

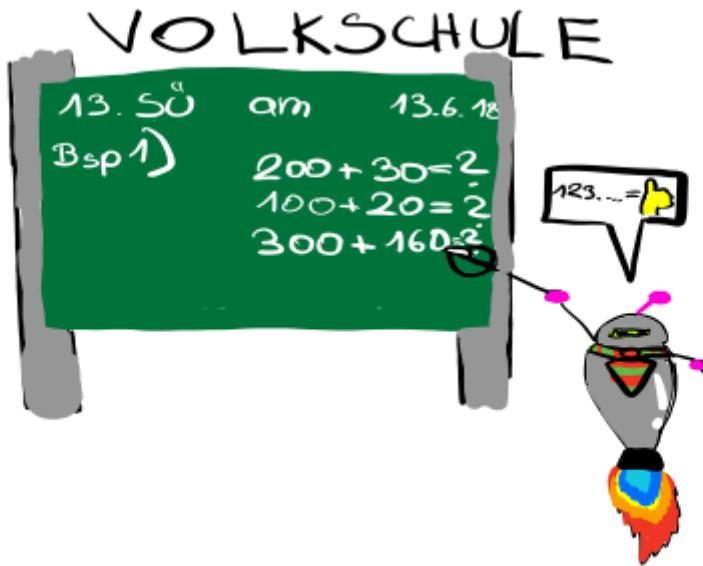
# Machine Learning: Basic Principles

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## Abstract

This tutorial is based on the lecture notes for, and the plentiful student feedback received from, the courses “Machine Learning: Basic Principles” and “Artificial Intelligence”, which I have co-taught since 2015 at Aalto University. The aim is to provide an accessible introduction to some of the main concepts and methods within machine learning. Many of the current systems which are considered as (artificially) intelligent are based on combinations of few basic machine learning methods. After formalizing the main building blocks of a machine learning problem, some popular algorithmic design patterns for machine learning methods are discussed in some detail. In order to improve accessibility of the main concepts, we mostly avoid the use of probabilistic (interpretations of) models.



“Machine Learning Class” by Helene Jung

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# 1 Introduction

This tutorial discusses some key techniques for building **artificial intelligent (AI)** systems which act **rational** in the sense of pursuing an **overarching (long-term) goal**.

AI Principle: Based on the perceived environment, compute **actions** (decisions) which allow to maximize a long-term **return**.

The actual implementation of this principle requires, of course, to have a precise definition of what is meant by “perceived environment”, “actions” and “return”. We highlight that those definitions are essentially a **design choice** which have to be made by an AI scientist or engineer which is facing a particular application domain. Let us consider some application domains where AI systems can be used:

- a **forest fire management system**: perceptions given by satellite images and local observations (using sensors or “crowd sensing”); actions amount to issuing warnings and bans of open fire; return is reduction of number of forest fires.
- an **emission reduction system** for combustion engines: perceptions given by various measurements (such as temperature, fuel consistency); actions amount to varying fuel feed and timing and the amount of recycled exhaust gas; return is measured in reduction of emissions.
- a **severe weather warning service**: perceptions given by weather radar; actions are preventive measures taken by farmers or power grid operators; return is measured by savings in damage costs (see <https://www.munichre.com/>)
- an automated **benefit application system** for a social insurance institute (like “Kela” in Finland): perceptions given by information about application and applicant; actions are either accept or reject the application; return is measured in reduction of processing time (applicants like to get decisions quickly)
- a **personal diet assistant**: perceived environment is the food preferences of the app user and their health condition; actions amount to personalized suggestions for healthy and yummy food; return is the increase in well-being (or the reduction in public spending for health-care).
- the **cleaning robot** Rumba (see Figure 1) perceives its environment using different sensors (distance sensors, on-board camera); actions amount to choosing different moving directions (“north”, “south”, “east”, “west”); return might be the amount of cleaned floor area within a particular time period.
- a **personal health assistant**: perceptions given by current health condition (blood values, weight,...), lifestyle (preferred food, exercise plan); actions amount to personalized suggestions for changing lifestyle habits (less meat, more jogging,...); return is measured via level of well-being (or the reduction in public spending for health-care).

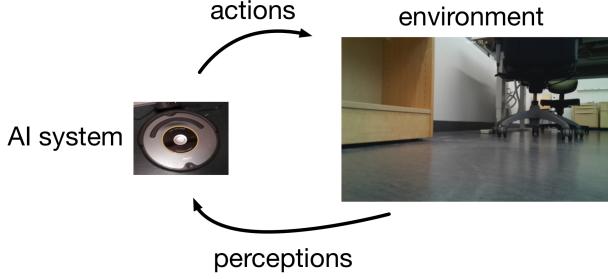


Figure 1: A cleaning robot should choose actions (corresponding to moving in different directions) in order to maximize the return measured in the amount of cleaned floor area per day.

- **government-system** for a community: perceived environment is constituted by current economic and demographic indicators (unemployment rate, budget deficit, age distribution, . . . ); actions involve the design of tax and employment laws, public investment in infrastructure, organisation of health-care system; return might be determined by the gross domestic product, the budget deficit or the gross national happiness (cf. [https://en.wikipedia.org/wiki/Gross\\_National\\_Happiness](https://en.wikipedia.org/wiki/Gross_National_Happiness)).

Finding optimal (or good) decisions typically requires first to get some insights. Consider the cleaning robot Rumba (see Figure 2) which has to find its way through a crowded office room in order to clean the floor. In order to choose good actions, which amount to the different directions to move next, Rumba has to find out its current location within the room using only low-level information such as raw sensor readings or simple features of snapshots obtained by an on-board camera. The task of determining **higher-level insights** (we refer to these insights as “labels” in what follows), such as your current location within the Aalto university main building, from **low-level perceptions** (we refer to these perceptions as “features” in what follows), such as measurements of distance sensors or snapshots generated by an on-board camera, is a key problem studied within the field of **machine learning (ML)**. Loosely speaking, **ML methods address low-level tasks** within an AI system. The predictions (or “inferences”) produced by ML methods can be used as the input to higher-level AI functions such as **logical reasoning**.

In order to apply ML methods, we first need to formalize a particular ML task by defining the relevant **features** of the raw data, the **labels** we are interested in and a **loss function** for measuring how good a particular ML method performs (see Section 2). Besides features, labels and loss function we also highlight the importance of restricting the class of potential predictor maps from features to labels. This restricted class of **computationally feasible** maps is referred to as the **hypothesis space** in what follows. As we will discuss in Section 3, many well-known ML methods are obtained as combinations of particular choices for feature and label space, loss function and hypothesis space.

In Section 4 we introduce and discuss the principle of **empirical risk minimization (ERM)** which amounts to choosing an optimal predictor based on minimizing the average loss (or empirical risk) incurred over **labeled training data**. A wide range of current ML methods can be interpreted as an instance of ERM. In Section 5 we elaborate on a main algorithmic workhorse of modern ML algorithms, i.e., **gradient descent (GD)** which is an iterative method for solving the ERM problem in order to find good predictors. We then discuss in Section 6 the basic idea of validating

an ML method by trying it out on labeled data (so called “validation data”) which is different from the training data used within ERM. As detailed in Section 7.1, a main reason for doing validation is to detect and avoid **overfitting** which causes poor performance of ML methods.

The main focus of this tutorial is on supervised learning methods which assign labels to each data point and require the availability of some data points for which the label is known. However, in some ML applications there is no reason for assigning labels and each data point is only characterized by its features. The resulting ML methods are then called **unsupervised ML methods**. In Section 8, we will study an important family of unsupervised ML methods which amount to **clustering** data points into coherent groups (clusters). In Section 9, we discuss another important unsupervised ML problem referred to as **feature learning**, which amounts to learning few relevant features for data points in a high-dimensional space.

**Prerequisites.** We assume some familiarity with basic concepts of linear algebra, real analysis and probability theory. For a quick review of those concepts, we recommend [1, Chapter 2-4].

**Notation.** We mainly follow the notational conventions used in [1]. In particular, boldface upper case letters (such as  $\mathbf{A}, \mathbf{X}, \dots$ ) denote matrices while boldface lower case letters (such as  $\mathbf{y}, \mathbf{x}, \dots$ ) denote vectors. The generalized identity matrix  $\mathbf{I}_{d \times r} \in \{0, 1\}^{d \times r}$  is a diagonal matrix with ones on the main diagonal. The norm of a vector  $\mathbf{x} = (x_1, \dots, x_d)^T$  is denoted  $\|\mathbf{x}\| = \sqrt{\sum_{r=1}^d x_r^2}$ . We denote the set constituted by the indexed elements  $\mathbf{z}^{(i)}$  as  $\{\mathbf{z}^{(i)}\}_{i=1}^N = \{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}\}$ . If  $\mathbf{z}^{(1)} = 4$  and  $\mathbf{z}^{(2)} = 1$ , then  $\{\mathbf{z}^{(i)}\}_{i=1}^2 = \{4, 1\}$ .

## 2 The Components of an ML Problem (and its Solution)

Consider the cleaning robot “Rumba” in Figure 2, which has to clean the office room B329. For simplicity, we model this office room as a plain rectangular area (see Figure 3) in what follows. We discretise the office floor using small squares or “cells”. A particular cell within room B329 is represented by the coordinate pair  $\langle m, y \rangle$  with coordinates  $m \in \{1, \dots, K\}$  and  $y \in \{1, \dots, L\}$ .



Figure 2: The cleaning robot “Rumba”.

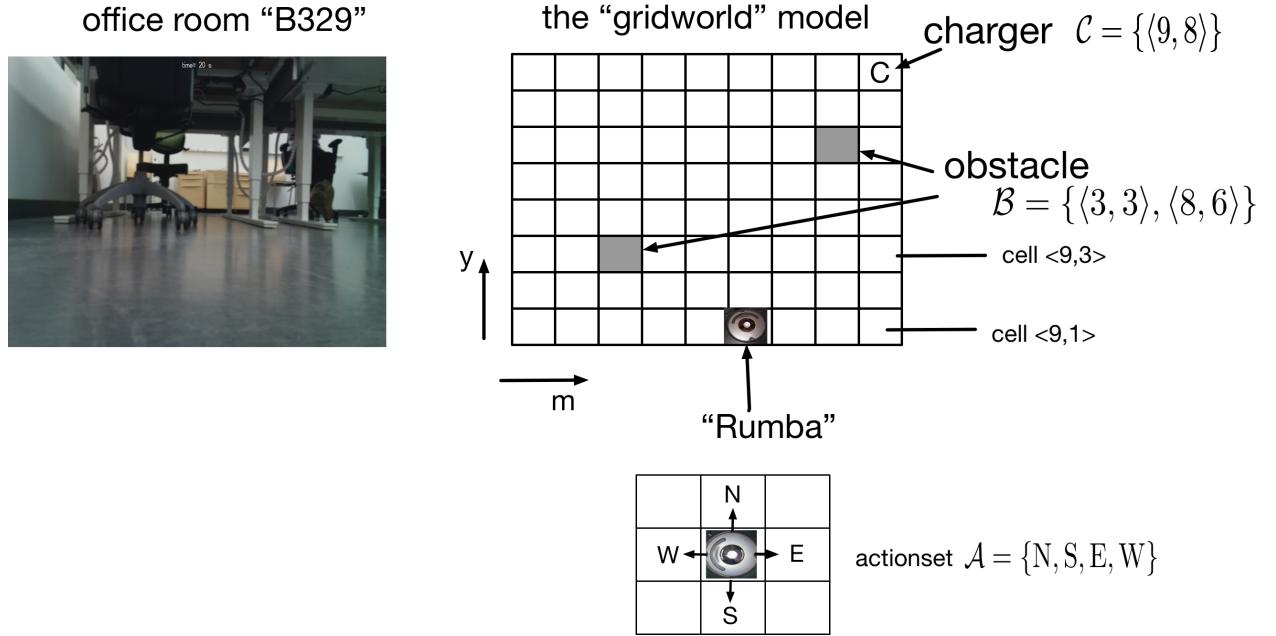


Figure 3: The office room, which Rumba has to keep tidy, and a simple gridworld model of the room’s floor space.

From time to time, Rumba has to visit a charging station in order to charge its battery. In order to reach a charging station, Rumba can choose from different actions each of which corresponding to a particular direction into which it can move next (see Figure 3). The optimal action at a particular time  $t$  depends on the current location  $\langle m_t, y_t \rangle$  of Rumba. However, it

turns out that determining the precise location within a typical office room is far from trivial (see <http://www.indooratlas.com/how-it-works/>). Therefore, let us now assume that Rumba has to predict (or infer) its location, i.e., the coordinates  $m_t$  and  $y_t$ , using solely the information contained in the snapshots generated by a simple on-board camera.

We will use this particular ML application to illustrate how to formally define an ML problem. This formal notion of an ML problem involves three main components (see Figure 4)

- the data with underlying **feature and label space**
- a **hypothesis space** which contains all feasible (given the available computational resources) maps (called “predictors” or “classifiers”) from feature to label space
- a **loss function** which is used to measure the quality of a particular predictor (or classifier).

Each of these components allows for different design choices and many ML methods are derived by using compositions of particular choices for these components (see Section 3).

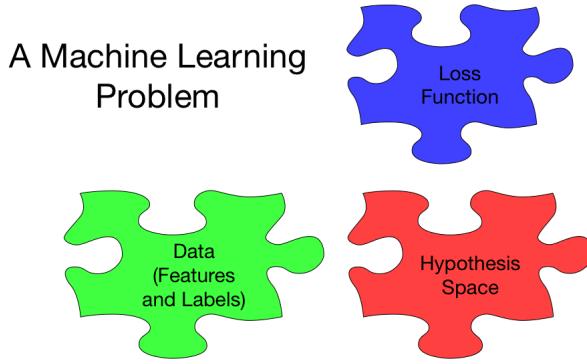


Figure 4: A formal ML problem consists of (i) a particular choice of features (space) and label (space) of data points, (ii) a hypothesis space which consists of the (computationally) feasible predictor maps from features to labels and (iii) a loss function which is used to assess the quality of a particular predictor.

## 2.1 The Data: Features and Labels

Consider a snapshot, denoted as  $\mathbf{z}^{(t)}$ , taken by Rumba’s on-board camera at time  $t$ . Let us assume that the on-board camera stores the snapshots as simple RGB bitmaps containing  $512 \times 512$  pixels. In principle we can feed with a RGB bitmap file directly into ML methods which then predict the coordinate  $y_t$  based on the image. However, it is often much more efficient not to feed an ML method directly with the raw data point (such as RGB bitmap files), but rather with a more compact set of characteristic properties of the data point  $\mathbf{z}^{(t)}$  which are called **features**. We denote them mostly as  $x$  (when it is a single number) or  $\mathbf{x}$  (when the features are several numbers). A possible choice of features for RGB bitmaps is the average greenness, blueness and redness obtained by summing over all pixels.

Besides its features, a data point can often be associated with a particular **label** (also referred to as “output” or “target”) denoted  $y$ . The label  $y$  of a data point is the particular information

we are eventually interested in, but which is more difficult to obtain compared to the features  $\mathbf{x}$  of the data point. In general, obtaining accurate label information requires manual (costly) expert labor. Acquiring labels might involve sending out a team of marine biologists to the Baltic sea [2], running a particle physics experiment at the European organization for nuclear research (CERN) [3], running animal testing in pharmacology [4], or manually determining the location of Rumba within the office room it has to clean (see Figure 6). Thus, in many application domains we do not have accurate label information for most of the data points but have to guess or predict the labels based on the features of a data point.

Interestingly, as observed in [5], some of the most successful ML methods have been devised in application domains where label information can be acquired easily. In particular, ML methods for speech recognition and machine translation can make use of massive labeled datasets collected throughout various channels (media, international institutions like European parliament).

If data is considered the oil of the 21st century, **labeled data** is the **premium fuel** while **unlabeled data** would correspond to **crude oil**.

### 2.1.1 Feature Space

In what follows, we represent the snapshot  $\mathbf{z}^{(i)}$  taken by Rumba’s on-board camera at time  $i$  using the feature vector

$$\mathbf{x}^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)})^T \in \mathbb{R}^d.$$

The feature vector  $\mathbf{x}^{(i)}$  contains  $d$  individual features  $x_1^{(i)}, \dots, x_d^{(i)}$ . In principle, we can use as a feature any quantity which can be determined (computed) directly from the data point  $\mathbf{z}^{(i)}$ . In particular, we could define a feature  $x_1^{(i)}$  using the red colour component of the pixel at location  $(10, 100)$  in the snapshot  $\mathbf{z}^{(i)}$ , while another feature  $x_2^{(i)}$  could be the number of pixels in the snapshot whose greenness is above a certain threshold. Alternatively, as depicted in Figure 5, we could use as features the red, green and blue components of each pixel in the snapshot.

The set of all possible values that the feature vector can take on is sometimes referred to as **feature space**, which we denote as  $\mathcal{X}$ . Many ML methods are based on using the Euclidean space  $\mathbb{R}^d$  as the features space. In contrast, it is also possible to use a finite set as the feature space. This can be useful for **network-structured datasets** where the data points can be compared with each other by some application-specific notion of similarity [6, 7, 8]. Here, the feature space is identified with the node set of an “empirical graph” whose nodes represent individual data points along with its similarities (encoded in the edges of the graph). In general, we can choose an arbitrary set as the feature space  $\mathcal{X}$ . In order to obtain efficient ML methods, we typically use a feature space  $\mathcal{X}$  which has some mathematical structure such as a notion of distance or an algebraic structure (such as addition and multiplication).

In what follows, we will focus on using the feature space  $\mathcal{X} = \mathbb{R}^d$  with some fixed dimension  $d$ . If we use the RGB intensities (modelled as real numbers for simplicity) of the pixels within a (rather small)  $512 \times 512$  bitmap, we end up with a feature space  $\mathcal{X} = \mathbb{R}^d$  of (rather large) dimension  $d = 3 \cdot 512^2$ . Indeed, for each of the  $512 \cdot 512$  pixels we obtain 3 numbers which encode the red, green and blue colour intensity of the respective pixel (see Figure 5).

Choosing “good” features (and feature space  $\mathcal{X}$ ) for the data points arising within a particular ML application is far from trivial and might be the most difficult task within the overall ML application. The family of ML methods known as **kernel methods** [9] is based on constructing

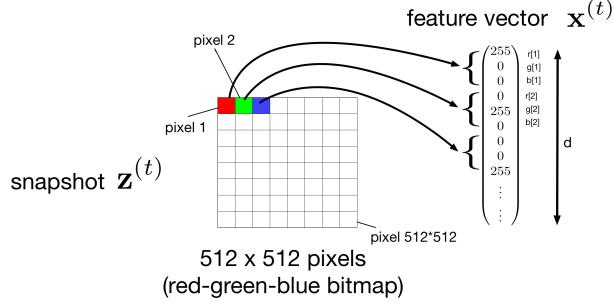


Figure 5: If the snapshot  $\mathbf{z}^{(i)}$  is stored as a  $512 \times 512$  RGB bitmap, we could use as features  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  the red-, green- and blue component of each pixel in the snapshot. The length of the feature vector would then be  $d = 3 \cdot 512 \cdot 512 \approx 786000$ .

efficient features by applying high-dimensional **feature maps**. A recent breakthrough achieved by modern ML methods, which are known as **deep learning methods** (see Section 3.9), is their ability to automatically learn good features without requiring too much manual engineering (“tuning”) [1]. We will discuss the very basic ideas behind such **feature learning** methods in Section 9 but for now assume the task of selecting good features already solved. In particular, we have access to a suitable feature vector  $\mathbf{x}^{(t)}$  which describes the snapshot  $\mathbf{z}^{(t)}$  taken by Rumba at time  $t$ .

### 2.1.2 Label Space

Our main focus for the rest of this paper is the design and analysis of ML methods which allow to predict the label  $y$ , e.g., the current location  $y_t$  of a cleaning robot (see Figure 6), or a data point based solely on its features  $\mathbf{x}$ , e.g., characterizing the current snapshot of an on-board camera (see Figure 6). The set of all possible values the label  $y$  can take is known as the **label space**, denoted as  $\mathcal{Y}$ , of an ML problem. For the indoor localisation problem for cleaning robots, the label space might be the finite set  $\{1, \dots, K\}$ . It is common to refer to ML problems involving a discrete (finite or countably infinite) label space as **classification problems**. Examples of classification problems are: detecting presence of a tumour in a tissue, classifying persons according to their age group or associating the on-board camera image of a mower robot to one of the categories “grass”, “tiles” or “soil”.

The definition (choice) of the labels corresponds to formulating the particular research question we want to have answered. Some questions (label choices) are more difficult to answer while others are easier to answer. We could model the label  $y_t$  also as a real number such that the label space is the set  $\mathbb{R}$  of real numbers. It is common to call ML problems (methods) involving a continuous label space (e.g.,  $\mathcal{Y} = \mathbb{R}$ ) **regression problems (methods)**.

In the end, both features and labels are just specific properties of individual data points which can be defined freely to some extent. However, the handling of these two types of quantities in practice is fundamentally different. While features are typically easy to compute or measure (such as the total greenness of a webcam snapshot), determining the correct label often requires much more effort including human expert labor.<sup>1</sup> Therefore, in many applications we have a lot of data

<sup>1</sup>There are marketplaces where you can offer or buy human labelling workforce. One such marketplace is <https://www.mturk.com>.

points whose features we can access easily but the labels are known for few data points only. In general, labeled data is a scarce resource. In the extreme case, we do not have any labels available. However, even in the absence of any labeled information ML methods can be useful for extracting relevant information out of the features only. These ML methods which do not require any label information are referred to as **unsupervised ML methods** (which will be discussed in Section 8 and Section 9).

As discussed next, many ML methods aim at constructing (or finding) a “good” predictor  $h : \mathcal{X} \rightarrow \mathcal{Y}$  which takes the features  $\mathbf{x} \in \mathcal{X}$  of a data point as its input and outputs a predicted label (or output, or target)  $\hat{y} = h(\mathbf{x}) \in \mathcal{Y}$ . A good predictor should be such that  $\hat{y} \approx y$ , i.e., the predicted label  $\hat{y}$  is close (with small error  $\hat{y} - y$ ) to the true underlying label  $y$ .

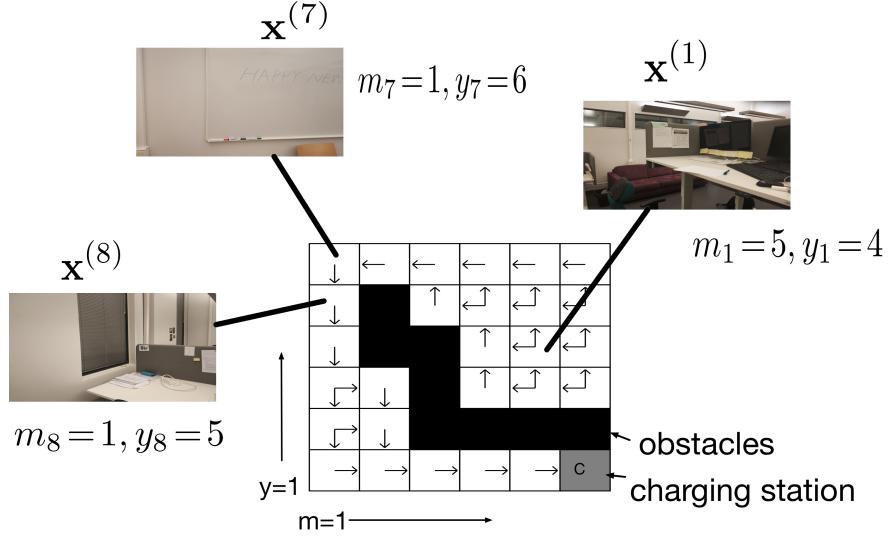


Figure 6: The cleaning robot Rumba is collecting snapshots  $\mathbf{z}^{(i)}$ , each of which is represented by the feature vector  $\mathbf{x}^{(i)}$  and labeled with the  $y$ -coordinate  $y^{(i)}$  of Rumba’s location at time  $i$ .

### 2.1.3 Example: Cryptocurrencies

Let us illustrate the concept of features and labels in the context of predicting cryptocurrency prices. In particular, we are interested in predicting the price of the cryptocurrency “Bitcoin” at a particular day based solely on the price of another cryptocurrency “Ethereum” on the same day. For solving this task, we have some historic data  $\mathbb{X}$  at our disposal. This data is available in the form of two “csv” files, one file for Bitcoin and one file for Ethereum (see Figure 7).

The available dataset  $\mathbb{X}$  is constituted by the data points  $\mathbf{z}^{(i)}$  which correspond to all the information contained in the  $i$ -th row of both files. Thus, the data point  $\mathbf{z}^{(i)}$  contains the closing and opening prices as well as the traded volumes of both currencies at a particular day  $i$  (see Figure 7). Since we are interested in predicting the price of Bitcoin, we use the Bitcoin closing price at the  $i$ -th day to define the label (or output, or target)  $y^{(i)}$  of data point  $\mathbf{z}^{(i)}$ . The prediction should be based solely on the closing price of Ethereum on the same day. Thus, we use the closing price of Ethereum as the feature  $x^{(i)}$  characterizing the data point  $\mathbf{z}^{(i)}$ .

Date	Open	High	Low	Close	Adj Close	Volume
2015-08-06	278	279.6	274.28	277.89	277.89	$1.19 \cdot 10^7$
2015-08-07	277.89	278.92	257.42	258.6	258.6	$2.23 \cdot 10^7$
2015-08-08	258.6	266.75	258.56	263.87	263.87	$1.52 \cdot 10^7$
2015-08-09	263.87	266.63	260.52	263.3	263.3	$1.29 \cdot 10^7$
2015-08-10	263.3	269.9	261.44	269.03	269.03	$1.37 \cdot 10^7$
2015-08-11	269.03	271.5	263.66	267.66	267.66	$1.52 \cdot 10^7$
2015-08-12	267.66	268.39	261.28	263.44	263.44	$1.5 \cdot 10^7$
2015-08-13	263.44	267.22	260.21	265.03	265.03	$1.39 \cdot 10^7$
2015-08-14	265.03	266.55	259.38	260.52	260.52	$1.03 \cdot 10^7$
2015-08-15	260.52	261.92	254.57	257.12	257.12	$1.79 \cdot 10^7$
2015-08-16	257.12	259.93	252.87	257.13	257.13	$1.24 \cdot 10^7$

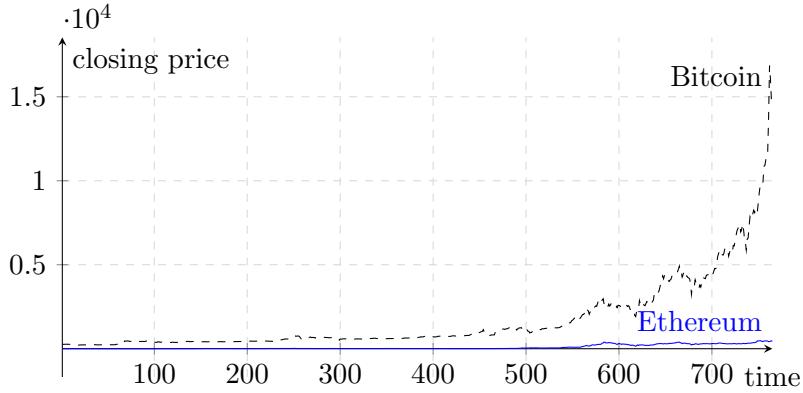
(a)

Date	Open	High	Low	Close	Adj Close	Volume
2015-08-06	0.67	3	0.67	3	3	371
2015-08-07	3	3	0.15	1.2	1.2	1,438
2015-08-08	1.2	1.2	1.2	1.2	1.2	0
2015-08-09	1.2	1.2	1.2	1.2	1.2	0
2015-08-10	1.2	1.2	0.65	0.99	0.99	7,419
2015-08-11	0.99	1.29	0.91	1.29	1.29	2,376
2015-08-12	1.29	1.88	1.26	1.88	1.88	4,923
2015-08-13	1.88	2.1	1.79	1.79	1.79	11,070
2015-08-14	1.79	1.79	1.5	1.79	1.79	14,812
2015-08-15	1.79	1.79	0.5	1.37	1.37	10,794
2015-08-16	1.37	1.59	1.25	1.3	1.3	6,063

(b)

Figure 7: Historic recordings of (a) Bitcoin and (b) Ethereum statistics.

**Normalization.** In order to get intuition about the relation between the closing prices  $x^{(i)}$  and  $y^{(i)}$  of Bitcoin and Ethereum, we plot them as a function of time (time series) in Figure 8.

Figure 8: Time series of Bitcoin closing price  $x^{(i)}$  and Ethereum closing price  $y^{(i)}$ .

As evident from Figure 8, comparing the raw closing prices between Bitcoin and Ethereum is difficult because of the significantly different value ranges of Bitcoin and Ethereum prices. Therefore, we normalize (or scale) the closing prices according to

$$x_{\text{scaled}}^{(i)} := \frac{x^{(i)}}{\max_{j=1,\dots,N} x^{(j)}}, \text{ and } y_{\text{scaled}}^{(i)} := \frac{y^{(i)}}{\max_{j=1,\dots,N} y^{(j)}}. \quad (1)$$

The normalization (1) results in features  $x_{\text{scaled}}^{(i)}$  and labels  $y_{\text{scaled}}^{(i)}$  in the same value range  $[0, 1]$ . We depict the time series of normalized closing prices in Figure 9, which suggests that the closing prices might be correlated.

**Scatterplot.** In order to get more insight into the relation between feature  $x^{(i)}$  and label  $y^{(i)}$ , it can be helpful to generate a scatter plot as shown in Figure 10. A scatter plot depicts the data points  $\mathbf{z}^{(i)} = (x^{(i)}, y^{(i)})$  in a two-dimensional plane with the axes representing the values of feature  $x$  and label  $y$ . From Figure 10, it seems that the relation between feature  $x$  and label  $y$  is non-linear. In particular, for larger feature values  $x$ , the values of the label  $y$  are almost constant.

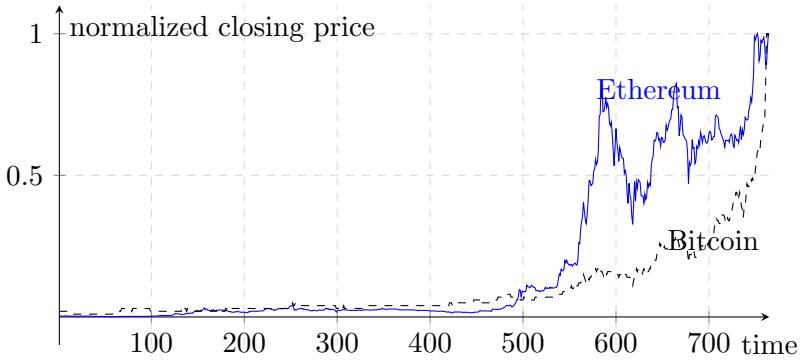


Figure 9: Normalized closing prices  $x_{\text{scaled}}^{(i)}$  and  $y_{\text{scaled}}^{(i)}$  of Bitcoin and Ethereum, respectively.

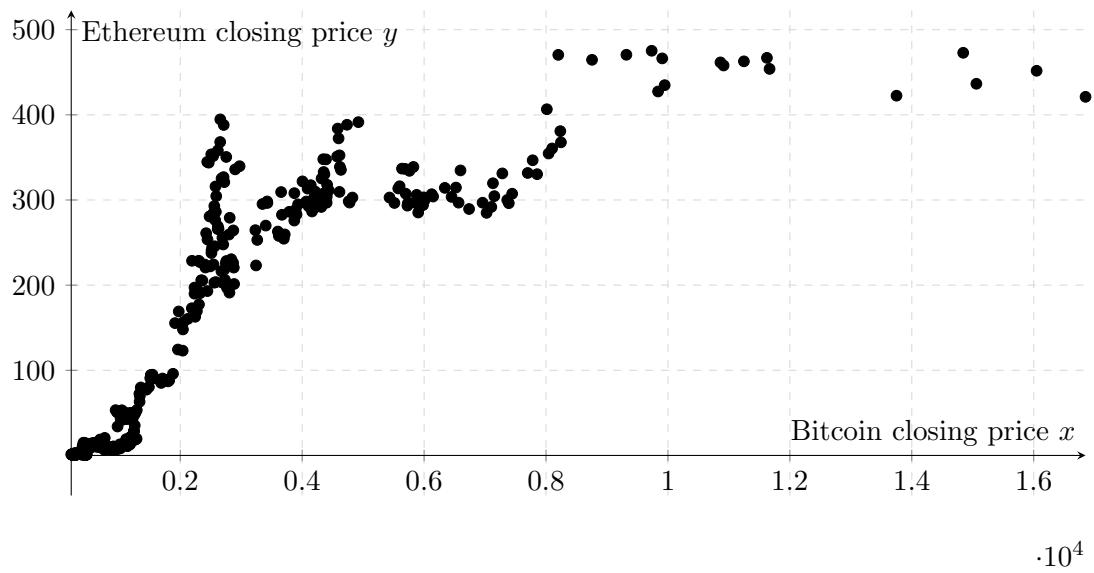


Figure 10: A scatterplot of data points  $(x^{(i)}, y^{(i)})$  with Bitcoin closing price  $x^{(i)}$  and Ethereum closing price  $y^{(i)}$  at the  $i$ -th day. Each data point  $(x^{(i)}, y^{(i)})$  is depicted by a dot located at the point with coordinates  $x^{(i)}$  and  $y^{(i)}$ .

## 2.2 Hypothesis Space

Let us consider again the cleaning robot Rumba (see Figure 1). Here, the goal is to predict the coordinate  $y^{(i)} \in \mathbb{R}$  (which is the label) of Rumba’s location at time  $i$  based solely on some features  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  of the snapshot  $\mathbf{z}^{(i)}$  taken by the on-board camera of Rumba at time  $i$ . In order to have any chance to solve this task, we must assume (or hypothesize) an underlying relation between the features  $\mathbf{x}^{(i)}$  and the coordinate (label)  $y^{(i)}$ . We will represent this relation between features  $\mathbf{x}^{(i)}$  and label  $y^{(i)}$  of a data point (e.g., the snapshot taken by Rumba at time  $i$ ) using a **hypothesis**  $h : \mathcal{X} \rightarrow \mathcal{Y}$ , which maps the feature vector of the snapshot to a predicted label  $\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$ .

A reasonable hypothesis  $h$  should approximate the true label ( $y$ -coordinate)  $\hat{y}^{(i)}$  as accurately as possible, i.e.,  $\hat{y}^{(i)} \approx y^{(i)}$ . Note that computing the prediction  $h(\mathbf{x})$  of the label  $y$  based on features  $\mathbf{x}$  amounts to the evaluation of a map  $h(\cdot)$  for the particular argument  $\mathbf{x}$  (see Figure 11). This seems trivial, but in many ML applications the feature  $\mathbf{x}$  and the predictor  $h(\cdot)$  can be very complex objects. Using feature vectors with millions of entries is not an exception. Much of ML theory revolves around the analysis and design of automated methods for finding good predictors  $h$  which can be evaluated efficiently.

