

A Gentle Introduction to Supervised Machine Learning

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Abstract

This tutorial is based on the lecture notes for the courses “Machine Learning: Basic Principles” and “Artificial Intelligence”, which I have taught during fall 2017 and spring 2018 at Aalto university. The aim is to provide an accessible introduction to some of the main concepts and methods within supervised machine learning. Most of the current systems which are considered as (artificially) intelligent are based on some form of supervised machine learning. After discussing the main building blocks of a formal machine learning problem, some of the most popular algorithmic design patterns for machine learning methods are presented.

1 Introduction

This tutorial discusses some powerful techniques which can be used to build artificial intelligent (AI) systems which act rational in the sense of following an overarching goal.

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

The actual implementation of this principle requires, of course, to have a precise definition for 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 could be used (beneficially?):

- a **routing app** for Helsinki (similar to <https://www.reittiopas.fi/>): given the perceived specification of origin and destination as well as current traffic situation in Helsinki, determine optimal route plan; actions are particular choices of which means of transport to use and in what order; the return is derived from (reciprocal) trip duration (we prefer to reach the goal as fast as possible).
- a **chess AI**: perceived environment is the current constellation of all chess figures; actions are possible moves of the chess figures; return is the probability of winning.
- 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

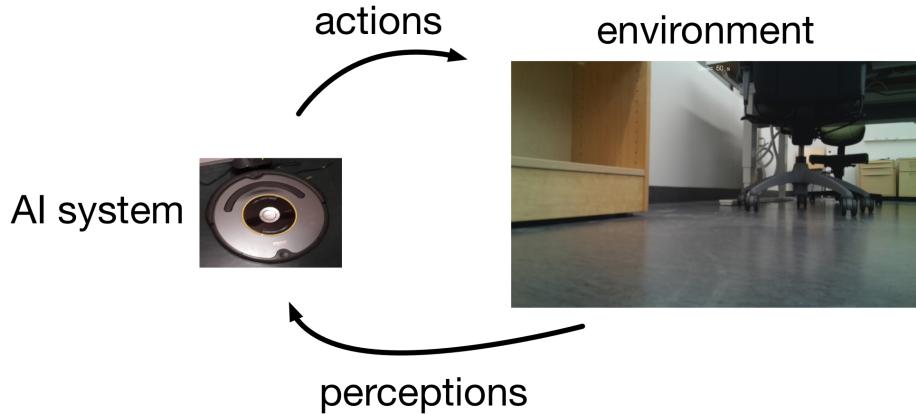


Figure 1: A cleaning robot should choose actions (corresponding to moving in different directions) in order to maximize the return measured in the amount of cleaned floor area per day.

("north", "south", "east", "west"); return might be the amount of cleaned floor area within a particular time period.

- **food waste avoidance:** we are currently wasting more edible food than what would be required to feed all starving people. A food avoidance system perceives the current consumer behaviour using various channels (social media, sales statistics of retailers) and choose optimally actions for when, where and what food to produce as well as how to distribute the food. The actions are chosen to maximize a particular choice for the return, e.g., the return can be measured by the amount of wasted food.
- **government-system** for Finland: perceived environment is constituted by current economic statistics (unemployment rate, budget deficit, ...); 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).

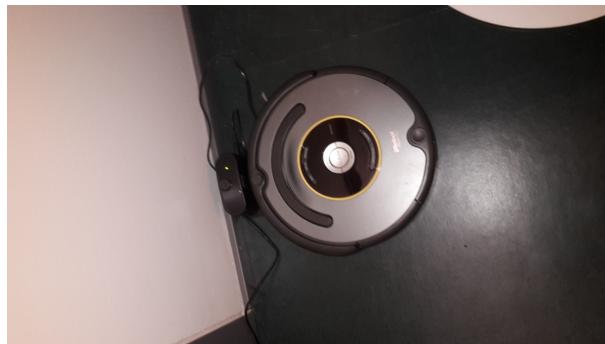


Figure 2: The cleaning robot “Rumba”.

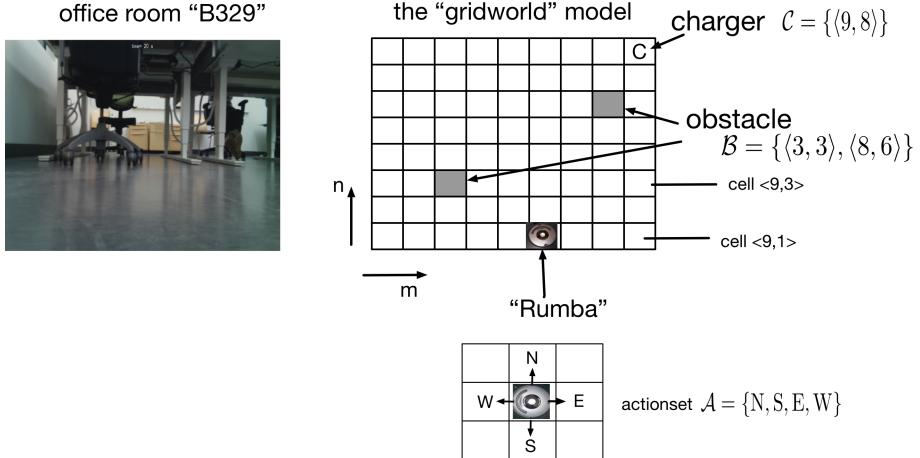


Figure 3: The office room, which Rumba has to keep tidy, and a simple gridworld model of the room’s floor space.

The task of determining **higher-level facts** or properties, e.g., your current location within the Aalto university main building, from **low-level perception**, e.g., measurements of distance sensors or snapshots generated by an on-board camera, is a key problem studied within the field of **machine learning (ML)**. In a certain sense, 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 functions such as logical reasoning.

In what follows, we discuss some basic ML techniques that enable the cleaning robot Rumba (see Figure 2) to predict its current location within the room using low-level data, e.g., simple features of snapshots obtained by an on-board camera. These methods require first to formalize the 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).

In Section 3 we introduce and discuss the principle of empirical risk minimization (ERM) which amounts to choosing a ML method based on minimizing the average loss incurred for labeled training data. A wide range of ML methods can be interpreted as an instance of ERM. In Section 4 we elaborate on a main algorithmic workhorse of modern ML algorithms, i.e., gradient descent which is an iterative method for solving the ERM problem. We then discuss in Section 5 the basic idea of validating a ML method by trying it out on labeled data which is different from the training data used within empirical risk minimization. As detailed in Section 6, a main reason for doing validation is to detect and avoid overfitting causing poor performance of ML methods.

2 The Elements of a ML Problem

Consider the cleaning robot “Rumba”, as depicted 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 $\langle m, n \rangle$ with integer valued coordinates $m \in \{1, \dots, K\}$ and $n \in \{1, \dots, L\}$.

