

Mathematics for Machine Learning

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1. INTRODUCTION

We discuss motivations for studying the mathematics behind machine learning, give an outline of the content of the course, and mention the references which were used in putting it together.

Machine learning is a term which is commonly heard and spoken, and one less commonly understood. This is in part due to the rapid growth in experimental machine learning techniques, and the lagging in mathematical explanations of these techniques. Another prominent reason is that the mathematical understanding of machine learning can, in enterprise settings, be considered as ‘less useful’ or ‘less relevant’. Some people may also perceive the inner workings of machine learning to be a ‘black box’, and a subject which they couldn’t understand.

We will focus on tackling the final obstruction. The perception of the value of understanding finds itself in the hands of others, but the understanding in question is firmly in our own. There are only a few mathematical concepts needed to gain a working understanding of machine learning, and we will cover these as they are needed.

We hope to present a self-contained course, covering the key topics in detail, gradually working towards popular models and algorithms which are seen in real-world machine learning applications. We will place a heavy focus on examples, ones which are hopefully relevant and familiar to the reader, rooting the work we are completing in the context of its application.

For those interested in reading more than we have time to cover, we recommend the work of Schwartz et al.[3], Bishop[1], and Faisal et al.[2], all of which were to a lesser or greater extent consulted in the writing of this course.

1.1 WHAT IS LEARNING?

Sometimes, it is those concepts of which we have an intuitive idea which are hardest to rigorously define. What does it mean to learn? What does it mean to have learned? What does it mean to understand? These are all relevant questions in the theory of machine learning, especially the first, and we will first consider them in the context of human learning.

In the loosest sense, *learning* is the process of converting past experiences into applicable knowledge. For humans, the input to this learning can come in any number of formats. For example, we could consider the knowledge obtained from reading a book. What exactly is the process occurring in the mind of the reader which allows them to retain, and importantly, re-apply this information. We note that the process is decidedly not memorisation. As a child who has memorised their times tables cannot claim the ability of multiplication, the reader who cannot call upon knowledge in unseen circumstances cannot claim to fully understand what they have read. This gives a good hint as to an important facet of learning systems; *generalisation*.

For machines, the process is not dissimilar. The input for a learning algorithm is data, and the output (the expertise) are some tuned parameters which allow the model produce outputs from unseen data in the future. There is more nuance to this, but as we move towards mathematical rigour, it will be useful to keep this in mind.

1.2 STRUCTURE OF THE COURSE

As previously mentioned, there are only few mathematical concepts which are absolutely necessary for understanding machine learning. An overview of the structure of this course is as follows,

- Linear Algebra

- Multivariable calculus
- Probability
- Optimisation
- Linear regression
- Logistic regression

Those familiar with the above topics may note that this course is structured in a ‘bottom-up’ fashion – we build on the theory as we move forwards. This is somewhat in contrast to other machine learning courses which take a ‘top-down’ approach in which the theory behind the application is uncovered as it is encountered. Both of these strategies have their strengths, and courses which are mathematically inclined typically take the same approach as us. It is however necessary to have patience with this approach. If you have previously only encountered machine learning in a practical, hands-on setting, you may struggle to understand how the early chapters of this course fit into the wider picture, but eventually all will be clear.

2. LINEAR ALGEBRA

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3. MULTIVARIABLE CALCULUS

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3.1 INTRODUCTION

4. PROBABILITY

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5. LEARNING PROBLEMS

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We now aim to combine the concepts which we have thus far encountered, and construct a formal definition for a learning problem. We will begin by defining the necessary inputs, and the desired outputs, before working towards the fundamental definition of PAC learnability, which will allow us to have some notion of the possibility of learning a certain problem.

5.1 INTRODUCTION

We begin the chapter by laying out an example which we will reference and build around throughout. Suppose that you are a loaner, aiming to determine if an arbitrary loanee will or will not default on the loan you give them. We phrase the problem deliberately in this manner, to emphasize the simplistic scenario in which we are working – the value of the loan is predetermined, and the goal is to provide a binary classification of loanees.

What information will be useful in this task? How will we determine if our solution is adequate? How will we provide a useful notation to describe the problem?