**Shazaam.** Consider the ML problem underlying a music information retrieval smartphone app [10]. Such an app aims at identifying the song-title based on a short audio recording of (an interpretation of a) the song obtained via the microphone of a smartphone. Here, the feature vector  $\mathbf{x}$  represents the sampled audio signal and the label  $y$  is a particular song title out of a huge music database. What is the length  $d$  of the feature vector  $\mathbf{x} \in \mathbb{R}^d$  if its entries are the signal amplitudes of a 20 second long recording which is sampled at a rate of 44 kHz?

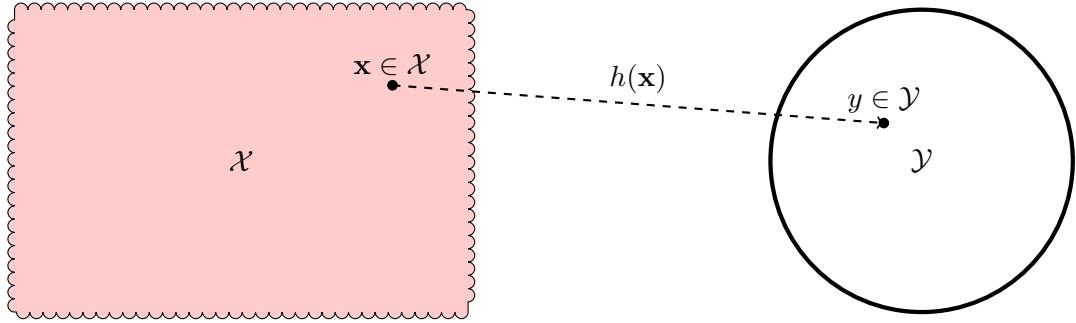


Figure 11: A hypothesis  $h$  is nothing but a map from the feature space  $\mathcal{X}$  into the label space  $\mathcal{Y}$  of an ML problem.

In principle, we could use any map  $h : \mathbb{R}^d \rightarrow \mathbb{R}$  to predict the coordinate  $y^{(i)}$  based on the snapshot features  $\mathbf{x}^{(i)}$  (see Figure 12) at time  $i$ . However, given **limited computational resources**,<sup>2</sup> it might be beneficial to restrict the resulting ML methods to a small subset of computationally feasible (“affordable”) predictor functions. This subset of “affordable” predictors is sometimes referred to as the **hypothesis space** (or **concept class**). In what follows, we will mainly focus on

<sup>2</sup>See a price list for computing resources at <https://aws.amazon.com/ec2/pricing/on-demand/>.

**linear prediction methods** which use the hypothesis space

$$\mathcal{H} := \{h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R} : h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{x}^T \mathbf{w} \text{ with some weight vector } \mathbf{w} \in \mathbb{R}^d\}. \quad (2)$$

Each element of this hypothesis space  $\mathcal{H}$  is a linear map (function)  $h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R}$  which maps the feature vector  $\mathbf{x} \in \mathbb{R}^d$  to the predicted label (or output)  $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{x}^T \mathbf{w} \in \mathbb{R}$ . For  $d = 1$ , where the feature vector reduces to one single feature  $x$ , the hypothesis space (2) consists of all maps  $h^{(w)}(x) = wx$  with some weight  $w \in \mathbb{R}$  (see Figure 13).

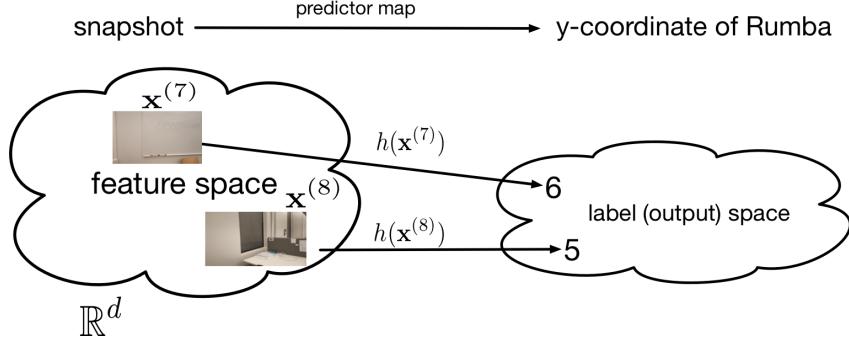


Figure 12: A predictor (hypothesis)  $h : \mathcal{X} \rightarrow \mathcal{Y}$  takes the feature vector  $\mathbf{x}^{(t)} \in \mathcal{X}$  (e.g., representing the snapshot taken by Rumba at time  $t$ ) as input and outputs a predicted label  $\hat{y}_t = h(\mathbf{x}^{(t)})$  (e.g., the predicted  $y$ -coordinate of Rumba at time  $t$ ). A key problem studied within ML is how to automatically learn a good (accurate) predictor  $h$  such that  $y_t \approx h(\mathbf{x}^{(t)})$ .

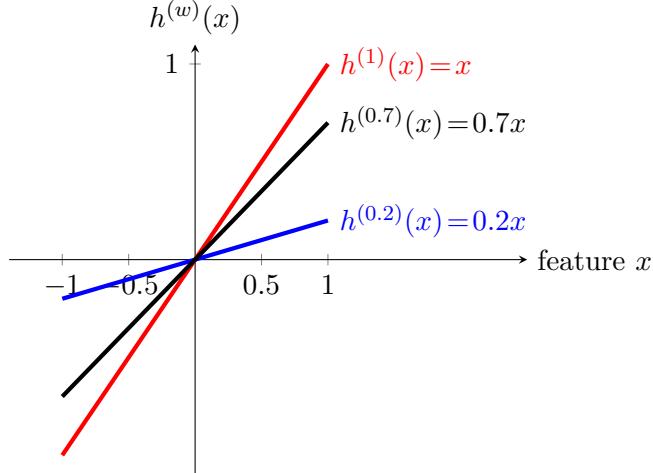


Figure 13: Three particular members of the hypothesis space  $\mathcal{H} = \{h^{(w)} : \mathbb{R} \rightarrow \mathbb{R}, h^{(w)}(x) = w \cdot x\}$  which consists of all linear functions of the scalar feature  $x$ . We can parametrize this hypothesis space conveniently using the weight  $w \in \mathbb{R}$  as  $h^{(w)}(x) = w \cdot x$ .

Note that each element of the hypothesis space  $\mathcal{H}$  in (2) is parametrized (indexed) by a particular value of the weight vector  $\mathbf{w} \in \mathbb{R}^d$ . In particular, each map  $h^{(\mathbf{w})}$  is fully specified by the weight vector  $\mathbf{w}$ . Thus, instead of searching a good hypothesis directly in the function space  $\mathcal{H}$  (its elements are functions!), we can equivalently search over all possible weight vectors  $\mathbf{w} \in \mathbb{R}^d$ .

We highlight that the choice of the hypothesis space, i.e., which subset of maps  $h : \mathcal{X} \rightarrow \mathcal{Y}$  to be considered, is a **design choice**. The AI engineer has to choose a suitable hypothesis space for a given particular ML application. As with the choice of what features to use, finding a good choice of the hypothesis space typically requires a good understanding of the particular application (domain expertise). Sometimes the most relevant aspect for choosing a particular hypothesis space is the available computational infrastructure. If we only have a spreadsheet program at our disposal then it might be useful to consider a hypothesis space of maps which can be represented by spread sheets in the form of look-up tables (see Figure 1). The particular hypothesis space (2) constituted by linear maps is only one possible choice, which can be quite useful in many applications but might be less suitable for other applications.

We highlight that the elements of the hypothesis space  $\mathcal{H}$  are maps  $h$  from the feature space to the label space of a given ML problem. In other words, a particular hypothesis  $h$  is a map that takes a feature vector  $\mathbf{x}$  as input and outputs a predicted (or estimated) label  $h(\mathbf{x})$ . If the label space is discrete, such as  $\{-1, 1\}$  for a binary classification problem, we sometimes use the term **classifier** instead of hypothesis. For regression problems involving a continuous label space (such as  $\mathbb{R}$ ) it is common to refer to a hypothesis as a **predictor**. However, in the end, a classifier (or a predictor (or a hypothesis)) is nothing but a **map from the feature space to the label space of an ML problem**.

For a discrete label space  $\mathcal{Y}$ , which is used in classification problems, we can characterize a particular classifier using its **decision boundary** which contains all the border points between the different regions  $\mathcal{R}_{\hat{y}}$  of the feature space  $\mathcal{X}$ . The region  $\mathcal{R}_{\hat{y}}$  contains the feature values  $\mathbf{x} \in \mathcal{X}$  which are mapped to the same predicted label  $\hat{y} \in \mathcal{Y}$ .

If the label space is  $\mathcal{Y} = \{-1, 1\}$  (yielding a binary classification problem), a particular hypothesis  $h$  partitions the feature space  $\mathcal{X}$  into two regions  $\mathcal{R}_1 = \{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) \geq 0\}$  and  $\mathcal{R}_{-1} = \{\mathbf{x} \in \mathcal{X} : h(\mathbf{x}) < 0\}$ . Thus, the overall feature space  $\mathcal{X}$  decomposes into two half-spaces  $\mathcal{R}_1$  and  $\mathcal{R}_{-1}$  which are separated by the hyperplane  $\{\mathbf{x} : h(\mathbf{x}) = 0\}$ , which is also the decision boundary obtained from  $h$ .

Sometimes, these two regions can be represented quite efficiently by only specifying the boundary (“decision boundary”) between those two regions. For binary classifications problems with label space  $\mathcal{Y} = \{-1, 1\}$ , the family of **linear classifiers**, which includes logistic regression (see Section 3.4), the SVM (see Section 3.5) and naive Bayes’ classifiers (see Section 3.6), uses a hypothesis space which is composed of maps whose decision boundary is a hyperplane  $\{\mathbf{x} : \mathbf{w}^T \mathbf{x} = b\}$  (see Figure 14).

**Exercise.** Given the hyperplane  $\mathcal{C} = \{\mathbf{x} : \mathbf{w}^T \mathbf{x} = 1\}$  with vector  $\mathbf{w} = (1, 0, 0, 1)^T$ , can you find a hypothesis  $h : \mathbb{R}^4 \rightarrow \mathbb{R}$  of the form  $h(\mathbf{x}) = \mathbf{u}^T \mathbf{x} + g$  with some vector  $\mathbf{u} \in \mathbb{R}^4$  and constant  $g$ , such that  $h(\mathbf{x}) \geq 0$  for all  $\mathbf{x}$  above  $\mathcal{C}$  and  $h(\mathbf{x}) < 0$  for all  $\mathbf{x}$  below  $\mathcal{C}$ ?

In principle, the question of which hypothesis space to use is a design choice, which has to be made individually for a given ML application and the available **computational resources**. One important aspect guiding this choice is the computational framework used for implementing the resulting ML methods. If we use a **spreadsheet program** as the computational engine, we could define a hypothesis space by collecting all predictors  $h : \mathcal{X} \rightarrow \mathcal{Y}$  which can be implemented by a spreadsheet (see Table 1) having two columns, one for the input value and one for the output value, and a maximum number of rows (the maximum number corresponds to the quantization interval). If we instead use the programming language Python as the computational engine, we can obtain a

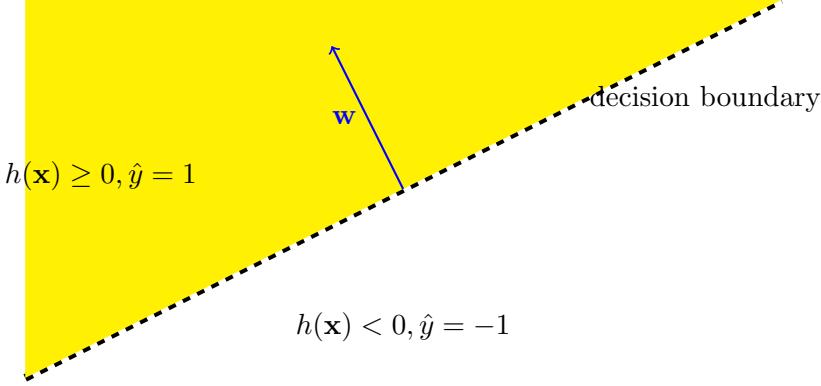


Figure 14: A hypothesis  $h : \mathcal{X} \rightarrow \mathcal{Y}$  for a binary classification problem with label space  $\mathcal{Y} = \{-1, 1\}$  can be represented conveniently via the decision boundary (dashed line) which separates all feature vectors  $\mathbf{x}$  with  $h(\mathbf{x}) \geq 0$  from the region of feature vectors with  $h(\mathbf{x}) < 0$ . If the decision boundary is a hyperplane  $\{\mathbf{x} : \mathbf{w}^T \mathbf{x} = b\}$  (with normal vector  $\mathbf{w} \in \mathbb{R}^d$ ), we refer to the map  $h$  as a **linear classifier**.

hypothesis class by collecting all possible Python subroutines with one input (scalar feature) and one output argument and having less than 100 lines of code (see Figure 17).

The largest possible choice for the hypothesis space  $\mathcal{H}$  of an ML problem using feature space  $\mathcal{X}$  and label space  $\mathcal{Y}$  is the set  $\mathcal{Y}^\mathcal{X}$  constituted by all maps from the feature space  $\mathcal{X}$  to the label space  $\mathcal{Y}$ .<sup>3</sup> The choice  $\mathcal{H} = \mathcal{Y}^\mathcal{X}$  is rarely used in practice since this space is simply too large to work within a reasonable amount of computational resources. Instead, the hypothesis space  $\mathcal{H}$  is typically a (very small) subset of  $\mathcal{Y}^\mathcal{X}$  (see Figure 16). However, choosing the hypothesis space too small might result in poor performance of the overall ML method, as we might not find any suitable predictor (or classifier)  $h \in \mathcal{H}$  which allows to represent the true underlying relationship between features  $\mathbf{w}$  and label  $y$  of data points.

Consider the dataset depicted in Figure 10 consisting of historic information about cryptocurrency prices. Each data point (depicted by a dot) corresponds to the cryptocurrency statistics of one particular day. The  $i$ -th data point is characterized using the feature  $x^{(i)}$  being the closing price of Bitcoin at day  $i$  and the label  $y^{(i)}$  being the closing price of Ethereum at the same day.

As indicated by Figure 10, the relation  $x \mapsto y$  cannot be well explained by a linear function but rather some non-linear function. Therefore, it might be useful to consider a hypothesis space which contains non-linear maps. In particular, we might consider a hypothesis space which is constituted by polynomials, e.g.,  $h(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3$ , of a given maximum degree. In Figure 15, we show a particular predictor which belongs to this larger hypothesis space. We will consider ML problems using a hypothesis space of polynomial functions of a scalar feature in Section 3.2.

In general the (design) choice for the hypothesis space  $\mathcal{H}$  has to balance between two contradicting goals:

- It has to be **sufficiently large** to represent the true underlying relation between the features and the label of the data points arising in an ML problem.

---

<sup>3</sup>The elements of  $\mathcal{Y}^\mathcal{X}$  are maps  $h : \mathcal{X} \rightarrow \mathcal{Y}$ .

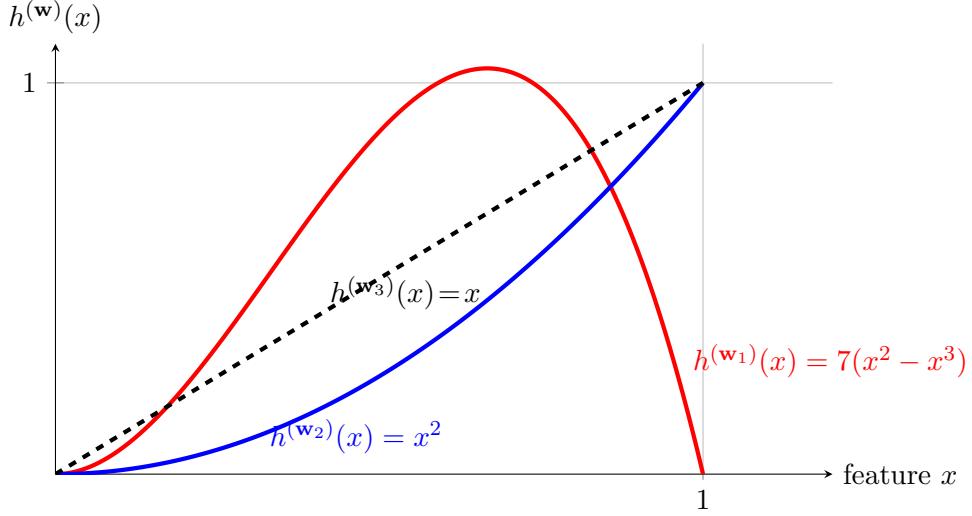


Figure 15: Three particular members of the hypothesis space  $\mathcal{H}_{\text{poly}}^{(3)}$  (see (14)) which consists of polynomials of degree at most 3.

- It has to be **sufficiently small** such that, given the available computational resources, it can be efficiently searched over to find good predictors according to some criterion (see Section 2.3 and Section 4). This requirement implies also that the maps  $h(\mathbf{x})$  contained in  $\mathcal{H}$  can be evaluated (computed) efficiently [11]. Another important reason for not choosing the hypothesis space  $\mathcal{H}$  not too large is to avoid overfitting (see 7.1) the training data which is used to pick a good predictor map out of  $\mathcal{H}$ . If the hypothesis space  $\mathcal{H}$  is too large than just by luck we will find a predictor which performs well over a training dataset. However, such a predictor will yield poor performance on other data, which is different from the training data.

The second aspect becomes relevant already for (seemingly) simple ML problems. Indeed, consider Rumba which has to predict if it is moving towards a charging station at time  $i$ , which is encoded by the label  $y^{(i)} = -1$  or not, encoded by  $y^{(i)} = 1$ . In order to determine if it is moving towards a charging station, Rumba can only use the snapshot  $\mathbf{z}^{(i)}$  generated by its on-board camera at time  $i$ . The snapshot is available as a black-white bitmap consisting of  $512 \times 512$  pixels. In order to construct a classifier, we represent the snapshot using a feature vector  $\mathbf{x}^{(i)} \in \{0, 1\}^d$  of length  $d = 512^2$  (see Figure 5). If we would use as hypothesis space  $\mathcal{H}_{\text{BW}}$  the set of all possible maps from the feature space  $\mathcal{X} = \{0, 1\}^{512^2}$  (representing a BW bitmap) into the label space  $\mathcal{Y} = \{-1, 1\}$ , we would end up with a hypothesis space containing  $2^{|\mathcal{X}|} = 2^{2^{512^2}}$  elements. Thus, the naive choice of a hypothesis space (which is to consider all possible maps from feature to label space) for this (quite small) ML problem would already result in a hypothesis space  $\mathcal{H}_{\text{BW}}$  with more elements than the estimated number of atoms in the visible universe (which is around  $10^{80}$ ).

Using such a large hypothesis space might become computationally intractable given limited resources. Indeed, ML methods amount to searching over the hypothesis space for the best or optimal hypothesis  $h \in \mathcal{H}$  (see Section 5). If the hypothesis space is too large, then this search (see Section 4) takes too long (we do not want to have Rumba taking one year to clean the office room). Moreover, having a large hypothesis space  $\mathcal{H}$  typically implies that it will contain very complicated predictors  $h \in \mathcal{H}$ . In order to predict the label  $y$  of a data point  $\mathbf{x}$  we need to evaluate the predictor

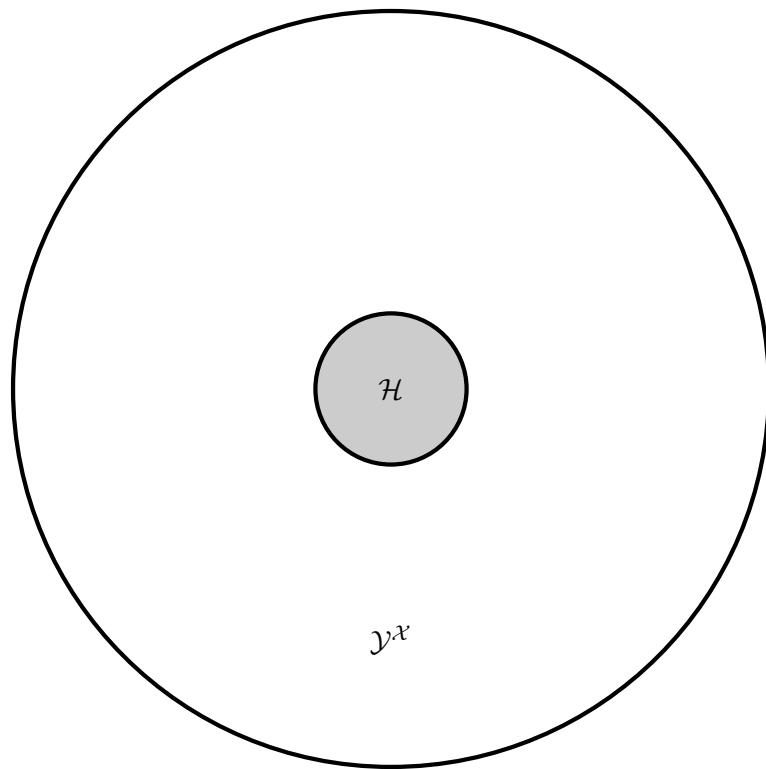


Figure 16: The hypothesis space  $\mathcal{H}$  is typically a small subset of the (extremely large) set  $\mathcal{Y}^{\mathcal{X}}$  which is constituted by all possible maps from feature space  $\mathcal{X}$  into the label space  $\mathcal{Y}$ .

feature $x$	predicted label (output)
0	0
1/10	10
2/10	3
:	:
1	22.3

Table 1: A spread sheet representing of a hypothesis map  $h$  in the form of a look-up table. The value  $h(x)$  is given by the entry in the second column of the row whose first column entry is  $x$ .

which might become intractable for highly complicated maps  $h \in \mathcal{H}$  (consider a map which is a look up table consisting of billions of rows). Thus, it might be useful to use a hypothesis space which does not include all possible maps from feature space  $\mathcal{X}$  to label space  $\mathcal{Y}$  but rather only a subset of **computationally feasible** (affordable), given the available computational resources, maps  $h : \mathcal{X} \rightarrow \mathcal{Y}$ .

Consider again the cleaning robot Rumba which, based on the features  $\mathbf{x}^{(i)} \in 2^{512 \times 512}$  (black-/white bitmap) of the on-board camera snapshot, has to determine if it moves towards a charging station ( $y^{(i)} = 1$ ) or not ( $y^{(i)} = -1$ ). Instead of searching for a good classifier  $h$  among all possible maps in  $\mathcal{H}_{\text{BW}}$  from feature space  $\mathcal{X} = \{0, 1\}^{512 \times 512}$  to label space  $\mathcal{Y} = \{-1, 1\}$ , we could use a smaller hypothesis space  $\mathcal{H}_{\text{small}} \subseteq \mathcal{H}_{\text{BW}}$  consisting of all maps which depend only on the top-left  $3 \times 3$  pixels in the snapshot.

It will be sometimes convenient to allow the hypothesis  $h$  to take on also values that do not belong to the label space  $\mathcal{Y}$ . In particular, we will consider binary classification problems (see Section 3.4) with label space  $\mathcal{Y} = \{-1, 1\}$  and use hypothesis maps  $h : \mathcal{X} \rightarrow \mathbb{R}$  which can take on values outside the label space  $\mathcal{Y} = \{-1, 1\}$ . This is useful since the absolute value of  $h(\mathbf{x})$  can represent a level of confidence in the resulting predicted label  $\hat{y}$  which is typically obtained as the sign of  $h(\mathbf{x})$ , i.e.,

$$\hat{y} = \begin{cases} 1 & \text{if } h(\mathbf{x}) \geq 0 \\ -1 & \text{if } h(\mathbf{x}) < 0. \end{cases} \quad (3)$$

Consider two data points  $(\mathbf{x}^{(1)}, y^{(1)})$  and  $(\mathbf{x}^{(2)}, y^{(2)})$  with binary labels  $y^{(1)} = y^{(2)} = 1$  which we classify using a hypothesis map  $h$  yielding the values  $h(\mathbf{x}^{(1)}) = 10$  and  $h(\mathbf{x}^{(2)}) = 1/100$ . While the resulting labels are the same  $\hat{y}^{(1)} = 1$  and  $\hat{y}^{(2)} = 1$  for both data points, we are much more confident in the classification of  $\mathbf{x}^{(1)}$  while the classification of  $\mathbf{x}^{(2)}$  seems not very reliable.

### 2.3 Loss Function and Empirical Risk

Let us consider a particular ML problem which revolves around predicting the label  $y \in \mathcal{Y}$  (such as a coordinate of the current location of Rumba) of a data point (such as the current snapshot  $\mathbf{z}$  delivered by the on-board camera of Rumba) based on its features  $\mathbf{x} \in \mathcal{X}$  (see Figure 5). This prediction is done by applying a hypothesis  $h$  (called “predictor” for continuous label space  $\mathcal{Y}$  or “classifier” for discrete label space  $\mathcal{Y}$ ), to the features  $\mathbf{x}$  yielding a predicted (or estimated) label  $\hat{y} = h(\mathbf{x})$ . Taking into account the available computational resources, we have defined the hypothesis space  $\mathcal{H}$  which consists of all **computationally feasible** predictor maps  $h$ . The next

hypothesis space  $\mathcal{H}$

```
def predictor_map1(x):
    return x*x
```

```
def predictor_map3(x):
    return 5*x
```

```
def predictor_map2(x):
    return 3*x*x*x
```

```
def predictor_map4(x):
    return 5
```

Figure 17: Example of a hypothesis space  $\mathcal{H}$  which consists of four predictor maps which are implemented using the programming language Python.

obvious question is: which predictor map  $h$  out of all the maps in the hypothesis space  $\mathcal{H}$  is the best for the ML problem at hand?

We want to assess the quality of a particular predictor  $h$  (“is it any good?”) in its ability to predict the label  $y$  based on features  $\mathbf{x}$  of a data point. To this end, we need to define a measure of the **loss** (or error) incurred by using the particular predictor  $h(\mathbf{x})$  when the true label is  $y$ . More formally, we define a loss function  $\mathcal{L} : \mathcal{X} \times \mathcal{Y} \times \mathcal{H} \rightarrow \mathbb{R}$  which measures the loss  $\mathcal{L}((\mathbf{x}, y), h)$  incurred by predicting the label  $y$  of a data point using the prediction  $h(\mathbf{x})$ . The concept of loss functions is best understood by considering some particular examples.

For numeric labels  $y \in \mathbb{R}$ , arising within regression problems with continuous label space  $\mathcal{Y} = \mathbb{R}$ , a popular choice for the loss function is the **squared error loss** (see Figure 18)

$$\mathcal{L}((\mathbf{x}, y), h) := (y - h(\mathbf{x}))^2. \quad (4)$$

The squared error loss (4) is quite natural for ML problems involving a continuous (numeric) label or output  $y \in \mathbb{R}$  (e.g., the closing price of the cryptocurrency “Bitcoin” at a particular day) which has to be predicted using a predictor  $h(\mathbf{x}) \in \mathbb{R}$ . However, for classification problems using a discrete label space, such as in binary classification where  $\mathcal{Y} = \{-1, 1\}$ , the squared error  $(y - h(\mathbf{x}))^2$  is not a useful measure of the quality of a classifier  $h(\mathbf{x})$ . Indeed, if we consider the classifier  $h(\mathbf{x})$  delivering a real-number, we would like to punish wrong classifications, e.g., if the true label is  $y = -1$  and the classifier produces a large positive number, e.g.,  $h(\mathbf{x}) = 1000$ . On the other hand, for a true label  $y = -1$ , we do not want to punish a classifier  $h$  which yields a large negative number, e.g.,  $h(\mathbf{x}) = -1000$ . However, this is exactly happening for the squared error loss. In

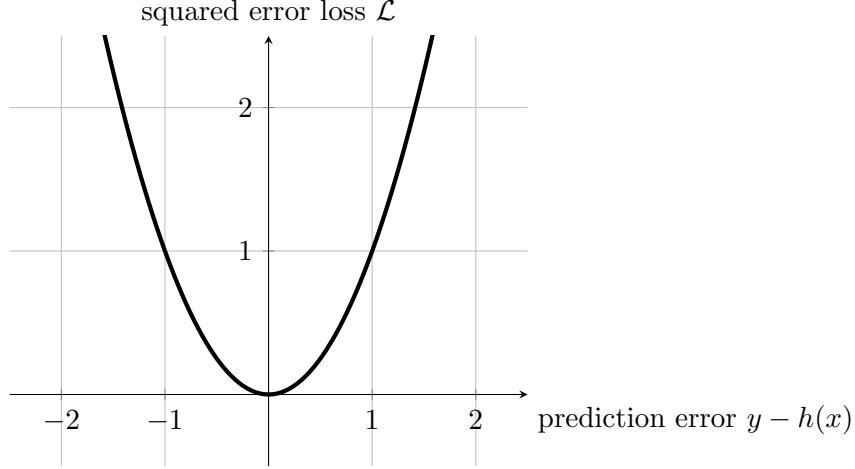


Figure 18: A widely used choice for the loss function in regression problems (with label space  $\mathcal{Y} = \mathbb{R}$ ) is the squared error loss  $L((\mathbf{x}, y), h) := (y - h(\mathbf{x}))^2$ . Note that in order to evaluate the loss function for a given hypothesis  $h$ , so that we can tell if  $h$  is any good, we need to know the feature  $\mathbf{x}$  and the label  $y$  of the data point.

Figure 19, we depict a dataset consisting of 5 labeled data points with binary labels represented by circles (for  $y = 1$ ) and squares (for  $y = -1$ ). Under the squared error loss, the classifier  $h_1$ , which does not separate the two classes perfectly, would have a smaller loss than the classifier  $h_2$  which perfectly separates the two classes. Thus, the squared error loss is rarely used for classification problems involving a discrete label space  $\mathcal{Y}$ .

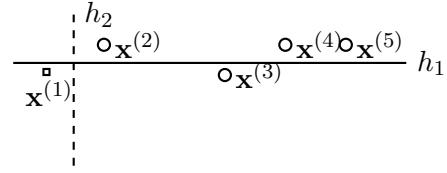


Figure 19: Using the squared error loss would result in preferring the classifier  $h_1$  over  $h_2$ .

In what follows we present some popular choices for the loss function suitable for ML problems with binary labels, i.e., the label space  $\mathcal{Y}$  has two different elements. While the representation of the label values is completely irrelevant, it will be notationally convenient to consider a particular “encoding” of the two label values using the numbers  $-1$  and  $1$ . The formulas of the loss functions we present now only apply to this encoding. However, the modification of these formulas to a different encoding (e.g., using  $0$  and  $1$ ) is straightforward.

Consider the problem of detecting forest fires as early as possible using webcam snapshots such as the one depicted in Figure 20. A particular snapshot is characterized by the features  $\mathbf{x}$  and the label  $y \in \mathcal{Y} = \{-1, 1\}$  with  $y = 1$  if the snapshot shows a forest fire and  $y = -1$  if there is no forest fire. We would like to find or learn a classifier  $h(\mathbf{x})$  which takes the features  $\mathbf{x}$  as input and provides a classification according to  $\hat{y} = 1$  if  $h(\mathbf{x}) > 0$  and  $\hat{y} = -1$  if  $h(\mathbf{x}) \leq 0$ . Ideally we would



Figure 20: A webcam snapshot taken near a ski resort in Lapland.

like to have  $\hat{y} = y$ , which suggests to use the **0/1 loss** (see Figure 21)

$$\mathcal{L}((\mathbf{x}, y), h) := \begin{cases} 1 & \text{if } yh(\mathbf{x}) < 0 \\ 0 & \text{else.} \end{cases} \quad (5)$$

The 0/1 loss is conceptually appealing as it approximates the misclassification (error) probability  $P(y \neq \hat{y})$  with  $\hat{y} = \text{sign}\{h(\mathbf{x})\}$ . Indeed, if we interpret the data points  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  as i.i.d. realizations of some underlying random vector  $\mathbf{x} \in \mathcal{X}$  and random label  $y \in \{-1, 1\}$ , we have

$$(1/N)\mathcal{L}((\mathbf{x}, y), h) \approx P(y \neq \hat{y}) \quad (6)$$

with high probability for sufficiently large sample size  $N$ . The approximation (6) is a direct consequence of the law of large numbers, which is a central result in probability theory (see [12]).

In view of (6), the 0/1 loss seems the most natural choice for assessing the quality of a classifier if our goal is to enforce correct classification ( $\hat{y} = y$ ). However, this appealing theoretical property of the 0/1 loss comes at the cost of high computational complexity. Indeed, for a particular data point  $(\mathbf{x}, y)$ , the 0/1 loss (5) is neither convex nor differentiable when viewed as a function of the classifier  $h$ . Thus, using the 0/1 loss for binary classification problems typically involves advanced optimization methods for solving the resulting learning problem (see Section 3.6).

In order to “cure” the non-convexity of the 0/1 loss we approximate it by a convex loss function. This convex approximation results in the **hinge loss** (see Figure 21)

$$\mathcal{L}((\mathbf{x}, y), h) := \max\{0, 1 - y \cdot h(\mathbf{x})\}. \quad (7)$$

While the hinge loss solves the non-convexity of the 0/1 loss it still is a non-differentiable function of the classifier  $h$ . The next example of a loss function for classification problems cures also the non-differentiability issue.

As a third example for a loss function which is useful for binary classification problems we mention the **logistic loss** (used within logistic regression, see Section 3.4)

$$\mathcal{L}((\mathbf{x}, y), h) := \log(1 + \exp(-yh(\mathbf{x}))). \quad (8)$$

For a fixed feature vector  $\mathbf{x}$  and label  $y$  both, the hinge and the logistic loss function are **convex functions** of the hypothesis  $h$ . However, while the logistic loss (8) depends **smoothly** on  $h$  (such that we could define a derivative of the loss with respect to  $h$ ), the hinge loss (7) is **non-smooth** which makes it more difficult to minimize.

Thus, while ML methods based on the logistic loss function (such as logistic regression in Section 3.4), can make use of simple **gradient descent methods** (see Section 5), ML methods based on the hinge loss (such as support vector machines [13]) have to make use of more advanced tools for solving the resulting learning problem (see Section 4).