In order to model the behaviour of Rumba, we define the state s_t of Rumba at time t as the

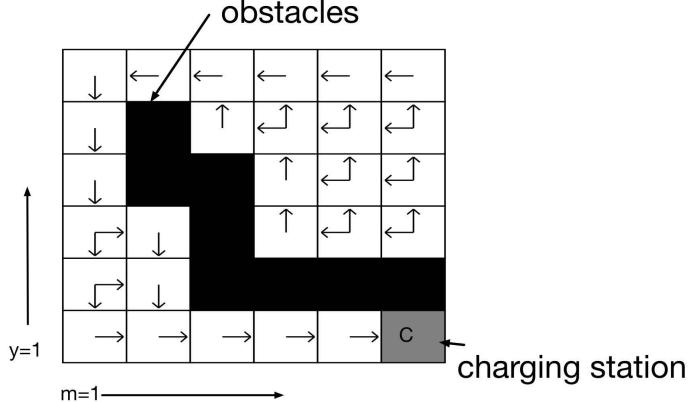


Figure 4: The optimal policy for Rumba when operating in office room “B329”.

cell $\langle m_t, n_t \rangle$ at which Rumba resides at time t . The state-space \mathcal{S} of Rumba is constituted by all possible states (cells) it can occupy, i.e.,

$$\mathcal{S} = \{\langle m, n \rangle \mid m \in \{1, \dots, K\}, n \in \{1, \dots, L\}\}. \quad (1)$$

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 take different actions $a \in \mathcal{A} = \{N, S, E, W\}$, which correspond to four directions into which it can move next (see Figure 3).

Let us assume that we have an up-to-date room plan for the office B329, i.e., this plan tells us precisely which cells of the floor are occupied by stuff and where to find charging stations. Using this knowledge, we can define a transition model (which is part of the MDP model) which describes how Rumba will behave when taking actions (e.g., it cannot move into obstacles and never leaves a charger). There are simple, yet quite efficient, methods based on the theory of Markov decision processes (MDP) [1], which allow to compute an optimal policy π for Rumba in order to reach a charging station as quickly as possible. In particular, such a policy $\pi : \mathcal{S} \rightarrow \mathcal{A}$ indicates the best action $\pi(s)$ for Rumba to take when it is in state $s \in \mathcal{S}$. We illustrate the optimal policy obtained for the particular room B329 in Figure 3. The arrow in cell $\langle m, n \rangle$ indicate the action which Rumba should take when it is currently in the corresponding grid cell or state $s = \langle m, n \rangle$, in order to reach the charging station as quickly as possible.

In order to implement (or execute) a policy π , which maps its current state s_t to its next action a_t , the cleaning robot Rumba needs to determine its current coordinates m_t, n_t within the gridworld office. However, it turns out that determining the precise location within a typical office room is far from trivial (cf. <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, n_t , using solely the information contained in the snapshots Rumba obtained by a cheap on-board camera.

2.1 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 512×512 pixels. In principle this bitmap image file can be fed into ML methods which then predict the coordinate n_t based on the snapshot. However, it is often much more efficient to feed a ML method not directly

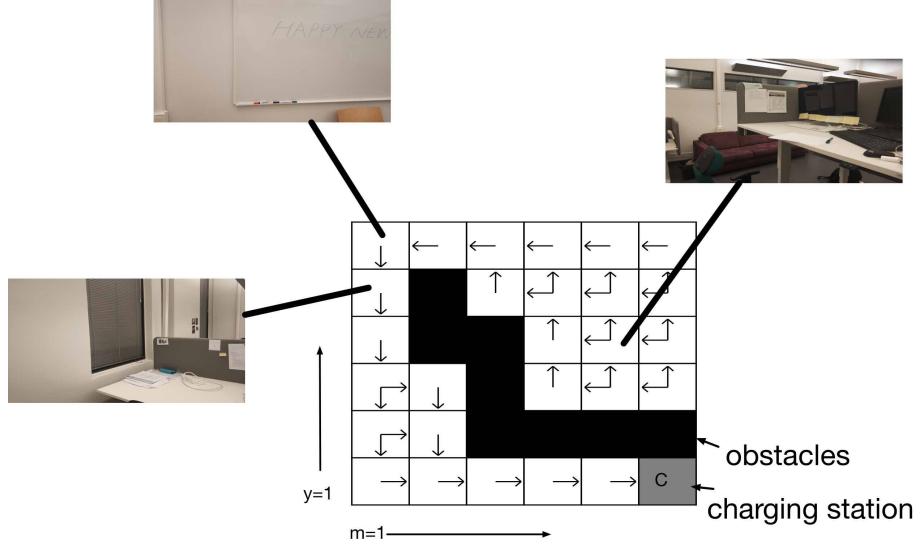


Figure 5: Several snapshots taken using the on-board camera Rumba while moving around in office “B329”.

using the raw format of the data point (such as RGB bitmaps), but rather a more compact set of characteristic properties of the data point which are called **features**.

Thus, we represent the snapshot $\mathbf{z}^{(t)}$ using the feature vector

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

which contains the individual features $x_i^{(t)}$. In principle, we can use as a feature any quantity which can be determined (computed) directly from the data point $\mathbf{z}^{(t)}$. E.g., we could define a feature $x_1^{(t)}$ using the red colour component of the pixel at location $(10, 100)$ in the snapshot $\mathbf{z}^{(t)}$, while another feature $x_2^{(t)}$ could be the number of pixels in the snapshot whose greenness is above a certain threshold. Alternatively, as depicted in Figure 6, we could use as features the red, green and blue components of each pixel in the snapshot.

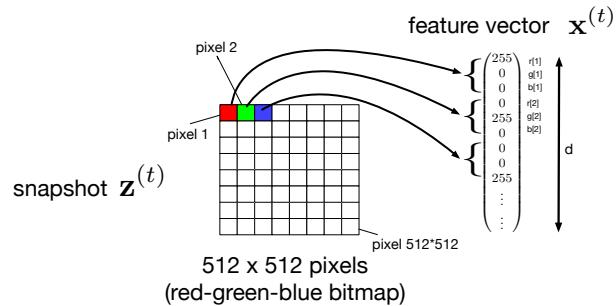


Figure 6: If the snapshot $\mathbf{z}^{(t)}$ is stored as a 512×512 RGB bitmap, we could use as features $\mathbf{x}^{(t)} \in \mathbb{R}^d$ the red-, green- and blue intensities of each pixel in the snapshot. The size of the feature vector would then be $d = 3 \cdot 512 \cdot 512$.

Choosing good features of data points arising within a particular ML application is far from trivial and might be even the most difficult task within the overall ML application. A recent breakthrough achieved by modern ML methods, which are referred to as **deep learning methods**, is that (to some extend) they can automatically learn good features without requiring too much manual tuning [2]. However, within this chapter, we will assume that the task of selecting good features is already solved and we have access to a suitable feature vector $\mathbf{x}^{(t)}$ which describes the snapshot $\mathbf{z}^{(t)}$.

In what follows, we will consider ML methods which will allow Rumba to determine its current location $s_t = \langle m_t, n_t \rangle$ solely from the features $\mathbf{x}^{(t)}$ of the snapshot $\mathbf{z}^{(t)}$. We consider the coordinates m_t and n_t of Rumba's location s_t as the **label (or output, or target)** associated with the snapshot $\mathbf{z}^{(t)}$ at time t (see Figure 7). For the sake of simplicity, let us focus on the subproblem of determining only the coordinate n_t of Rumba's current location in what follows. The adaption of the discussed methods in order to find the other coordinate m_t is trivial.

