

Working Title
University of Oslo



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Abstract

Abstract goes here [e.g. 1, page 300].

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Chapter 1

Introduction

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Chapter 2

Quantum Mechanics

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Chapter 3

Manybody Quantum Mechanics

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Chapter 4

Molecular Dynamics

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Chapter 5

Machine learning

Machine learning is the study of algorithms and statistical models employed by computing systems capable of performing tasks without explicit instruction. While traditional algorithms rely on some specified input and a ruleset for determining the output, machine learning is instead concerned with a set of generic algorithms which can find patterns in a broad class of data sets. This section will give a brief overview of machine learning, and more specifically the class of algorithms known as neural networks, and will follow closely the review by [Mehta et. al.] which the reader is encouraged to seek out.

Examples of machine learning problems include identifying objects in images, transcribing text from audio and making film recommendations to viewers based on their watch history. Machine learning problems are often subdivided into estimation and prediction problems. In both cases, we choose some observable \mathbf{x} (e.g. the period of a pendulum) related to some parameters $\boldsymbol{\theta}$ (e.g. the length and the gravitational constant) through a model $p(\mathbf{x}|\boldsymbol{\theta})$ that describes the probability of observing \mathbf{x} given $\boldsymbol{\theta}$. Subsequently we perform an experiment to obtain a dataset \mathbf{X} and use these data to fit the model. Fitting the model means finding the parameters $\hat{\boldsymbol{\theta}}$ that provide the best explanation for the data. *Estimation* problems are concerned with the accuracy of $\hat{\boldsymbol{\theta}}$, whereas prediction problems are concerned with the ability of the model $p(\mathbf{x}|\boldsymbol{\theta})$ to make new predictions. Physics has traditionally been more concerned with the estimation of model parameters, while in this thesis we will be focused on the accuracy of the model.

Many problems in machine learning are defined by the same set of ingredients. The first is the dataset $\mathcal{D} = (\mathbf{X}, \mathbf{Y})$, where \mathbf{X} is a matrix containing

observations of the independent variables \mathbf{x} , and \mathbf{Y} is a matrix containing observations of dependent variables. Second is a model $\mathbf{F} : \mathbf{x} \rightarrow \mathbf{y}$ which is a function of the parameters $\boldsymbol{\theta}$. Finally we have a cost function $\mathcal{C}(\mathbf{Y}, \mathbf{F}(\mathbf{X}; \boldsymbol{\theta}))$ that judges the performance of our model at generating predictions.

In the case of linear regression we consider a set of independent observations $\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_N]$ related to a set of dependent observations $\mathbf{y} = (y_1, y_2, \dots, y_N)$ through a linear model $f(\mathbf{x}; \boldsymbol{\theta}) = x_1 \cdot w_1 + x_2 \cdot w_2 + \dots + x_P \cdot w_P$, with parameters $\boldsymbol{\theta} = (w_1, w_2, \dots, w_P)$. The cost function is the well known sum of least squares $\mathcal{C}(\mathbf{y}, f(\mathbf{X}; \boldsymbol{\theta})) = \sum_i^N (y_i - f(\mathbf{x}_i; \boldsymbol{\theta}))^2$ and the best fit is chosen as the set of parameters which minimize this cost function: $\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \mathcal{C}(\mathbf{Y}, f(\mathbf{X}; \boldsymbol{\theta}))$.

5.0.1 Basics of statistical learning

Statistical learning theory is a field of statistics dealing with the problem of making predictions from data. We begin with an unknown function $y = f(x)$ and our goal is to develop a function $h(x)$ such that $h \sim f$. We fix a hypothesis set \mathcal{H} that the algorithm is willing to consider. The expected error of a particular h over all possible inputs x and outputs y is:

$$E[h] = \int_{X \times Y} \mathcal{C}(h(x), y) \rho(x, y) dx dy,$$

where \mathcal{C} is a cost function and $\rho(x, y)$ is the joint probability distribution for x and y . This is known as the *expected error*. Since this is impossible to compute without knowledge of the probability distribution ρ , we instead turn to the *empirical error*. Given n data points the empirical error is given as:

$$E_S[h] = \frac{1}{n} \sum_i^n \mathcal{C}(h(x_i), y_i).$$

The *generalization error* is defined as the difference between the expected and empirical errors:

$$G = E[h] - E_S[h].$$

We say an algorithm is able to learn from data or *generalize* if

$$\lim_{n \rightarrow \infty} G = 0.$$

We are in general unable to compute the expected error, and therefore unable to compute the generalization error. The most common approach known as *cross-validation* is to estimate the generalization error by subdividing our dataset into a *training* set and a *test* set. The value of the cost function on the training set is called the *in-sample* error and the value of the cost function on the test set the *out-of-sample* error.

5.0.2 Neural networks

5.0.3 Optimization

Chapter 6

Conclusion

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Appendix A

Appendix Title

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- [1] Albert Einstein. “Zur Elektrodynamik bewegter Körper. (German) [On the electrodynamics of moving bodies]”. In: *Annalen der Physik* 322.10 (1905), pp. 891–921. DOI: <http://dx.doi.org/10.1002/andp.19053221004>.