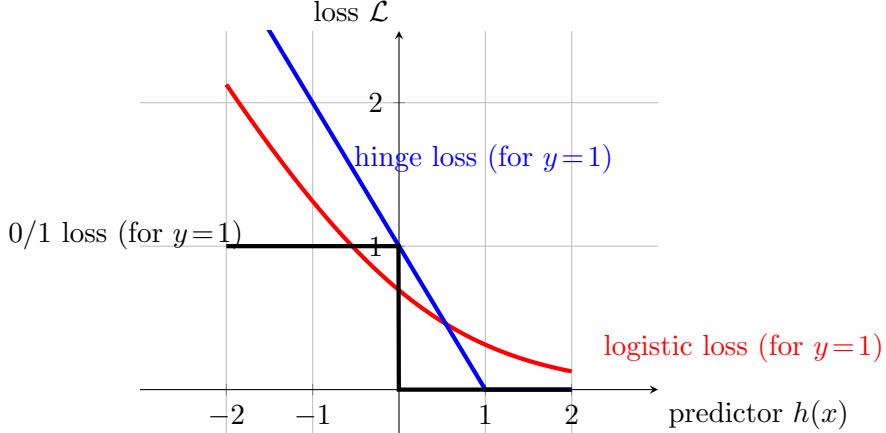


Figure 21: Some popular loss functions for binary classification problems with label space  $\mathcal{Y} = \{-1, 1\}$ . Note that the more correct a decision, i.e., the more positive  $h(x)$  is (when  $y = 1$ ), the smaller is the loss. In particular, all depicted loss functions tend to 0 monotonically with increasing  $h(x)$ .

**Exercise.** How would Figure 21 change if we consider the loss functions for a data point  $z = (x, y)$  with known label  $y = -1$ ?

Let us emphasize that, very much as the choice of features and hypothesis space, the question of which particular loss function to use within an ML method is a **design choice**, which has to be tailored to the application at hand. What qualifies as a useful loss function depends heavily on the overall goal we wish to achieve using ML methods. Thus, there is no useful concept of “optimal loss function”. In general, different loss functions are preferable for different ML applications.

An important aspect guiding the choice of loss function is the computational complexity of the resulting ML method. Indeed, the basic idea behind ML methods is quite simple: learn (find) the particular hypothesis out of a given hypothesis space which yields the smallest loss (on average). The difficulty of the resulting optimization problem (see Section 4) depends crucially on the properties of the chosen loss function. Some loss functions allow to use very simple but efficient iterative methods for solving the optimization problem underlying an ML method (see Section 5).

In order to evaluate the loss  $\mathcal{L}((\mathbf{x}, y), h)$  incurred by a particular predictor  $h \in \mathcal{H}$ , we need to know the feature vector  $\mathbf{x}$  and the true underlying label  $y$ . Therefore, we need to collect labeled

data points. For the an indoor positioning application, these labeled data points could be on-board camera snapshots with features  $\mathbf{x}^{(i)}$  and for which we know the true  $y$ -coordinate  $y^{(i)}$  of the cleaning robot Rumba (see Figure 6).

Let us assume we have collected a bunch of labeled snapshots  $\mathbf{z}^{(i)}$  during the first  $N$  time steps  $i = 1, \dots, N$ . Each snapshot is characterized by the features  $\mathbf{x}^{(i)}$  and the label  $y^{(i)}$ . We collect these labeled snapshots into the **(training) dataset**

$$\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N.$$

Having labeled data allows to compute the **empirical (average) risk** (see Figure 22) of a particular predictor  $h$ :

$$\mathcal{E}(h|\mathbb{X}) := (1/N) \sum_{i=1}^N \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h), \quad (9)$$

with some **loss function**  $\mathcal{L}((\mathbf{x}, y), h)$ . For the particular choice of squared error loss (4), the empirical risk in (9) becomes the **mean squared error**

$$\mathcal{E}(h|\mathbb{X}) = (1/N) \sum_{i=1}^N (y^{(i)} - h(\mathbf{x}^{(i)}))^2. \quad (10)$$

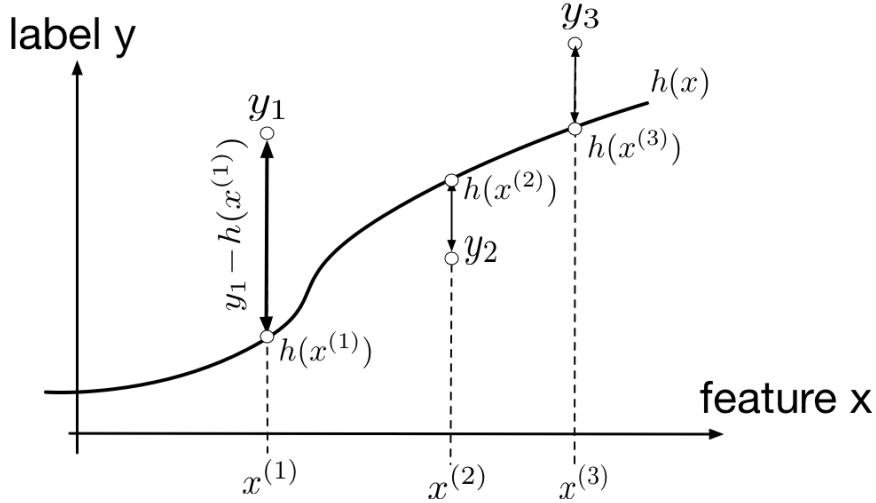


Figure 22: We can evaluate the quality of a particular predictor  $h \in \mathcal{H}$  by measuring the prediction error  $y - h(\mathbf{x})$  obtained for a labeled data point  $\mathbf{z} = (\mathbf{x}, y)$ . For the Rumba application, these labeled data points could be a bunch of snapshots  $\mathbf{z}^{(i)} = (\mathbf{x}^{(i)}, y^{(i)})$ , for  $i = 1, \dots, N$ , with feature vectors  $\mathbf{x}^{(i)}$  and known  $y$ -coordinate  $y^{(i)}$  of the position where the  $i$ -th snapshot has been taken.

### 3 Some Examples

After introducing the main components of a formal ML problem in Section 2, we now detail how different combinations of particular choices for these components yield some of the most popular models of ML problems.

#### 3.1 (Least Squares) Linear Regression

A linear regression problem is based on the feature space  $\mathcal{X} = \mathbb{R}^d$ , a continuous label (output) space  $\mathcal{Y} = \mathbb{R}$  (it is a regression method) and the linear hypothesis space

$$\mathcal{H}^{(d)} = \{h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R} : h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}, \text{ with some weight vector } \mathbf{w} \in \mathbb{R}^d\}. \quad (11)$$

The quality of a particular predictor  $h^{(\mathbf{w})}$  is measured by the squared error loss (4). Based on labeled training data  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , linear regression amounts to finding a predictor  $\hat{h}$  which minimizes the average squared error loss (mean squared error) (see (4))

$$\begin{aligned} \hat{h} &= \underset{h \in \mathcal{H}^{(d)}}{\operatorname{argmin}} \mathcal{E}(h | \mathbb{X}) \\ &\stackrel{(10)}{=} \underset{h \in \mathcal{H}^{(d)}}{\operatorname{argmin}} (1/N) \sum_{i=1}^N (y^{(i)} - h(\mathbf{x}^{(i)}))^2. \end{aligned} \quad (12)$$

Since the hypothesis space  $\mathcal{H}^{(d)}$  is parametrized by the weight vector  $\mathbf{w}$  (see (11)), we can rewrite (12) as an optimization problem directly over the weight vector  $\mathbf{w}$ :

$$\begin{aligned} \mathbf{w}_{\text{opt}} &= \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} (1/N) \sum_{i=1}^N (y^{(i)} - h^{(\mathbf{w})}(\mathbf{x}^{(i)}))^2 \\ &\stackrel{h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}}{=} \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} (1/N) \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2. \end{aligned} \quad (13)$$

The optimization problems (12) and (13) are equivalent in the following sense: Any optimal weight vector  $\mathbf{w}_{\text{opt}}$  which solves (13), can be used to construct an optimal predictor  $\hat{h}$ , which solves (12), via  $\hat{h}(\mathbf{x}) = h^{(\mathbf{w}_{\text{opt}})}(\mathbf{x}) = \mathbf{w}_{\text{opt}}^T \mathbf{x}$ .

#### 3.2 Polynomial Regression

Consider an ML problem involving data points which are characterized by a single numeric feature  $x \in \mathbb{R}$  (the feature space is  $\mathcal{X} = \mathbb{R}$ ) and a numeric label  $y \in \mathbb{R}$  (the label space is  $\mathcal{Y} = \mathbb{R}$ ). We observe a bunch of labeled data points which are depicted in Figure 23.

The geometry of the data points depicted in Figure 23 suggests that the relation  $x \mapsto y$  between feature  $x$  and label  $y$  is highly non-linear. For such non-linear relations between features and labels it is useful to consider a hypothesis space which is constituted by polynomial functions

$$\mathcal{H}_{\text{poly}}^{(d)} = \{h^{(\mathbf{w})} : \mathbb{R} \rightarrow \mathbb{R} : h^{(\mathbf{w})}(x) = \sum_{r=1}^{d+1} w_r x^{r-1}, \text{ with some } \mathbf{w} = (w_1, \dots, w_{d+1})^T \in \mathbb{R}^{d+1}\}. \quad (14)$$

Indeed, we can approximate any non-linear relation  $y = h(x)$  very accurate by using a polynomial  $\sum_{r=1}^d w_r x^{r-1}$  of sufficiently large degree  $d$ .<sup>4</sup>

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<sup>4</sup>The precise formulation of this statement is known as the “Stone-Weierstrass Theorem” [14, Thm. 7.26].

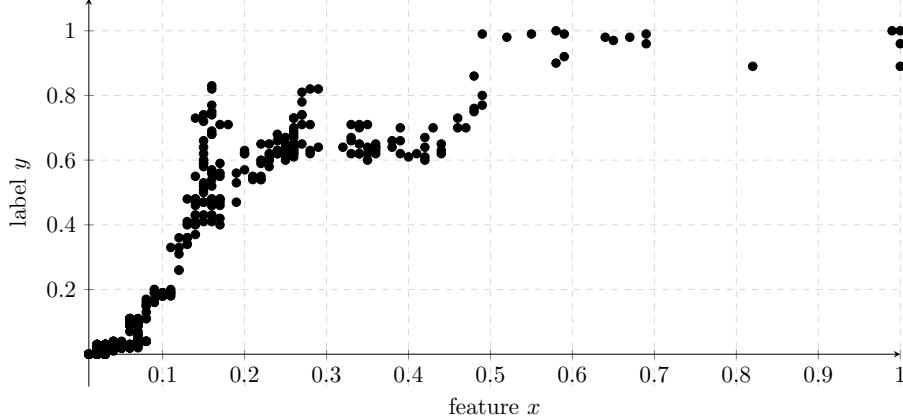


Figure 23: A scatterplot of data points  $(x^{(i)}, y^{(i)})$ .

As for linear regression (see Section 3.1), we measure the quality of a predictor by the squared error loss (4). Based on labeled training data  $\mathbb{X} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$ , with scalar features  $x^{(i)}$  and labels  $y^{(i)}$ , polynomial regression amounts to minimizing the average squared error loss (mean squared error) (see (4)):

$$\min_{h \in \mathcal{H}_{\text{poly}}^{(d)}} (1/N) \sum_{i=1}^N (y^{(i)} - h(\mathbf{w})(x^{(i)}))^2. \quad (15)$$

It is useful to interpret polynomial regression as a combination of a feature map (transformation) (see Section 2.1.1) and linear regression (see Section 3.1). Indeed, any polynomial predictor  $h(\mathbf{w}) \in \mathcal{H}_{\text{poly}}^{(d)}$  can be written as the concatenation of the feature map

$$\phi(x) \mapsto (1, x, \dots, x^d)^T \in \mathbb{R}^{d+1} \quad (16)$$

and a linear map  $g(\mathbf{w}) : \mathbb{R}^{d+1} \rightarrow \mathbb{R} : \mathbf{x} \mapsto \mathbf{w}^T \mathbf{x}$ , i.e.,

$$h(\mathbf{w})(x) = g(\mathbf{w})(\phi(x)). \quad (17)$$

Thus, given a labeled dataset  $\mathbb{X} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$ , we can implement polynomial regression by first applying the feature map  $\phi$  (see (16)) to the scalar features  $x^{(i)}$ , resulting in the feature vectors

$$\mathbf{x}^{(i)} = \phi(x^{(i)}) = (1, x^{(i)}, \dots, (x^{(i)})^d)^T \in \mathbb{R}^{d+1}, \quad (18)$$

and then applying linear regression as in Section 3.1. In particular, by inserting (17) into (15), we end up with a linear regression problem (13) with feature vectors (18). Thus, while a predictor  $h(\mathbf{w}) \in \mathcal{H}_{\text{poly}}^{(d)}$  is a non-linear function  $h(\mathbf{w})(x)$  of the original feature  $x$ , it is a linear function, given explicitly by  $g(\mathbf{w})(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$  (see (17)), of the transformed features  $\mathbf{x}$  (see (18)).

### 3.3 Gaussian Basis Regression

As we have discussed in Section 3.2, we can extend the basic linear regression problem by first transforming the features  $x$  using a vector-valued feature map  $\phi : \mathbb{R} \rightarrow \mathbb{R}^d$  and then applying a

weight vector  $\mathbf{w}$  to the transformed features  $\phi(x)$ . For polynomial regression, the feature map is constructed using powers  $x^l$  of the scalar feature  $x$ . However, we can use also other functions (different from polynomials) to construct the feature map  $\phi$ .

In principle, we can extend linear regression using an arbitrary feature map  $\phi(x) = (\phi_1(x), \dots, \phi_d(x))^T$  with the scalar maps  $\phi_j : \mathbb{R} \rightarrow \mathbb{R}$  which are referred to as **basis functions**. The choice of basis functions depends heavily on the particular application and the underlying relation between features and labels of the observed data points. The basis functions underlying polynomial regression are  $\phi_j(x) = x^j$ . Another popular choice for the basis functions is to use “shifted Gaussians”

$$\phi_{\sigma,\mu}(x) = \exp(-(1/(2\sigma^2))(x-\mu)^2) \quad (19)$$

with the variance  $\sigma^2$  and shift  $\mu$  being design parameters.

Thus, we obtain Gaussian basis linear regression by combining the feature map

$$\phi(x) = (\phi_{\sigma,\mu_1}(x), \dots, \phi_{\sigma,\mu_d}(x))^T \quad (20)$$

with linear regression (see Figure 24). The resulting hypothesis space is then

$$\mathcal{H}_{\text{Gauss}}^{(d)} = \{h^{(\mathbf{w})} : \mathbb{R} \rightarrow \mathbb{R} : h^{(\mathbf{w})}(x) = \sum_{j=1}^d w_j \phi_{\sigma,\mu_j}(x) \text{ with weights } \mathbf{w} = (w_1, \dots, w_d)^T\}. \quad (21)$$

Note that we obtain a different hypothesis space  $\mathcal{H}_{\text{Gauss}}$  for different choices of the variance  $\sigma^2$  and shifts  $\mu_j$  used for the Gaussian function in (19). These parameters have to be chosen suitably for the ML application at hand (e.g., using model selection techniques discussed in Section 6.2). The hypothesis space (21) is parameterized by the weight vector  $\mathbf{w} \in \mathbb{R}^d$  such that each particular element of  $\mathcal{H}_{\text{Gauss}}$  corresponds to a particular choice of the weight vector  $\mathbf{w}$ .

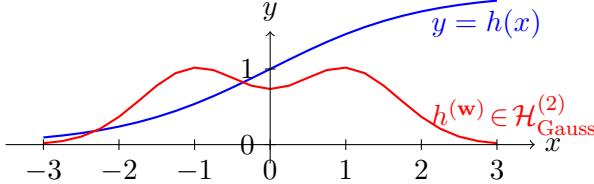


Figure 24: The true relation  $x \mapsto y = h(x)$  (blue) between feature  $x$  and label  $y$  is highly non-linear.

**Exercise.** Try to approximate the hypothesis map depicted in Figure 33 by an element of  $\mathcal{H}_{\text{Gauss}}$  (see (21)) using  $\sigma = 1/10$ ,  $d = 10$  and  $\mu_j = -1 + (2j/10)$ .

### 3.4 Logistic Regression

Logistic regression is a classification method based on the feature space  $\mathcal{X} = \mathbb{R}^d$ , binary label space  $\mathcal{Y} = \{-1, 1\}$  and the linear hypothesis space  $\mathcal{H}^{(d)}$  (see (11)), which we already encountered within linear regression in Section 3.1. At first sight, using classifiers  $h \in \mathcal{H}^{(d)}$  seems to be an overkill since a linear map  $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$ , with some weight vector  $\mathbf{w} \in \mathbb{R}^d$ , can take on any real number. In contrast, the label  $y \in \{-1, 1\}$ , which we are eventually interested in, takes on only one of the two real numbers 1 and  $-1$ . However, it turns out to be quite useful to use classifier maps  $h$  which can take on arbitrary real numbers. Indeed, we can always threshold the value  $h(\mathbf{x})$  according to (3)

to obtain a predicted label  $\hat{y} \in \{-1, 1\}$ . Moreover, the absolute value  $|h(\mathbf{x})|$  indicates how reliable the classification is.

Within logistic regression, we assess the quality of a particular classifier  $h^{(\mathbf{w})} \in \mathcal{H}^{(d)}$  using the logistic loss (8). In particular, given some labeled training data  $\mathbb{X} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$ , logistic regression amounts to minimizing the empirical risk

$$\begin{aligned}\mathcal{E}(\mathbf{w}|\mathbb{X}) &= (1/N) \sum_{i=1}^N \log(1 + \exp(-y^{(i)} h^{(\mathbf{w})}(\mathbf{x}^{(i)}))) \\ h^{(\mathbf{w})}(\mathbf{x}) &\stackrel{=} {=} \mathbf{w}^T \mathbf{x} \quad (1/N) \sum_{i=1}^N \log(1 + \exp(-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)})).\end{aligned}\quad (22)$$

Once we have found the optimal weight vector  $\mathbf{w}_{\text{opt}}$  which minimizes (22), we can classify a data point based on its features  $\mathbf{x}$  according to

$$\hat{y} = \begin{cases} 1 & \text{if } h^{(\mathbf{w})}(\mathbf{x}) \geq 0 \\ -1 & \text{otherwise.} \end{cases}\quad (23)$$

### 3.5 Support Vector Machines

Support vector machines (SVM) are a family of classification methods which use the hinge loss (7) to evaluate the quality of a given classifier  $h \in \mathcal{H}$ . The most basic variant of SVM applies to ML problems with feature space  $\mathcal{X} = \mathbb{R}^d$ , label space  $\mathcal{Y} = \{-1, 1\}$  and the hypothesis space  $\mathcal{H}^{(d)}$  (11), which is also underlying linear regression (see Section 3.1) and logistic regression (see Section 3.4).

While, there are many different variants of the SVM we focus here on the **soft-margin** SVM [9, Chapter 2]. The soft-margin SVM is a classification method which uses the loss function

$$\begin{aligned}\mathcal{L}((\mathbf{x}, y), h^{(\mathbf{w})}) &:= \max\{0, 1 - y \cdot h^{(\mathbf{w})}(\mathbf{x})\} + \lambda \|\mathbf{w}\|^2 \\ h^{(\mathbf{w})}(\mathbf{x}) &\stackrel{=} {=} \mathbf{w}^T \mathbf{x} \quad \max\{0, 1 - y \cdot \mathbf{w}^T \mathbf{x}\} + \lambda \|\mathbf{w}\|^2\end{aligned}\quad (24)$$

with a tuning parameter  $\lambda > 0$ .

According to [9, Chapter 2], a classifier  $h^{(\mathbf{w}_{\text{SVM}})}$  minimizing the loss (24), averaged over some labeled data points  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , is such that its decision boundary (the set of points  $\mathbf{x}$  satisfying  $\mathbf{w}_{\text{SVM}}^T \mathbf{x} = 0$ ) has the largest possible distance (margin) to the two classes  $\mathcal{C}_1 = \{\mathbf{x}^{(i)} : y^{(i)} = 1\}$  and  $\mathcal{C}_2 = \{\mathbf{x}^{(i)} : y^{(i)} = -1\}$ . As depicted in Figure 25, the margin between the decision boundary and the classes  $\mathcal{C}_1$  and  $\mathcal{C}_2$  is typically determined by few data points (such as  $\mathbf{x}^{(6)}$  in Figure 25) which are closest to the decision boundary. Such data points are referred to as **support vectors** and fully determine the resulting classifier  $h^{(\mathbf{w}_{\text{SVM}})}$  or, in other words, once the support vectors are identified the remaining data points become irrelevant for learning the classifier  $h^{(\mathbf{w}_{\text{SVM}})}$ .

We highlight that both, the SVM and logistic regression amount to linear classifiers  $h^{(\mathbf{w})} \in \mathcal{H}^{(d)}$  (see (11)) whose decision boundary is a hyperplane in the feature space  $\mathcal{X} = \mathbb{R}^d$  (see Figure 14). The difference between SVM and logistic regression is the loss function used for evaluating the quality of a particular classifier  $h^{(\mathbf{w})} \in \mathcal{H}^{(d)}$ . The SVM uses the hinge loss (7) which is the best convex approximation to the 0/1 loss (5). Thus, we expect the classifier obtained by the SVM to yield a smaller classification error probability  $P(\hat{y} \neq y)$  (with  $\hat{y} = 1$  if  $h(\mathbf{x}) > 0$  and  $\hat{y} = -1$  otherwise) compared to logistic regression which uses the logistic loss (8).

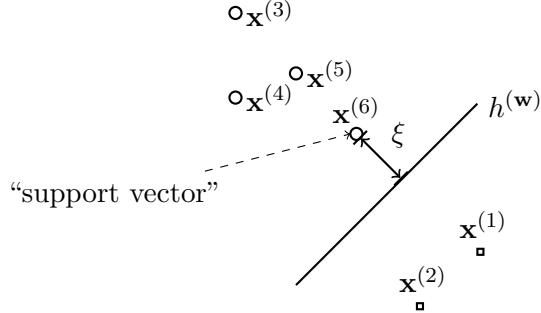


Figure 25: The SVM is based on the hinge loss and aims at finding a classifier  $h(\mathbf{w})$  whose decision boundary has largest possible margin  $\xi$  to the different classes.

The statistical superiority of the SVM comes at the cost of increased computational complexity. In particular, the hinge loss (7) is non-differentiable which prevents the use of simple gradient-based methods (see Section 5) and requires more advanced optimization methods. In contrast, the logistic loss (8) is convex and differentiable which allows to apply simple iterative methods for minimization of the loss (see Section 5).

The logistic loss has an interesting representation if we model the label  $y \in \{-1, 1\}$  as a random variable with probability  $P(\{\}y = 1\}$  which is parameterized using a linear predictor  $h(\mathbf{w})(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$  via

$$\log P(\{\}y = 1\}/(1 - P(\{\}y = 1\}) = \mathbf{w}^T \mathbf{x}, \quad (25)$$

or, equivalently,

$$P(\{\}y = 1\} = 1/(1 + \exp(-\mathbf{w}^T \mathbf{x})). \quad (26)$$

A standard approach to choosing the weight vector  $\mathbf{w}$  is based on maximizing the probability of the observed dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  under the probabilistic model (26). If we assume the labels  $y^{(i)}$  to be statistically independent, this yields

$$\hat{\mathbf{w}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmax}} P(\{\}y^{(i)}\}_{i=1}^N \stackrel{(a)}{=} \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmax}} \prod_{i=1}^N P(\{\}y^{(i)}) \stackrel{(\text{??})}{=} \quad (27)$$

### 3.6 Bayes' Classifier

Consider a classification problem involving data points characterized by features  $\mathbf{x} \in \mathcal{X}$  and associated with labels  $y \in \mathcal{Y}$  out of a discrete label space  $\mathcal{Y}$ . The family of Bayes' classifier methods is based on ML problems using the 0/1 loss (5) for assessing the quality of classifiers  $h$ .

The goal of ML is to find (or learn) a classifier  $h : \mathcal{X} \rightarrow \mathcal{Y}$  such that the predicted (or estimated) label  $\hat{y} = h(\mathbf{x})$  agrees with the true label  $y \in \mathcal{Y}$  as much as possible. Thus, it is reasonable to assess the quality of a classifier  $h$  using the 0/1 loss (5). If we model the data points, with its features  $\mathbf{x}$  and label  $y$ , as i.i.d. random variables, the 0/1 loss approximates the misclassification (or error) probability  $P_{\text{err}} = P(y \neq h(\mathbf{x}))$ .

An important subclass of Bayes' classifiers uses the hypothesis space (11) which is also underlying logistic regression (see Section 3.4) and the SVM (see Section 3.5). Thus, logistic regression, the SVM and Bayes' classifiers yield linear classifiers (see Figure 14) which partition the feature

space  $\mathcal{X}$  into two half-spaces: one half-space consists of all feature vectors  $\mathbf{x}$  which result in the predicted label  $\hat{y} = 1$  and the other half-space constituted by all feature vectors  $\mathbf{x}$  which result in the predicted label  $\hat{y} = -1$ . The difference between these three linear classifiers is how they choose these half-spaces by using different loss-functions. We will discuss Bayes' classifier methods in more detail in Section 4.3.

### 3.7 Kernel Methods

Consider some ML (classification or regression) problem with an underlying feature space  $\mathcal{X}$ . In order to predict the label  $y \in \mathcal{Y}$  of a data point based on its features  $\mathbf{x} \in \mathcal{X}$ , we apply a predictor  $h$  selected out of some hypothesis space. Sometimes it is beneficial to add a pre-processing step before applying the predictor  $h$ .

The family of kernel methods is based on transforming the features  $\mathbf{x}$  to new features  $\hat{\mathbf{x}} \in \mathcal{X}'$  which belong to a (typically very) high-dimensional space  $\mathcal{X}'$  [9]. It is not uncommon that, while the original feature space is a low-dimensional Euclidean space (e.g.,  $\mathcal{X} = \mathbb{R}^2$ ), the transformed feature space  $\mathcal{X}'$  is an infinite-dimensional function space.

The rationale behind transforming the original features into a new (higher-dimensional) feature space  $\mathcal{X}'$  is to reshape the intrinsic geometry of the feature vectors  $\mathbf{x}^{(i)} \in \mathcal{X}$  such that the transformed feature vectors  $\hat{\mathbf{x}}^{(i)}$  have a “simpler” geometry (see Figure 26).

Different kernel methods are then obtained by formulating different (more basic) ML problems (such as linear regression or logistic regression) using this transformed features  $\hat{\mathbf{x}} = \phi(\mathbf{x})$ . A key challenge within kernel methods is the choice of the feature map  $\phi : \mathcal{X} \rightarrow \mathcal{X}'$  which maps the original feature vector  $\mathbf{x}$  to a new feature vector  $\hat{\mathbf{x}} = \phi(\mathbf{x})$ .

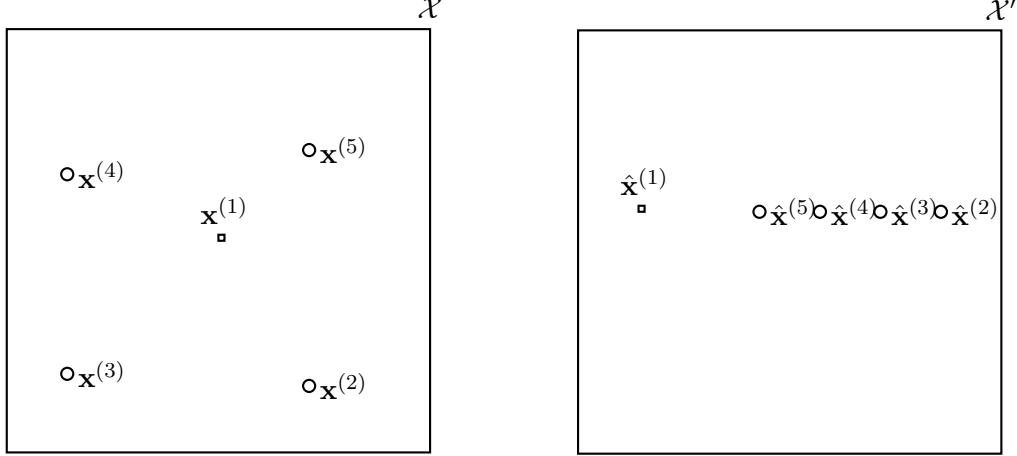


Figure 26: Applying the feature map  $\phi$  within a binary classification problem can turn a dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}_{i=1}^5$  which cannot be separated by a linear classifier into a dataset  $\widehat{\mathbb{X}} = \{\hat{\mathbf{x}}^{(i)}\}_{i=1}^5$  which can be separated linearly (by a linear classifier) in the new feature space  $\widehat{\mathbb{X}}$ .

### 3.8 Decision Trees

A decision tree is a symbolic description of a hypothesis  $h : \mathcal{X} \rightarrow \mathcal{Y}$  which maps the features  $\mathbf{x} \in \mathcal{X}$  to a predicted label  $h(\mathbf{x}) \in \mathcal{Y}$  [13]. While decision trees can be used for arbitrary feature space  $\mathcal{X}$  and label space  $\mathcal{Y}$ , we will discuss them for the particular feature space  $\mathcal{X} = \mathbb{R}^2$ . Here, a decision tree describes how a feature vector  $\mathbf{x} = (x_1, x_2)^T$  is mapped to a predicted label  $h(\mathbf{x})$ .

We have depicted an example of a decision tree in Figure 27. The decision tree consists of nodes which are connected by directed edges. It is useful to think of a decision tree as a step-by-step instruction (a “recipe”) for how to compute the predictor value  $h(\mathbf{x})$  given the input feature  $\mathbf{x} \in \mathcal{X}$ . This computation starts at the **root node** and ends at one of the **leaf nodes**. A leaf node  $m$ , which does not have any outgoing edges, corresponds to a certain subset or “region”  $\mathcal{R}_m \subseteq \mathcal{X}$  of the feature space. The hypothesis  $h$  associated with a decision tree is constant over the regions  $\mathcal{R}_m$ , such that  $h(\mathbf{x}) = h_m$  for all  $\mathbf{x} \in \mathcal{R}_m$  and some fixed number  $h_m \in \mathbb{R}$ . In general, there are two types of nodes in a decision tree:

- decision (or test) nodes, which correspond to particular “tests” about the feature vector  $\mathbf{x}$  (e.g., “is the norm of  $\mathbf{x}$  larger than 10” which can be rephrased as the condition “ $\|\mathbf{x}\| > 10$ ”).
- leaf nodes, which correspond to subsets of the feature space.

The particular decision tree depicted in Figure 27 consists of two decision nodes (including the root node) and three leaf nodes.

Given limited computational resources, we need to restrict ourselves to decision trees which are not too large. We can define a particular hypothesis space by collecting all decision trees which uses the tests “ $\|\mathbf{x} - \mathbf{u}\| \leq r$ ” and “ $\|\mathbf{x} - \mathbf{v}\| \leq r$ ” (for fixed vectors  $\mathbf{u}$  and  $\mathbf{v}$  and fixed radius  $r > 0$ ) and depth not larger than 2.<sup>5</sup> In order to assess the quality of different decision trees we need to use a loss function which can be chosen arbitrarily. We emphasize that decision trees can be combined with an arbitrary loss function.

In general, we are not interested in one particular decision tree only but in a large set of different decision trees from which we choose the most suitable given some data (see Section 4.2). We can define a hypothesis space by collecting predictor maps  $h$  represented by a set of decision trees (such as depicted in Figure 28). A typical strategy is to fix a set of “elementary tests” on the input feature vector, e.g.,  $\|\mathbf{x}\| > 3$ ,  $x_3 < 1$  or a continuous ensemble of test such as  $\{x_2 > \eta\}_{\eta \in [0, 10]}$ . We then build a hypothesis space by considering all decision trees not exceeding a maximum depth and whose decision nodes implement one of those elementary tests.

A decision tree represents a map  $h : \mathcal{X} \rightarrow \mathcal{Y}$ , which is piecewise-constant on clusters (or regions) of the feature space  $\mathcal{X}$ . These non-overlapping regions form a partitioning of the feature space. Each leaf node of a decision tree corresponds to one particular region. By allowing for large decision trees involving many different tests, we can represent very complicated partitions that resemble any given labeled dataset (see Figure 29).

This is quite different from ML problems using the linear hypothesis space (11), such as linear regression, logistic regression or SVM. Such linear maps have a rather simple geometry, since a linear map is constant along hyperplanes. In particular, linear classifiers partition the feature-space into two half-spaces (see Figure 14). In particular, given a labeled dataset, we can construct

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<sup>5</sup>The depth of a decision tree is the maximum number of hops it takes to reach a leaf node starting from the root and following the arrows. The decision tree depicted in Figure 27 has depth 2.

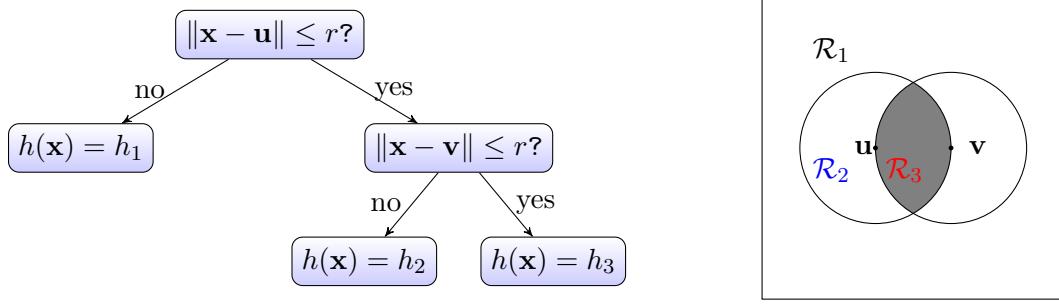


Figure 27: A decision tree represents a hypothesis  $h$  which is constant over subsets  $\mathcal{R}_m$  of the feature space such that  $h(\mathbf{x}) = h_m$  for all  $\mathbf{x} \in \mathcal{R}_m$ . Each subset  $\mathcal{R}_m \subseteq \mathcal{X}$  corresponds to one of the leaf nodes of the decision tree.

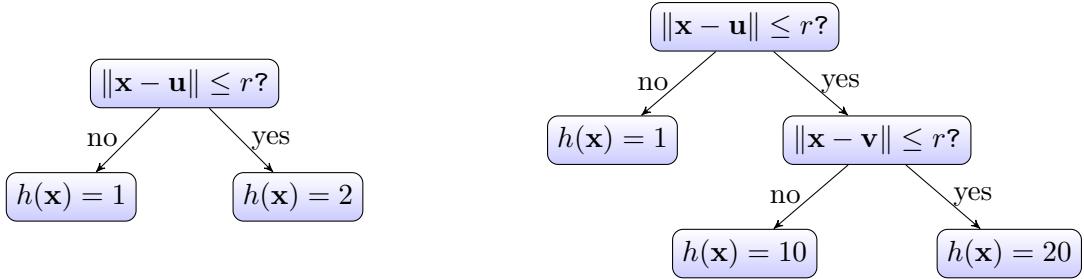


Figure 28: A hypothesis space  $\mathcal{H}$  consists of two decision trees with depth at most 2 and using the tests  $||\mathbf{x} - \mathbf{u}|| \leq r$  and  $||\mathbf{x} - \mathbf{v}|| \leq r$  with a fixed radius  $r$  and points  $\mathbf{u}$  and  $\mathbf{v}$ .

a decision tree which partitions the feature space such that each data point belongs to a different cluster.