A ML method aims at constructing (or finding) a good predictor map $h : \mathbb{R}^d \rightarrow \mathbb{R}$ which takes the feature vector $\mathbf{x}^{(t)} \in \mathbb{R}^d$ as its input and delivers as its output a predicted label (or output or target) $\hat{n}_t = h(\mathbf{x}^{(t)})$. A good predictor map should be such that $\hat{n}_t \approx n_t$, i.e., the predicted label \hat{n}_t is close (in some sense) to the true underlying label n_t .

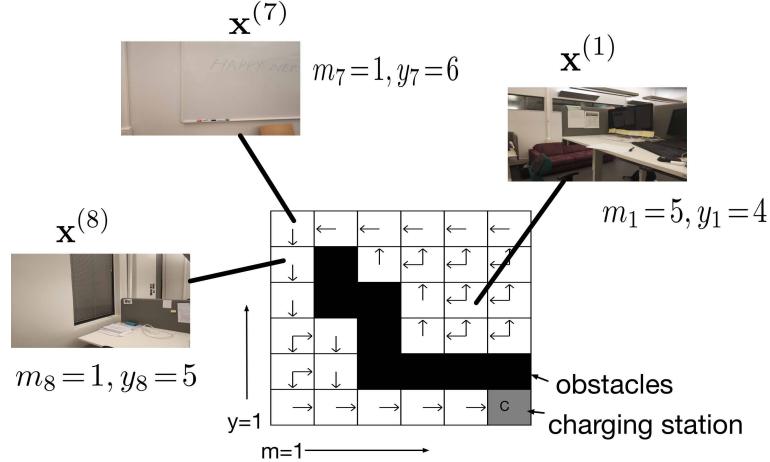


Figure 7: The cleaning robot Rumba is collecting snapshots $\mathbf{z}^{(t)}$, each of which is represented by the feature vector $\mathbf{x}^{(t)}$ and labeled with the coordinate n_t of Rumba, at time t .

2.2 Hypothesis Space

Remember our goal is to predict the coordinate $n_t \in \mathbb{R}$ of Rumba's location at time t based solely on the features $\mathbf{x}^{(t)} \in \mathbb{R}^d$ of the snapshot taken by the on-board camera of Rumba at time t . To this end we will construct a predictor map (or hypothesis) $h(\mathbf{x}^{(t)})$ which maps the feature vector of the snapshot to a predicted value $\hat{n}_t = h(\mathbf{x}^{(t)})$ which should approximate the true coordinate n_t as accurate as possible, i.e., $\hat{n}_t = n_t$. Much of ML theory and algorithms revolve around the analysis and design of automated methods for finding good predictors $h(\cdot)$.

In principle, we could use any map $h : \mathbb{R}^d \rightarrow \mathbb{R}$ as a predictor for the coordinate n_t based on the snapshot features $\mathbf{x}^{(t)}$ (see Figure 8). However, given limited computational resources, we should be

able to quickly search over all possible candidate predictors. To this end, it might be beneficial to restrict the ML methods to a small subset of “allowed” predictor functions. This subset of allowed predictors is called the **hypothesis space** of a ML method. In what follows, we will mainly focus on **linear prediction methods** which use the hypothesis space

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

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 $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^d$ 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 9).

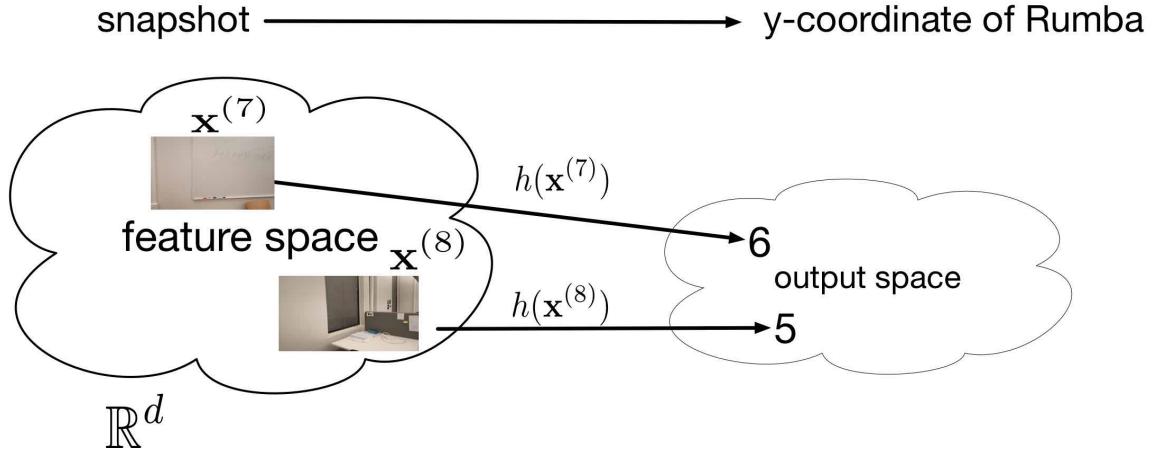


Figure 8: A predictor map $h : \mathbb{R}^d \rightarrow \mathbb{R}$ takes the feature vector $\mathbf{x}^{(t)} \in \mathbb{R}^d$ (e.g., representing the snapshot taken by Rumba at time t) as input and outputs a predicted label $\hat{n}_t = h(\mathbf{x}^{(t)})$ (e.g., the predicted coordinate of Rumba at time t). A key problem studied within ML is how to automatically learn a good (accurate) predictor map such that $n_t \approx h(\mathbf{x}^{(t)})$.

Note that each element of the hypothesis space \mathcal{H} in (2) is parametrized (indexed) by a particular value of the weight vector $\mathbf{w} \in \mathbb{R}^d$, i.e., each map $h^{(\mathbf{w})}$ is fully specified by the weight vector \mathbf{w} . Thus, instead of searching for good predictors 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 predictor maps are considered allowed, for a particular ML method is a design choice. The AI engineer has to choose a suitable hypothesis space individually for each particular ML application. The particular hypothesis space (2) constituted by linear predictor maps is only one possible choice, which however can be quite useful in many applications.

Another class of predictor maps $h : \mathbb{R}^d \rightarrow \mathbb{R}$ mapping a feature vector \mathbf{x} to a predicted label (output) $h(\mathbf{x})$, which has proven extremely powerful in a wide range of applications, e.g., image captioning or automated translation, is based on a **network representation** of a predictor map. In particular, we might define a predictor map $h^{(\mathbf{w})} : \mathbb{R}^d \rightarrow \mathbb{R}$ using an **artificial neural network** (ANN) structure as depicted in Figure 10. The feature vector \mathbf{x} is fed into the input units, each of which reads in one feature x_i . 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 (neuron) in the middle

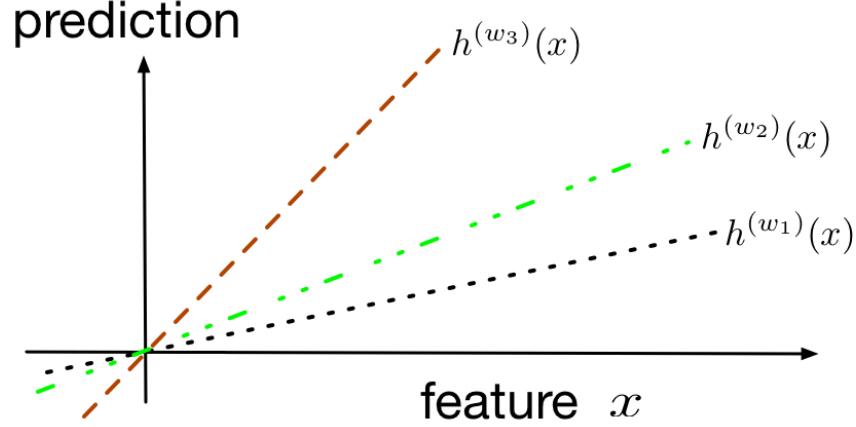


Figure 9: The hypothesis space \mathcal{H} which is constituted by all linear maps $h^{(w)}(x) = xw$ of the single feature x .