5.2 A FORMAL LEARNING MODEL (BASIC)

5.2.1 LEARNING INPUT

The learner of a statistical learning problem has access to the following,

- Domain set: an arbitrary set which we typically label by \mathcal{X} . This set is nothing more than the objects to which we aim to assign labels. In the example outlined in the previous section, this set \mathcal{X} is the set of potential loanees.
- Label set: A set which we typically label by \mathcal{Y} . This is the set of possible labels, e.g., {default, no default}. Of course, it is more common to denote the possible labels simply by integers, and in our binary classification example, we will take $\mathcal{Y} = \{\pm 1\}$.
- Training data: a finite sequence of pairs $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, i.e., a sequence of labelled objects. In our case, this will be a sequence of past loaners together with information relating to their repayment. We will tend to denote the training data by $\mathcal{S} = ((x_1, y_1), \dots, (x_m, y_m))$, where m is the size of the training data.

REMARK. It is important to note that the training data is described as a sequence rather than a set. This is a rather nuanced point, and not one which we will dedicate much thought to. The reason for such pedanticity is that there exist learning algorithms which are dependent on the order of the training points, and there is no necessity for \mathcal{S} to be duplicate free.

It is however still common to refer to \mathcal{S} as the training set.

5.2.2 LEARNING OUTPUT

- Prediction rule: the only output from a statistical learning problem is a function $h : \mathcal{X} \rightarrow \mathcal{Y}$. We also refer to the function as a hypothesis, and is a rule which the learner can use to label new elements of the domain space.

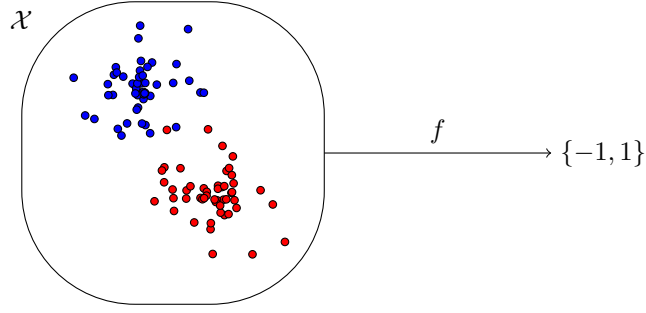


Figure 5.1: The training set \mathcal{S} is the collection of points in \mathcal{X} for which we have labels. The function f is the true labelling function.

If we are considering an algorithm \mathcal{A} , then we will denote by $\mathcal{A}(\mathcal{S})$ or $h_{\mathcal{S}}$ the output hypothesis of the algorithm.

5.2.3 A DATA GENERATING MODEL

It is important to consider how exactly the training data is generated, as this is integral to how we consider the learning to occur. We assume that there is some probability distribution \mathcal{D} over \mathcal{X} which, importantly, the learner does not know about. For the time being, we also make the assumption that there is some ‘correct’ labelling function $f : \mathcal{X} \rightarrow \mathcal{Y} : x_i \mapsto y_i$, which maps the object x_i to its correct label in every case. Explicitly,

$$f(x_i) = y_i \quad \forall i.$$

In every learning scenario, it is exactly this function f which the learner aims to obtain. In our example, we can suppose that we have past data, \mathcal{S} which provides a source of truth in the way that each of the training examples is an individual of whom we *know* the loaning outcome.

5.2.4 MEASURE OF SUCCESS

The final element of our formal learning model is the means to quantify the success of our learning, or more strictly our hypothesis, h . In our classification problem, the error of the hypothesis h is defined to be the probability that for a given data point $x \in \mathcal{X}$, the predicted classification is not the same as the ‘correct’ classification. Notatively,

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

REMARK. The notation of $L_{\mathcal{D},f}$ is well chosen since it makes clear the dependence of the error of the classifier on the underlying distribution \mathcal{D} and correct classification function f , although if the context is clear we will omit this for brevity.

It is also common to refer to the probability $L_{\mathcal{D},f}(h)$ as the ‘risk’, and we will often refer to it as such.

5.3 EMPIRICAL RISK MINIMISATION (INTERMEDIATE)

We now have a good idea about the inputs, outputs and measures of success of a formal learning problem. The natural next step is to explore the strategy by which we can solve such problems.

It maybe initially seems obvious that we would like to minimise the risk, explicitly reducing the probability of incorrect classification, implicitly bringing our hypothesis output h closer to the true

classifier f . Although this is the right idea, the learner is limited by their knowledge of the problem. In particular, the learner knows nothing of the distribution \mathcal{D} , nothing of the true classifier f , and hence nothing of the risk $L_{\mathcal{D},f}$. As a result, we must construct a different quantity which we would like to minimise.

