can obtain very different results on the same data set. It is sometimes stated that the influence of the prior is benign and in the limit, the prior is “washed out” by the data, as indicated by certain consistency results for the Bayesian approach (Berger, 1985). However, this argument is somewhat misleading. On a finite data set, the whole point of the prior is that it should bias our inference towards solutions that we consider more likely. So it is maybe appropriate to say that the Bayesian approach is a convenient method for *updating* our beliefs about solutions which we had before taking into account the data. Among Bayesian practitioners it is generally accepted that even though priors are “wrong”, most of the time they are quite useful in that Bayesian averaging over parameters leads to good generalization behavior. One point in favor of working with prior distributions is that they are a nice tool to invoke assumptions on the underlying problem in a rather explicit way. In practice, whether or not we should apply Bayesian methods thus depends on whether we are able to encode our prior knowledge in the form of a distribution over solutions.

On the other hand, SLT is arguably more explicit about model complexity, an issue which in Bayesian framework is a little harder to spot. As an example for how model complexity is dealt with in the Bayesian framework, consider the posterior distribution (20) and the MAP problem (21). We rewrite this problem by taking the negative logarithm, in which case the product becomes a sum and the maximization problem becomes a minimization problem:

$$\operatorname{argmin}_{\alpha \in A} (-\log P(\alpha) - \log P(\text{data} \mid \alpha)).$$

(Note that we are a bit sloppy here: applying the logarithm can be interpreted as a re-parameterization of the problem. One can show that MAP solutions are not invariant under such re-parameterizations.) Now we are given a sum of two terms which have an interpretation similar to the approaches we have seen so far. One could say that the second term $\log P(\text{data} \mid \alpha)$ describes the model fit to the data, that is it plays a similar role as the training error R_{emp} in the standard SLT approach, or the quantity $L(\text{data} \mid f)$ in the minimum description length framework. Continuing with this analogy, the other term $P(\alpha)$ would then be the term corresponding to the “complexity” of f . But how is the prior probability related to complexity? The general idea is as follows. It is a simple fact from coding theory that there exist much fewer “simple” models than “complicated” models. For example, a “simple” model class described by one parameter $\alpha \in \{1, 2, 3, \dots, 100\}$ contains 100 models, whereas a slightly less simple model class using two such parameters already contains $100^2 = 10000$ models. That is, the number of models increases dramatically with the complexity of the model class. Now assume we want to assign a prior distribution to the parameters. For finite model classes as above, a prior distribution simply assigns a certain probability value to each of the models in the class, and those probability values have to sum to 1. In case of the first model mentioned above, we need to assign 100 numbers to the parameters α . If we do the same for the second model, we have 10000 probabilities to assign. Now note that in order to make them sum to 1, the individual prior values per parameter tends to be much smaller in the second case than in the first case, simply because the second case requires many more parameters than the first one. On a higher level, the consequence is that prior probabilities assigned to elements of “complex” model classes tend to be much lower than prior probabilities for elements of “simple” model classes. Hence, the negative logarithm of the priors of complex function classes is high, whereas the same quantity for simple model classes is low. All in all, as in the standard SLT approach, the Bayesian framework implicitly deals with overfitting by looking at the trade-off between data fit and model complexity.

The literature on general Bayesian statistics is huge. A classic is Cox (1961), which introduces the fundamental axioms that allow to express beliefs using probability calculus. Jaynes (2003) puts those axioms to work and addresses many practical and philosophical concerns. Another general treatment of Bayesian statistics can be found in O’Hagan (1994). A gentle introduction into Bayesian methods for machine learning can be found in Tipping (2003), a complete monograph on machine learning with a strong focus on Bayesian methods is Bishop (2006).

10 The VC dimension, Popper’s dimension, and the number of parameters

We have seen that for statistical learning theory, it is crucial that one controls the capacity of the class of hypotheses from which one chooses the solution of a learning process. The best known measure of capacity is a combinatorial quantity termed the VC dimension. Corfield et al. (2005) have pointed out that the VC dimension is related to Popper’s notion of the dimension of a theory. Popper’s dimension of a theory is defined as follows (for a discussion of the terms involved, we refer to Popper (1959), Corfield et al. (2005)):

If there exists, for a theory t , a field of singular (but not necessarily basic) statements such that, for some number d , the theory cannot be falsified by any d -tuple of the field, although it can be falsified by certain $(d + 1)$ -tuples, then we call d the characteristic number of the theory with respect to that field. All statements of the field whose degree of composition is less than d , or equal to d , are then compatible with the theory, and permitted by it, irrespective of their content. (Popper, 1959, p. 130)