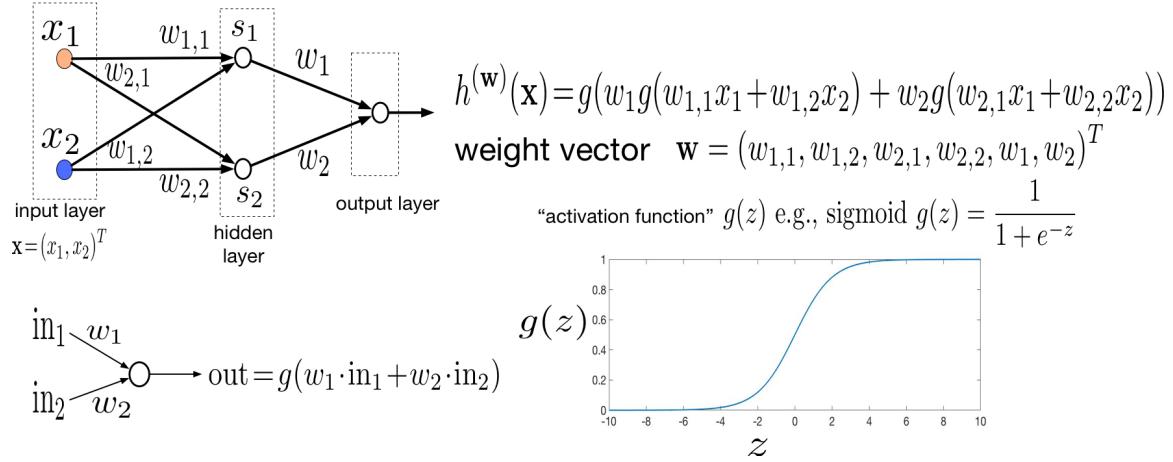


Figure 10: ANN representation of a predictor map $h^{(\mathbf{w})}(\mathbf{x})$ which maps the input (feature) vector $\mathbf{x} = (x_1, x_2)^T$ to a predicted label (output) $h^{(\mathbf{w})}(\mathbf{x})$.

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

Table 1: A spread sheet implementation of a predictor $h(x)$ which maps the feature $x \in [0, 1]$ to the predicted label (output) $h(x)$.

(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 function of a neuron is a weighted combination of the nodes in the previous layer. E.g., the activation for the neuron s_1 is $z = w_{1,1}x_1 + w_{1,2}x_2$.

It turns out that using a simple non-linear activation function $g(z)$ (e.g., the sigmoid function $g(z) = \frac{1}{1+e^{-z}}$) as 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 which is associated with a typical ANN, 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 [2, Ch. 6.4.1.].

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 [2] for an in-depth introduction to deep learning methods).

On a more practical level, we can derive classes of predictor maps (a hypothesis space) directly from the properties of the particular computational framework used for implementing the predictor maps: If we use a spreadsheet program as the computational engine, we could define a hypothesis space by collecting all predictor maps which can be implemented by a lookup table (see Table 1) having two columns, one for the input value and one for the output value, and at 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 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.

2.3 Loss Function and Empirical Risk

In order to assess the quality of a particular predictor $h(\mathbf{x})$ (“is it any good?”) of the label y based on features \mathbf{x} , we require a measure for the error (or loss) incurred by using the particular predictor $h(\mathbf{x})$ when the true label is y . For real-valued labels $y \in \mathbb{R}$, a common choice is the **squared error loss** (see Figure 11)

$$L((\mathbf{x}, y), h) := (y - h(\mathbf{x}))^2. \quad (3)$$

We refer to ML problems involving a real-valued label (e.g., temperature or probabilities of an event) as **regression problems**.

For ML applications using binary-valued labels $y \in \{-1, 1\}$, a popular choice is the **hinge loss** (see Figure 11)

$$L((\mathbf{x}, y), h) := \max\{0, 1 - y \cdot h(\mathbf{x})\}. \quad (4)$$

We refer to ML problems involving a discrete-valued label y , i.e., the label y can take on values only from a finite set, as **classification problems**. Examples of classification problems are, e.g., detecting presence of a tumour in a tissue or classifying persons according to their age group.

In principle, the loss function used within a ML method is a **design parameter** which has to be chosen suitably for a particular application.

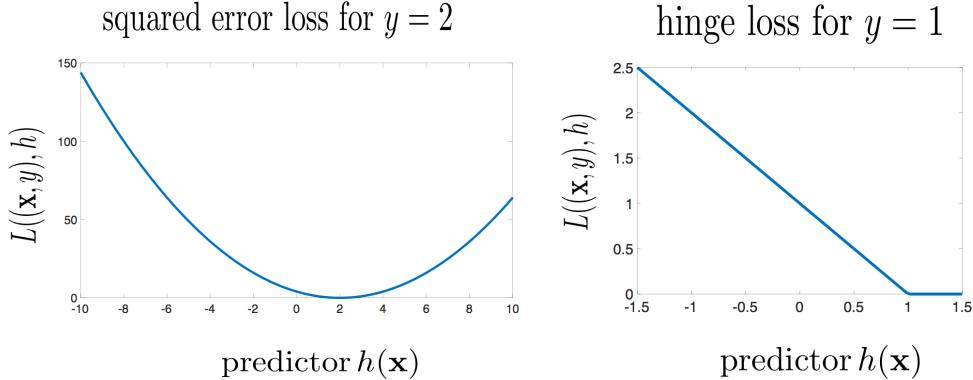


Figure 11: Two popular choices for the loss function: (Left) the squared error loss $L((\mathbf{x}, y), h) := (y - h(\mathbf{x}))^2$ is often used for predicting continuous (numerical) variables (e.g., the coordinate of the current location of Rumba); (Right) the hinge loss $L((\mathbf{x}, y), h) := \max\{0, 1 - yh(\mathbf{x})\}$ is often used for **classification problems** where the goal is to predict a discrete-valued variable (e.g., a binary variable $y \in \{-1, 1\}$).

In order to evaluate the loss $L((\mathbf{x}, y), h)$ 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, e.g., snapshots with features $\mathbf{x}^{(t)}$ and for which we know the true coordinate n_t of Rumba's location.