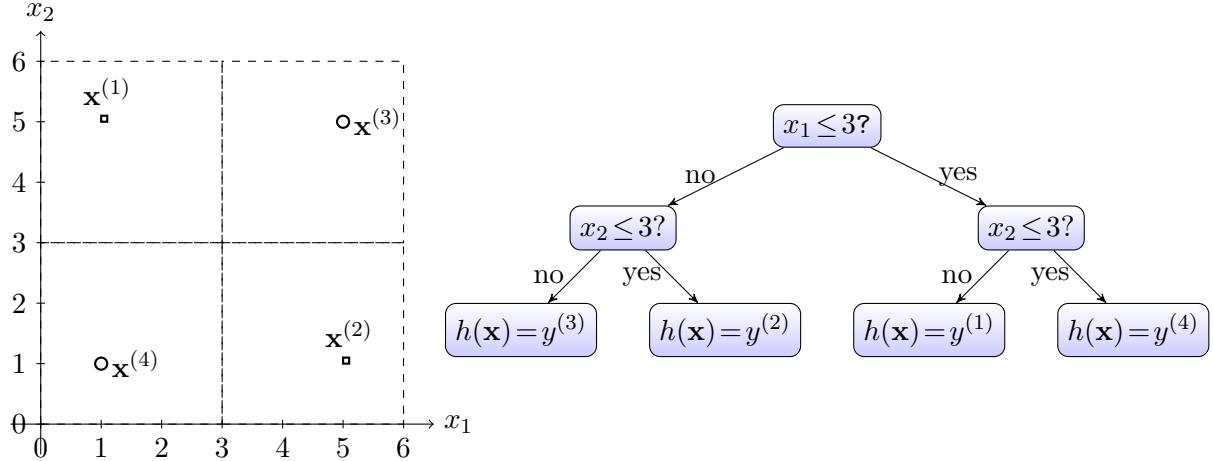


Figure 29: Using a decision tree we can construct a map  $h$  such that  $h(\mathbf{x}^{(i)}) = y^{(i)}$  for a given labeled dataset  $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ .

### 3.9 Artificial Neural Networks – Deep Learning

Another example of a hypothesis space, which has proven useful in a wide range of applications, e.g., image captioning or automated translation, is based on a **network representation** of a predictor  $h : \mathbb{R}^d \rightarrow \mathbb{R}$ . In particular, we can define a predictor  $h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R}$  using an **artificial neural network** (ANN) structure as depicted in Figure 30. A feature vector  $\mathbf{x} \in \mathbb{R}^d$  is fed into the

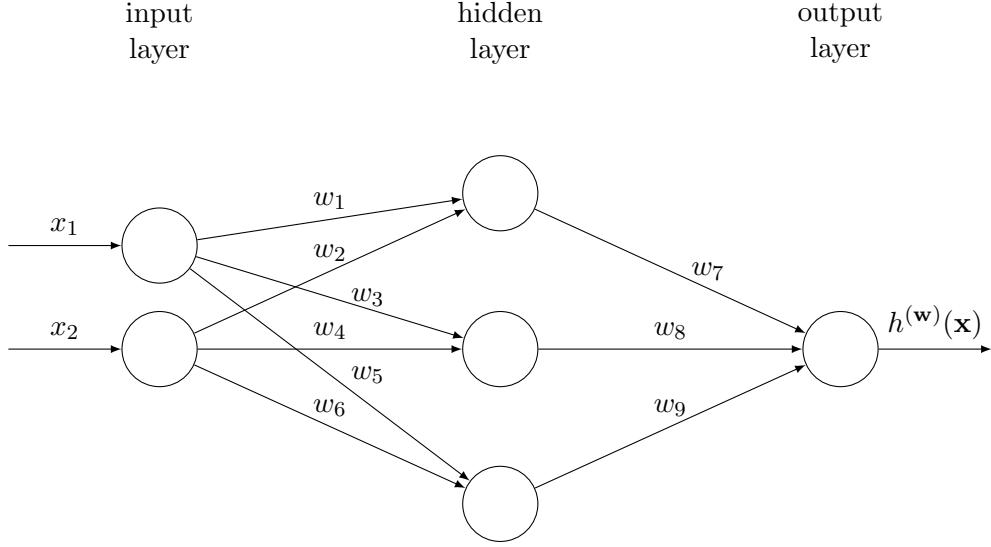


Figure 30: ANN representation of a predictor  $h^{(\mathbf{w})}(\mathbf{x})$  which maps the input (feature) vector  $\mathbf{x} = (x_1, x_2)^T$  to a predicted label (output)  $h^{(\mathbf{w})}(\mathbf{x})$ .

input units, each of which reads in one single feature  $x_i \in \mathbb{R}$ . The features  $x_i$  are then multiplied with the weights  $w_{j,i}$  associated with the link between the  $i$ -th input node (“neuron”) with the  $j$ -th node in the middle (hidden) layer. The output of the  $j$ -th node in the hidden layer is given by  $s_j = g(\sum_{i=1}^d w_{j,i}x_i)$  with some (typically highly non-linear) **activation function**  $g(z)$ . The input (or activation)  $z$  for the activation (or output)  $g(z)$  of a neuron is a weighted (linear) combination  $\sum_{i=1}^d w_{j,i}s_i$  of the outputs  $s_i$  of the nodes in the previous layer. For the ANN depicted in Figure 30, the activation of the neuron  $s_1$  is  $z = w_{1,1}x_1 + w_{1,2}x_2$ .

Two popular choices for the activation function used within ANNs are the **sigmoid function**  $g(z) = \frac{1}{1+\exp(-z)}$  or the **rectified linear unit**  $g(z) = \max\{0, z\}$ . An ANN with many, say 10, hidden layers, is often referred to as a **deep neural network** and the obtained ML methods are known as **deep learning** methods (see [1] for an in-depth introduction to deep learning methods).

It turns out that using a simple non-linear activation function  $g(z)$  as the building block for ANNs allows to represent an extremely large class of predictor maps  $h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R}$ . The hypothesis space generated by a given ANN structure, i.e., the set of all predictor maps which can be implemented by a given ANN and suitable weights  $\mathbf{w}$ , tends to be much larger than the hypothesis space (2) of linear predictors using weight vectors  $\mathbf{w}$  of the same length [1, Ch. 6.4.1.]. It can be shown that already ANN with one sufficiently large hidden layer can approximate an arbitrary

map  $h : \mathcal{X} \rightarrow \mathcal{Y} = \mathbb{R}$  to any desired accuracy [15]. However, it turns out that using several layers with few neurons, instead of one single layer containing many neurons, is computationally favorable [16].

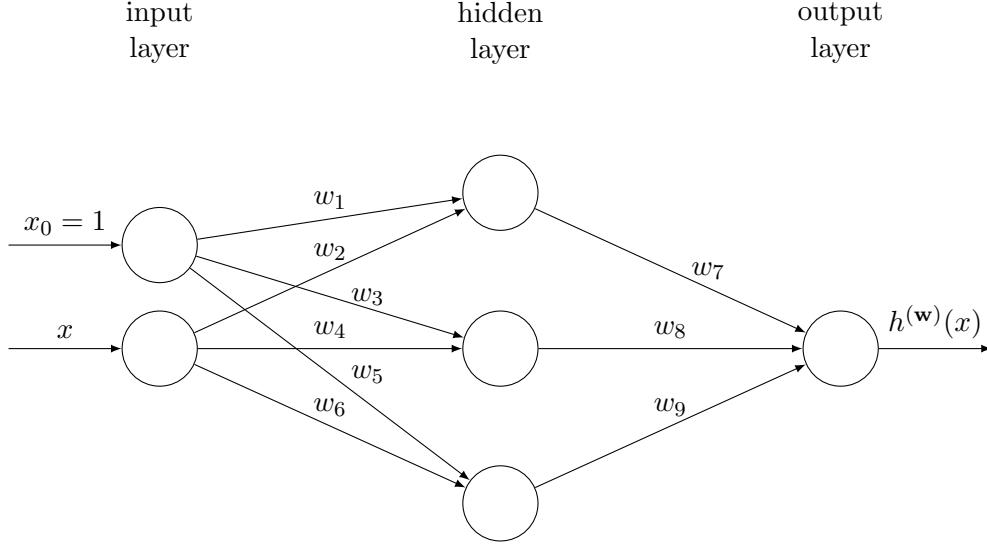


Figure 31: This ANN with one hidden layer defines a hypothesis space consisting of all maps  $h^{(\mathbf{w})}(x)$  obtained by implementing the ANN with different weight vectors  $\mathbf{w} = (w_1, \dots, w_9)^T$ .

**Exercise.** Consider the simple ANN structure in Figure 31 using the “ReLU” activation function  $g(z) = \max\{z, 0\}$  (see Figure 32). Show that there is a particular choice for the weights  $\mathbf{w} = (w_1, \dots, w_9)^T$  such that the resulting hypothesis map  $h^{(\mathbf{w})}(x)$  is a triangle as depicted in Figure 33. Can you also find a choice for the weights  $\mathbf{w} = (w_1, \dots, w_9)^T$  that produce the same triangle shape if we replace the ReLU activation function with the linear function  $g(z) = 10 \cdot z$ ?

The recent success of ML methods based on ANN with many hidden layers (which makes them deep) might be attributed to the fact that the network representation of hypothesis maps is beneficial for the computational implementation of ML methods. First, we can evaluate a map  $h^{(\mathbf{w})}$  represented by an ANN efficiently using modern parallel and distributed computing infrastructure via message passing over the network. Second, the ANN representation also allows to efficiently evaluate changes of weights  $\mathbf{w}$ . In particular, the gradient of the overall loss or empirical risk (see Section 5) can be obtained via a message passing procedure known as **back-propagation** [1].

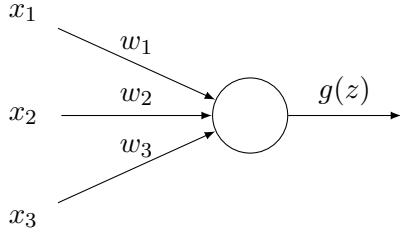


Figure 32: Each single neuron of the ANN depicted in Figure 31 implements a weighted summation  $z = \sum_i w_i x_i$  of its inputs  $x_i$  followed by applying a non-linear activation function  $g(z)$ .

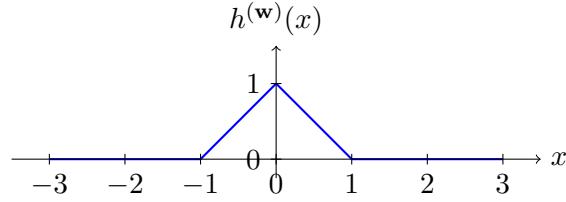


Figure 33: A hypothesis map with the shape of a triangle.

### 3.10 Maximum Likelihood

In many applications it is useful to model the observed data points  $\mathbf{z}^{(i)}$  as realizations of a random variable  $\mathbf{z}$  with probability distribution  $P(\mathbf{z}; \mathbf{w})$  which depends on some parameter vector  $\mathbf{w} \in \mathbb{R}^d$ . A principled approach to estimating the vector  $\mathbf{w}$  based on several independent and identically distributed (i.i.d.) realizations  $\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}$  is **maximum likelihood estimation** [17]. Maximum likelihood estimation can be interpreted as an ML problem with a hypothesis space parameterized by the weight vector  $\mathbf{w}$ , i.e., each element  $h^{(\mathbf{w})}$  of the hypothesis space  $\mathcal{H}$  corresponds to one particular choice for the weight vector  $\mathbf{w}$ , and loss function

$$\mathcal{L}(\mathbf{z}, h^{(\mathbf{w})}) := -\log P(\mathbf{z}; \mathbf{w}). \quad (28)$$

A widely used choice for the probability distribution  $P(\mathbf{z}; \mathbf{w})$  is a multivariate normal distribution with mean  $\boldsymbol{\mu}$  and covariance matrix  $\boldsymbol{\Sigma}$ , both of which constitute the weight vector  $\mathbf{w} = (\boldsymbol{\mu}, \boldsymbol{\Sigma})$  (we have to reshape the matrix  $\boldsymbol{\Sigma}$  suitably into a vector form). Given some i.i.d. data points  $\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}$ , we obtain the maximum likelihood estimates  $\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}$  of the mean and the covariance matrix by minimizing the empirical risk (see (28))

$$\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}} = \underset{\boldsymbol{\mu}, \boldsymbol{\Sigma}}{\operatorname{argmin}} (1/N) \sum_{i=1}^N -\log P(\mathbf{z}^{(i)}; (\boldsymbol{\mu}, \boldsymbol{\Sigma})). \quad (29)$$

The resulting estimates are

$$\hat{\boldsymbol{\mu}} = (1/N) \sum_{i=1}^N \mathbf{z}^{(i)}, \text{ and } \hat{\boldsymbol{\Sigma}} = (1/N) \sum_{i=1}^N (\mathbf{z}^{(i)} - \hat{\boldsymbol{\mu}})(\mathbf{z}^{(i)} - \hat{\boldsymbol{\mu}})^T. \quad (30)$$

### 3.11 $k$ -Nearest Neighbours

The class of  $k$  nearest neighbour ( $k$ -NN) predictors (with continuous label space, e.g.,  $\mathcal{Y} = \mathbb{R}$ ) or classifiers (with discrete label space  $\mathcal{Y} = \{-1, 1..\}$ ) is defined for feature spaces with an intrinsic notion of distance of a metric (such that  $\mathcal{X}$  is a metric space [14]). A prime example of such a metric space is  $\mathbb{R}^d$  with the Euclidean metric induced by the distance  $\|\mathbf{x} - \mathbf{y}\| = \sqrt{\sum_{r=1}^d (x_r - y_r)^2}$  between two vectors  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ .

The hypothesis space underlying  $k$ -NN problems consists of all maps  $h : \mathcal{X} \rightarrow \mathcal{Y}$  such that the function value  $h(\mathbf{x})$  for a particular feature vector  $\mathbf{x}$  depends only on the (labels of the)  $k$  nearest data points of some labeled training dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ . In contrast to the ML problems discussed above in Section 3.1 - Section 3.9, the hypothesis space of  $k$ -NN depends on the training data  $\mathbb{X}$ .

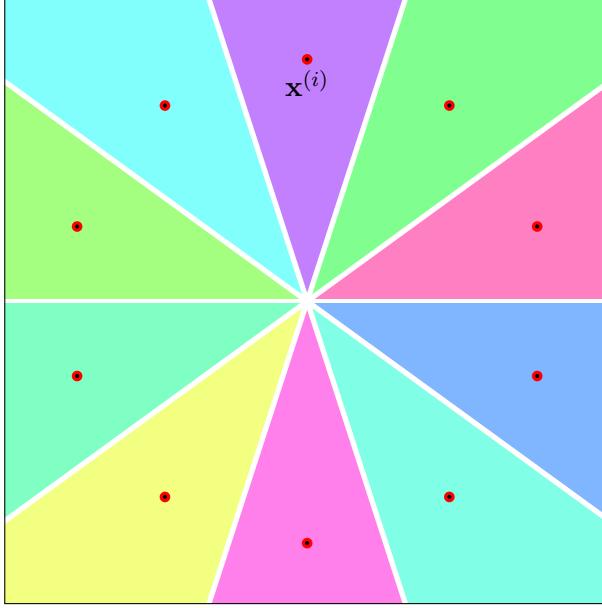


Figure 34: A hypothesis map  $h$  for  $k$ -NN with  $k = 1$  and feature space  $\mathcal{X} = \mathbb{R}^2$ . The hypothesis map is constant on regions (indicated by the coloured areas) located around data points  $\mathbf{x}^{(i)}$  indicated by a dot) of a dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}$ .

### 3.12 Network Lasso

Some important ML applications involve datasets which can be represented efficiently by an **empirical graph**  $\mathcal{G} = (\mathcal{V}, \mathcal{E})$  whose nodes  $\mathcal{V}$  represent individual data points  $\mathbf{x}^{(i)}$ . For example, the node  $i \in \mathcal{V}$  might represent a (super-)pixel in image processing, a neuron of a neural network [1] or a social network user profile [18].

These applications naturally suggest a notion of similarity between individual data points, e.g., the profiles of befriended social network users or greyscale values of neighbouring image pixels. These domain-specific notions of similarity are represented by the edges of the empirical graph  $\mathcal{G}$ , i.e., the nodes  $i, j \in \mathcal{V}$  representing similar data points  $\mathbf{x}^{(i)}$  and  $\mathbf{x}^{(j)}$  are connected by an undirected

edge  $\{i, j\} \in \mathcal{E}$ . We denote the neighbourhood of the node  $i \in \mathcal{V}$  by  $\mathcal{N}(i) := \{j \in \mathcal{V} : \{i, j\} \in \mathcal{E}\}$ .

In some applications it is possible to quantify the extent to which data points  $\mathbf{x}^{(i)}$  and  $\mathbf{x}^{(j)}$  are similar, e.g., via the Euclidean distance  $\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|$ . Given two similar data points  $i, j \in \mathcal{V}$ , which are connected by an edge  $\{i, j\} \in \mathcal{E}$ , we will quantify the strength of their connection by the edge weight  $W_{i,j} > 0$  which we collect in the symmetric weight matrix  $\mathbf{W} \in \mathbb{R}_+^{N \times N}$ . The absence of an edge between nodes  $i, j \in \mathcal{V}$  is encoded by a zero weight  $W_{i,j} = 0$ . Thus the edge structure of the empirical graph  $\mathcal{G}$  is fully specified by the support (locations of the non-zero entries) of the weight matrix  $\mathbf{W}$ .

Beside the empirical graph structure  $\mathcal{G}$ , a dataset typically conveys additional information, e.g., features, labels or model parameters. We represent this additional information by a graph signal defined over  $\mathcal{G}$ . A graph signal  $h[\cdot]$  is a map  $\mathcal{V} \rightarrow \mathbb{R}$ , which associates every node  $i \in \mathcal{V}$  with the signal value  $h[i] \in \mathbb{R}$  which represents a label  $y$  characterizing the data point.

Most methods for processing graph signals rely on a signal model which is inspired by a clustering hypothesis [19]. In particular, the graph signals obtained in some important application domains are smooth in the sense of having similar signal values  $h[i] \approx h[j]$  at nodes  $i, j \in \mathcal{V}$ , which belong to the same well-connected region (“cluster”) of the empirical graph. The clusterdness of a graph signal  $h[\cdot]$  can be measured by the total variation (TV):

$$\|h\|_{\text{TV}} = \sum_{\{i,j\} \in \mathcal{E}} W_{i,j} |h(i) - h(j)|. \quad (31)$$

Examples of application domains involving clustered graph signals are digital signal processing where time samples at adjacent time instants are strongly correlated for sufficiently high sampling rate. Moreover, many image processing methods rely on close-by pixels tending to be coloured likely which amounts to a clustered graph signal over the grid graph (representing the pixels).

The recently introduced network Lasso (nLasso) amounts to a formal ML problem involving network-structured data which can be represented by an empirical graph  $\mathcal{G}$ . In particular, the hypothesis space of nLasso is constituted by graph signals on  $\mathcal{G}$ :

$$\mathcal{H} = \{h : \mathcal{V} \rightarrow \mathcal{Y}\}. \quad (32)$$

The loss function of nLasso is a combination of squared error and TV (see (31))

$$\mathcal{L}((\mathbf{x}, y), h) = (y - h(\mathbf{x}))^2 + \lambda \|h\|_{\text{TV}}. \quad (33)$$

The regularization parameter  $\lambda$  allows to trade-off a small prediction error  $y - h(\mathbf{x})$  against clusterdness of the predictor  $h$ .

### 3.13 Logistic Network Lasso

The logistic network Lasso [20, 8] amounts to a classification problem involving network-structured data. As within the network Lasso (see Section 3.12), we consider network-structured datasets with associated empirical graph  $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{W})$ . Each data point  $\mathbf{z}$  has some features  $\mathbf{x}$  and is associated with a label  $y \in \mathcal{Y}$ , taking on values from a discrete label space  $\mathcal{Y}$ . The simplest setting is binary classification where each data point has a binary label  $y \in \{-1, 1\}$ . The hypothesis space underlying logistic network Lasso is given by the graph signals on the empirical graph:

$$\mathcal{H} = \{h : \mathcal{V} \rightarrow \mathcal{Y}\} \quad (34)$$

and the loss function is a combination of logistic loss and TV (which quantifies smoothness)

$$\mathcal{L}((\mathbf{x}, y), h) = -\log(1 + \exp(-yh(\mathbf{x}))) + \lambda\|h\|_{\text{TV}}. \quad (35)$$

## 4 Empirical Risk Minimization

As detailed in Section 2, the formal specification of an ML problem involves the feature space  $\mathcal{X}$  and label space  $\mathcal{Y}$  of the data points, a hypothesis space  $\mathcal{H}$  of possible predictor maps from features  $\mathbf{x}$  to labels  $y$ , and a loss function  $\mathcal{L}((\mathbf{x}, y), h)$  which is used to measure the quality of a particular predictor map  $h \in \mathcal{H}$ . In essence, ML methods automate the process of finding (or learning) a good (accurate) hypothesis map out of  $\mathcal{H}$ . Thus, in a certain sense, ML methods are just particular optimization methods.

In particular, for a given hypothesis space (e.g., the space of linear maps (2)) and labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , we would like to find the particular predictor within  $\mathcal{H}$  which minimizes the empirical risk (9). Thus, we end up with an **empirical risk minimization (ERM) problem**

$$\begin{aligned}\hat{h} &= \underset{h \in \mathcal{H}}{\operatorname{argmin}} \mathcal{E}(h|\mathbb{X}) \\ &\stackrel{(9)}{=} \underset{h \in \mathcal{H}}{\operatorname{argmin}} \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h).\end{aligned}\quad (36)$$

The task of solving (36) amounts to learning (finding) a good predictor  $\hat{h}$  by “training” it on the dataset  $\mathbb{X}$ , which is therefore referred to as the **training dataset**.

Solving the optimization problem (36) provides two things. First, the minimizer  $\hat{h}$  defines a predictor which performs well, i.e., incurs a small loss on average on the labeled dataset  $\mathbb{X}$ . Second, the corresponding objective value  $\mathcal{E}(\hat{h}|\mathbb{X})$  (the “training error”) indicates how accurate the predictions of  $\hat{h}$  will be. However, as we will discuss in Section 7.1, for certain ML problems, the training error  $\mathcal{E}(\hat{h}|\mathbb{X})$  obtained for the dataset  $\mathbb{X}$  can be very different from the general accuracy of  $\hat{h}$  when applied to new data points which are not contained in  $\mathbb{X}$ .

Given a parameterization  $h^{(\mathbf{w})}(\mathbf{x})$  of the predictor maps in the hypothesis space  $\mathcal{H}$ , such as within linear regression (2) or for ANNs (see Figure 30), we can reformulate the optimization problem (36) (with optimization domain being a function space!) as an optimization directly over the weight vector:

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}) \text{ with } f(\mathbf{w}) := \mathcal{E}(h^{(\mathbf{w})}|\mathbb{X}). \quad (37)$$

The objective function  $f(\mathbf{w})$  in (37) is the empirical risk  $\mathcal{E}(h^{(\mathbf{w})}|\mathbb{X})$  achieved by  $h^{(\mathbf{w})}$  when applied to the data points in the dataset  $\mathbb{X}$ .

The two formulations (37) and (36) are fully equivalent for a parametrized hypothesis space  $\mathcal{H}$ . In particular, given the optimal weight vector  $\mathbf{w}_{\text{opt}}$  solving (37), the predictor  $h^{(\mathbf{w}_{\text{opt}})}$  is an optimal predictor solving (36).

The idea of learning a good predictor map via ERM (36) conforms with the notion of learning by “trial and error”: Some instructor or supervisor provides snapshots  $\mathbf{z}^{(i)}$  with features  $\mathbf{x}^{(i)}$  and known labels  $y^{(i)}$ . We then try out some predictor map  $h$  in order to tell the label  $y^{(i)}$  only from the snapshot features  $\mathbf{x}^{(i)}$  and determine the (training) error  $\mathcal{E}(h|\mathbb{X})$  incurred. If the error  $\mathcal{E}(h|\mathbb{X})$  is too large we try out another predictor map  $h'$  instead of  $h$  with the hope of achieving a smaller training error  $\mathcal{E}(h'|\mathbb{X})$ .

This principle of learning by supervision, i.e., using labeled data points (“training examples”), could also be used to model the development of language in human brains (“concept learning”). Consider a child, who should learn the concept “tractor” (see Figure 4). We could try to show many different pictures to the child and for each picture say “tractor” or “no tractor”. Based on this

“labeled data”, the child tries to learn the relation between features of an image and the presence (or absence) of a tractor in the image.



Figure 35: A bunch of labeled images. The label  $y$  of an image indicates if a tractor is shown ( $y = 1$ ) or not ( $y = -1$ ).

We highlight that the precise shape of the objective function  $f(\mathbf{w})$  in (37) depends heavily on the parametrization of the predictor functions, i.e., how does the predictor  $h^{(\mathbf{w})}$  vary with the weight vector  $\mathbf{w}$ . Moreover, the shape of  $f(\mathbf{w})$  depends also on the choice for the loss function  $\mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h)$ . As depicted in Figure 36, the different combinations of predictor parametrisation and loss functions can result in objective functions with fundamentally different properties such that their optimization is more or less difficult.

The objective function  $f(\mathbf{w})$  for the ERM obtained for linear regression (see Section 3.1) is differentiable and convex and can therefore be minimized using simple iterative gradient descent methods (see Section 5). In contrast, the objective function  $f(\mathbf{w})$  of ERM obtained for the SVM (see Section 3.5) is non-differentiable but still convex. The minimization of such functions is more challenging but still tractable as there exist efficient convex optimization methods which do not require differentiability of the objective function [21]. The objective function  $f(\mathbf{w})$  obtained for ANN tends to be **highly non-convex** but still differentiable for particular activation functions. The optimization of non-convex objective function is in general more difficult than optimizing convex objective functions. However, it turns out that despite the non-convexity, iterative gradient based methods can still be successfully applied to solve the ERM [1]. Even more challenging is the ERM obtained for decision trees or Bayes’ classifiers which amount to non-differentiable and non-convex objective functions.

In what follows, we discuss the structure of the ERM obtained for three particular ML problems: In Section 4.1, we discuss the ERM obtained for linear regression (see Section 3.1). The

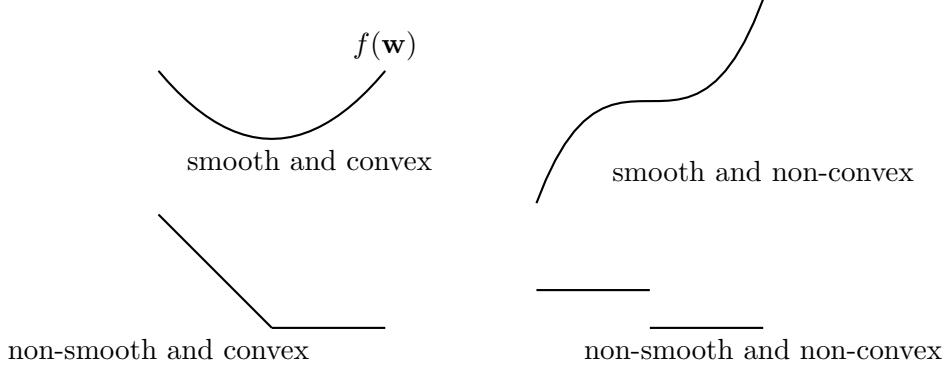


Figure 36: Different types of objective functions obtained for ERM in different settings.

resulting ERM has appealing properties as it amounts to minimizing a differentiable (smooth) and convex function which can be done efficiently using efficient gradient based methods (see Section 5). We then discuss in Section 4.2 the ERM obtained for decision trees which yields a discrete optimization problem and is therefore fundamentally different from the smooth ERM obtained for linear regression. In particular, we cannot apply gradient based methods (see Section 5) to solve them but have to rely on discrete search methods. Finally, in Section 4.3, we discuss how Bayes' methods can be used to solve the non-convex and non-differentiable ERM problem obtained for classification problems with the 0/1 loss (5).

#### 4.1 ERM for Linear Regression

Let us now focus on linear regression problem (see Section 3.1) which is based on the particular combination of squared error loss (4) and linear predictor maps of the form  $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$ . For this particular combination, we can rewrite the ERM problem (37) as

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}) \text{ with objective function } f(\mathbf{w}) := (1/|\mathbb{X}|) \sum_{(\mathbf{x}, y) \in \mathbb{X}} (y - \mathbf{x}^T \mathbf{w})^2. \quad (38)$$

Here,  $|\mathbb{X}|$  denotes the cardinality (number of elements) of the set  $\mathbb{X}$ . The objective function  $f(\mathbf{w})$  in (38) has some appealing properties, since it is convex and smooth (see Section 5).

It will be useful to rewrite the ERM problem (38) using matrix and vector representations of the feature vectors  $\mathbf{x}^{(i)}$  and labels  $y^{(i)}$  contained in the dataset  $\mathbb{X}$ . To this end, we stack the labels  $y^{(i)}$  and the feature vectors  $\mathbf{x}^{(i)}$ , for  $i = 1, \dots, N$ , into a “label vector”  $\mathbf{y}$  and “feature matrix”  $\mathbf{X}$  as follows

$$\mathbf{y} = (y^{(1)}, \dots, y^{(N)})^T \in \mathbb{R}^N, \text{ and } \mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})^T \in \mathbb{R}^{N \times d}. \quad (39)$$

This allows us to rewrite the objective function in (38) more compactly as

$$f(\mathbf{w}) = (1/N) \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2. \quad (40)$$

Using (40), we can rewrite the optimization problem (38) as a quadratic problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \underbrace{(1/2)\mathbf{w}^T \mathbf{Q}\mathbf{w} - \mathbf{q}^T \mathbf{w}}_{=f(\mathbf{w})} \text{ with } \mathbf{Q} = (1/N)\mathbf{X}^T \mathbf{X}, \mathbf{q} = (1/N)\mathbf{X}^T \mathbf{y}. \quad (41)$$

Since  $f(\mathbf{w})$  is a differentiable and convex function, a necessary and sufficient condition for some  $\mathbf{w}_0$  to satisfy  $f(\mathbf{w}_0) = \min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w})$  is the **zero-gradient condition** [22, Sec. 4.2.3]

$$\nabla f(\mathbf{w}_{\text{opt}}) = \mathbf{0}. \quad (42)$$

Combining (41) with (42), yields the following sufficient and necessary condition for a weight vector  $\mathbf{w}_{\text{opt}}$  to solve the ERM (38):

$$(1/N)\mathbf{X}^T \mathbf{X} \mathbf{w}_{\text{opt}} = (1/N)\mathbf{X}^T \mathbf{y}. \quad (43)$$

It can be shown that, for any given feature matrix  $\mathbf{X}$  and label vector  $\mathbf{y}$ , there always exists at least one optimal weight vector  $\mathbf{w}_{\text{opt}}$  which solves (43). The optimal weight vector might not be unique, such that there are several different vectors which achieve the minimum in (38). However, any optimal solution  $\mathbf{w}_{\text{opt}}$ , which solves (43), achieves the same minimum empirical risk

$$\mathcal{E}(h^{(\mathbf{w}_{\text{opt}})} | \mathbb{X}) = \min_{\mathbf{w} \in \mathbb{R}^d} \mathcal{E}(h^{(\mathbf{w})} | \mathbb{X}) = \|(\mathbf{I} - \mathbf{P})\mathbf{y}\|^2. \quad (44)$$

Here, we used the orthogonal projection matrix  $\mathbf{P} \in \mathbb{R}^{N \times N}$  on the linear span of the feature matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})^T \in \mathbb{R}^{N \times d}$  (see (39)).<sup>6</sup>

If the feature matrix  $\mathbf{X}$  (see (39)) has full column rank, implying invertibility of the matrix  $\mathbf{X}^T \mathbf{X}$ , the projection matrix  $\mathbf{P}$  is given explicitly as

$$\mathbf{P} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T.$$

Moreover, in this case, the solution of (43) is unique and given by

$$\mathbf{w}_{\text{opt}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}. \quad (45)$$

The closed-form solution (45) requires the inversion of the  $d \times d$  matrix  $\mathbf{X}^T \mathbf{X}$ . Computing the inverse can be computationally challenging for large feature length  $d$  (see Figure 5 for a simple ML problem where the feature length is almost a million). Moreover, inverting a matrix which is close to singular typically introduces numerical errors.

In Section 5.3, we will discuss an alternative method for computing (approximately) the optimal weight vector  $\mathbf{w}_{\text{opt}}$  which does not require any matrix inversion. This alternative method, referred to as “gradient descent”, is based on constructing a sequence  $\mathbf{w}^{(0)}, \mathbf{w}^{(1)}, \dots$  of increasingly accurate approximations of  $\mathbf{w}_{\text{opt}}$ . Two particular benefits of using this iterative method, instead of using the formula (45), for computing  $\mathbf{w}_{\text{opt}}$  are (i) it is computationally cheaper and (ii) it also works when the matrix  $\mathbf{X}$  is not full rank in which case the formula (45) becomes invalid.

## 4.2 ERM for Decision Trees

Let us now consider the ERM problem (36) for a regression problem with label space  $\mathcal{Y} = \mathbb{R}$ , feature space  $\mathcal{X} = \mathbb{R}^d$  and using a hypothesis space defined by decision trees (see Section 3.8). In stark contrast to the ERM problem obtained for linear or logistic regression, the ERM problem obtained for decision trees amounts to a **discrete optimization problem**. Consider the particular hypothesis space  $\mathcal{H}$  depicted in Figure 28. This hypothesis space contains a finite number of predictor maps, each map corresponding to a particular decision tree.

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<sup>6</sup>The linear span  $\text{span}(\mathbf{A})$  of a matrix  $\mathbf{A} = (\mathbf{a}^{(1)}, \dots, \mathbf{a}^{(N)}) \in \mathbb{R}^{d \times N}$  is the subspace of  $\mathbb{R}^d$  consists of all possible linear combinations of the columns  $\mathbf{a}^{(r)}$  of  $\mathbf{A}$ .