DEFINITION 5.1 (Empirical risk). Given a training sequence $\mathcal{S} = ((x_1, y_1), \dots, (x_m, y_m))$, the *empirical risk* with respect to \mathcal{S} is defined and denoted by,

$$L_{\mathcal{S}}(h) := \frac{|\{i \in \{1, \dots, m\} : h(x_i) \neq y_i\}|}{m}$$

This definition is basic in spite of its verbosity. The numerator is expressing the process of counting misclassifications on the training set, and we are dividing by the size of the training set to ensure that $L_{\mathcal{S}}$ is bounded between 0 and 1.

The empirical risk is a good quantity to consider in learning problems since it is related to the training data available to us, i.e., “the snapshot of the world available to the learner”[3]. So, our strategy of learning comes down to minimising the empirical risk – finding a hypothesis h , which agrees well with f on the training set. Learning by this strategy is called *empirical risk minimisation*, referred to by ERM.

5.3.1 OVERFITTING

We now explore a pitfall into which many learning algorithms fall, and one which we will illustrate using the framework so far developed in this chapter, working again with the example of loaning.

EXAMPLE 5.2. In order to illustrate overfitting in the ERM paradigm, we suppose that the underlying distribution \mathcal{D} on loan applicants \mathcal{X} is uniform, that is, the correct classification of the feature space is half-half between default (1) and non-default (−1).

It may seem initially that the process of finding an ERM hypothesis is challenging, but this is not actually the case. We can find a scenario agnostic ERM hypothesis,

$$h_{\mathcal{S}}(x) = \begin{cases} y_i & \text{if } \exists i \in \{1, \dots, m\} \text{ s.t. } x_i = x \\ 1 & \text{otherwise} \end{cases}$$

What exactly is this hypothesis doing? If the selected data point $x \in \mathcal{X}$ can be found in the training set \mathcal{S} , then the hypothesis returns the label which is assigned to x in the training set. Otherwise, the hypothesis returns 1, i.e., predicts that the loanee will be good for their loan and won’t default. This hypothesis $h_{\mathcal{S}}$ is ERM since it agrees exactly with the labels provided in the dataset, and hence has $L_{\mathcal{S}}(h_{\mathcal{S}}) = 0$ – there is zero probability of the hypothesis incorrectly classifying an instance of the training set. However, if the hypothesis returns −1 on only a finite number of instances, then $L_{\mathcal{D},f}(h_{\mathcal{S}}) = 1/2$.

We have found a hypothesis which according to our strategy provides perfect learning, but in reality, performs very badly. That is, the hypothesis cannot generalise. It is ‘overfitted’ to the training set.

The previous example outlines a clear failure of the ERM paradigm, but we shouldn’t let this provide obstruction to its use in total; instead we will find ways to reprimand its issues.

5.4 LIMITING THE HYPOTHESIS SPACE

One way to address the problem of overfitting in ERM is to limit the possible hypotheses which we will output from learning. In particular, the learner should explicitly define a set of possible predictors.

We call this set the *hypothesis class*, and typically label it by \mathcal{H} , which contains hypotheses of the form we have seen previously; functions $h : \mathcal{X} \rightarrow \mathcal{Y}$.

In order to distinguish the ERM learning rule from the hypothesis restricted analogue, we use $\text{ERM}_{\mathcal{H}}$. Furthermore, we can understand the $\text{ERM}_{\mathcal{H}}$ learning rule as minimisation of the empirical risk over the set of hypotheses. That is,

$$\text{ERM}_{\mathcal{H}}(\mathcal{S}) \in \arg \min_{h \in \mathcal{H}} \{L_{\mathcal{S}}(h)\}.$$

NOTATION. For those who haven't seen it before, the notation $\arg \min_{x \in \mathbb{R}} \{f(x)\}$ denotes the value (or set of values) of x in the set \mathbb{R} which minimises the function f . So, in our case, we are looking for the hypothesis h in the hypothesis set \mathcal{H} which minimises the empirical risk function $L_{\mathcal{S}}$.

It is natural to ask how exactly a learner should go about limiting/defining a hypothesis set. The restriction to a certain set of hypotheses should be based on some prior knowledge of the problem, the process of choosing this hypothesis set is referred to as *inductive bias*. It should also be fully considered whether or not the restricted hypothesis set is a good one; will the restriction actually prevent overfitting of the learner? We will explore some examples in this direction later on.