Let us assume we have collected a bunch of labeled snapshots during the first N time steps $t = 1, \dots, N$. We collect the snapshots into the **labeled dataset**

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

Having labeled data allows to compute the **empirical (average) risk** (see Figure 12) of a particular predictor h :

$$\mathcal{E}(h|\mathbb{X}) := (1/N) \sum_{(\mathbf{x}, y) \in \mathbb{X}} L((\mathbf{x}, y), h), \quad (5)$$

with some **loss function** $L((\mathbf{x}, y), h)$. For the particular choice of squared error loss (3), the empirical risk in (5) becomes the **mean squared error**

$$\mathcal{E}(h|\mathbb{X}) = (1/N) \sum_{(\mathbf{x}, y) \in \mathbb{X}} (y - h(\mathbf{x}))^2. \quad (6)$$

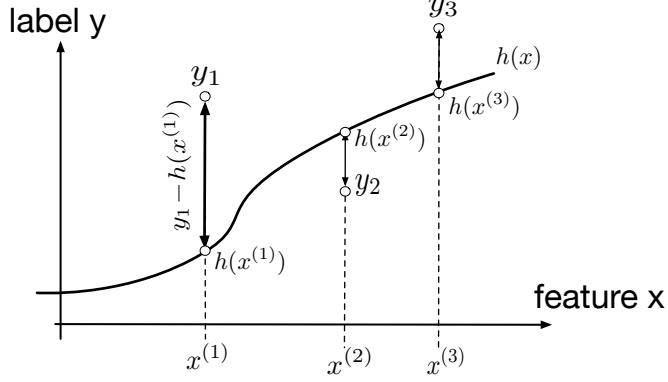


Figure 12: We can evaluate the quality of a predictor $h(\mathbf{x})$ by computing the prediction error $n_t - h(\mathbf{x}^{(t)})$ for labeled data points $(\mathbf{x}^{(t)}, n_t)$. These labeled data points could be, e.g., a bunch of snapshots with feature vectors $\mathbf{x}^{(t)}$ for which it is known at which coordinate n_t these snapshots have been taken.

3 Empirical Risk Minimization

For a given hypothesis space, e.g., the space of linear maps (2), we would like to find the particular predictor within \mathcal{H} which minimizes the empirical risk. Thus, we end up with an **empirical risk minimization (ERM) problem**

$$\hat{h} = \operatorname{argmin}_{h \in \mathcal{H}} \mathcal{E}(h|\mathbb{X}). \quad (7)$$

Solving the optimization problem (7) 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 $\mathcal{E}(\hat{h}|\mathbb{X})$, i.e., the empirical risk achieved by \hat{h} , gives us a measure of how accurate the predictions of \hat{h} will be. However, as we will discuss below, in certain settings the empirical risk $\mathcal{E}(\hat{h}|\mathbb{X})$ obtained for the data set \mathbb{X} might give only little indication on how well the predictor \hat{h} performs on new data points which are not contained in \mathbb{X} .

Using a parameterization $h^{(\mathbf{w})}(\mathbf{x})$ of the predictor maps, e.g., for linear predictors (2) or for ANNs (see Figure 10), we can rewrite (7) as an optimization directly over the weight vector:

$$\mathbf{w}_{\text{opt}} = \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^d} f(\mathbf{w}) \text{ with } f(\mathbf{w}) := \mathcal{E}(h^{(\mathbf{w})}|\mathbb{X}). \quad (8)$$

The objective function $f(\mathbf{w})$ in (8) is the empirical risk $\mathcal{E}(h^{(\mathbf{w})}|\mathbb{X})$ incurred by using the predictor $h^{(\mathbf{w})}$ to predict the labels n_t from the features $\mathbf{x}^{(t)}$ of the data points in the labeled dataset \mathbb{X} .

The idea of learning a good predictor map via ERM (7) conforms with the notion of learning by “trial and error”: Some instructor or supervisor provides snapshots $\mathbf{z}^{(t)}$ with features $\mathbf{x}^{(t)}$ and known labels n_t . We then try out different predictor maps h in order to tell the label n_t only from the snapshot features $\mathbf{x}^{(t)}$ and determine the error $\mathcal{E}(h|\mathbb{X})$ incurred. If the error $\mathcal{E}(h|\mathbb{X})$ is too large we consider another predictor map h' instead of h .

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 which should learn the concept “tractor” (see Figure 3). 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.

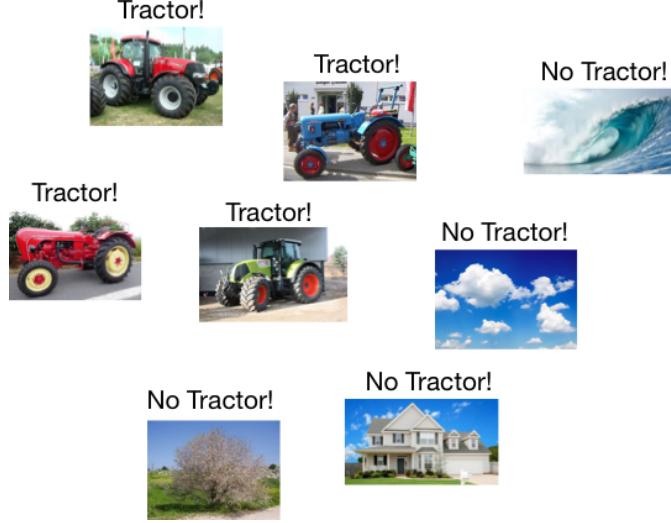


Figure 13: A bunch of labeled images. The label of an image indicates if a tractor is shown or not.

We highlight that the precise shape of the objective function $f(\mathbf{w})$ in (8) 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 $L((\mathbf{x}^{(t)}, n_t), h)$. The different combinations of predictor parametrisation and loss functions can result in objective functions whose optimization is more or less difficult. E.g., the objective function obtained for predictor maps parameterized using an ANN tends to be **highly non-convex**. The optimization of non-convex objective function is in general much more difficult than optimizing convex objective functions.

In what follows, we focus on the particular combination of squared error loss (3) 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 (8) as

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} f(\mathbf{w}) \text{ with objective function } f(\mathbf{w}) := (1/|\mathbb{X}|) \sum_{(\mathbf{x}, y) \in \mathbb{X}} (y - \mathbf{x}^T \mathbf{w})^2. \quad (9)$$

The objective function $f(\mathbf{w})$ in (9) has some appealing properties (see Figure 14): First, it is a **differentiable** function with a gradient $\nabla f(\mathbf{w})$ which provides a linear approximation around a point \mathbf{w}_0 as

$$f(\mathbf{w}) \approx f(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^T \nabla f(\mathbf{w}_0) \text{ for all } \mathbf{w} \text{ close to } \mathbf{w}_0. \quad (10)$$

Secondly, it is a **convex** (“bowl-shaped”) function, which means that any local minimum must be global minimum [3]. Note that while the hinge loss (4) is also convex, it is not differentiable.