For the small hypothesis space  $\mathcal{H}$  in Figure 28, the ERM problem is easy since we just have to evaluate the empirical risk for each of the elements in  $\mathcal{H}$  and pick the one yielding the smallest. However, in ML applications we typically use significantly larger hypothesis spaces and then discrete optimization tends to be more complicated compared to smooth optimization which can be solved by (variants of) gradient descent (see Section 5).

A popular approach to ERM for decision trees is to use greedy algorithms which try to expand (grow) a given decision tree by adding new branches to leaf nodes in order to reduce the empirical risk (see [23, Chapter 8] for more details).

The idea behind many decision tree learning methods is quite simple: try out expanding a decision tree by replacing a leaf node with a decision node (implementing another “test” on the feature vector) in order to reduce the overall empirical risk as much as possible.

Consider the labeled dataset  $\mathbb{X}$  depicted in Figure 37 and a given decision tree for predicting the label  $y$  based on the features  $\mathbf{x}$ . We start with a very simple tree shown in the top of Figure 37. Then we try out growing the tree by replacing a leaf node with a decision node. According to Figure 37, replacing the right leaf node results in a decision tree which is able to perfectly represent the training dataset (it achieves zero empirical risk).

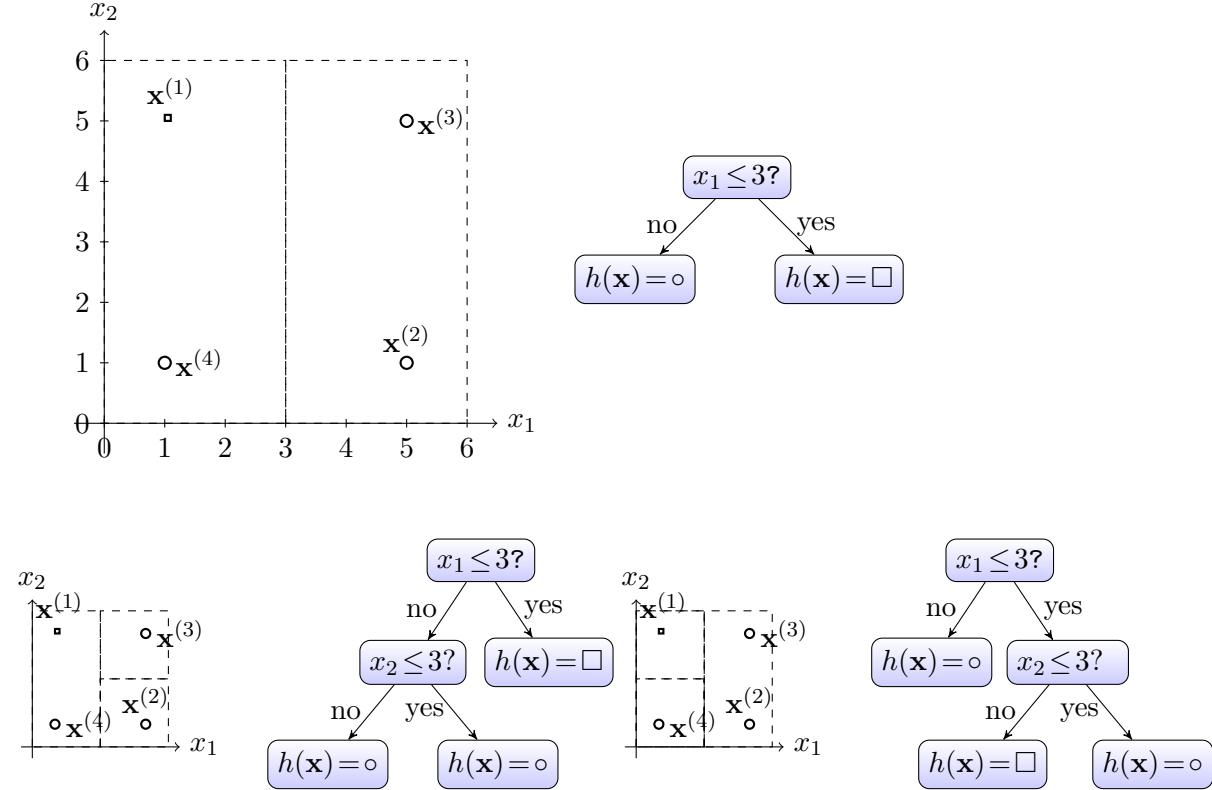


Figure 37: Given the labeled dataset and a decision tree in the top row, we would like to grow the decision tree by expanding it at one of its two leaf nodes. The resulting new decision trees obtained by expanding different leaf node is shown in the bottom row.

One important aspect of learning decision trees from labeled data is the question of when to

stop growing. A natural stopping criterion might be obtained from the limitations in computational resources, i.e., we can only afford to use decision trees up to certain maximum depth. Beside the computational limitations, we also face statistical limitations for the maximum size of decision trees. Indeed, if we allow very large decision trees, which represent highly complicated maps, we might end up overfitting the training data (see Figure 29 and Section 7.1) which is detrimental for the prediction performance of decision trees obtained for new data (which has not been used for training or growing the decision tree).

### 4.3 ERM for Bayes' Classifiers

The family of Bayes' classifiers is based on using the 0/1 loss (5) for measuring the quality of a classifier  $h$ . The resulting ERM is

$$\begin{aligned}\hat{h} &= \operatorname{argmin}_{h \in \mathcal{H}} (1/N) \sum_{i=1}^N \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h) \\ &\stackrel{(5)}{=} \operatorname{argmin}_{h \in \mathcal{H}} (1/N) \sum_{i=1}^N \mathcal{I}(h(\mathbf{x}^{(i)}) \neq y^{(i)}).\end{aligned}\quad (46)$$

Note that the objective function of this optimization problem is non-smooth (non differentiable) and non-convex (see Figure 36). This prevents us from using standard gradient based optimization methods (see Section 5) to solve (46).

We will now approach the ERM (46) via a different route by interpreting the data points  $(\mathbf{x}^{(i)}, y^{(i)})$  as realizations of i.i.d. random variables which are distributed according to some probability distribution  $p(\mathbf{x}, y)$ . As discussed in Section 2.3, the empirical risk obtained using 0/1 loss approximates the error probability  $P(\hat{y} \neq y)$  with the predicted label  $\hat{y} = 1$  for  $h(\mathbf{x}) > 0$  and  $\hat{y} = -1$  otherwise (see (6)). Thus, we can approximate the ERM (46) as

$$\hat{h} \stackrel{(6)}{\approx} \operatorname{argmin}_{h \in \mathcal{H}} P(\hat{y} \neq y). \quad (47)$$

Note that the hypothesis  $h$ , which is the optimization variable in (47), enters into the objective function of (47) via the definition of the predicted label  $\hat{y}$ , which is  $\hat{y} = 1$  if  $h(\mathbf{x}) > 0$  and  $\hat{y} = -1$  otherwise.

It turns out that if we would know the probability distribution  $p(\mathbf{x}, y)$ , which is required to compute  $P(\hat{y} \neq y)$ , the solution of (47) can be found easily via elementary Bayesian decision theory [24]. In particular, the optimal classifier  $h(\mathbf{x})$  is such that  $\hat{y}$  achieves the maximum a-posteriori probability  $p(\hat{y}|\mathbf{x})$  of the label being  $\hat{y}$ , given (or conditioned on) the features  $\mathbf{x}$ . However, since we do not know the probability distribution  $p(\mathbf{x}, y)$ , we have to estimate (or approximate) it from the observed data points  $(\mathbf{x}^{(i)}, y^{(i)})$  which are modelled as i.i.d. random variables distributed according to  $p(\mathbf{x}, y)$ .

The estimation of  $p(\mathbf{x}, y)$  can be based on a particular probabilistic model for the features and labels which depends on certain parameters and then determining the parameters using maximum likelihood (see Section 3.10). A widely used probabilistic model is based on Gaussian random vectors. In particular, conditioned on the label  $y$ , we model the feature vector  $\mathbf{x}$  as a Gaussian

vector with mean  $\boldsymbol{\mu}_y$  and covariance  $\boldsymbol{\Sigma}$ , i.e.,

$$p(\mathbf{x}|y) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_y, \boldsymbol{\Sigma}).^7 \quad (48)$$

Note that the mean vector of  $\mathbf{x}$  depends on the label such that for  $y = 1$  the mean of  $\mathbf{x}$  is  $\boldsymbol{\mu}_1$ , while for data points with label  $y = -1$  the mean of  $\mathbf{x}$  is  $\boldsymbol{\mu}_{-1}$ . In contrast, the covariance matrix  $\boldsymbol{\Sigma} = \mathbb{E}\{(\mathbf{x} - \boldsymbol{\mu}_y)(\mathbf{x} - \boldsymbol{\mu}_y)^T|y\}$  of  $\mathbf{x}$  is the same for both values of the label  $y \in \{-1, 1\}$ . Note that, while conditioned on  $y$  the random vector  $\mathbf{x}$  is Gaussian, the marginal distribution of  $\mathbf{x}$  is a Gaussian mixture model (see Section 8.2). For this probabilistic model of features and labels, the optimal classifier (which minimizes the error probability  $P(\hat{y} \neq y)$ ) is given as  $\hat{y} = 1$  for  $h(\mathbf{x}) > 0$  and  $\hat{y} = -1$  for  $h(\mathbf{x}) \leq 0$  using the classifier map

$$h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} \text{ with the weight vector } \mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_{-1}). \quad (49)$$

Carefully note that this expression is only valid if the matrix  $\boldsymbol{\Sigma}$  is invertible.

We cannot implement the classifier (49) directly, since we do not know the true values of the class-specific mean vectors  $\boldsymbol{\mu}_1$ ,  $\boldsymbol{\mu}_{-1}$  and covariance matrix  $\boldsymbol{\Sigma}$ . Therefore, we have to replace those unknown parameters with some estimates  $\hat{\boldsymbol{\mu}}_1$ ,  $\hat{\boldsymbol{\mu}}_{-1}$  and  $\hat{\boldsymbol{\Sigma}}$ , like the maximum likelihood estimates which are given by (see (30))

$$\begin{aligned} \hat{\boldsymbol{\mu}}_1 &= (1/N_1) \sum_{i=1}^N \mathcal{I}(y^{(i)} = 1) \mathbf{x}^{(i)}, \\ \hat{\boldsymbol{\mu}}_{-1} &= (1/N_{-1}) \sum_{i=1}^N \mathcal{I}(y^{(i)} = -1) \mathbf{x}^{(i)}, \\ \hat{\boldsymbol{\mu}} &= (1/N) \sum_{i=1}^N \mathbf{x}^{(i)}, \\ \text{and } \hat{\boldsymbol{\Sigma}} &= (1/N) \sum_{i=1}^N (\mathbf{z}^{(i)} - \hat{\boldsymbol{\mu}})(\mathbf{z}^{(i)} - \hat{\boldsymbol{\mu}})^T, \end{aligned} \quad (50)$$

with  $N_1 = \sum_{i=1}^N \mathcal{I}(y^{(i)} = 1)$  denoting the number of data points with label  $y = 1$  ( $N_{-1}$  is defined similarly). Inserting the estimates (50) into (49) yields the (implementable) Bayes classifier

$$h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} \text{ with the weight vector } \mathbf{w} = \hat{\boldsymbol{\Sigma}}^{-1}(\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_{-1}). \quad (51)$$

We highlight that the classifier (51) is only well-defined if the estimated covariance matrix  $\hat{\boldsymbol{\Sigma}}$  (50) is invertible. This requires to use a sufficiently large number of training data points such that  $N \geq d$ .

Using the route via maximum likelihood estimation, we arrived at (51) as an approximate solution to the ERM (46). The final classifier (51) turns out to be a linear classifier very much like logistic regression and SVM. In particular, the classifier (51) partitions the feature space  $\mathbb{R}^d$

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<sup>7</sup>We use the shorthand  $\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$  to denote the probability density function

$$p(\mathbf{x}) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

of a Gaussian random vector  $\mathbf{x}$  with mean  $\boldsymbol{\mu} = \mathbb{E}\{\mathbf{x}\}$  and covariance matrix  $\boldsymbol{\Sigma} = \mathbb{E}\{(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\}$ .

into two halfspaces: one for  $\hat{y} = 1$  and one for  $\hat{y} = -1$  (see Figure 14). Thus, the Bayes' classifier (51) belongs to the same family (of linear classifiers) as logistic regression and the SVM. These three classification methods differ only in the way of choosing the decision boundary (see Figure 14) separating the two half-spaces in the feature space.

It turns out that accuracy of the estimate  $\hat{\Sigma}$  (30) for the covariance matrix requires a number of data points which is on the order of  $d^2$  which might be infeasible in applications with only few data points. Moreover, the maximum likelihood estimate  $\hat{\Sigma}$  (50) is not invertible whenever  $N < d$  such that the expression (51) becomes useless in this case. A helpful approach is then to make additional simplifying assumptions such as requiring the covariance to be diagonal  $\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_d^2)$ . This is equivalent to modelling the individual features  $x_1, \dots, x_d$  as conditionally independent, given the label  $y$  of a data point (this special case of a Bayes' classifier is referred to as **naive Bayes** classifier).

We finally highlight that the classifier (51) is obtained using the generative model (48) for the data. Therefore, Bayes' classifiers belong to the family of generative ML methods which involve modelling the data generation. In contrast, logistic regression and SVM do not require a generative model for the data points but aim directly at finding the relation between features  $\mathbf{x}$  and label  $y$  of a data point. These methods belong therefore to the family of discriminative ML methods. Generative methods such as Bayes' classifier are preferable for applications with only very limited amounts of labeled data. Indeed, having a generative model such as (48) allows to synthetically generate more labeled data by generating random features and labels according to the probability distribution (48). We refer to [25] for a more detailed comparison between generative and discriminative methods.

## 5 Gradient Descent

In the following, we will mainly focus on ML problems with hypothesis space  $\mathcal{H}$  consisting of predictor maps  $h^{(\mathbf{w})}$  which are parametrized by a weight vector  $\mathbf{w} \in \mathbb{R}^d$ . Moreover, for a given data point with features  $\mathbf{x}$  and label  $y$ , the loss function  $\mathcal{L}((\mathbf{x}, y), h^{(\mathbf{w})})$  depends smoothly on the weight vector  $\mathbf{w}$ . This requirement on the loss function is not too restrictive as many important ML problems, including linear regression (see Section 3.1) and logistic regression (see Section 3.4), result in a smooth loss function.<sup>8</sup>

For a smooth loss function, the resulting ERM (see (37))

$$\begin{aligned}\mathbf{w}_{\text{opt}} &= \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \mathcal{E}(h^{(\mathbf{w})} \mid \mathbb{X}) \\ &= (1/N) \underbrace{\sum_{i=1}^N \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})})}_{:=f(\mathbf{w})}\end{aligned}\quad (52)$$

is a **smooth optimization problem**. A smooth optimization problem is of the form

$$\min_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w}) \quad (53)$$

with a smooth function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  of the vector argument  $\mathbf{w} \in \mathbb{R}^d$ . It turns out that a smooth function  $f(\mathbf{w})$  can be approximated locally around a point  $\mathbf{w}_0$  using a hyperplane, which passes through the point  $(\mathbf{w}_0, f(\mathbf{w}_0))$  and having normal vector  $\mathbf{n} = (\nabla f(\mathbf{w}_0), -1)$  (see Figure 38). Indeed, basic analysis yields the following linear approximation (around a point  $\mathbf{w}_0$ ) [14]

$$f(\mathbf{w}) \approx f(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^T \nabla f(\mathbf{w}_0) \text{ for all } \mathbf{w} \text{ close to } \mathbf{w}_0. \quad (54)$$

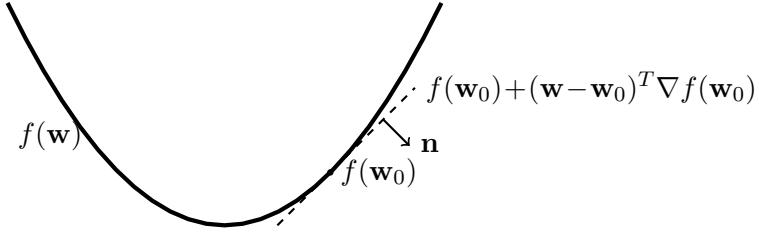


Figure 38: A smooth function  $f(\mathbf{w})$  can be approximated locally around a point  $\mathbf{w}_0$  using a hyperplane whose normal vector  $\mathbf{n} = (\nabla f(\mathbf{w}_0), -1)$  is determined by the gradient  $\nabla f(\mathbf{w}_0)$ .

### 5.1 The Basic GD Step

We now discuss a very simple, yet quite powerful, algorithm for finding the weight vector  $\mathbf{w}_{\text{opt}}$  which solves continuous optimization problems like (52). Let us assume we have already some

<sup>8</sup>A smooth function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  has continuous partial derivatives of all orders. In particular, we can define the gradient  $\nabla f(\mathbf{w})$  for a smooth function  $f(\mathbf{w})$  at every point  $\mathbf{w}$ .

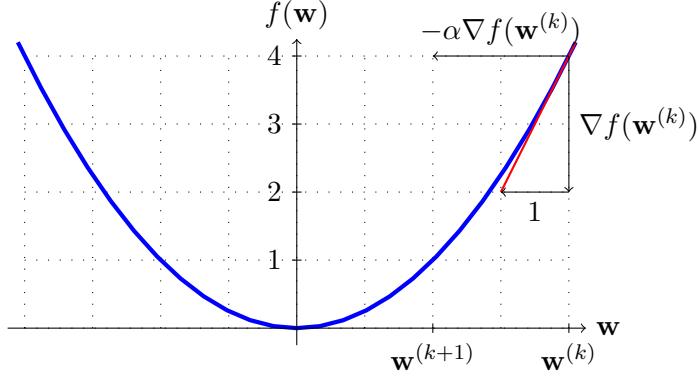


Figure 39: The GD step (55) amounts to a shift by  $-\alpha \nabla f(\mathbf{w}^{(k)})$ .

guess (or approximation)  $\mathbf{w}^{(k)}$  for the optimal weight vector  $\mathbf{w}_{\text{opt}}$  and would like to improve it to a new guess  $\mathbf{w}^{(k+1)}$  which yields a smaller value of the objective function  $f(\mathbf{w}^{(k+1)}) < f(\mathbf{w}^{(k)})$ . For a differentiable objective function  $f(\mathbf{w})$ , we can use the approximation  $f(\mathbf{w}^{(k+1)}) \approx f(\mathbf{w}^{(k)}) + (\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)})^T \nabla f(\mathbf{w}^{(k)})$  (cf. (54)) for  $\mathbf{w}^{(k+1)}$  not too far away from  $\mathbf{w}^{(k)}$ . Thus, we should be able to enforce  $f(\mathbf{w}^{(k+1)}) < f(\mathbf{w}^{(k)})$  by choosing

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha \nabla f(\mathbf{w}^{(k)}) \quad (55)$$

with a sufficiently small **step size**  $\alpha > 0$  (a small  $\alpha$  ensures that the linear approximation (54) is valid). Then, we repeat this procedure to obtain  $\mathbf{w}^{(k+2)} = \mathbf{w}^{(k+1)} - \alpha \nabla f(\mathbf{w}^{(k+1)})$  and so on.

The update (55) amounts to a **gradient descent (GD) step**. It turns out that for a convex differentiable objective function  $f(\mathbf{w})$  and sufficiently small step size  $\alpha$ , the iterates  $f(\mathbf{w}^{(k)})$  obtained by repeating the GD steps (55) converge to a minimum, i.e.,  $\lim_{k \rightarrow \infty} f(\mathbf{w}^{(k)}) = f(\mathbf{w}_{\text{opt}})$  (see Figure 39). When the GD step is used within an ML method (see Section 5.3 and Section 3.4), the step size  $\alpha$  is also referred to as the **learning rate**.

In order to implement the GD step (55) we need to choose the step size  $\alpha$  and we need to be able to compute the gradient  $\nabla f(\mathbf{w}^{(k)})$ . Both tasks can be very challenging for an ML problem. The success of deep learning methods, which are based on ANN representation of predictor maps (see Section 3.9), can be attributed to some extend to the ability of computing the gradient  $\nabla f(\mathbf{w}^{(k)})$  efficiently via the back-propagation method [1]. For the particular case of linear regression (see Section 3.1) and logistic regression (see Section 5.4), we will present precise conditions on the step size  $\alpha$  which guarantee convergence of GD in Section 5.3 and Section 5.4. Moreover, the objective functions  $f(\mathbf{w})$  arising within linear and logistic regression allow for closed-form expressions of the gradient  $\nabla f(\mathbf{w})$ .

## 5.2 Choosing Step Size

The choice of the step size  $\alpha$  in the GD step (55) has a significant influence on the performance of Algorithm 1. If we choose the step size  $\alpha$  too large, the GD steps (55) diverge (see Figure 40-(b)) and in turn, Algorithm 1 to fail in delivering an approximation of the optimal weight vector  $\mathbf{w}_{\text{opt}}$  (see (58)). If we choose the step size  $\alpha$  too small (see Figure 40-(a)), the updates (55) make

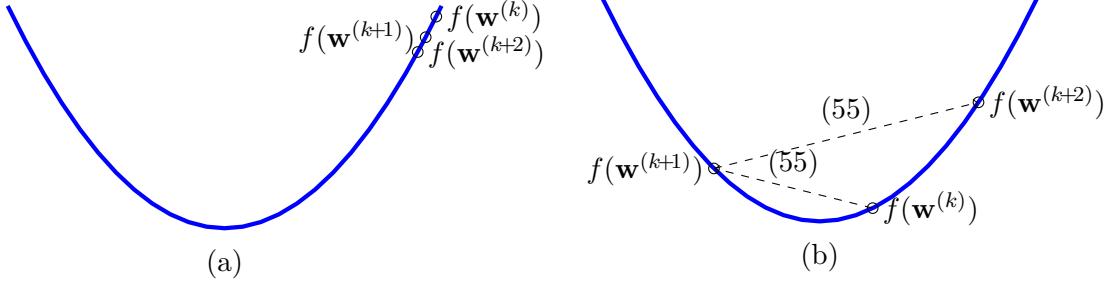


Figure 40: Effect of choosing learning rate  $\alpha$  in GD step (55) too small (a) or too large (b). If the steps size  $\alpha$  in the GD step (55) is chosen too small, the iterations make only very little progress towards the optimum. If the learning rate  $\alpha$  is chosen too large, the iterates  $\mathbf{w}^{(k)}$  might not converge at all (it might happen that  $f(\mathbf{w}^{(k+1)}) > f(\mathbf{w}^{(k)})$ !).

only very little progress towards approximating the optimal weight vector  $\mathbf{w}_{\text{opt}}$ . Again, this will typically make Algorithm 1 failing in delivering a good approximation of  $\mathbf{w}_{\text{opt}}$ .

The optimal choice of the step size  $\alpha$  of GD can be a challenging task and many sophisticated approaches have been proposed for its solution (see [1, Chapter 8]). We will restrict ourselves to a simple sufficient condition on the step size which guarantees convergence of the GD iterations  $\mathbf{w}^{(k)}$  for  $k = 1, 2, \dots$ . In particular, for a convex and smooth objective function  $f(\mathbf{w})$ , the iterates generated by the GD step (55) converge to an optimum  $\mathbf{w}_{\text{opt}}$  if the step size  $\alpha$  satisfies [26]

$$\alpha \leq \frac{1}{\lambda_{\max}(\nabla^2 f(\mathbf{w}))} \text{ for all } \mathbf{w} \in \mathbb{R}^d. \quad (56)$$

Here, we use the Hessian matrix  $\nabla^2 f(\mathbf{w}) \in \mathbb{R}^{d \times d}$  of a smooth function  $f(\mathbf{w})$  whose entries are the second-order partial derivatives  $\frac{\partial^2 f(\mathbf{w})}{\partial w_i \partial w_j}$  of the function  $f(\mathbf{w})$ . It is important to note that (56) guarantees convergence for every possible initialization  $\mathbf{w}^{(0)}$  of the GD iterations.

Note that while it might be computationally challenging to determine the maximum eigenvalue  $\lambda_{\max}(\nabla^2 f(\mathbf{w}))$  for arbitrary  $\mathbf{w}$ , it might still be feasible to find an upper bound  $U$  for the maximum eigenvalue. If we know an upper bound  $U \geq \lambda_{\max}(\nabla^2 f(\mathbf{w}))$  (valid for all  $\mathbf{w} \in \mathbb{R}^d$ ), the step size  $\alpha = 1/U$  still ensures convergence of the GD iteration.

### 5.3 GD for Linear Regression

We can now formulate a full-fledged ML algorithm for solving a linear regression problem (see Section 3.1). This algorithm amounts to finding the optimal weight vector  $\mathbf{w}_{\text{opt}}$  for a linear predictor (see (11)) of the form

$$h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}. \quad (57)$$

The optimal weight vector  $\mathbf{w}_{\text{opt}}$  for (57) should minimize the empirical risk (under squared error loss (4))

$$\mathcal{E}(h^{(\mathbf{w})} | \mathbb{X}) \stackrel{(37)}{=} (1/N) \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2, \quad (58)$$

incurred by the predictor  $h(\mathbf{w})(\mathbf{x})$  when applied to the labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ . Thus,  $\mathbf{w}_{\text{opt}}$  is obtained as the solution of a particular smooth optimization problem (53), i.e.,

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}) \text{ with } f(\mathbf{w}) = (1/N) \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2. \quad (59)$$

In order to apply GD (55) to solve (59), and to find the optima weight vector  $\mathbf{w}_{\text{opt}}$ , we need to compute the gradient  $\nabla f(\mathbf{w})$ . The gradient of the objective function in (59) is given by

$$\nabla f(\mathbf{w}) = -(2/N) \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)}) \mathbf{x}^{(i)}. \quad (60)$$

By inserting (60) into the basic GD iteration (55), we obtain Algorithm 1.

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**Algorithm 1** “Linear Regression via GD”

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**Input:** labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  containing feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and labels  $y^{(i)} \in \mathbb{R}$ ;  
GD step size  $\alpha > 0$ .  
**Initialize:** set  $\mathbf{w}^{(0)} := \mathbf{0}$ ; set iteration counter  $k := 0$   
1: **repeat**  
2:      $k := k + 1$  (increase iteration counter)  
3:      $\mathbf{w}^{(k)} := \mathbf{w}^{(k-1)} + \alpha(2/N) \sum_{i=1}^N (y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}) \mathbf{x}^{(i)}$  (do a GD step (55))  
4: **until** convergence  
**Output:**  $\mathbf{w}^{(k)}$  (which approximates  $\mathbf{w}_{\text{opt}}$  in (59))

---

Let us have a closer look on the update in step 3 of Algorithm 1, which is

$$\mathbf{w}^{(k)} := \mathbf{w}^{(k-1)} + \alpha(2/N) \sum_{i=1}^N (y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}) \mathbf{x}^{(i)}. \quad (61)$$

The update (61) has an appealing form as it amounts to correcting the previous guess (or approximation)  $\mathbf{w}^{(k-1)}$  for the optimal weight vector  $\mathbf{w}_{\text{opt}}$  by the correction term

$$(2\alpha/N) \sum_{i=1}^N \underbrace{(y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)})}_{e^{(i)}} \mathbf{x}^{(i)}. \quad (62)$$

The correction term (62) is a weighted average of the feature vectors  $\mathbf{x}^{(i)}$  using weights  $(2\alpha/N) \cdot e^{(i)}$ . These weights consist of the global factor  $(2\alpha/N)$  (that applies equally to all feature vectors  $\mathbf{x}^{(i)}$ ) and a sample-specific factor  $e^{(i)} = (y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)})$ , which is the prediction (approximation) error obtained by the linear predictor  $h(\mathbf{w}^{(k-1)})(\mathbf{x}^{(i)}) = (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}$  when predicting the label  $y^{(i)}$  from the features  $\mathbf{x}^{(i)}$ .

We can interpret the GD step (61) as an instance of “learning by trial and error”. Indeed, the GD step amounts to “trying out” the predictor  $h(\mathbf{x}^{(i)}) = (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}$  and then correcting the weight vector  $\mathbf{w}^{(k-1)}$  according to the error  $e^{(i)} = y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}$ .

The choice of the step size  $\alpha$  used for Algorithm 1 can be based on the sufficient condition (56) with the Hessian  $\nabla^2 f(\mathbf{w})$  of the objective function  $f(\mathbf{w})$  underlying linear regression (see (59)). This Hessian is given explicitly as

$$\nabla^2 f(\mathbf{w}) = (1/N)\mathbf{X}^T\mathbf{X}, \quad (63)$$

with the feature matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})^T \in \mathbb{R}^{N \times d}$  (see (39)). Note that the Hessian (63) does not depend on the weight vector  $\mathbf{w}$ !

Comparing (63) with (56), one particular strategy for choosing the step size in Algorithm 1 is to (i) compute the matrix product  $\mathbf{X}^T\mathbf{X}$ , (ii) compute the maximum eigenvalue  $\lambda_{\max}((1/N)\mathbf{X}^T\mathbf{X})$  of this product and (iii) set the step size to  $\alpha = 1/\lambda_{\max}((1/N)\mathbf{X}^T\mathbf{X})$ . Sometimes it might be computationally challenging to determine the maximum eigenvalue  $\lambda_{\max}((1/N)\mathbf{X}^T\mathbf{X})$  but it might be easier to find an upper bound  $U$  for the maximum eigenvalue.<sup>9</sup> If we know an upper bound  $U \geq \lambda_{\max}((1/N)\mathbf{X}^T\mathbf{X})$ , the step size  $\alpha = 1/U$  still ensures convergence of the GD iteration. Consider a dataset  $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  with normalized features, i.e.,  $\|\mathbf{x}^{(i)}\| = 1$  for all  $i = 1, \dots, N$ . Then, by elementary linear algebra, one can verify the upper bound  $U = 1$ , i.e.,  $1 \geq \lambda_{\max}((1/N)\mathbf{X}^T\mathbf{X})$ . We can then ensure convergence of the GD iterations  $\mathbf{w}^{(k)}$  (see (61)) by choosing the step size  $\alpha = 1$ .

## 5.4 GD for Logistic Regression

As discussed in Section 3.4, the classification method logistic regression amounts to constructing a classifier  $h^{(\mathbf{w}_{\text{opt}})}$  by minimizing the empirical risk (22) obtained for a labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , with features  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and binary labels  $y^{(i)} \in \{-1, 1\}$ . Thus, logistic regression amounts to an instance of the smooth optimization problem (53), i.e.,

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}) \text{ with } f(\mathbf{w}) = (1/N) \sum_{i=1}^N \log(1 + \exp(-y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)})). \quad (64)$$

In order to apply GD (55) to solve (64), we need to compute the gradient  $\nabla f(\mathbf{w})$ . The gradient of the objective function in (64) is given by

$$\nabla f(\mathbf{w}) = (1/N) \sum_{i=1}^N \frac{-y^{(i)}}{1 + \exp(y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)})} \mathbf{x}^{(i)}. \quad (65)$$

By inserting (65) into the basic GD iteration (55), we obtain Algorithm 2.

Let us have a closer look on the update in step 3 of Algorithm 2, which is

$$\mathbf{w}^{(k)} := \mathbf{w}^{(k-1)} + \alpha(1/N) \sum_{i=1}^N \frac{y^{(i)}}{1 + \exp(y^{(i)}(\mathbf{w}^{(k-1)})^T\mathbf{x}^{(i)})} \mathbf{x}^{(i)}. \quad (66)$$

The update (66) has an appealing form as it amounts to correcting the previous guess (or approximation)  $\mathbf{w}^{(k-1)}$  for the optimal weight vector  $\mathbf{w}_{\text{opt}}$  by the correction term

$$(\alpha/N) \sum_{i=1}^N \underbrace{\frac{y^{(i)}}{1 + \exp(y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)})}}_{e^{(i)}} \mathbf{x}^{(i)}. \quad (67)$$

---

<sup>9</sup>The problem of computing a full eigenvalue decomposition of  $\mathbf{X}^T\mathbf{X}$  has essentially the same complexity as solving the ERM problem directly via (43), which we want to avoid by using the “cheaper” GD algorithm.

---

**Algorithm 2** “Logistic Regression via GD”

---

**Input:** labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  containing feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and labels  $y^{(i)} \in \mathbb{R}$ ;

GD step size  $\alpha > 0$ .

**Initialize:** set  $\mathbf{w}^{(0)} := \mathbf{0}$ ; set iteration counter  $k := 0$

1: **repeat**

2:      $k := k + 1$  (increase iteration counter)

3:      $\mathbf{w}^{(k)} := \mathbf{w}^{(k-1)} \alpha (1/N) \sum_{i=1}^N \frac{y^{(i)}}{1 + \exp(y^{(i)} (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)})} \mathbf{x}^{(i)}$  (do a GD step (55))

4: **until** convergence

**Output:**  $\mathbf{w}^{(k)}$  (which approximates the optimal weight vector  $\mathbf{w}_{\text{opt}}$  defined in (64))

---

The correction term (67) is a weighted average of the feature vectors  $\mathbf{x}^{(i)}$ , each of those vectors is weighted by the factor  $(\alpha/N) \cdot e^{(i)}$ . These weighting factors consist of the global factor  $(\alpha/N)$  (that applies equally to all feature vectors  $\mathbf{x}^{(i)}$ ) and a sample-specific factor  $e^{(i)} = \frac{y^{(i)}}{1 + \exp(y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)})}$ , which quantifies the error of the classifier  $h^{(\mathbf{w}^{(k-1)})}(\mathbf{x}^{(i)}) = (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}$  when predicting applied to a data point with the label  $y^{(i)} \in \{-1, 1\}$  and the features  $\mathbf{x}^{(i)} \in \mathbb{R}^d$ .

As for GD in linear regression, we can use the sufficient condition (56) (which guarantees convergence of GD) for guiding the choice of the step size  $\alpha$  used for Algorithm 2. In order to apply condition (56), we need to determine the Hessian  $\nabla^2 f(\mathbf{w})$  matrix of the objective function  $f(\mathbf{w})$  underlying logistic regression (see (64)). Some basic calculus reveals (see [13, Ch. 4.4.])

$$\nabla^2 f(\mathbf{w}) = (1/N) \mathbf{X}^T \mathbf{D} \mathbf{X}. \quad (68)$$

Here, we used the feature matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})^T \in \mathbb{R}^{N \times d}$  (see (39)) and the diagonal matrix  $\mathbf{D} = \text{diag}\{d_1, \dots, d_N\} \in \mathbb{R}^{N \times N}$  with diagonal elements

$$d_i = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}^{(i)})} \left( 1 - \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x}^{(i)})} \right). \quad (69)$$

We highlight that, in contrast to the Hessian (63) obtained for the objective function arising in linear regression, the Hessian (68) varies with the weight vector  $\mathbf{w}$ . This makes the analysis of Algorithm 2 and the optimal choice of step size somewhat more difficult compared to Algorithm 1. However, since the diagonal entries (69) take values in the interval  $[0, 1]$ , for normalized features (with  $\|\mathbf{x}^{(i)}\| = 1$ ) the step size  $\alpha = 1$  ensures convergence of the GD updates (66) to the optimal weight vector  $\mathbf{w}_{\text{opt}}$  solving (64).

