

Mathematical Machine Learning

Yahya SALEH, Tizian WENZEL, Kamal SHARMA

March 7, 2024

Contents

I Introduction	v
I.1 Examples of supervised learning	v
I.1.1 Curse of Dimensionality	v
I.1.2 Underfitting, overfitting, or just right?	v
I.2 A formal definition of learning	v
II Empirical Risk Minimization Principles	vii
III Machine Learning Models	ix
III.1 Neural Networks	ix
III.2 Kernel Methods	ix
IV Modern Machine Learning	xi
V Modern Mathematical Machine Learning	xiii
VI Bibliography	xv

Introduction

Underlying the success of artificial intelligence are learning algorithms, i.e., algorithms that learn from data to perform a certain task. We start this book by two concrete examples of supervised learning algorithms. In the first example we consider the problem of approximating functions from pointwise evaluations using linear regression. In the second example we look at the task of classifying hand-written digits. In these two examples we identify and familiarize ourselves with the main components of learning algorithms; *datasets*, a *hypothesis class*, and *optimization algorithms*. We further identify important aspects of supervised learning algorithms, such as overfitting, and underfitting. Finally, we motivate in these two examples problems at the forefront of research in mathematical machine learning, namely *the curse of dimensionality (CoD)* and double/multiple descent phenomenon.

I.1 Examples of supervised learning

[1] Approximating smooth functions from point evaluations
Classifying hand-written digits.

I.1.1 Curse of Dimensionality

I.1.2 Underfitting, overfitting, or just right?

I.2 A formal definition of learning

Wait! What is what?

Here is a list of questions that help you check your understanding of key concepts inside this chapter?

Empirical Risk Minimization Principles

Machine Learning Models

III.1 Neural Networks

III.2 Kernel Methods

Modern Machine Learning

Modern Mathematical Machine Learning

Bibliography

- [1] Y. Saleh, V. Sanjay, A. Iske, A. Yachmenev, and J. Küpper, “Active learning of potential-energy surfaces of weakly bound complexes with regression-tree ensembles”, **155** (2021), 144109, arXiv: 2104.00708 [physics].