It will be useful to rewrite the ERM problem (9) using matrix and vector representations of the feature vectors $\mathbf{x}^{(t)}$ and labels n_t contained in the dataset \mathbb{X} . To this end, we stack the labels n_t and the feature vectors $\mathbf{x}^{(t)}$, for $t = 1, \dots, N$, into a “label vector” \mathbf{n} and “feature matrix” \mathbf{X} as follows

$$\mathbf{n} = (n_1, \dots, n_N)^T \in \mathbb{R}^N, \text{ and } \mathbf{X} = (\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)})^T \in \mathbb{R}^{N \times d}. \quad (11)$$

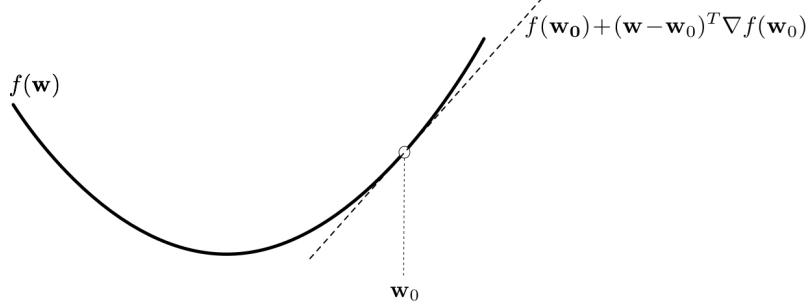


Figure 14: A convex (“bowl-shaped”) and differentiable function $f(\mathbf{w})$.

This allows us to rewrite the objective function in (9) as

$$f(\mathbf{w}) = (1/N)\|\mathbf{n} - \mathbf{X}\mathbf{w}\|_2^2$$

where $\|\mathbf{v}\|_2^2 = \sum_{i=1}^N v_i^2$ denotes the squared Euclidean norm of a vector $\mathbf{v} = (v_1, \dots, v_N)^T \in \mathbb{R}^N$.

4 Gradient Descent

Let us now introduce a very simple, yet quite powerful, algorithm for finding the weight vector \mathbf{w}_{opt} which solves the optimization problem (9). Assume we have already some guess (or approximation) $\mathbf{w}^{(k)}$ for \mathbf{w}_{opt} and would like to improve it, i.e., find a new guess $\mathbf{w}^{(k+1)}$ which yields a smaller value of the objective function, i.e., $f(\mathbf{w}^{(k+1)}) < f(\mathbf{w}^{(k)})$. 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. (10)) 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

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha \nabla f(\mathbf{w}^{(k)}) \quad (12)$$

with a sufficiently small positive **step size** α (a small α ensures that the linear approximation (10) 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 (12) amounts to a **gradient descent (GD) step**. It turns out that for a convex differentiable objective function $f(\mathbf{w})$ and sufficiently small positive step size α , the iterates $f(\mathbf{w}^{(k)})$ obtained by repeating the GD steps (12) converge to a minimum, i.e., $\lim_{k \rightarrow \infty} f(\mathbf{w}^{(k)}) = f(\mathbf{w}_{\text{opt}})$ (see Figure 15).

We can now formulate a full-fledged ML algorithm which amounts to finding the optimal weight vector \mathbf{w}_{opt} for a linear predictor of the form $h^{(\mathbf{w})}(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$. The optimal weight vector \mathbf{w}_{opt} should minimize the empirical risk $f(\mathbf{w}) = \mathcal{E}(h^{(\mathbf{w})} | \mathbb{X})$ (cf. (8)) incurred by the predictor $h^{(\mathbf{w})}$ when applied to the labeled dataset $\mathbb{X} = \{(\mathbf{x}^{(t)}, n_t)\}_{t=1}^N$.

It turns out to be extremely fruitful for the analysis of this learning algorithm to view at it from fixed-point theory. Indeed, we can rewrite the GD step (12) as the fixed-point iteration [4]

$$\mathbf{w}^{(k)} = \mathcal{P}\mathbf{w}^{(k-1)}$$

with the “GD operator” $\mathcal{P} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ defined as

$$\mathbf{w} \mapsto \mathcal{P}\mathbf{w} := \mathbf{w} - \alpha \nabla f(\mathbf{w}).$$

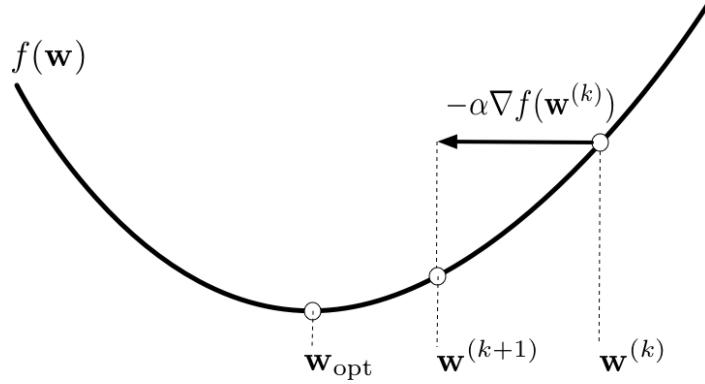


Figure 15: We can find the minimum of a convex and differentiable function $f(\mathbf{w})$ by repeatedly performing GD steps (12) with a sufficiently small step size α .

Algorithm 1 “Linear Regression via GD”

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

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: $\mathbf{w}^{(k)} := \mathbf{w}^{(k-1)} - \alpha \nabla f(\mathbf{w}^{(k-1)})$ (do a GD step (12))
- 4: **until** convergence

Output: $\mathbf{w}^{(k)}$ (which approximates \mathbf{w}_{opt} in (8))

Learning Rate. The choice of the step size α in the GD update (12) has a significant influence on the performance of Algorithm I. In particular, the step size controls the speed (or rate) at which the iterates $\mathbf{w}^{(k)}$ improve (with increasing iteration number k) in their ability to yield a good linear predictor $h(\mathbf{w}^{(k)})$. The quality of the predictor $h(\mathbf{w}^{(k)})$, obtained from the weight vector $\mathbf{w}^{(k)}$ after k iterations, is the corresponding objective value $f(\mathbf{w}^{(k)})$, which is the empirical risk incurred by applying the predictor $h(\mathbf{w}^{(k)})$ to the data set \mathbb{X} (cf. (9)). Therefore, the step size α is sometimes also referred to as the **learning rate** of the ML algorithm.

Choosing Right Step Size. As illustrated in Figure 16, choosing the learning rate α too small could lead to requiring an unreasonably large number of GD steps to come close to an optimal weight vector \mathbf{w}_{opt} (there might be several different weight vectors \mathbf{w}_{opt}). On the other hand, and even more serious, if we choose the learning rate α too large, then GD might not converge at all but, e.g., oscillate or diverge ($f(\mathbf{w}^{(k)}) \rightarrow \infty$).

Many (quite) sophisticated techniques for optimally tuning the learning rate in order to ensure fast convergence of the iterates $\mathbf{w}^{(k)}$ have been proposed [3]. Let us mention one sufficient condition on the learning rate α which guarantees the GD iterates $\mathbf{w}^{(k)}$ to converge to an optimum weight vector \mathbf{w}_{opt} , i.e., which minimizes the objective function $f(\mathbf{w})$ (9). In particular, convergence of GD is guaranteed for any learning rate which satisfies $\alpha \leq \frac{N}{2\rho(\mathbf{X}^T \mathbf{X})}$ where $\rho(\mathbf{X}^T \mathbf{X})$ denotes the **spectral radius** of the square matrix $\mathbf{X}^T \mathbf{X}$, i.e., the largest magnitude of the eigenvalues of $\mathbf{X}^T \mathbf{X}$.