## 5.5 Data Normalization

The convergence speed of the GD steps (55), i.e., the number of steps required to reach the minimum of the objective function (38) within a prescribed accuracy, depends crucially on the condition number  $\kappa(\mathbf{X}^T \mathbf{X})$ . This condition number is defined as the ratio

$$\kappa(\mathbf{X}^T \mathbf{X}) := \lambda_{\max}/\lambda_{\min} \quad (70)$$

between the largest and smallest eigenvalue of the matrix  $\mathbf{X}^T \mathbf{X}$ .

The condition number is only well defined if the columns of the feature matrix  $\mathbf{X}$  (cf. (39)), which are precisely the feature vectors  $\mathbf{x}^{(i)}$ , are linearly independent. In this case the condition number is lower bounded as  $\kappa(\mathbf{X}^T \mathbf{X}) \geq 1$ .

It can be shown that the GD steps (55) converge faster for smaller condition number  $\kappa(\mathbf{X}^T \mathbf{X})$  [27]. Thus, GD will be faster for datasets with a feature matrix  $\mathbf{X}$  such that  $\kappa(\mathbf{X}^T \mathbf{X}) \approx 1$ . It is therefore often beneficial to pre-process the feature vectors using a **normalization** (or **standardization**) procedure as detailed in Algorithm 3.

---

**Algorithm 3** “Data Normalization”

---

**Input:** labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$

1: remove sample means  $\bar{\mathbf{x}} = (1/N) \sum_{i=1}^N \mathbf{x}^{(i)}$  from features, i.e.,

$$\mathbf{x}^{(i)} := \mathbf{x}^{(i)} - \bar{\mathbf{x}} \text{ for } i = 1, \dots, N$$

2: normalise features to have unit variance, i.e.,

$$\hat{x}_j^{(i)} := x_j^{(i)} / \hat{\sigma} \text{ for } j = 1, \dots, d \text{ and } i = 1, \dots, N$$

with the empirical variance  $\hat{\sigma}_j^2 = (1/N) \sum_{i=1}^N (x_j^{(i)})^2$

**Output:** normalized feature vectors  $\{\hat{\mathbf{x}}^{(i)}\}_{i=1}^N$

---

The preprocessing implemented in Algorithm 3 reshapes (transforms) the original feature vectors  $\mathbf{x}^{(i)}$  into new feature vectors  $\hat{\mathbf{x}}^{(i)}$  such that the new feature matrix  $\hat{\mathbf{X}} = (\hat{\mathbf{x}}^{(1)}, \dots, \hat{\mathbf{x}}^{(N)})^T$  tends to be well-conditioned, i.e.,  $\kappa(\hat{\mathbf{X}}^T \hat{\mathbf{X}}) \approx 1$ .

**Exercise.** Consider the dataset with feature vectors  $\mathbf{x}^{(1)} = (100, 0)^T \in \mathbb{R}^2$  and  $\mathbf{x}^{(2)} = (0, 1/10)^T$  which we stack into the matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \mathbf{x}^{(2)})^T$ . What is the condition number of  $\mathbf{X}^T \mathbf{X}$ ? What is the condition number of  $(\hat{\mathbf{X}})^T \hat{\mathbf{X}}$  with the matrix  $\hat{\mathbf{X}} = (\hat{\mathbf{x}}^{(1)}, \hat{\mathbf{x}}^{(2)})^T$  constructed from the normalized feature vectors  $\hat{\mathbf{x}}^{(i)}$  delivered by Algorithm 3.

## 5.6 Stochastic GD

Consider an ML problem with a hypothesis space  $\mathcal{H}$  which is parametrized by a weight vector  $\mathbf{w} \in \mathbb{R}^d$  (such that each element  $h^{(\mathbf{w})}$  of  $\mathcal{H}$  corresponds to a particular choice of  $\mathbf{w}$ ) and a loss function  $\mathcal{L}((\mathbf{x}, y), h^{(\mathbf{w})})$  which depends smoothly on the weight vector  $\mathbf{w}$ . The resulting ERM (52) amounts to a smooth optimization problem which can be solved using GD (55).

Note that the gradient  $\nabla f(\mathbf{w})$  obtained for the optimization problem (52) has a particular structure. Indeed, the gradient is a sum

$$\nabla f(\mathbf{w}) = (1/N) \sum_{i=1}^N \nabla f_i(\mathbf{w}) \text{ with } f_i(\mathbf{w}) := \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})}). \quad (71)$$

Evaluating the gradient  $\nabla f(\mathbf{w})$  (e.g., within a GD step (55)) by computing the sum in (71) can be computationally challenging for at least two reasons. First, computing the sum exactly is challenging for extremely large datasets with  $N$  in the order of billions. Second, for datasets which

are stored in different datacenters located all over the world, the summation would require huge amount of network resources and also put limits on the rate by which the GD steps (55) can be executed.

**ImageNet.** The “ImageNet” database contains more than  $10^6$  images [28]. These images are labeled according to their content (e.g., does the image show a dog?). Let us assume that each image is represented by a (rather small) feature vector  $\mathbf{x} \in \mathbb{R}^d$  of length  $d = 1000$ . Then, if we represent each feature by a floating point number, performing only one single GD update (55) per second would require at least  $10^9$  FLOPS.

The idea of **stochastic GD (SGD)** is quite simple: Replace the exact gradient  $\nabla f(\mathbf{w})$  by some approximation which can be computed easier than (71). Moreover, the term “stochastic” in the name SGD hints already at the use of particular approximation techniques which involve randomness (stochastic approximations). In the most basic form of SGD, we approximate the gradient  $\nabla f(\mathbf{w})$  by a randomly selected component  $\nabla f_{\hat{i}}(\mathbf{w})$  in (71), with the index  $\hat{i}$  being chosen randomly out of  $\{1, \dots, N\}$ . Thus, SGD amounts to iterating the update

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha \nabla f_{\hat{i}}(\mathbf{w}^{(k)}). \quad (72)$$

It is important to repeat the random selection of the index  $\hat{i}$  during each new iteration.

Note that SGD replaces the summation over all training data points in the GD step (55) just by the random selection of one particular summand. The resulting savings in computational complexity can be significant in applications where a large number of data points is stored in a distributed fashion. However, this saving in computational complexity comes at the cost of introducing a non-zero gradient noise

$$\varepsilon = \nabla f(\mathbf{w}) - \nabla f_{\hat{i}}(\mathbf{w}), \quad (73)$$

into the SGD updates. In order avoid the accumulation of the gradient noise (73) while running SGD updates (72) the step size  $\alpha$  needs to be gradually decreased, e.g., using  $\alpha = 1/k$  with  $k$  being the iteration counter (see [29]).

## 6 Model Validation and Selection

Consider some ML algorithm (such as Algorithm 1), which learns a predictor  $\hat{h}$  via ERM (36) based on some labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ . It is then important to monitor or **to validate** the performance of the predictor  $\hat{h}$  on new data points  $(\mathbf{x}, y)$  (which are not contained in  $\mathbb{X}$ ). In particular, we need to validate the predictor  $\hat{h}$  to make sure that it **generalizes** well to new data.

Indeed, the ultimate goal of ML methods is to find a predictor  $\hat{h}$  which is accurate when applied to a new unlabeled data point for which we do not know the label  $y$  but only the features  $\mathbf{x}$  (if we would know the label, then there is no point in learning predictors which estimate the label). A good indicator for the accuracy of a predictor is the empirical risk (training error)  $\mathcal{E}(\hat{h}|\mathbb{X})$  incurred over the labeled training dataset  $\mathbb{X}$ . However, there are situations where the training error  $\mathcal{E}(\hat{h}|\mathbb{X})$  is quite small but the prediction error  $y - \hat{h}(\mathbf{x})$  obtained for new data  $(\mathbf{x}, y)$  is unacceptably large. This situation is referred to as **overfitting** and the reasons for this to happen will be discussed in Section 7.1.

Validation is useful not only for verifying if the predictor generalises well to new data (in particular detecting overfitting) but also for guiding model selection. In what follows, we mean by model selection the problem of selecting a particular hypothesis space out of a whole ensemble of potential hypothesis spaces  $\mathcal{H}_1, \mathcal{H}_2, \dots$

### 6.1 How to Validate a Predictor?

Consider an ML problem using a hypothesis space  $\mathcal{H}$ . We have chosen a particular predictor  $\hat{h} \in \mathcal{H}$  by ERM (36) using a labeled dataset (the training set). The basic idea of validating the predictor  $\hat{h}$  is simple: compute the empirical risk of  $\hat{h}$  over another set of data points  $(\mathbf{x}, y)$  which have not been already used for training. It is very important to validate the predictor  $\hat{h}$  using labeled data points which do not belong to the dataset which has been used to learn  $\hat{h}$  (e.g., via ERM (36)). This is reasonable since the predictor  $\hat{h}$  tends to “look better” on the training set than for other data points, since it is optimized precisely for the data points in the training set.

A golden rule of ML practice: try always to use different data points for the training (see (36)) and the validation of a predictor  $\hat{h}$ !

A very simple recipe for implementing learning and validation of a predictor based on one single labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  is as follows (see Figure 41):

1. randomly divide (“split”) the entire dataset  $\mathbb{X}$  of labeled snapshots into two disjoint subsets  $\mathbb{X}^{(\text{train})}$  (the “training set”) and  $\mathbb{X}^{(\text{val})}$  (the “validation set”):  $\mathbb{X} = \mathbb{X}^{(\text{train})} \cup \mathbb{X}^{(\text{val})}$  (see Figure 41).
2. learn a predictor  $\hat{h}$  via ERM using the training data  $\mathbb{X}^{(\text{train})}$ , i.e., compute (cf. (36))

$$\begin{aligned}\hat{h} &= \underset{h \in \mathcal{H}}{\operatorname{argmin}} \mathcal{E}(h|\mathbb{X}^{(\text{train})}) \\ &= \underset{h \in \mathcal{H}}{\operatorname{argmin}} (1/N_{\text{train}}) \sum_{(\mathbf{x}, y) \in \mathbb{X}^{(\text{train})}} \mathcal{L}((\mathbf{x}, y), h)\end{aligned}\tag{74}$$

with corresponding **training error**

$$\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{train})}) = (1/N_{\text{train}}) \sum_{i=1}^{N_{\text{train}}} \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), \hat{h}) \quad (75)$$

3. validate the predictor  $\hat{h}$  obtained from (74) by computing the empirical risk

$$\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})}) = (1/N_{\text{val}}) \sum_{(\mathbf{x}, y) \in \mathbb{X}^{(\text{val})}} \mathcal{L}((\mathbf{x}, y), \hat{h}) \quad (76)$$

obtained when applying the predictor  $\hat{h}$  to the **validation dataset**  $\mathbb{X}^{(\text{val})}$ . We might refer to  $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})})$  as the **validation error**.

The choice of the split ratio  $|\mathbb{X}^{(\text{val})}|/|\mathbb{X}^{(\text{train})}|$ , i.e., how large should the training set be relative to the validation set is often based on experimental tuning. It seems difficult to make a precise statement on how to choose the split ratio which applies broadly to different ML problems [30].

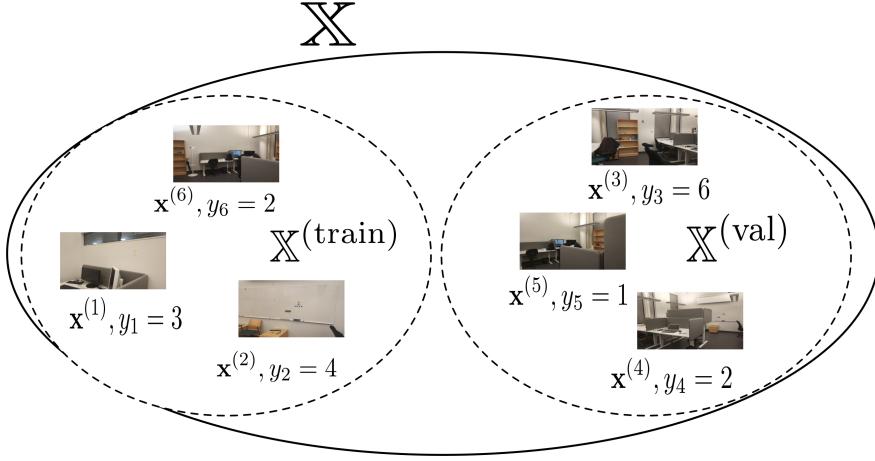


Figure 41: If we have only one single labeled dataset  $\mathbb{X}$ , we split it into a **training set**  $\mathbb{X}^{(\text{train})}$  and a **validation set**  $\mathbb{X}^{(\text{val})}$ . We use the training set in order to learn (find) a good predictor  $\hat{h}(\mathbf{x})$  by minimizing the empirical risk  $\mathcal{E}(h|\mathbb{X}^{(\text{train})})$  (see (36)). In order to validate the performance of the predictor  $\hat{h}$  on new data, we compute the empirical risk  $\mathcal{E}(h|\mathbb{X}^{(\text{val})})$  incurred by  $\hat{h}(\mathbf{x})$  for the validation set  $\mathbb{X}^{(\text{val})}$ . We refer to the empirical risk  $\mathcal{E}(h|\mathbb{X}^{(\text{val})})$  obtained for the validation set as the **validation error**.

The basic idea of randomly splitting the available labeled data into training and validation sets is underlying many validation techniques. A popular extension of the above approach, which is known as  $k$ -fold cross-validation, is based on repeating the splitting into training and validation sets  $k$  times. During each repetition, this method uses different subsets for training and validation. We refer to [13, Sec. 7.10] for a detailed discussion of  $k$ -fold cross-validation.

## 6.2 Model Selection

We will now discuss how to use the validation principle of Section 6.1 to perform model selection. As discussed in Section 2, the choice of the hypothesis space from which we select a predictor map

(e.g., via solving the ERM (36)) is a design choice. However, it is often not obvious what a good choice for the hypothesis space is. Rather, we often try out different choices  $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_M$  for the hypothesis space.

Consider a prediction problem where the relation between feature  $x$  and  $y$  is non-linear (see, e.g., Figure 10). We might then use polynomial regression (see Section 3.2) using the hypothesis space  $\mathcal{H}_{\text{poly}}^{(d)}$  with some maximum degree  $d$ . For each value of the maximum degree  $d$  we get a different hypothesis space:  $\mathcal{H}_1 = \mathcal{H}_{\text{poly}}^{(0)}, \mathcal{H}_2 = \mathcal{H}_{\text{poly}}^{(1)}, \dots, \mathcal{H}_M = \mathcal{H}_{\text{poly}}^{(M-1)}$ . Or, instead of polynomial regression, we might use Gaussian basis regression (see Section 3.3), with different choices for the variance  $\sigma$  and shifts  $\mu$  of the Gaussian basis function (19), e.g.,  $\mathcal{H}_1 = \mathcal{H}_{\text{Gauss}}^{(2)}$  with  $\sigma = 1$  and  $\mu_1 = 1$  and  $\mu_2 = 2$ ,  $\mathcal{H}_2 = \mathcal{H}_{\text{Gauss}}^{(2)}$  with  $\sigma = 1/10, \mu_1 = 10, \mu_2 = 20$ .

A principled approach for choosing a hypothesis space out of a given a set of candidates  $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_M$  is as follows:

- randomly divide (split) the entire dataset  $\mathbb{X}$  of labeled snapshots into two disjoint subsets  $\mathbb{X}^{(\text{train})}$  (the “training set”) and  $\mathbb{X}^{(\text{val})}$  (the “validation set”):  $\mathbb{X} = \mathbb{X}^{(\text{train})} \cup \mathbb{X}^{(\text{val})}$  (see Figure 41).
- for each hypothesis space  $\mathcal{H}_l$  learn predictor  $\hat{h}_l \in \mathcal{H}_l$  via ERM (36) using training data  $\mathbb{X}^{(\text{train})}$ :

$$\begin{aligned}\hat{h}_l &= \underset{h \in \mathcal{H}_l}{\operatorname{argmin}} \mathcal{E}(h | \mathbb{X}^{(\text{train})}) \\ &= \underset{h \in \mathcal{H}_l}{\operatorname{argmin}} (1/N_{\text{train}}) \sum_{i=1}^{N_{\text{train}}} \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h)\end{aligned}\quad (77)$$

- compute the validation error of  $\hat{h}_l$

$$\mathcal{E}(\hat{h}_l | \mathbb{X}^{(\text{val})}) = (1/N_{\text{val}}) \sum_{i=1}^{N_{\text{val}}} \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), \hat{h}_l) \quad (78)$$

obtained when applying the predictor  $\hat{h}_l$  to the **validation dataset**  $\mathbb{X}^{(\text{val})}$ .

- pick the hypothesis space  $\mathcal{H}_l$  resulting in the smallest validation error  $\mathcal{E}(\hat{h}_l | \mathbb{X}^{(\text{val})})$

### 6.3 Bias, Variance and Generalization within Linear Regression

A core problem or challenge within ML is the verification (or validation) if a predictor or classifier which works well on a labeled training dataset will also work well (generalize) to new data points. In practice we can only validate by using different data points than for training an ML method via ERM. However, if we can find some generative probabilistic model which well explains the observed data points  $\mathbf{z}^{(i)}$  we can study the generalization ability via probability theory.

In order to study generalization within a linear regression problem (see Section 3.1), we will invoke a **probabilistic toy model** for the data arising in an ML application. In particular, we assume that any observed data point  $\mathbf{z} = (\mathbf{x}, y)$  with features  $\mathbf{x} \in \mathbb{R}^d$  and label  $y \in \mathbb{R}$  can be considered as an i.i.d. realization of a Gaussian random vector. The feature vector  $\mathbf{x}$  is assumed to

have zero mean and covariance being the identity matrix, i.e.,  $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ . The label  $y$  of a data point is related to its features  $\mathbf{x}$  via a **linear Gaussian model**

$$y = \mathbf{w}_{\text{true}}^T \mathbf{x} + \varepsilon, \text{ with noise } \varepsilon \sim \mathcal{N}(0, \sigma^2). \quad (79)$$

The noise variance  $\sigma^2$  is assumed fixed (non-random) and known. Note that the error component  $\varepsilon$  in (79) is intrinsic to the data (within our toy model) and cannot be overcome by any ML method. We highlight that this model for the observed data points might not be accurate for a particular ML application. However, this toy model will allow us to study some fundamental behaviour of ML methods.

In order to predict the label  $y$  from the features  $\mathbf{x}$  we will use predictors  $h$  that are linear maps of the first  $r$  features  $x_1, \dots, x_r$ . This results in the hypothesis space

$$\mathcal{H}^{(r)} = \{h^{(\mathbf{w})}(\mathbf{x}) = (\mathbf{w}^T, \mathbf{0})\mathbf{x} \text{ with } \mathbf{w} \in \mathbb{R}^r\}. \quad (80)$$

The design parameter  $r$  determines the size of the hypothesis space  $\mathcal{H}^{(r)}$  and allows to control the computational complexity of the resulting ML method which is based on the hypothesis space  $\mathcal{H}^{(r)}$ . For  $r < d$ , the hypothesis space  $\mathcal{H}^{(r)}$  is a proper subset of the space of linear predictors (2) used within linear regression (see Section 3.1). Note that each element  $h^{(\mathbf{w})} \in \mathcal{H}^{(r)}$  corresponds to a particular choice of the weight vector  $\mathbf{w} \in \mathbb{R}^r$ .

The quality of a particular predictor  $h^{(\mathbf{w})} \in \mathcal{H}^{(r)}$  is measured via the mean squared error  $\mathcal{E}(h^{(\mathbf{w})} \mid \mathbb{X}^{(\text{train})})$  incurred over a labeled training set  $\mathbb{X}^{(\text{train})} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N_{\text{train}}}$ . Within our toy model (see (79), (81) and (82)), the training data points  $(\mathbf{x}^{(i)}, y^{(i)})$  are i.i.d. copies of the data point  $\mathbf{z} = (\mathbf{x}, y)$ . In particular, each of the data points in the training dataset is statistically independent from any other data point  $(\mathbf{x}, y)$  (which has not been used for training). However, the training data points  $(\mathbf{x}^{(i)}, y^{(i)})$  and any other (new) data point  $(\mathbf{x}, y)$  share the same probability distribution (a multivariate normal distribution):

$$\mathbf{x}, \mathbf{x}^{(i)} \text{ i.i.d. with } \mathbf{x}, \mathbf{x}^{(i)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (81)$$

and the labels  $y^{(i)}, y$  are obtained as

$$y^{(i)} = \mathbf{w}_{\text{true}}^T \mathbf{x}^{(i)} + \varepsilon^{(i)}, \text{ and } y = \mathbf{w}_{\text{true}}^T \mathbf{x} + \varepsilon \quad (82)$$

with i.i.d. noise  $\varepsilon, \varepsilon^{(i)} \sim \mathcal{N}(0, \sigma^2)$ .

As discussed in Section 4, the training error  $\mathcal{E}(h^{(\mathbf{w})} \mid \mathbb{X}^{(\text{train})})$  is minimized by the predictor  $h^{(\hat{\mathbf{w}})}(\mathbf{x}) = \hat{\mathbf{w}}^T \mathbf{I}_{r \times d} \mathbf{x}$ , with weight vector

$$\hat{\mathbf{w}} = (\mathbf{X}_r^T \mathbf{X}_r)^{-1} \mathbf{X}_r^T \mathbf{y} \quad (83)$$

with feature matrix  $\mathbf{X}_r$  and label vector  $\mathbf{y}$  defined as

$$\mathbf{X}_r = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N_{\text{train}})})^T \mathbf{I}_{d \times r} \in \mathbb{R}^{N_{\text{train}} \times r}, \text{ and } \mathbf{y} = (y^{(1)}, \dots, y^{(N_{\text{train}})})^T \in \mathbb{R}^{N_{\text{train}}}. \quad (84)$$

It will be convenient to tolerate a slight abuse of notation and denote by  $\hat{\mathbf{w}}$  both, the length- $r$  vector (83) as well as the zero padded length- $d$  vector  $(\hat{\mathbf{w}}^T, \mathbf{0})^T$ . This allows us to write the predictor  $h^{(\hat{\mathbf{w}})}(\mathbf{x})$  as

$$h^{(\hat{\mathbf{w}})}(\mathbf{x}) = \hat{\mathbf{w}}^T \mathbf{x}. \quad (85)$$

We highlight that the formula (83) for the optimal weight vector  $\hat{\mathbf{w}}$  is only valid if the matrix  $\mathbf{X}_r^T \mathbf{X}_r$  is invertible. However, it can be shown that within our toy model (see (81)), this is true with probability one whenever  $N_{\text{train}} \geq r$ . In what follows, we will consider the case of having more training samples than the dimension of the hypothesis space, i.e.,  $N_{\text{train}} > r$  such that the formula (83) is valid (with probability one). The case  $N_{\text{train}} \leq r$  will be studied in Section 7.1.

The optimal weight vector  $\hat{\mathbf{w}}$  (see (83)) depends on the training data  $\mathbb{X}^{(\text{train})}$  via the feature matrix  $\mathbf{X}_r$  and label vector  $\mathbf{y}$  (see (84)). Therefore, since we model the training data as random, the weight vector  $\hat{\mathbf{w}}$  (83) is a random quantity. For each different realization of the training dataset, we obtain a different realization of the optimal weight  $\hat{\mathbf{w}}$ .

Within our toy model, which relates the features  $\mathbf{x}$  of a data point to its label  $y$  via (79), the best case would be if  $\hat{\mathbf{w}} = \mathbf{w}_{\text{true}}$ . However, in general this will not happen since we have to compute  $\hat{\mathbf{w}}$  based on the features  $\mathbf{x}^{(i)}$  and noisy labels  $y^{(i)}$  of the data points in the training dataset  $\mathbb{X}$ . Thus, we typically have to face a non-zero **estimation error**

$$\Delta \mathbf{w} := \hat{\mathbf{w}} - \mathbf{w}_{\text{true}}. \quad (86)$$

Note that this estimation error is a random quantity since the learnt weight vector  $\hat{\mathbf{w}}$  (see (83)) is random.

**Bias and Variance.** As we will see below, the prediction quality achieved by  $h^{(\hat{\mathbf{w}})}$  depends crucially on the **mean squared estimation error (MSE)**

$$\mathcal{E}_{\text{est}} := \mathbb{E}\{\|\Delta \mathbf{w}\|_2^2\} = \mathbb{E}\{\|\hat{\mathbf{w}} - \mathbf{w}_{\text{true}}\|_2^2\}. \quad (87)$$

It is useful to characterize the MSE  $\mathcal{E}_{\text{est}}$  by decomposing it into two components, one component (the ‘‘bias’’) which depends on the choice  $r$  for the hypothesis space and another component (the ‘‘variance’’) which only depends on the distribution of the observed feature vectors  $\mathbf{x}^{(i)}$  and labels  $y^{(i)}$ . It is then not too hard to show that

$$\mathcal{E}_{\text{est}} = \underbrace{\|\mathbf{w}_{\text{true}} - \mathbb{E}\{\hat{\mathbf{w}}\}\|_2^2}_{\text{‘‘bias’’ } B^2} + \underbrace{\mathbb{E}\|\hat{\mathbf{w}} - \mathbb{E}\{\hat{\mathbf{w}}\}\|_2^2}_{\text{‘‘variance’’ } V} \quad (88)$$

The bias term in (88), which can be computed as

$$B^2 = \|\mathbf{w}_{\text{true}} - \mathbb{E}\{\hat{\mathbf{w}}\}\|_2^2 = \sum_{l=r+1}^d w_{\text{true},l}^2, \quad (89)$$

measures the distance between the ‘‘true predictor’’  $h^{(\mathbf{w}_{\text{true}})}(\mathbf{x}) = \mathbf{w}_{\text{true}}^T \mathbf{x}$  and the hypothesis space  $\mathcal{H}^{(r)}$  (see (80)) of the linear regression problem. The bias is zero if  $w_{\text{true},l} = 0$  for any index  $l = r+1, \dots, d$ , or equivalently if  $h^{(\mathbf{w}_{\text{true}})} \in \mathcal{H}^{(r)}$ . We can guarantee  $h^{(\mathbf{w}_{\text{true}})} \in \mathcal{H}^{(r)}$  only if we use the largest possible hypothesis space  $\mathcal{H}^{(r)}$  with  $r = d$ . For  $r < d$ , we cannot guarantee a zero bias term since we have no access to the true underlying weight vector  $\mathbf{w}_{\text{true}}$  in (79). In general, the bias term decreases for increasing model size  $r$  (see Figure 42). We also highlight that the bias term does not depend on the variance  $\sigma^2$  of the noise  $\varepsilon$  in our toy model (79).

Let us now consider the variance term in (88). Using the properties of our toy model (see (79), (81) and (82))

$$V = \mathbb{E}\{\|\hat{\mathbf{w}} - \mathbb{E}\{\hat{\mathbf{w}}\}\|_2^2\} = \sigma^2 \text{trace}\{\mathbb{E}\{(\mathbf{X}_r^T \mathbf{X}_r)^{-1}\}\}. \quad (90)$$

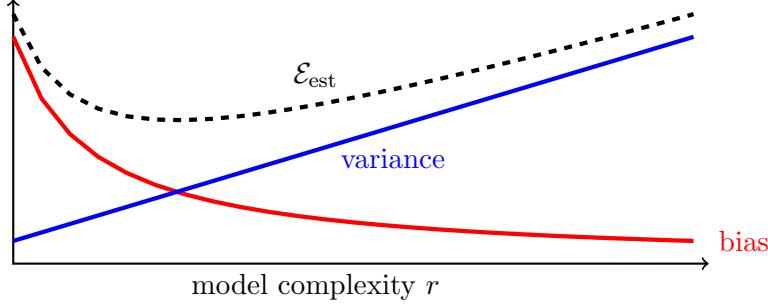


Figure 42: The estimation error  $\mathcal{E}_{\text{est}}$  incurred by linear regression can be decomposed into a bias term  $B^2$  and a variance term  $V$  (see (88)). These two components depend on the model complexity  $r$  in an opposite manner resulting in a bias-variance tradeoff.

By (81), the matrix  $(\mathbf{X}_r^T \mathbf{X}_r)^{-1}$  is random and distributed according to an **inverse Wishart distribution** [31]. In particular, for  $N_{\text{train}} > r + 1$ , its expectation is obtained as

$$\mathbb{E}\{(\mathbf{X}_r^T \mathbf{X}_r)^{-1}\} = 1/(N_{\text{train}} - r - 1) \mathbf{I}_{r \times r}. \quad (91)$$

By inserting (91) and  $\text{trace}\{\mathbf{I}_{r \times r}\} = r$  into (90),

$$V = \mathbb{E}\{\|\hat{\mathbf{w}} - \mathbb{E}\{\hat{\mathbf{w}}\}\|_2^2\} = \sigma^2 r / (N_{\text{train}} - r - 1). \quad (92)$$

As indicated by (92), the variance term increases with increasing model complexity  $r$  (see Figure 42). This behaviour is in stark contrast to the bias term which decreases with increasing  $r$ . The opposite dependency of bias and variance on the model complexity is known as the **bias-variance tradeoff**. Thus, the choice of model complexity  $r$  (see (80)) has to balance between small variance and small bias term.

**Generalization.** In most ML applications, we are primarily interested in how well a predictor  $h^{(\hat{\mathbf{w}})}$ , which has been learnt from some training data  $\mathbb{X}$  (see (36)), predicts the label  $y$  of a new datapoint (which is not contained in the training data  $\mathbb{X}$ ) with features  $\mathbf{x}$ . Within our linear regression model, the prediction (approximation guess or estimate)  $\hat{y}$  of the label  $y$  is obtained using the learnt predictor  $h^{(\hat{\mathbf{w}})}$  via

$$\hat{y} = \hat{\mathbf{w}}^T \mathbf{x}. \quad (93)$$

Note that the prediction  $\hat{y}$  is a random variable since (i) the feature vector  $\mathbf{x}$  is modelled as a random vector (see (81)) and (ii) the optimal weight vector  $\hat{\mathbf{w}}$  (see (83)) is random. In general, we cannot hope for a perfect prediction but have to face a non-zero prediction error

$$\begin{aligned} e_{\text{pred}} &:= \hat{y} - y \\ &\stackrel{(93)}{=} \hat{\mathbf{w}}^T \mathbf{x} - y \\ &\stackrel{(79)}{=} \hat{\mathbf{w}}^T \mathbf{x} - (\mathbf{w}_{\text{true}}^T \mathbf{x} + \varepsilon) \\ &= \Delta \mathbf{w}^T \mathbf{x} - \varepsilon. \end{aligned} \quad (94)$$

Note that, within our toy model (see (79), (81) and (82)), the prediction error  $e_{\text{pred}}$  is a random variable since (i) the label  $y$  is modelled as a random variable (see (79)) and (ii) the prediction  $\hat{y}$  is random.

Since, within our toy model (82),  $\varepsilon$  is zero-mean and independent of  $\mathbf{x}$  and  $\hat{\mathbf{w}} - \mathbf{w}_{\text{true}}$ , we obtain the **average predictor error** as

$$\begin{aligned}
\mathcal{E}_{\text{pred}} &= \mathbb{E}\{e_{\text{pred}}^2\} \\
&\stackrel{(94),(79)}{=} \mathbb{E}\{\Delta\mathbf{w}^T \mathbf{x}\mathbf{x}^T \Delta\mathbf{w}\} + \sigma^2 \\
&\stackrel{(a)}{=} \mathbb{E}\{\mathbb{E}\{\Delta\mathbf{w}^T \mathbf{x}\mathbf{x}^T \Delta\mathbf{w} \mid \mathbb{X}\}\} + \sigma^2 \\
&\stackrel{(b)}{=} \mathbb{E}\{\Delta\mathbf{w}^T \Delta\mathbf{w}\} + \sigma^2 \\
&\stackrel{(86),(87)}{=} \mathcal{E}_{\text{est}} + \sigma^2 \\
&\stackrel{(88)}{=} B^2 + V + \sigma^2. \tag{95}
\end{aligned}$$

Here, step (a) is due to the law of total expectation [12] and step (b) uses that, conditioned on the dataset  $\mathbb{X}$ , the feature vector  $\mathbf{x}$  of a new data point (not belonging to  $\mathbb{X}$ ) has zero mean and covariance matrix  $\mathbf{I}$  (see (81)).

Thus, as indicated by (95), the average (expected) prediction error  $\mathcal{E}_{\text{pred}}$  is the sum of three contributions: (i) the bias  $B^2$ , (ii) the variance  $V$  and (iii) the noise variance  $\sigma^2$ . The bias and variance, whose sum is the estimation error  $\mathcal{E}_{\text{est}}$ , can be influenced by varying the model complexity  $r$  (see Figure 42) which is a design parameter. The noise variance  $\sigma^2$  is the intrinsic accuracy limit of our toy model (79) and is not under the control of the ML engineer. It is impossible for any ML method (no matter how clever it is engineered) to achieve, on average, a small prediction error than the noise variance  $\sigma^2$ .

We finally highlight that our analysis of bias (89), variance (92) and the average prediction error (95) achieved by linear regression only applies if the observed data points are well modelled as realizations of random vectors according to (79), (81) and (82). The usefulness of this model for the data arising in a particular application has to be verified in practice by some validation techniques [32, 33].

An alternative approach for analyzing bias, variance and average prediction error of linear regression is to use simulations. Here, we generate a number of i.i.d. copies of the observed data points by some random number generator [34]. Using these i.i.d. copies, we can replace exact computations (expectations) by empirical approximations (sample averages).

## 6.4 Diagnosis

Consider a predictor  $\hat{h}$  obtained from ERM (36) with training error  $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{train})})$  and validation error  $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})})$ . By comparing the two numbers  $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{train})})$  and  $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})})$  with some desired or tolerated error  $E_0$ , we can get some idea of how to adapt the current ERM approach (see (36)) to improve performance:

- $\mathcal{E}(h|\mathbb{X}^{(\text{train})}) \approx \mathcal{E}(h|\mathbb{X}^{(\text{val})}) \approx E_0$ : There is not much to improve regarding prediction accuracy since we achieve the desired error on both training and validation set.
- $\mathcal{E}(h|\mathbb{X}^{(\text{val})}) \gg \mathcal{E}(h|\mathbb{X}^{(\text{train})}) \approx E_0$ : The ERM (36) results in a hypothesis  $\hat{h}$  with sufficiently small training error but when applied to new (validation) data the performance of  $\hat{h}$  is significantly worse. This is an indicator of overfitting which can be addressed by regularization techniques (see Section 7.1).