Corfield et al. (2005) argue that although this definition sounds similar to the VC dimension, there is a crucial difference which could either be attributed to an error on Popper’s side, or to a difference between statistical learning and “active” learning: in Popper’s definition, it is enough to find one $(d + 1)$ -tuple that falsifies a theory. E.g, the “theory” that two classes of data can be separated by a hyperplane could be falsified by three collinear points labeled “+1”, “−1”, and “+1”. In the definition of the VC dimension, on the other hand, it is required that there exists no $(d + 1)$ -tuple of points which can be shattered, i.e., for any $(d + 1)$ -tuple of points, there exists some labeling such that it falsifies the hyperplane, say. The VC dimension of separating hyperplanes in \mathbb{R}^n is $n + 1$, while the Popper dimension of separating hyperplanes is always 2, independent of n . Whilst one could fix this by adding some noise to the points in the Popper dimension, thus ruling out the existence of non-generic configurations, it may be more interesting to relate the difference between the two definitions to the fact that for Popper, the scientist trying to perform induction is actively looking for points, or experiments, that might be able to falsify the current hypothesis, while Vapnik and Chervonenkis devised their capacity measure to characterize the generalization error of a learning procedure where the incoming measurement points are generated randomly according to a certain probability distribution.

Interestingly, Popper also discusses the link between his capacity measure and the number of a parameters in an algebraic characterization of a hypothesis class (Corfield et al., 2005), stating that “[...] the number of freely determinable parameters of a set of curves by which a theory is represented is characteristic for the degree of falsifiability [...]” (cited after Corfield et al. (2005)). From the point of view of statistical learning theory, Popper here falls into the same trap hole as classical statistics sometimes does. In learning theory, it is not the number of parameters but the capacity which determines the generalization ability. Whilst the number of parameters sometimes coincides with, e.g., the VC dimension (the above mentioned hyperplanes being an example), there are also important cases where this is not true. For instance, it has been pointed out that the class of thresholded sine waves on \mathbb{R} , parameterized by a single real frequency parameter, has infinite VC dimension (Vapnik, 1995).

We conclude with Corfield et al. (2005) that Popper has at an astonishingly early point in time identified some of the crucial aspects of what constitutes the capacity of a class of hypothesis. If he had had the full developments of statistical learning theory at his disposal, he might have been able to utilize them to address certain other shortcomings of his approach, in particular by

using bounds of statistical learning theory to make statements about certain notions of reliability or generalization ability of theories.

11 Conclusion

At first glance, methods for machine learning are impressive in that they automatically extract certain types of “knowledge” from empirical data. The above description, however, has shown that in fact, none of this knowledge is created from scratch.

In the Bayesian view of machine learning, the data only serves to update one’s prior — we start with a probability distribution over hypothesis, and end of up with a somewhat different distribution that reflects what we have seen in between. For a subjective Bayesian, learning is thus nothing but an update of one’s beliefs which is consistent with the rules of probability theory. Statements regarding how well the inferred solution works are generally not made, nor are they necessary — for an orthodox Bayesian.

In the framework of statistical learning theory, on the other hand, we start with a class of hypotheses, and use the empirical data to select one hypothesis from the class. One can show that if the data generating mechanism is benign, then we can assert that the difference between the training error and test error of a hypothesis from the class is small. “Benign” here can take different guises; typically it refers to the fact that there is a stationary probability law that independently generates all individual observations, however other assumptions (e.g., on properties of the law) can also be incorporated. The class of hypothesis plays a role analogous to the prior, however, it does not need to reflect one’s beliefs. Rather, the statements that we obtain are conditional on that class in the sense that if the class is bad (in the sense that the “true” function cannot be approximated within the class, or in the sense that there is no “true” function, e.g., the data is completely random) then the result of our learning procedure will be unsatisfactory in that the upper bounds on the test error will be too large. Typically, either the training error will be too large, or the confidence term, depending on the capacity of the function class, will be too large. It is appealing, however, that statistical learning theory generally avoids metaphysical statements about aspects of the “true” underlying dependency, and thus is precise by referring to the difference between training and test error.

While the above are the two main theoretical schools of machine learning, there are other variants some of which we have briefly mentioned in this article. Importantly, none of them get away without making assumptions, and learning is never a process that starts from a tabula rasa and automatically generates knowledge.

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