Convergence Speed and Data Normalization. Moreover, it turns out that the convergence speed of the GD updates (12), i.e., the number of iterations necessary to reach the minimum of

the objective function (9) within a prescribed accuracy, depends on the condition number $\kappa(\mathbf{X}^T \mathbf{X})$ which is defined as the ratio between the largest and smallest eigenvalue of the matrix $\mathbf{X}^T \mathbf{X}$.

Note that the condition number is only well defined if the columns of the feature matrix \mathbf{X} (cf. (11)), which are precisely the feature vectors $\mathbf{x}^{(t)}$ contained in the labeled dataset $\mathbb{X} = \{(\mathbf{x}^{(t)}, n_t)\}_{t=1}^N$, are linearly independent. In this case the condition number is lower bounded by one, i.e., for any feature matrix \mathbf{X} with linearly independent columns we have $\kappa(\mathbf{X}^T \mathbf{X}) \geq 1$. It can be shown that the GD updates (12) converge faster for smaller condition number $\kappa(\mathbf{X}^T \mathbf{X})$ [4]. 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 raw data (original feature vectors) using a **normalization** (or **standardization**) procedure.

Algorithm 2 “Data Normalization”

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

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

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

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

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

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

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

The preprocessing implemented in Algorithm 2 reshapes (transforms) the original feature vectors $\mathbf{x}^{(t)}$ into new feature vectors $\hat{\mathbf{x}}^{(t)}$ 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., $\kappa(\hat{\mathbf{X}}^T \hat{\mathbf{X}}) \approx 1$.

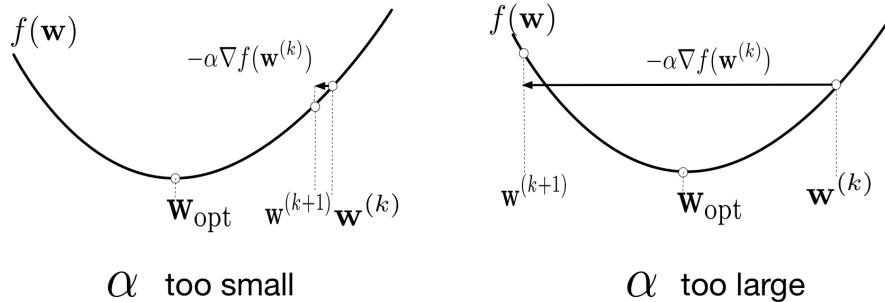


Figure 16: Left: if the learning rate α in the GD step (12) is chosen too small, the iterations make only very little progress towards the optimum. right: if the learning rate α is chosen too large, the iterates $\mathbf{w}^{(k)}$ might not converge at all (it might happen that $f(\mathbf{w}^{(k+1)}) > f(\mathbf{w}^{(k)})$!).

5 Validation

Let us assume we have used some ML algorithm, e.g., Algorithm I above, which delivered a predictor \hat{h} by optimizing its empirical risk obtained for the labeled dataset $\mathbb{X} = \{(\mathbf{x}^{(t)}, n_t)\}_{t=1}^N$ which consists of the features and labeled of the snapshots collected by Rumba during time $t = 1, \dots, N$. It is then important to monitor or **to validate** the performance of the predictor $h(\mathbf{x})$ on new data points.

For the validation of the predictor \hat{h} , we need to apply it to labeled snapshots, i.e., with known label n_t , 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 (7)). The intuition behind this guideline is that the predictor \hat{h} tends to “look better” on the training set than for many 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 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 $\mathbb{X} = \{(\mathbf{x}^{(t)}, n_t)\}_{t=1}^N$ is as follows (see Figure 17):

- divide the entire dataset \mathbb{X} of labeled snapshots into two disjoint subsets $\mathbb{X}^{(\text{train})}$ (which is often referred to as the “training set”) and $\mathbb{X}^{(\text{val})}$ (which is often referred to as the “validation set”): $\mathbb{X} = \mathbb{X}^{(\text{train})} \cup \mathbb{X}^{(\text{val})}$.
- learn a predictor \hat{h} via ERM using the training data $\mathbb{X}^{(\text{train})}$, i.e., compute (cf. (7))

$$\begin{aligned}\hat{h} &= \underset{h \in \mathcal{H}}{\operatorname{argmin}} \mathcal{E}(h | \mathbb{X}^{(\text{train})}) \\ &\stackrel{(6)}{=} \underset{h \in \mathcal{H}}{\operatorname{argmin}} (1 / |\mathbb{X}^{(\text{train})}|) \sum_{(\mathbf{x}, y) \in \mathbb{X}^{(\text{train})}} (y - h(\mathbf{x}))^2\end{aligned}\quad (13)$$

with corresponding **training error** $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{train})})$.

- validate the predictor \hat{h} obtained from (13) by computing the empirical risk $\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{val})})$ obtained when applying \hat{h} to the **validation dataset** $\mathbb{X}^{(\text{val})}$, i.e., the **validation error**

$$\mathcal{E}(\hat{h} | \mathbb{X}^{(\text{val})}) = (1 / |\mathbb{X}^{(\text{val})}|) \sum_{(\mathbf{x}, y) \in \mathbb{X}^{(\text{val})}} (y - \hat{h}(\mathbf{x}))^2.$$

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

The choice of the split ratio, 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 precise statements on how to choose the split ratio which would apply to a wide range of different ML problems.

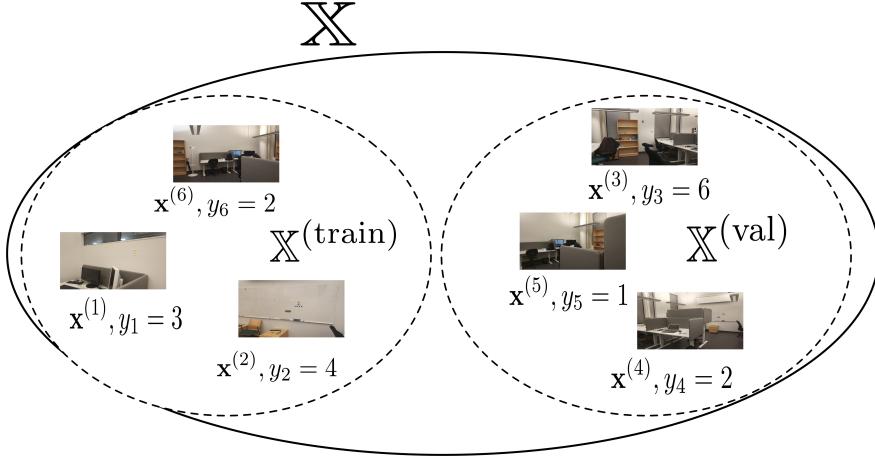


Figure 17: If we have only one single labeled dataset \mathbb{X} , we split it into a **training set** $\mathbb{X}^{(\text{train})}$ and a **validation set** $\mathbb{X}^{(\text{val})}$. We use the training set in order to learn (find) a good predictor $h(\mathbf{x})$ by minimizing the training error, i.e., the empirical risk $\mathcal{E}(h|\mathbb{X}^{(\text{train})})$ obtained for the training set. In order to verify or validate the performance of the predictor on new data, we compute the empirical risk of $h(\mathbf{x})$ over the validation set. We refer to the empirical risk $\mathcal{E}(h|\mathbb{X}^{(\text{val})})$ obtained for the validation set as the validation error.