EXAMPLE 5.3. A natural way to limit the potential hypotheses is to limit the size of the hypothesis set. That is, we may impose a finiteness condition on \mathcal{H} . We could let \mathcal{H} be the set of all predictors which can be implemented via python programs of at most 10^{32} characters. There are a number of other common examples.

REMARK. What is to say that this restriction solves the problem? There is a whole host of machinery needed in order to prove that this is the case, and for the sake of maintaining the introductory nature of this course, we decide to pass up on work in this direction. This is a very interesting topic, and those interested should read on *PAC learnability*.

5.5 GENERALISATION

There are many more types of learning problems which we would like to consider – not everything can be as simple as a binary classification problem after all. We will now list some other common learning problems, and how they apply to the framework which we have laid out.

5.5.1 MULTICLASS CLASSIFICATION

This is the most natural generalisation of the framework which we have explored. We are now thinking of $\mathcal{Y} = \{1, \dots, n\}$ where n is the number of classes which we may assign each $x \in \mathcal{X}$ to. There are some small changes we need to make to the rest of the framework, particularly for the risk functions.

PROBLEM 5.1. Consider the example of document classification. Describe each part of the learning framework in this case.

SOLUTION 5.1. • Domain set: the collection of documents which we aim to classify. To be exact, each $x \in \mathcal{X}$ is some multidimensional object which encodes the properties/features of the document which we would like to classify on. For example, x may contain information on the length of the document, key words, source of the document etc. Can you think of any other possible features?

• Label set: the possible labels which we will assign to the document. In this case, one possible

label set is,

$$\mathcal{Y} = \{\text{sport, news, science, finance}\}.$$

- Training data: this is the same as before.
- Learning output: this is the same as before.
- Measure of success: this is an interesting one. In some sense, it makes sense to consider the same risk function as before,

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

It shouldn't be automatically accepted as appropriate however. It is now possible that f and h disagree in *different* ways. In particular, it should be considered whether a misclassification of a finance document as a news document is *as* unsuccessful as the misclassification of a finance document as a sport document.

In order to construct an alternative risk function, we need some measure of the proximity of two different classifications, and although this is beyond the scope of this introductory course, it is an interesting thing to ponder on.

5.5.2 REGRESSION

5.6 EXERCISES

5.6.1 EXERCISES (BASIC)

PROBLEM 5.2. What are the elements of a statistical learning problem which the learner has access to?

SOLUTION 5.2. There are three elements of the problem which the learner has access to,

- Domain set
- Label set
- Training data

You could make an argument that the training data which is available to the learner is representative of the access which the learner has to the domain set \mathcal{X} . If the learner had full access to \mathcal{X} , learning by memorisation would be a successful method.

5.6.2 EXERCISES (INTERMEDIATE)

5.6.3 EXERCISES (CHALLENGING)

6. CONVEX LEARNING PROBLEMS

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Another common method of limiting the hypothesis space is by asserting it to be convex. We will explore learning problems in this area in the following chapter, encountering some challenging associated concepts.

6.1 CONVEXITY

DEFINITION 6.1 (Convex set). A set C is said to be *convex* if for every pair of points $a, b \in C$, the following inclusion holds,

$$\{\lambda a + (1 - \lambda)b : \lambda \in [0, 1]\} \subseteq C$$

There is a good geometric intuition for this definition. In particular, the set which must be included in C describes the straight line from a to b . So, a set C is convex if and only if it contains every straight line between any two points. See the figure below.

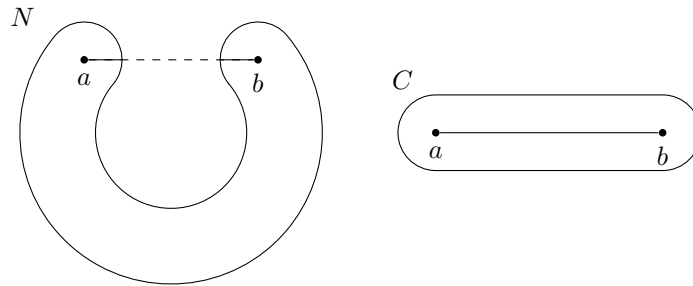


Figure 6.1: The set C is convex, but since we can find a line which is not contained in the set N , this set is not convex.

7. OPTIMISATION THEORY

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8. LINEAR REGRESSION

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9. LOGISTIC REGRESSION

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