- $\mathcal{E}(h|\mathbb{X}^{(\text{train})}) \gg \mathcal{E}(h|\mathbb{X}^{(\text{val})})$ : There seemingly went something wrong with the solution of the ERM (36), since the training error obtained by solving the ERM (36) should always be smaller than the validation error. One particular reason could be that the optimization method, such as GD, is not working properly, e.g., due to improper choice of the step size for the GD step (55).

## 7 Overfitting and Regularization

A main reason for validating predictors is to detect **overfitting**. The phenomenon of overfitting is one of the key obstacles for the successful application of ML methods. Loosely speaking, overfitting refers to a situation where the ERM approach can be highly misleading. Note that the ERM principle only makes sense if the empirical risk (or training error, see (9)) incurred by a predictor over some labeled data  $\mathbb{X} = \{\mathbf{z}^{(i)} = (\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , is also an indicator for the average prediction error (see (95)) achieved when applied to new data. When overfitting, the empirical risk obtained for the training dataset can be very different from the average prediction error.

A predictor  $h : \mathbb{R}^d \rightarrow \mathbb{R}$  overfits the training data if it has a **small training error** (empirical risk obtained by applying the predictor to the training set) but a **large average prediction error** on other data points, which are different from the data points used to train the predictor.

A main cause for overfitting within the ERM approach (see Section 4) is that the hypothesis space  $\mathcal{H}$  is chosen too large. If the hypothesis space is too large, ML methods based on solving the ERM (36) can choose from so many different maps  $h \in \mathcal{H}$  (from features  $\mathbf{x}$  to label  $y$ ) that just by luck it will find a good one for a given training dataset. However, the resulting small empirical risk on the training dataset is highly misleading since if a predictor was good for the training dataset just “by accident”, we can not expect that it will be any good for other data points.

It seems reasonable to avoid overfitting by pruning the hypothesis space  $\mathcal{H}$ , i.e., removing some of its elements. In particular, instead of solving (36) we solve the restricted ERM

$$\hat{h} = \underset{h \in \mathcal{H}'}{\operatorname{argmin}} \mathcal{E}(h|\mathbb{X}) \text{ with the pruned hypothesis space } \mathcal{H}' \subset \mathcal{H}. \quad (96)$$

Another approach to avoid overfitting is to regularize the ERM (36) by adding a penalty term  $\mathcal{R}(h)$  which somehow measures the complexity or non-regularity of a predictor map  $h$  using a non-negative number  $\mathcal{R}(h) \in \mathbb{R}_+$ . We then obtain the regularized ERM

$$\hat{h} = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \mathcal{E}(h|\mathbb{X}) + \mathcal{R}(h). \quad (97)$$

The additional term  $\mathcal{R}(h)$  aims at approximating (or anticipating) the increase in the empirical risk of a predictor  $\hat{h}$  when it is applied to new data points, which are different from the dataset  $\mathbb{X}$  used to learn the predictor  $\hat{h}$  by (97).

The two approaches (96) and (97), for making ERM (36) robust against overfitting are closely related. In particular, these two approaches are, in a certain sense, **dual** to each other: for a given restriction  $\mathcal{H}' \subset \mathcal{H}$  we can find a penalty  $\mathcal{R}(h)$  term such that the solutions of (96) and (97) coincide. Similarly for a many popular types of penalty terms  $\mathcal{R}(h)$ , we can find a restriction  $\mathcal{H}' \subset \mathcal{H}$  such that the solutions of (96) and (97) coincide. This statements can be made precise using the theory of duality for optimization problems (see [35]).

In what follows we will analyze the occurrence of overfitting in Section 7.1 and then discuss in Section 7.2 how to avoid overfitting using regularization.

### 7.1 Overfitting

Let us illustrate the phenomenon of overfitting using a simplified model for how a human child learns the concept “tractor”. In particular, this learning task amounts to finding an association (or predictor) between an image and the fact if the image shows a tractor or not. In order to teach this

association to a child, we show it many pictures and tell for each picture if there is a “tractor” or if there is “no tractor” depicted. Consider that we have taught the child using the image collection  $\mathbb{X}^{(\text{train})}$  depicted in Figure 43. For some reason, one of the images is labeled erroneously as “tractor” but actually shows an ocean wave. As a consequence, if the child is good in memorizing images, it might predict the presence of tractors whenever looking at a wave (Figure 7.1).



Figure 43: A (misleading) training dataset  $\mathbb{X}^{(\text{train})} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N_{\text{train}}}$  consisting of  $N_{\text{train}} = 9$  images. The  $i$ -th image is characterized by the feature vector  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and labeled with  $y^{(i)} = 1$  (if image depicts a tractor) or with  $y^{(i)} = -1$  (if image does not depict a tractor).

For the sake of the argument, we assume that the child uses a linear predictor  $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$ , using the features  $\mathbf{x}$  of the image, and encodes the fact of showing a tractor by  $y = 1$  and if it is not showing a tractor by  $y = -1$ . In order to learn the weight vector, we use ERM with squared error loss over the training dataset, i.e., its learning process amounts to solving the ERM problem (38) using the labeled training dataset  $\mathbb{X}^{(\text{train})}$ . If we stack the feature vectors  $\mathbf{x}^{(i)}$  and labels  $y^{(i)}$  into the matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N_{\text{train}})})$  and vector  $\mathbf{y} = (y^{(1)}, \dots, y^{(N_{\text{train}})})^T$ , the optimal linear predictor is obtained for the weight vector solving (43) and the associated training error is given by (44), which we repeat here for convenience:

$$\mathcal{E}(h^{(\mathbf{w}_{\text{opt}})} | \mathbb{X}^{(\text{train})}) = \min_{\mathbf{w} \in \mathbb{R}^d} \mathcal{E}(h^{(\mathbf{w})} | \mathbb{X}^{(\text{train})}) = \|(\mathbf{I} - \mathbf{P})\mathbf{y}\|^2. \quad (98)$$

Here, we used the orthogonal projection matrix  $\mathbf{P}$  on the linear span  $\text{span}\{\mathbf{X}\}$  of the transposed feature matrix

$$\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N_{\text{train}})}) \in \mathbb{R}^{d \times N_{\text{train}}}. \quad (99)$$

Let us now study how overfitting arises whenever the sample size  $N$  is smaller or equal to the length  $d$  of the feature vectors  $\mathbf{x}$ , i.e., whenever

$$N_{\text{train}} \leq d. \quad (100)$$



Figure 44: The child, who has been taught the concept “tractor” using the image collection  $\mathbb{X}^{(\text{train})}$  in Figure 43, might “see” a lot of tractors during the next beach holiday.

In practice, a set of  $N_{\text{train}}$  feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  is typically linearly independent whenever (100) is satisfied. In this case, the span of the transposed feature matrix (99) coincides with  $\mathbb{R}^N$  which implies, in turn,  $\mathbf{P} = \mathbf{I}$ . Inserting  $\mathbf{P} = \mathbf{I}$  into (44) yields

$$\mathcal{E}(h^{(\mathbf{w}_{\text{opt}})} | \mathbb{X}^{(\text{train})}) = 0. \quad (101)$$

To sum up: as soon as the number of training examples  $N_{\text{train}} = |\mathbb{X}_{\text{train}}|$  is smaller than the size  $d$  of the feature vector  $\mathbf{x}$ , there is a linear predictor  $h^{(\mathbf{w}_{\text{opt}})}$  achieving **zero empirical risk** (see (101)) on the training data.

While this “optimal” predictor  $h^{(\mathbf{w}_{\text{opt}})}$  is perfectly accurate on the training data (the training error is zero!), it will typically incur a non-zero average prediction error  $y - h^{(\mathbf{w}_{\text{opt}})}(\mathbf{x})$  on new data points  $(\mathbf{x}, y)$  (which are different from the training data). Indeed, using a simple toy model for the data generation, we obtained the expression (95) for the average prediction error. This average prediction error is lower bounded by the noise variance  $\sigma^2$  which might be very large even the training error is zero. Thus, in case of overfitting, a small training error can be highly misleading regarding the average prediction error of a predictor.

A simple, yet quite useful, strategy to detect if a predictor  $\hat{h}$  overfits the training dataset  $\mathbb{X}^{(\text{train})}$ , is to compare the resulting training error  $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{train})})$  (see (75)) with the validation error  $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{val})})$  (see (76)). The validation error  $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{val})})$  is the empirical risk of the predictor  $\hat{h}$  on the validation dataset  $\mathbb{X}^{(\text{val})}$ . In case of overfitting, the validation error  $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{val})})$  is significantly larger than the training error  $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{train})})$ . The occurrence of overfitting for polynomial regression with degree  $d$  (see Section 3.2) chosen too large is depicted in Figure 45.

## 7.2 Regularization

As mentioned above, the overfitting of the training data  $\mathbb{X}^{(\text{train})} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N_{\text{train}}}$  might be caused by choosing the hypothesis space too large. Therefore, we can avoid overfitting by making

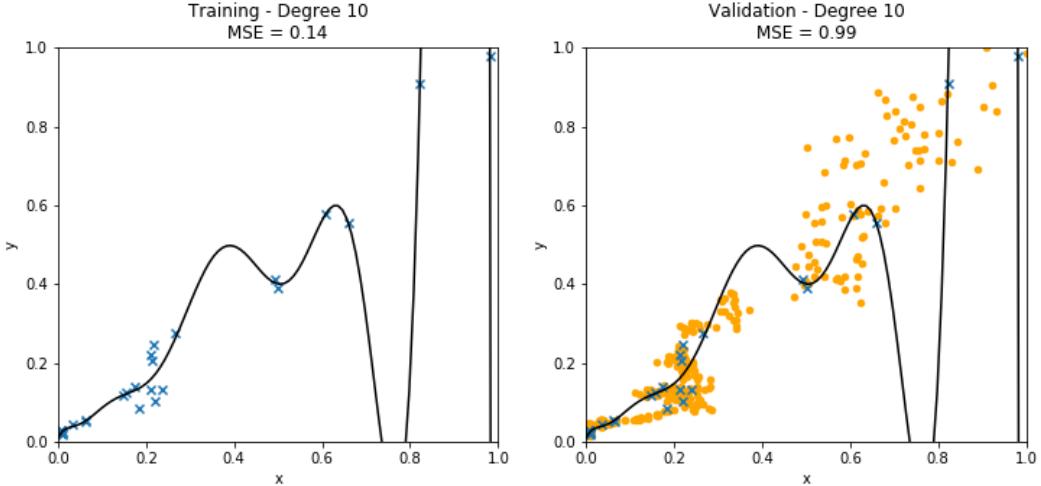


Figure 45: The training dataset consists of the blue crosses and can be almost perfectly fit by a high-degree polynomial. This high-degree polynomial gives only poor results for a different (validation) dataset indicated by the orange dots.

(pruning) the hypothesis space  $\mathcal{H}$  smaller to obtain a new hypothesis space  $\mathcal{H}_{\text{small}}$ . This smaller hypothesis space  $\mathcal{H}_{\text{small}}$  can be obtained by pruning, i.e., removing certain maps  $h$ , from  $\mathcal{H}$ .

A more general strategy is **regularization**, which amounts to modifying the loss function of an ML problem in order to favour a subset of predictor maps. Pruning the hypothesis space can be interpreted as an extreme case of regularization, where the loss functions become infinite for predictors which do not belong to the smaller hypothesis space  $\mathcal{H}_{\text{small}}$ .

In order to avoid overfitting, we have to augment our basic ERM approach (cf. (36)) by **regularization techniques**. According to [1], regularization aims at “any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error.” By generalization error, we mean the average prediction error (see (95)) incurred by a predictor when applied to new data points (different from the training set).

A simple but effective method to regularize the ERM learning principle, is to augment the empirical risk (58) of linear regression by the penalty term  $\mathcal{R}(h^{(\mathbf{w})}) := \lambda \|\mathbf{w}\|_2^2$ , which penalizes overly large weight vectors  $\mathbf{w}$ . Thus, we arrive at **regularized ERM**

$$\begin{aligned} \hat{\mathbf{w}}^{(\lambda)} &= \underset{h^{(\mathbf{w})} \in \mathcal{H}}{\operatorname{argmin}} [\mathcal{E}(h^{(\mathbf{w})} | \mathbb{X}^{(\text{train})}) + \lambda \|\mathbf{w}\|^2] \\ &= \underset{h^{(\mathbf{w})} \in \mathcal{H}}{\operatorname{argmin}} [(1/N_{\text{train}}) \sum_{i=1}^{N_{\text{train}}} \mathcal{L}((\mathbf{x}^{(i)}, y^{(i)}), h^{(\mathbf{w})}) + \lambda \|\mathbf{w}\|^2], \end{aligned} \quad (102)$$

with the regularization parameter  $\lambda > 0$ . The parameter  $\lambda$  trades a small training error  $\mathcal{E}(h^{(\mathbf{w})} | \mathbb{X})$  against a small norm  $\|\mathbf{w}\|$  of the weight vector. In particular, if we choose a large value for  $\lambda$ , then weight vectors  $\mathbf{w}$  with a large norm  $\|\mathbf{w}\|$  are “penalized” by having a larger objective function and are therefore unlikely to be a solution (minimizer) of the optimization problem (102).

Specialising (102) to the squared error loss and linear predictors yields **regularized linear**

**regression** (see (38)):

$$\hat{\mathbf{w}}^{(\lambda)} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \left[ (1/N_{\text{train}}) \sum_{i=1}^{N_{\text{train}}} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2 + \lambda \|\mathbf{w}\|_2^2 \right], \quad (103)$$

The optimization problem (103) is also known under the name **ridge regression** [13].

Using the feature matrix  $\mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N_{\text{train}})})^T$  and label vector  $\mathbf{y} = (y^{(1)}, \dots, y^{(N_{\text{train}})})^T$ , we can rewrite (103) more compactly as

$$\hat{\mathbf{w}}^{(\lambda)} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} \left[ (1/N_{\text{train}}) \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_2^2 \right]. \quad (104)$$

The solution of (104) is given by

$$\hat{\mathbf{w}}^{(\lambda)} = (1/N_{\text{train}})((1/N_{\text{train}})\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}. \quad (105)$$

This reduces to the closed-form expression (83) when  $\lambda = 0$  in which case regularized linear regression reduces to ordinary linear regression (see (103) and (38)). It is important to note that for  $\lambda > 0$ , the formula (105) is always valid, even when  $\mathbf{X}^T \mathbf{X}$  is singular (not invertible). This implies, in turn, that for  $\lambda > 0$  the optimization problem (104) (and (103)) have a unique solution (which is given by (105)).

Let us now study the effect of regularization on the resulting bias, variance and average prediction error incurred by the predictor  $h(\hat{\mathbf{w}}^{(\lambda)})(\mathbf{x}) = (\hat{\mathbf{w}}^{(\lambda)})^T \mathbf{x}$ . To this end, we will again invoke the simple probabilistic toy model (see (79), (81) and (82)) used already in Section 6.3. In particular, we interpret the training data  $\mathbb{X}^{(\text{train})} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N_{\text{train}}}$  as realizations of i.i.d. random variables according to (79), (81) and (82).

As discussed in Section 6.3, the average prediction error is the sum of three components: the bias, the variance and the noise variance  $\sigma^2$  (see (95)). The bias of regularized linear regression (103) is obtained as

$$B^2 = \|(\mathbf{I} - \mathbb{E}\{(\mathbf{X}^T \mathbf{X} + N\lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{X}\})\mathbf{w}_{\text{true}}\|_2^2. \quad (106)$$

For sufficiently large sample size  $N_{\text{train}}$  we can use the approximation

$$\mathbf{X}^T \mathbf{X} \approx N_{\text{train}} \mathbf{I} \quad (107)$$

such that (106) can be approximated as

$$\begin{aligned} B^2 &\approx \|(\mathbf{I} - (\mathbf{I} + \lambda \mathbf{I})^{-1})\mathbf{w}_{\text{true}}\|_2^2 \\ &= \sum_{l=1}^d \frac{\lambda}{1 + \lambda} w_{\text{true},l}^2. \end{aligned} \quad (108)$$

By comparing the (approximate) bias term (108) of regularized linear regression with the bias term (89) obtained for ordinary linear regression, we see that introducing regularization typically increases the bias. The bias increases with larger values of the regularization parameter  $\lambda$ .

For the variance of regularized linear regression (103), we obtain

$$V = (\sigma^2/N_{\text{train}}^2) \operatorname{trace} \mathbb{E}\{((1/N_{\text{train}})\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{X} ((1/N_{\text{train}})\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1}\}. \quad (109)$$

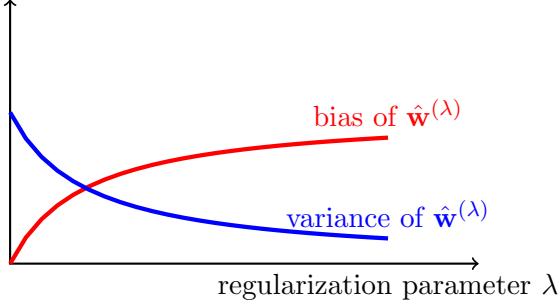


Figure 46: The bias and variance of regularized linear regression depend on the regularization parameter  $\lambda$  in an opposite manner resulting in a bias-variance tradeoff.

Using the approximation (107), which is reasonable for sufficiently large sample size  $N_{\text{train}}$ , we can approximate (109) as

$$V \approx \sigma^2(d/N_{\text{train}})(1/(1+\lambda)). \quad (110)$$

According to (110), the variance of regularized linear regression decreases with increasing regularization  $\lambda$ . Thus, as illustrated in Figure 46, the choice of  $\lambda$  has to balance between the bias  $B^2$  (108) (which increases with increasing  $\lambda$ ) and the variance  $V$  (110) (which decreases with increasing  $\lambda$ ). This is another instance of the bias-variance tradeoff (see Figure 42).

So far, we have only discussed the effect of regularization on the statistical properties (bias, variance, average prediction error) of the resulting ML method. However, regularization has also an effect on the computational properties of the resulting ML method. Note that the objective function in (104) is a smooth (infinitely often differentiable) convex function. Thus, as for linear regression, we can solve the regularization linear regression problem using GD (4) (see Algorithm 4). The effect of adding the regularization term  $\lambda\|\mathbf{w}\|_2^2$  to the objective function within linear regression is a **speed up of GD**. Indeed, we can rewrite (104) as the quadratic problem

$$\min_{\mathbf{w} \in \mathbb{R}^d} \underbrace{(1/2)\mathbf{w}^T \mathbf{Q} \mathbf{w} - \mathbf{q}^T \mathbf{w}}_{=f(\mathbf{w})} \text{ with } \mathbf{Q} = (1/N)\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}, \mathbf{q} = (1/N)\mathbf{X}^T \mathbf{y}. \quad (111)$$

This is similar to the quadratic problem (41) underlying linear regression but with different matrix  $\mathbf{Q}$ . It turns out that the convergence speed of GD (see (55)) applied to solving a quadratic problem of the form (111) depends crucially on the condition number  $\kappa(\mathbf{Q}) \geq 1$  of the psd matrix  $\mathbf{Q}$  [27]. In particular, GD methods are fast if the condition number  $\kappa(\mathbf{Q})$  is small (close to 1).

This condition number is given by  $\frac{\lambda_{\max}((1/N)\mathbf{X}^T \mathbf{X})}{\lambda_{\min}((1/N)\mathbf{X}^T \mathbf{X})}$  for ordinary linear regression (see (41)) and given by  $\frac{\lambda_{\max}((1/N)\mathbf{X}^T \mathbf{X}) + \lambda}{\lambda_{\min}((1/N)\mathbf{X}^T \mathbf{X}) + \lambda}$  for regularized linear regression (111). For increasing regularization parameter  $\lambda$ , the condition number obtained for regularized linear regression (111) tends to 1:

$$\lim_{\lambda \rightarrow \infty} \frac{\lambda_{\max}((1/N)\mathbf{X}^T \mathbf{X}) + \lambda}{\lambda_{\min}((1/N)\mathbf{X}^T \mathbf{X}) + \lambda} = 1. \quad (112)$$

Thus, according to (112), the GD implementation of regularized linear regression (see Algorithm 4) with a large value of the regularization parameter  $\lambda$  in (103) will converge faster compared to GD for linear regression (see Algorithm 1).

---

**Algorithm 4** “Regularized Linear Regression via GD”

---

**Input:** labeled dataset  $\mathbb{X} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$  containing feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and labels  $y^{(i)} \in \mathbb{R}$ ;

GD step size  $\alpha > 0$ .

**Initialize:** set  $\mathbf{w}^{(0)} := \mathbf{0}$ ; set iteration counter  $k := 0$

1: **repeat**

2:      $k := k + 1$  (increase iteration counter)

3:      $\mathbf{w}^{(k)} := (1 - \alpha\lambda)\mathbf{w}^{(k-1)} + \alpha(2/N) \sum_{i=1}^N (y^{(i)} - (\mathbf{w}^{(k-1)})^T \mathbf{x}^{(i)}) \mathbf{x}^{(i)}$  (do a GD step (55))

4: **until** convergence

**Output:**  $\mathbf{w}^{(k)}$  (which approximates  $\hat{\mathbf{w}}^{(\lambda)}$  in (104))

---

Let us finally point out a close relation between regularization (by adding the term  $\lambda\|\mathbf{w}\|^2$  in (102)) and model selection (see Section 6.2). It can be shown (see [35, Ch. 5]) that the regularized ERM (102) is equivalent to

$$\hat{\mathbf{w}}^{(\lambda)} = \underset{h^{(\mathbf{w})} \in \mathcal{H}^{(\lambda)}}{\operatorname{argmin}} (1/N_{\text{train}}) \sum_{i=1}^{N_{\text{train}}} (y^{(i)} - h^{(\mathbf{w})}(\mathbf{x}^{(i)}))^2 \quad (113)$$

with the restricted hypothesis space

$$\mathcal{H}^{(\lambda)} := \{h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R} : h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}, \text{ with some weight vector } \|\mathbf{w}\|^2 \leq C(\lambda)\} \subset \mathcal{H}^{(d)}. \quad (114)$$

For any given value  $\lambda$ , we can find a bound  $C(\lambda)$  such that solutions of (102) coincide with the solutions of (113). Thus, by solving the regularized ERM (102) we are performing implicitly model selection using a continuous ensemble (in contrast, to a discrete sequence of hypothesis spaces considered in Section 6.2) of hypothesis spaces  $\mathcal{H}^{(\lambda)}$  given by (114).

## 8 Clustering

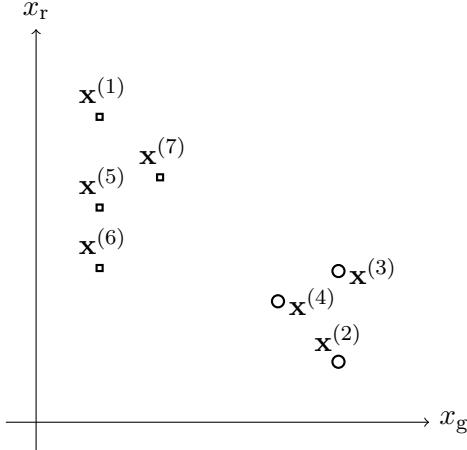


Figure 47: A scatterplot obtained from the features  $\mathbf{x}^{(i)} = (x_r^{(i)}, x_g^{(i)})^T$ , given by the redness  $x_r^{(i)}$  and greenness  $x_g^{(i)}$ , of some snapshots.

Up to now, we mainly considered ML methods which required some labeled training data in order to learn a good predictor or classifier. We will now start to discuss ML methods which do not make use of labels. These methods are often referred to as “unsupervised” since they do not require a supervisor (or teacher) which provides labels of some data points (which form the training set).

An important class of unsupervised methods, known as clustering methods, aims at grouping data points  $\mathbf{z}^{(i)}$ , for  $i = 1, \dots, N$ , into few **clusters** (subsets of data points). While there is no widely accepted definition of what is a cluster, we typically mean by a cluster a subset of data points which are more similar to each other than to other data points (belonging to different clusters). A variety of different clustering methods is obtained by using different choices for measuring “similarity” between data points.

In what follows we assume that data points  $\mathbf{z}^{(i)}$ , for  $i = 1, \dots, N$ , are characterized by feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^d$  and measure similarity between data points using the Euclidean distance  $\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|$ .<sup>10</sup> Thus, we consider two data points  $\mathbf{z}^{(i)}$  and  $\mathbf{z}^{(j)}$  similar if  $\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|$  is small. Moreover, we assume the number  $k$  of clusters prescribed.

Consider the scatter plot in Figure 47 which is obtained from the redness and greenness of several snapshots, which we would like to order into two groups: those snapshots which depict mostly grass and those which depict mostly something else than grass. We characterize a snapshot using the feature vector  $\mathbf{x} = (x_r, x_g)^T \in \mathbb{R}^2$  and the label  $y \in \{1, 2\}$  with  $y = 1$  if the snapshot shows grass and  $y = 2$  otherwise. If we were able to group the snapshots based solely on their features  $\mathbf{x}^{(i)}$  into  $k = 2$  groups  $\mathcal{C}_1$  (which correspond to grass snapshots) and  $\mathcal{C}_2$  (non-grass snapshots), we would need to acquire the label of one data point only. Indeed, given a perfect clustering, if we

<sup>10</sup>With a slight abuse of notation, we will occasionally denote a data point  $\mathbf{z}^{(i)}$  using its feature vector  $\mathbf{x}^{(i)}$ . In general, the feature vector is only part of a data point but for unsupervised methods we only have access to the feature vector of the data point.

know the label of one data point, we immediately know the label of all other data points in the same cluster. Moreover, we would also know the labels of the data points in the other cluster, since there are only two possible label values.

There are two main flavours of clustering methods:

- hard clustering (see Section 8.1)
- and soft clustering methods (see Section 8.2).

Within hard clustering, each data point  $\mathbf{x}^{(i)}$  belongs to one and only one cluster. In contrast, soft clustering methods assign a data point  $\mathbf{x}^{(i)}$  to several different clusters with varying degree of belonging (confidence).

Clustering methods determine for each data point  $\mathbf{z}^{(i)}$  a cluster assignment  $y^{(i)}$ . The cluster assignment  $y^{(i)}$  encodes to which cluster and to what extend the data point  $\mathbf{z}^{(i)}$  belongs to. For hard clustering with a prescribed number of  $k$  clusters, the cluster assignments  $y^{(i)} \in \{1, \dots, k\}$  represent the index of the cluster to which  $\mathbf{x}^{(i)}$  belongs.

In contrast, soft clustering allows each data point to belong to several different clusters. The degree with which data point  $\mathbf{x}^{(i)}$  belongs to cluster  $c \in \{1, \dots, k\}$  is denoted by the numbers  $y_c^{(i)} \in [0, 1]$ , which we stack into the vector  $\mathbf{y}^{(i)} = (y_1^{(i)}, \dots, y_k^{(i)})^T \in [0, 1]^k$ . Thus, while hard clustering generates non-overlapping clusters, the clusters produced by soft clustering methods may overlap.

We intentionally used the same symbol  $y^{(i)}$  used to denote the cluster assignments of a data point  $\mathbf{x}^{(i)}$  as we used to denote an associated label  $y^{(i)}$  in earlier sections. There is a strong conceptual link between clustering and classification.

We can interpret clustering as an extreme case of classification without having access to any labeled training data, i.e., we do not know the label of any data point.

Thus, in order to have any chance to find the correct labels (cluster assignments)  $y_c^{(i)}$  we have to rely solely on the intrinsic geometry of the data points which is given by the locations of the feature vectors  $\mathbf{x}^{(i)}$ .

## 8.1 Hard Clustering

A simple method for hard clustering is  $k$ -means which requires the number  $k$  of clusters to be specified before-hand. The idea underlying  $k$ -means is quite simple: First, given a current guess for the cluster assignments  $y^{(i)}$ , determine the cluster means  $\mathbf{m}^{(c)} = \frac{1}{|\{i:y^{(i)}=c\}|} \sum_{i:y^{(i)}=c} \mathbf{x}^{(i)}$  for each cluster.

Then, in a second step, update the cluster assignments  $y^{(i)} \in \{1, \dots, k\}$  for each data point  $\mathbf{x}^{(i)}$  based on the nearest cluster mean. By iterating these two steps we obtain Algorithm 5, which is known as “ $k$ -means”.

Here, in (115) we denote by  $\underset{c' \in \{1, \dots, k\}}{\operatorname{argmin}} \|\mathbf{x}^{(i)} - \mathbf{m}^{(c')}\|$  the set of all cluster indices  $c$  such that  $\|\mathbf{x}^{(i)} - \mathbf{m}^{(c)}\| = \min_{c' \in \{1, \dots, k\}} \|\mathbf{x}^{(i)} - \mathbf{m}^{(c')}\|$ .

The  $k$ -means algorithm requires the specification of initial choices for the cluster means  $\mathbf{m}^{(c)}$ , for  $c = 1, \dots, k$ . Unfortunately, there is no unique optimal strategy for the initialization but several heuristic strategies can be used. One approach to this initialization is to choose the cluster

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**Algorithm 5** “ $k$ -means”

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**Input:** dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ ; number  $k$  of clusters.

**Initialize:** choose initial cluster means  $\mathbf{m}^{(c)}$  for  $c = 1, \dots, k$ .

1: **repeat**

2:   for all  $i = 1, \dots, N$ , do

$$y^{(i)} \in \operatorname{argmin}_{c' \in \{1, \dots, k\}} \|\mathbf{x}^{(i)} - \mathbf{m}^{(c')}\| \text{ (update cluster assignments)} \quad (115)$$

3:   for all  $c = 1, \dots, k$  do

$$\mathbf{m}^{(c)} = \frac{1}{|\{i : y^{(i)} = c\}|} \sum_{i:y^{(i)}=c} \mathbf{x}^{(i)} \text{ (update cluster means)} \quad (116)$$

4: **until** convergence

**Output:** cluster assignments  $y^{(i)} \in \{1, \dots, k\}$

---

means as realizations of a random vector  $\mathbf{m}$  whose distribution is somehow matched to the dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}$ , e.g.,  $\mathbf{m} \sim \mathcal{N}(\hat{\mathbf{m}}, \hat{\mathbf{C}})$  with sample mean  $\hat{\mathbf{m}} = (1/N) \sum_{i=1}^N \mathbf{x}^{(i)}$  and the sample covariance  $\hat{\mathbf{C}} = (1/N) \sum_{i=1}^N (\mathbf{x}^{(i)} - \hat{\mathbf{m}})(\mathbf{x}^{(i)} - \hat{\mathbf{m}})^T$ . Another option is to choose the cluster means  $\mathbf{m}^{(c)}$  by randomly selecting  $k$  different data points  $\mathbf{x}^{(i)}$ . The cluster means might also be chosen by evenly partitioning the value range of the principal component of the dataset (see Section 9).

It can be shown that  $k$ -means implements a variant of empirical risk minimization. To this end we define the empirical risk (or “clustering error”)

$$\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X}) = (1/N) \sum_{i=1}^N \left\| \mathbf{x}^{(i)} - \mathbf{m}^{(y^{(i)})} \right\|^2. \quad (117)$$

Note that the empirical risk (117) depends on the current guess for the cluster means  $\{\mathbf{m}^{(c)}\}_{c=1,\dots,k}$  and cluster assignments  $\{y^{(i)}\}_{i=1,\dots,N}$ . The optimal cluster assignments and means minimize the empirical risk  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$ . Finding the global optimum of the function  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$  over all possible cluster assignments and cluster means is difficult as the function is non-convex.

However, the minimization of  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$  only partially by varying the cluster assignments  $\{y^{(i)}\}_{i=1}^N$  but with the cluster means  $\{\mathbf{m}^{(c)}\}_{c=1}^k$  held fixed is easy. Similarly, minimizing  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$  over the choices of cluster means with the cluster assignments held fixed is also quite simple. The  $k$ -means Algorithm 5 is exactly doing this: it is alternatively minimizing  $\mathcal{E}$  over all cluster means with the assignments  $\{y^{(i)}\}_{i=1}^N$  held fixed and minimizing  $\mathcal{E}$  over all cluster assignments with the cluster means  $\{\mathbf{m}^{(c)}\}_{c=1}^k$  held fixed. The interpretation of Algorithm 5 as an optimization method is useful for convergence diagnosis. In particular, we might terminate Algorithm 5 if the decrease of the objective function  $\mathcal{E}$  is below a prescribed (small) threshold.

A practical implementation of Algorithm 5 needs to fix three issues:

- Issue 1: We need to specify a tie-breaking strategy for the case that several indices  $c'$  achieve the minimum in the cluster assignment update (115).
- Issue 2: Moreover, we need to take care of the situation where no data points are associated

with cluster  $c$ , such that  $|\{i : y^{(i)} = c\}| = 0$  and the cluster means update (116) is not well defined for the cluster  $c$ .

- Issue 3: Finally, we also need to specify a particular criterion for termination (“checking convergence”).

The following algorithm fixes those three issues in a particular way [36].

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**Algorithm 6** “ $k$ -Means II” (a reformulation of the “Fixed Point Algorithm” presented in [36])

---

**Input:** dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ ; number  $k$  of clusters; prescribed tolerance  $\varepsilon \geq 0$ .

**Initialize:** choose initial cluster means  $\mathbf{m}^{(c)}$  for  $c = 1, \dots, k$  and assignments  $y^{(i)}$ ; iteration counter  $r := 0$ ; compute  $E^{(r)} = \mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N \mid \mathbb{X})$ ;

1: **repeat**

2:   for all data points  $i = 1, \dots, N$ , update cluster assignment

$$y^{(i)} := \min_{c' \in \{1, \dots, k\}} \left\{ \arg \min_{c'} \|\mathbf{x}^{(i)} - \mathbf{m}^{(c')}\| \right\} \text{ (update cluster assignments)} \quad (118)$$

3:   for all clusters  $c = 1, \dots, k$ , update activity indicator  $b^{(c)} = \begin{cases} 1 & \text{if } |\{i : y^{(i)} = c\}| > 0 \\ 0 & \text{else.} \end{cases}$

4:   for all  $c = 1, \dots, k$  with  $b^{(c)} = 1$ , update cluster means

$$\mathbf{m}^{(c)} = \frac{1}{|\{i : y^{(i)} = c\}|} \sum_{i:y^{(i)}=c} \mathbf{x}^{(i)} \text{ (update cluster means)} \quad (119)$$

5:    $r := r + 1$  (increment iteration counter)

6:    $E^{(r)} = \mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N \mid \mathbb{X})$  (see (117))

7: **until**  $E^{(r-1)} - E^{(r)} > \varepsilon$

**Output:** cluster assignments  $y^{(i)} \in \{1, \dots, k\}$  and cluster means  $\mathbf{m}^{(c)}$

---

The variables  $b^{(c)} \in \{0, 1\}$  indicate if cluster  $c$  is active ( $b^{(c)} = 1$ ) or cluster  $c$  is inactive ( $b^{(c)} = 0$ ), in the sense of having no data points assigned to it during the preceding cluster assignment step (118). Using these additional variables allows to ensure the cluster mean update step (119) to be well defined, since it is only applied to cluster  $c$  associated with at least one data point  $\mathbf{x}^{(i)}$ .