6 Overfitting and Regularization

One of the main arguments for validating predictors is that it allows 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 paradigm is misleading in the sense of favouring predictors $h : \mathbb{R}^d \rightarrow \mathbb{R}$, which have a **small training error** (empirical risk obtained by applying the predictor to the training set) but a **large prediction error** on other data points, which are different from the data points used to train the predictor.

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}_{misl} depicted in Figure 18. For some reason, one of the images is labeled wrong, i.e., it is labeled as “tractor” but shows an ocean wave. As a consequence, if the child is good in memorizing images, it might predict the presence of tractors whenever seeing a wave (Figure 6).

For the sake of the argument, we assume that the child uses a linear predictor $h(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$, 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, it may use ERM with squared error loss over the training data set, i.e., its learning process amounts to solving the ERM problem (9) using the labeled training dataset \mathbb{X}_{misl} .

It turns out that, under quite general conditions, the ERM problem can be solved perfectly, i.e., there is a predictor $h^{(\mathbf{w}_{\text{opt}})}$ achieving **zero empirical risk** $\mathcal{E}(h^{(\mathbf{w}_{\text{opt}})}|\mathbb{X}_{\text{misl}}) = 0$, as soon as the number of training examples $N_{\text{train}} = |\mathbb{X}_{\text{misl}}|$ is smaller than the size d of the feature vector \mathbf{x} , i.e.,



Figure 18: A (misleading) training data set $\mathbb{X}_{\text{misl}} = \{(\mathbf{x}^{(t)}, y_t)\}_{t=1}^N$ consisting of $N = 9$ images. The t -th image is characterized by the feature vector $\mathbf{x}^{(t)} \in \mathbb{R}^d$ and labeled according to if a tractor is shown ($y_t = 1$) or not ($y_t = -1$).

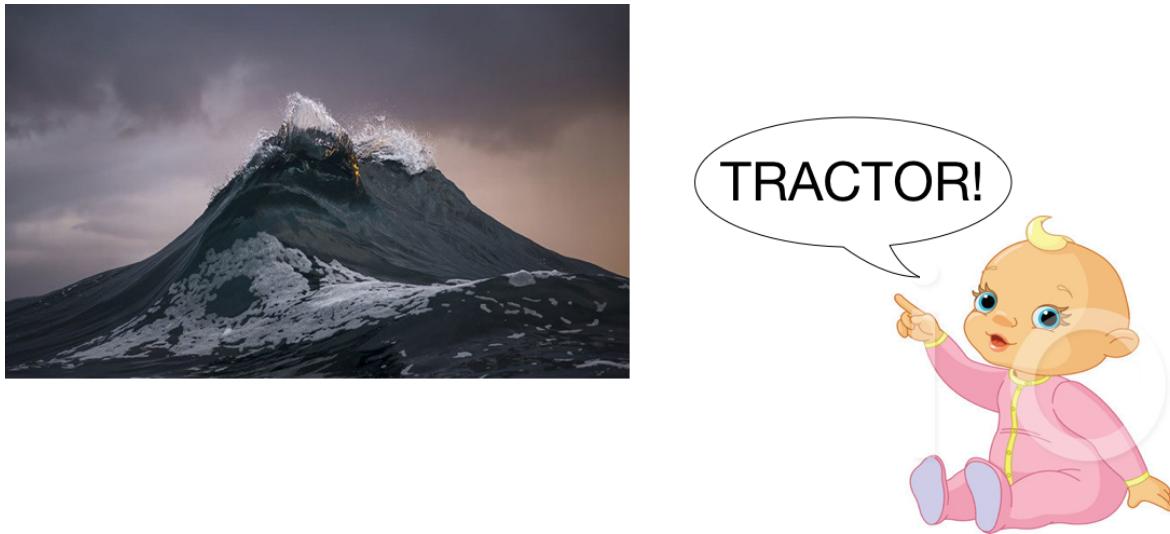


Figure 19: The child which has been taught the concept “tractor” using the image collection \mathbb{X}_{misl} might “see” a lot of tractors during the next beach holiday.

whenever

$$N_{\text{train}} \leq d.$$

However, this predictor $h^{(\mathbf{w}_{\text{opt}})}$ might be not useful for predicting the label of any image which is different from the images in the training set \mathbb{X}_{misl} . Thus, the predictor $h^{(\mathbf{w}_{\text{opt}})}$ overfits the dataset \mathbb{X}_{misl} .

A simple strategy to detect if a predictor \hat{h} overfits the dataset $\mathbb{X}^{(\text{train})}$ over which it is trained (e.g., via ERM (9)), is to compare the resulting training error $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{train})})$ with the validation error $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})})$, which is the empirical risk of the predictor \hat{h} obtained when applying it to the validation dataset $\mathbb{X}^{(\text{val})}$. In case of overfitting, the validation error $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{val})})$ is typically significantly larger than the training error $\mathcal{E}(\hat{h}|\mathbb{X}^{(\text{train})})$.

In order to avoid overfitting, we have to augment our basic ERM approach (cf. (7)) by **regularization techniques**. According to [2], regularization techniques aim 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 loss 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 by a regularization or penalty term $\lambda\|\mathbf{w}\|_2^2$, which penalizes overly large weight vectors \mathbf{w} . Thus, we arrive at regularized ERM

$$\begin{aligned} \mathbf{w} &= \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} [\mathcal{E}(h^{(\mathbf{w})}|\mathbb{X}) + \lambda\|\mathbf{w}\|_2^2] \\ &= \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} [(1/|\mathbb{X}|) \sum_{(\mathbf{x},y) \in \mathbb{X}} L((\mathbf{x},y), h^{(\mathbf{w})}) + \lambda\|\mathbf{w}\|_2^2], \end{aligned} \quad (14)$$

with the regularization parameter $\lambda > 0$. The parameter λ trades a small training error $\mathcal{E}(h^{(\mathbf{w})}|\mathbb{X})$ against a small norm $\|\mathbf{w}\|_2$ of the weight vector. In particular, if we choose a large value for λ , then weight vectors \mathbf{w} with a large norm $\|\mathbf{w}\|_2$ are “penalized” by having a larger objective function and are therefore unlikely to be a solution (minimizer) of the optimization problem (14).

Specialising (14) to the squared error loss and linear predictors yields the regularized linear regression problem (cf. (9)):

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} [(1/|\mathbb{X}|) \sum_{(\mathbf{x},y) \in \mathbb{X}} (y - \mathbf{x}^T \mathbf{w})^2 + \lambda\|\mathbf{w}\|_2^2],$$

which can be further simplified using the feature matrix \mathbf{X} and label vector \mathbf{y} (cf. (11)) as

$$\mathbf{w}_{\text{opt}} = \underset{\mathbf{w} \in \mathbb{R}^d}{\operatorname{argmin}} [(1/|\mathbb{X}|)\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2].$$

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