It can be shown that Algorithm 6 amounts to a fixed-point iteration

$$\{y^{(i)}\}_{i=1}^N \mapsto \mathcal{P}\{y^{(i)}\}_{i=1}^N \quad (120)$$

with some underlying operator  $\mathcal{P}$ . Thus, each iteration of Algorithm 6 amounts to an update of the cluster assignments  $y^{(i)}$  by applying the operator  $\mathcal{P}$ . By interpreting Algorithm 6 as a fixed-point iteration (120), the authors of [36, Thm. 2] present an elegant proof of the convergence of Algorithm 6 within a finite number of iterations (even for  $\varepsilon = 0$ ). What is more, after running Algorithm 6 for a finite number of iterations the cluster assignments  $\{y^{(i)}\}_{i=1}^N$  do not change anymore.

We illustrate the operation of Algorithm 6 in Figure 48. Each column corresponds to one iteration of Algorithm 6. The upper picture in each column depicts the update of cluster means while the lower picture shows the update of the cluster assignments during each iteration.

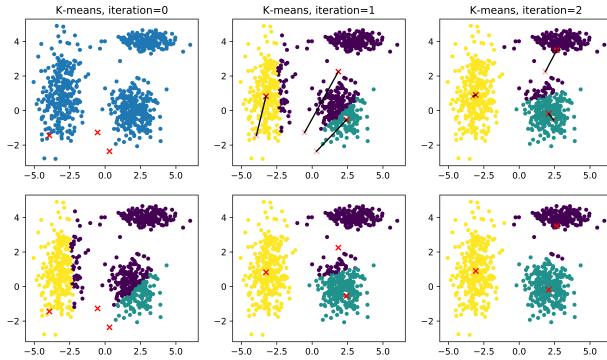


Figure 48: Evolution of cluster means and cluster assignments within  $k$ -means.

While Algorithm 6 is guaranteed to terminate after a finite number of iterations, the delivered cluster assignments and cluster means might only be (approximations) of local minima of the empirical error  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$  (see Figure 49). Therefore, in order to escape local minima, it is useful to run Algorithm 6 several times, each time using a different initialization for the cluster means and then pick the resulting cluster assignments  $\{y^{(i)}\}_{i=1}^N$  yielding the smallest value of  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$ .

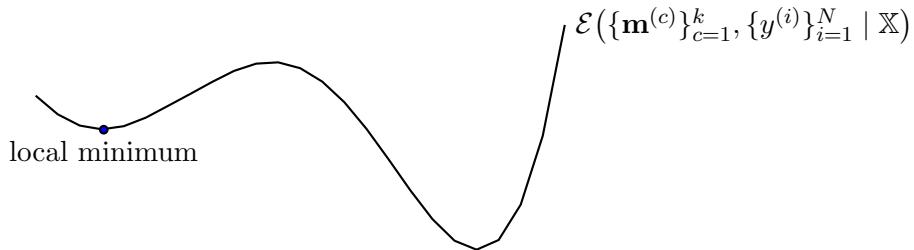


Figure 49: The empirical risk  $\mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$  underlying  $k$ -means (see (117)) is a non-convex function of the cluster means and assignments. It is therefore possible for  $k$ -means to get trapped around a local minimum.

Up till now, we have assumed the number  $k$  of clusters to be given before hand. However, in some applications it is not clear what a good choice for  $k$  can be. One approach to choosing the value of  $k$  is if the clustering method acts as a sub-module within an overall supervised ML system, which allows to implement some sort of validation. We could then try out different values of the number  $k$  and determine validation errors for each choice. Then, we pick the choice of  $k$  which results in the smallest validation error.

Another approach to choosing  $k$  is the so-called ‘‘elbow-method’’. This approach amounts to running  $k$ -means Algorithm 6 for different values of  $k$  resulting in the (approximate) optimum empirical error  $\mathcal{E}^{(k)} = \mathcal{E}(\{\mathbf{m}^{(c)}\}_{c=1}^k, \{y^{(i)}\}_{i=1}^N | \mathbb{X})$ . We then plot the minimum empirical error  $\mathcal{E}^{(k)}$  as a function of the number  $k$  of clusters. This plot typically looks like Figure 50, i.e., a steep decrease for small values of  $k$  and then flattening out for larger values of  $k$ . Finally, the choice of

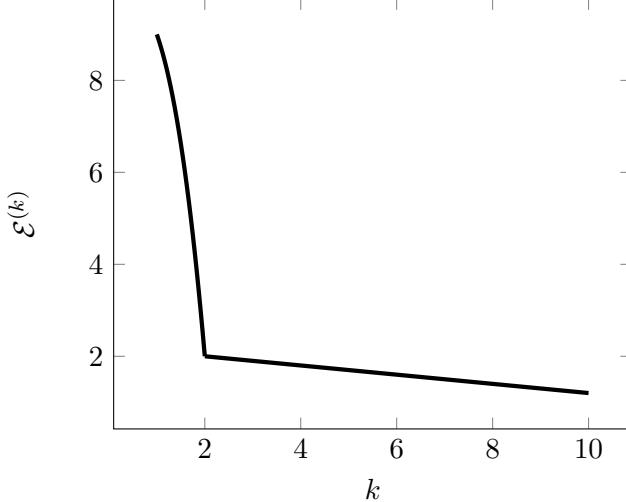


Figure 50: The clustering error  $\mathcal{E}^{(k)}$  achieved by  $k$ -means for increasing number  $k$  of clusters.

$k$  might be guided by some probabilistic model which penalizes larger values of  $k$ .

## 8.2 Soft Clustering

The cluster assignments obtained from hard-clustering methods, such as Algorithm 6, provide rather coarse-grained information. Indeed, even if two data points  $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$  are assigned to the same cluster  $c$ , their distances to the cluster mean  $\mathbf{m}^{(c)}$  might be very different. For some applications, we would like to have a more fine-grained information about the cluster assignments. In particular, we are interested in the degree by which a data point belongs to a particular cluster. The class of soft-clustering methods addresses this requirement by determining for each data point  $\mathbf{x}^{(i)}$  the degree by which it belongs to the different clusters  $c \in \{1, \dots, k\}$ .

In order to develop a soft clustering method, it is useful to interpret the observed data points  $\mathbf{x}^{(i)}$  as realizations of a random vector  $\mathbf{x}$ . The probability distribution of the random vector depends on the (hidden) cluster index  $c^{(i)} \in \{1, \dots, k\}$ , such that

$$P(\mathbf{x}^{(i)} | c^{(i)}) = \mathcal{N}(\boldsymbol{\mu}^{(c^{(i)})}, \boldsymbol{\Sigma}^{(c^{(i)})}) \quad (121)$$

with some (unknown!) cluster-specific mean vector  $\boldsymbol{\mu}^{(c)}$  and covariance matrix  $\boldsymbol{\Sigma}^{(c)}$  associated with cluster  $c$ . Thus, we consider  $\mathbf{x}^{(i)}$  drawn from some cluster, with index  $c^{(i)} \in \{1, \dots, k\}$ . Each cluster  $c \in \{1, \dots, k\}$  corresponds to a multivariate Gaussian distribution with mean  $\boldsymbol{\mu}^{(c)}$  and covariance matrix  $\boldsymbol{\Sigma}^{(c)}$ .

Since the true cluster indices  $c^{(i)}$  of data points  $\mathbf{x}^{(i)}$ , for  $i = 1, \dots, N$  are unknown, we model them as i.i.d. random variables. The probability distribution of the random variables  $c^{(i)}$  is characterized by the probabilities  $p_c = P(c^{(i)} = c)$  for  $c = 1, \dots, k$ . The overall probabilistic model (121) amounts to a **Gaussian mixture model** (GMM) since the marginal distribution  $P(\mathbf{x}^{(i)})$  is a mixture (superposition) of multivariate Gaussian distributions:

$$P(\mathbf{x}^{(i)}) = \sum_{c=1}^k P(c^{(i)} = c) \mathcal{N}(\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}). \quad (122)$$

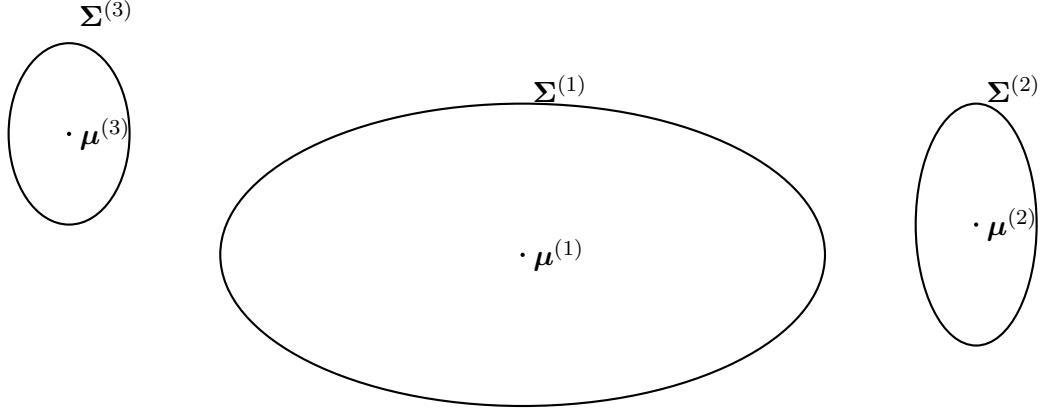


Figure 51: The GMM (122) yields a probability density function which is a weighted sum of multivariate normal distributions  $\mathcal{N}(\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)})$ . The weight of the  $c$ -th component is the cluster probability  $P(c^{(i)} = c)$ .

Using a GMM for the observed data  $\mathbf{x}^{(i)}$ , makes the clustering problem becoming a **statistical inference** or **parameter estimation problem** [37, 17]. In particular, we have to estimate (approximate) the true underlying cluster distribution  $p_c$ , means  $\boldsymbol{\mu}^{(c)}$  and covariances  $\boldsymbol{\Sigma}^{(c)}$  from the observed dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ . In what follows, we denote the estimates for those parameters by  $\hat{p}_c (\approx p_c)$ ,  $\mathbf{m}^{(c)} (\approx \boldsymbol{\mu}^{(c)})$  and  $\mathbf{C}^{(c)} (\approx \boldsymbol{\Sigma}^{(c)})$ , respectively. Based on the estimates for these parameters, we can then compute an estimate of the (a-posterior) probability

$$y_c^{(i)} = P(c^{(i)} = c \mid \mathbb{X}) \quad (123)$$

of the  $i$ -th data point  $\mathbf{x}^{(i)}$  belonging to cluster  $c$ , given the observed dataset  $\mathbb{X}$ .

It turns out that this estimation problem becomes significantly easier by operating in an alternating fashion: First, compute an estimate  $\hat{p}_c$  the cluster distribution  $p_c$  given a current estimate  $\mathbf{m}^{(c)}, \mathbf{C}^{(c)}$  for the cluster means and covariances. Then, given the current estimate  $\hat{p}_c$  for the cluster distribution  $p_c$ , update the estimates  $\mathbf{m}^{(c)}, \mathbf{C}^{(c)}$  of the cluster means and covariance matrices.

For ease of exposition, we consider the case of  $k = 2$  clusters  $c \in \{1, 2\}$ . The generalization to  $k > 2$  clusters is easy. We can then restrict ourselves to the cluster assignment  $y_1^{(i)}$  since  $y_2^{(i)} = 1 - y_1^{(i)}$ , since the vector entries  $\mathbf{y}^{(i)} = (y_1^{(i)}, y_2^{(i)})^T$  have to sum to one (any probability distribution has to sum to one). The cluster assignment probabilities can be written as  $p_1 = N_1/N$  and  $p_2 = N_2/N$  with  $N_1$  and  $N_2$  being interpreted as **effective sizes** of cluster  $c = 1$  and  $c = 2$ , respectively.

As for the  $k$ -means Algorithm 5, we can interpret the soft clustering Algorithm 7 as an instance of the ERM principle (Section 4). In particular, Algorithm 7 is a particular method for minimizing the empirical risk

$$\mathcal{E}(\{\mathbf{m}^{(c)}, \mathbf{C}^{(c)}, p_c\}_{c=1}^k \mid \mathbb{X}) = -\log \text{Prob}\{\mathbb{X}; \{\mathbf{m}^{(c)}, \mathbf{C}^{(c)}, p_c\}_{c=1}^k\}. \quad (125)$$

The interpretation of Algorithm 7 as a method for minimizing the empirical risk (125) suggests to use the decrease of the quantity  $-\log \text{Prob}\{\mathbb{X}; \{\mathbf{m}^{(c)}, \mathbf{C}^{(c)}, p_c\}_{c=1}^k\}$  for the termination criterion.

---

**Algorithm 7** “A Soft-Clustering Algorithm” [38]

---

**Input:** dataset  $\mathbb{X} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ ; number  $k$  of clusters.

**Initialize:** use initial guess for GMM parameters  $\{\mathbf{m}^{(c)}, \mathbf{C}^{(c)}, \hat{p}_r\}_{c=1}^k$

1: **repeat**

2:   for each sample  $\mathbf{x}^{(i)}$  and cluster  $c$ , update soft cluster assignments (degrees of belonging)

$$y_c^{(i)} = \frac{\hat{p}_c \mathcal{N}(\mathbf{x}^{(i)}; \mathbf{m}^{(c)}, \mathbf{C}^{(c)})}{\sum_{c'=1}^k \hat{p}_{c'} \mathcal{N}(\mathbf{x}^{(i)}; \mathbf{m}^{(c')}, \mathbf{C}^{(c')})} \quad (124)$$

3:   for each cluster  $c \in \{1, \dots, k\}$ , update estimates of GMM parameters:

- cluster probabilities  $\hat{p}_c = N_c/N$ , with effective cluster size  $N_c = \sum_{i=1}^N y_c^{(i)}$
- cluster means  $\mathbf{m}^{(c)} = \frac{1}{N_c} \sum_{i=1}^N y_c^{(i)} \mathbf{x}^{(i)}$
- cluster covariance matrices  $\mathbf{C}^{(c)} = \frac{1}{N_c} \sum_{i=1}^N y_c^{(i)} (\mathbf{x}^{(i)} - \mathbf{m}^{(c)}) (\mathbf{x}^{(i)} - \mathbf{m}^{(c)})^T$

4: **until** convergence

**Output:** soft cluster assignments  $\mathbf{y}^{(i)} = (y_1^{(i)}, \dots, y_k^{(i)})^T$

---

Similar to  $k$ -means Algorithm 5, also the soft clustering Algorithm 7 suffers from the problem of getting stuck in local minima of the empirical risk (125). As for  $k$ -means, a simple strategy to overcome this issue is to run Algorithm 7 several times, each time with a different initialization for the GMM parameter estimates  $\{\mathbf{m}^{(c)}, \mathbf{C}^{(c)}, \hat{p}_c\}_{c=1}^k$  and then picking the result which yields the smallest empirical risk (125).

We note that the empirical risk (125) underlying the soft-clustering Algorithm 7 is essentially a **log-likelihood function**. Thus, Algorithm 7 can be interpreted as an **approximate maximum likelihood** estimator for the true underlying GMM parameters  $\{\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, p_c\}_{c=1}^k$ . In particular, Algorithm 7 is an instance of a generic approximate maximum likelihood technique referred to as **expectation maximization** (EM) (see [13, Chap. 8.5] for more details). The interpretation of Algorithm 7 as a special case of EM allows to characterize the behaviour of Algorithm 7 using existing convergence results for EM methods [39].

We finally note that  $k$ -means hard clustering can be interpreted as an extreme case of soft-clustering Algorithm 7. Indeed, consider fixing the cluster covariance matrices  $\boldsymbol{\Sigma}^{(c)}$  within the GMM (121) to be the scaled identity:

$$\boldsymbol{\Sigma}^{(c)} = \sigma^2 \mathbf{I} \text{ for all } c \in \{1, \dots, k\}. \quad (126)$$

Then, for very small variance  $\sigma^2$  of the Gaussian components (see (122) and (126)), the update (124) tends to enforce  $y_c^{(i)} \in \{0, 1\}$ , i.e., each data point  $\mathbf{x}^{(i)}$  is associated to exactly one cluster  $c$ , whose cluster mean  $\mathbf{m}^{(c)}$  is closest to the data point  $\mathbf{x}^{(i)}$ . Thus, for  $\sigma^2 \rightarrow 0$ , the soft-clustering update (124) reduces to the hard cluster assignment update (115) of the  $k$ -means Algorithm 5.

## 9 Feature Learning

“To Make a Long Story Short”

A good part of this tutorial revolves around the problem of predicting the label  $y$  (e.g., the current location of Rumba) of a data point  $\mathbf{z}$  (e.g., a snapshot generated by the on-board camera of Rumba) based on some features  $\mathbf{x}$  (e.g., the total greenness) which characterize the data point  $\mathbf{z}$ . Intuitively, it should be beneficial to use more features since any observed properties of the data point can only help us in the task of predicting the label  $y$ . There are however two pitfalls in using a large number of features: the first one is a **computational pitfall** and the second one is a **statistical pitfall**.

Indeed, the longer the feature vector  $\mathbf{x}$ , the more computation (and storage) is required for executing the resulting ML method. Moreover, using a large number of features makes the resulting ML methods more prone to overfitting. Indeed, for linear regression it is essentially useless to use a feature vector  $\mathbf{x} \in \mathbb{R}^d$  whose length  $d$  exceeds the number  $N$  of labeled data points available for training (see Section 7.1). Thus, from a computational and statistical perspective, it is actually beneficial to use only a small number of features. However, the features have to be chosen such to retain most of the relevant information required for the prediction of the label  $y$ . Beside coping with overfitting and limited computational resources, feature learning can also be useful for data visualization. Indeed, if the resulting feature vector has length 2, we can use scatter plots to depict datasets.

We will now discuss some basic but powerful methods for efficiently constructing relevant features  $\mathbf{x}$  for a data point  $\mathbf{z}$ . Let us assume that the data point  $\mathbf{z}$  is represented by a large vector of length  $D$ . In order to obtain a small set of relevant features  $\mathbf{x} \in \mathbb{R}^d$ , we apply a linear operator to the data point:

$$\mathbf{x} = \mathbf{W}\mathbf{z}. \quad (127)$$

Here, the “compression” matrix  $\mathbf{W} \in \mathbb{R}^{d \times D}$  maps (in a linear fashion) the large vector  $\mathbf{z} \in \mathbb{R}^D$  to a smaller feature vector  $\mathbf{x} \in \mathbb{R}^d$ . In what follows, we consider particular choices for the matrix  $\mathbf{W}$ .

### 9.1 Principal Component Analysis

It is reasonable to choose the compression matrix  $\mathbf{W} \in \mathbb{R}^{d \times D}$  in (127) such that the resulting features  $\mathbf{x} \in \mathbb{R}^d$  allow to approximate the original data point as accurate as possible. We can approximate (or recover) the data point  $\mathbf{z} \in \mathbb{R}^D$  back from the features  $\mathbf{x}$  by applying a reconstruction operator  $\mathbf{R} \in \mathbb{R}^{D \times d}$ , which is chosen such that

$$\mathbf{z} \approx \mathbf{Rx} \stackrel{(127)}{=} \mathbf{RWz}. \quad (128)$$

The approximation error  $\mathcal{E}(\mathbf{W}, \mathbf{R} \mid \mathbb{X})$  resulting when (128) is applied to each data point in a dataset  $\mathbb{X} = \{\mathbf{z}^{(i)}\}_{i=1}^N$  is then

$$\mathcal{E}(\mathbf{W}, \mathbf{R} \mid \mathbb{X}) = (1/N) \sum_{i=1}^N \|\mathbf{z}^{(i)} - \mathbf{RWz}^{(i)}\|. \quad (129)$$

One can verify that the approximation error  $\mathcal{E}(\mathbf{W}, \mathbf{R} \mid \mathbb{X})$  can only be minimal if the compression matrix  $\mathbf{W}$  is of the form

$$\mathbf{W} = \mathbf{W}_{\text{PCA}} := (\mathbf{u}_1, \dots, \mathbf{u}_d)^T \in \mathbb{R}^{d \times D}, \quad (130)$$

with  $d$  orthonormal vectors  $\mathbf{u}_l$  which correspond to the  $d$  largest eigenvalues of the matrix

$$\mathbf{Q} := (1/N)\mathbf{Z}^T \mathbf{Z} \in \mathbb{R}^{D \times D} \quad (131)$$

with data matrix  $\mathbf{Z} = (\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)})^T \in \mathbb{R}^{N \times D}$ . By its very definition (131), the matrix  $\mathbf{Q}$  is positive semi-definite so that it allows for an eigenvalue decomposition (EVD) of the form [40]

$$\mathbf{Q} = (\mathbf{u}_1, \dots, \mathbf{u}_D) \begin{pmatrix} \lambda_1 & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & \dots & \lambda_D \end{pmatrix} (\mathbf{u}_1, \dots, \mathbf{u}_D)^T$$

with real-valued eigenvalues  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D \geq 0$  and orthonormal eigenvectors  $\{\mathbf{u}_r\}_{r=1}^D$ .

The features  $\mathbf{x}^{(i)}$ , obtained by applying the compression matrix  $\mathbf{W}_{\text{PCA}}$  (130) to the raw data points  $\mathbf{z}^{(i)}$ , are referred to as **principal components (PC)**. The overall procedure of determining the compression matrix (130) and, in turn, computing the PC vectors  $\mathbf{x}^{(i)}$  is known as **principal component analysis (PCA)** and summarized in Algorithm 8.

---

#### Algorithm 8 Principal Component Analysis (PCA)

---

**Input:** dataset  $\mathbb{X} = \{\mathbf{z}^{(i)} \in \mathbb{R}^D\}_{i=1}^N$ ; number  $d$  of PC.

- 1: compute EVD (132) yielding orthonormal eigenvectors  $(\mathbf{u}_1, \dots, \mathbf{u}_D)$  and decreasing eigenvalues  $\lambda_r$  for  $r = 1, \dots, D$
- 2: compute PC  $\mathbf{x}^{(i)} = \mathbf{W}_{\text{PCA}} \mathbf{z}^{(i)}$  with compression matrix (130)
- 3: compute approximation error  $\mathcal{E}^{(\text{PCA})} = \sum_{r=d+1}^D \lambda_r$  (see (132)).

**Output:** PC  $\mathbf{x}^{(i)}$  and approximation error  $\mathcal{E}^{(\text{PCA})}$ .

---

From a computational perspective, PCA Algorithm 8 effectively amounts to performing an EVD of the matrix  $\mathbf{Q} = \mathbf{Z}\mathbf{Z}^T$ . The EVD of  $\mathbf{Q}$  provides not only the optimal  $\mathbf{W}_{\text{PCA}}$ , the EVD (132) but also a measure for the information loss incurred by replacing the original data points  $\mathbf{z}^{(i)} \in \mathbb{R}^D$  with the smaller feature vector  $\mathbf{x}^{(i)} \in \mathbb{R}^d$ . In particular, this information loss is measured by the approximation error

$$\mathcal{E}^{(\text{PCA})} := \mathcal{E}(\mathbf{W}_{\text{PCA}}, \mathbf{R}_{\text{opt}} | \mathbb{X}) = \sum_{r=d+1}^D \lambda_r. \quad (132)$$

As depicted in Figure 52, the approximation error  $\mathcal{E}^{(\text{PCA})}$  depends on the number of PC  $d$  used in the feature transformation (127). The error is decreasing with increasing  $d$ . The maximum error  $\mathcal{E}^{(\text{PCA})} = (1/N) \sum_{i=1}^N \|\mathbf{z}^{(i)}\|^2$  is obtained for  $d = 0$  which amounts to completely ignoring the data points  $\mathbf{z}^{(i)}$ . For the other extreme case where  $d = D$ , which amounts to no compression at all, the approximation error is zero ( $\mathcal{E}^{(\text{PCA})} = 0$ ).

#### 9.1.1 How To Choose Number of PC?

two aspects

- for data visualization: use either  $d = 2$  or  $d = 3$
- computational budget: choose  $d$  sufficiently small such that computational complexity of overall ML method is feasible given the computational resources.

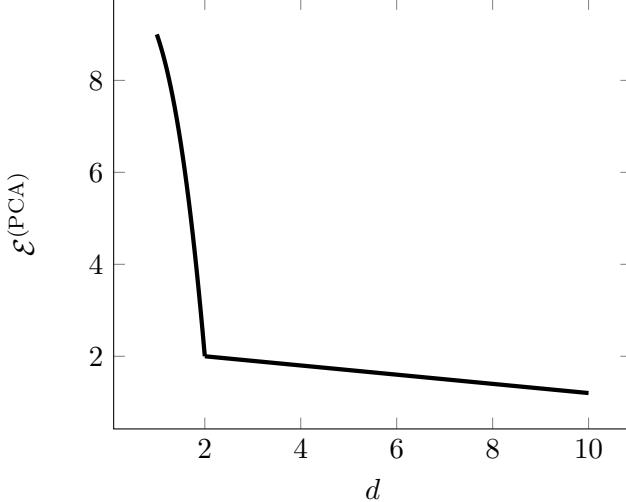


Figure 52: The reconstruction (approximation) error incurred by PCA for varying number  $d$  of PC.

- statistical budget: consider using PCA as a pre-processing step within a linear regression problem (see Section 3.1). Thus, we use the output  $\mathbf{x}^{(i)}$  of PCA as the feature vectors in linear regression. In order to avoid overfitting, we should choose  $d < N$  (see Section 7.1).
- approximation error: choose  $d$  such that approximation error  $\mathcal{E}^{(\text{PCA})}$  is reasonably small.

### 9.1.2 Data Visualisation

If we use PCA with  $d = 2$  PC, we obtain feature vectors  $\mathbf{x}^{(i)} = \mathbf{W}\mathbf{z}^{(i)}$  (see (127)) which can be illustrated as a scatter plot (see Section 2.1.3). Consider data points  $\mathbf{z}^{(i)}$  obtained from historic recordings of Bitcoin statistics (see Figure 7). Each data point  $\mathbf{z}^{(i)} \in \mathbb{R}^6$  is vector of length  $D = 6$ . It is difficult to visualise points in an Euclidean space  $\mathbb{R}^D$  of dimension  $D > 2$ . Therefore, in order to visualize data points, it is useful to apply PCA with  $d = 2$  PC. The resulting feature vectors  $\mathbf{x}^{(i)} \in \mathbb{R}^2$  can be depicted conveniently as a scatter plot (see Figure 53).

### 9.1.3 Extensions of PCA

There have been proposed several variants of the PCA method:

- **kernel PCA** [13, Ch.14.5.4]: combines PCA with a non-linear feature map (see Section 3.7).
- **robust PCA** [41]: modifies PCA to better cope with **outliers** in the dataset.
- **sparse PCA** [13, Ch.14.5.5]: requires each PC to involve **very few data attributes**  $z_j$ .
- **probabilistic PCA** [42, 43]: generalizes PCA by using a **probabilistic (generative) model** for the data.

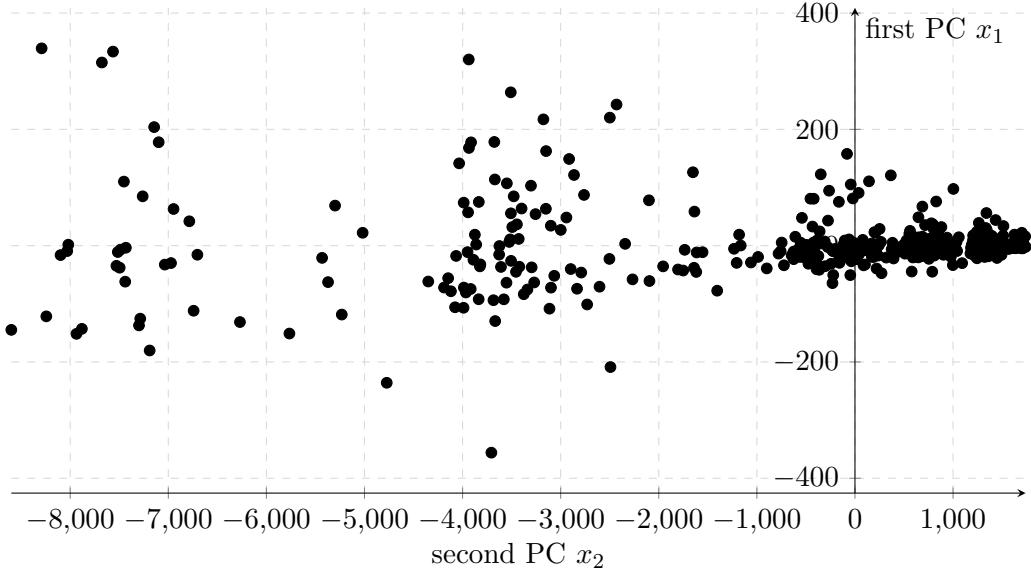


Figure 53: A scatterplot of feature vectors  $(x_1^{(i)}, x_2^{(i)})^T$  composed of the first two principal components of the Bitcoin statistics  $\mathbf{z}^{(i)}$  of the  $i$ -th day.

## 9.2 Linear Discriminant Analysis

Feature learning is typically used as a preprocessing step within some overall ML problem such as regression or classification. It can then be useful to exploit the availability of labeled data for the design of the compression matrix  $\mathbf{W}$  in (127). Note that PCA completely ignores any label information but only uses the features  $\mathbf{x}^{(i)}$  of the data points. For a binary classification problem, the compression matrix  $\mathbf{W}$  delivered by PCA can be highly suboptimal. A principled approach for choosing the compression matrix  $\mathbf{W}$  such that data points with different labels are well separated is **linear discriminant analysis** [13].

## 9.3 Random Projections

Note that PCA amounts to computing an EVD of the matrix  $\mathbf{XX}^T$  with the matrix  $\mathbf{X}$  containing the data points  $\mathbf{z}^{(i)} \in \mathbb{R}^D$  for  $i = 1, \dots, N$ . For a dimension  $D$  and sample size  $N$ , the overall computational complexity (amount of multiplications and additions) of lower bounded by  $\min\{D^2, N^2\}$  [44, 45]. This complexity of PCA can be prohibitive for ML applications with  $d$  and  $N$  being on the order of millions (which is already the case if the features are pixel values of a  $512 \times 512$  RGB bitmap, see Section 2.1.1). There is a surprisingly cheap alternative to PCA for finding a good choice for the compression matrix  $\mathbf{W}$  in (127). Indeed, a realization of a random matrix  $\mathbf{W}$  with entries i.i.d. according to a suitable probability distribution (such as the Bernoulli or Gaussian distribution) yields a good compression matrix  $\mathbf{W}$  (see (127)) with high probability [46, 47].

## 10 Glossary

- **classification problem:** an ML problem involving a discrete label space  $\mathcal{Y}$  (such as  $\mathcal{Y} = \{-1, 1\}$  for binary classification, or  $\mathcal{Y} = \{1, 2, \dots, K\}$  with  $K > 2$  for multi-class classification)
- **classifier:** a hypothesis map  $h : \mathcal{X} \rightarrow \mathcal{Y}$  for a discrete label space (e.g.,  $\mathcal{Y} = \{-1, 1\}$ );
- **condition number**  $\kappa(\mathbf{Q})$  of a matrix  $\mathbf{Q}$ : the ratio of largest to smallest eigenvalue of a psd matrix  $\mathbf{Q}$
- **csv file:** a text file which contains numerical values which are separated by particular symbols (e.g, comma)
- **data point:** an elementary unit of information such as a single pixel, a single image, a particular audio recording, a letter, a text document or an entire social network user profile.
- **dataset:** a collection of data points.
- **eigenvalue/eigenvector:** for a square matrix  $\mathbf{A} \in \mathbb{R}^{d \times d}$  we call a non-zero vector  $\mathbf{x} \in \mathbb{R}^d$  an eigenvector of  $\mathbf{A}$  if  $\mathbf{Ax} = \lambda \mathbf{x}$  with some  $\lambda \in \mathbb{R}$ , which we call an eigenvalue of  $\mathbf{A}$ .
- **features:** any measurements used to characterize a datapoint, e.g., the maximum amplitude of a sound recoding or the greenness of an RGB image.
- **hypothesis map:** a map (or function)  $h : \mathcal{X} \rightarrow \mathcal{Y}$  from the feature space  $\mathcal{X}$  to the label space  $\mathcal{Y}$ . Given a data point with features  $\mathbf{x}$  we use a hypothesis map to estimate (or approximate) the label  $y$  using the predicted label  $\hat{y} = h(\mathbf{x})$ . Machine learning is about automating the search for a good hypothesis map such that the error  $y - h(\mathbf{x})$  is small.
- **hypothesis space:** a set of maps  $h : \mathcal{X} \rightarrow \mathcal{Y}$  as its elements.
- **i.i.d.:** independent and identically distributed; e.g., “ $x, y, z$  are i.i.d. random variables” means that the joint probability distribution  $p(x, y, z)$  factors into the product  $p(x)p(y)p(z)$  with the marginal probability distribution  $p(\cdot)$  which is the same for all three variables  $x, y, z$ .
- **label:** some property of a data point which is of interest, such as the fact if a webcam snapshot shows a forest fire or not
- **loss function:** a function which associates a given data point  $(\mathbf{x}, y)$  with features  $\mathbf{x}$  and label  $y$  and hypothesis map  $h$  a number that quantifies the prediction error  $y - h(\mathbf{x})$
- **positive semi-definite (psd) matrix:** a positive semidefinite matrix  $\mathbf{Q}$ , i.e., a symmetric matrix  $\mathbf{Q} = \mathbf{Q}^T$  such that  $\mathbf{x}^T \mathbf{Q} \mathbf{x} \geq 0$
- **predictor:** a hypothesis map  $h : \mathcal{X} \rightarrow \mathcal{Y}$  for a continuous label space (e.g.,  $\mathcal{Y} = \mathbb{R}$ )
- **regression problem:** an ML problem involving a continuous label space  $\mathcal{Y}$  (such as  $\mathcal{Y} = \mathbb{R}$ )
- **training data:** a dataset which is used for finding a good hypothesis map  $h \in \mathcal{H}$  out of a hypothesis space  $\mathcal{H}$  (e.g., via empirical risk minimization)
- **validation data:** a dataset which is used for evaluating the quality of a predictor which has been learnt using some other (training) data

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