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Probabilistic Machine Learning

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Abstract

As a student of Scientific and Data Intensive Computing, I've created these notes while attending the **Probabilistic Machine Learning** course.

This course will cover the "*probabilistic side*" of machine learning. In particular, we will focus on the following topics:

- Basics of probability and probabilistic inference
- Probabilistic formulation of learning (Empirical Risk Minimization and PAC Learning)
- Graphical Models
- Inference with graphical models: belief propagation
- Hidden Markov Models for sequential data
- Bayesian Linear Regression and Classification, Laplace approximation, Model Selection
- Kernel Regression and Kernel functions, Gaussian Processes for regression (hints)
- Monte Carlo sampling
- Expectation Maximization and Variational Inference
- Bayesian Neural Networks
- Generative Modelling: Variational Autoencoders and Diffusion Processes

While these notes were primarily created for my personal study, they may serve as a valuable resource for fellow students and professionals interested in probabilistic machine learning.

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1 Introduction

1.1 Machine Learning

Machine learning is a field of computer science about **learning models**.

Models

Definition: *Model*

- A **Model** is a hypothesis that certain features of a system of interest are well replicated in another, simpler system.
- **Mathematical Model** is a model where the simpler system consists of a set of mathematical relations between objects (equations, inequalities, etc).
- A **Stochastic Model** is a mathematical model where the objects are probability distributions.

All modelling usually starts by defining a family of models indexed by some parameters, which are tweaked to reflect how well the feature of interest are replicated.

Machine learning deals with algorithms for automatic selection of a model from observations of the system.

Machine Learning

Definition: *Machine learning*

Machine learning explores the study and construction of algorithms that can learn from and make predictions on data.

Wikipedia

There are three main types of machine learning:

Generative and Discriminative Learning

- **Generative Learning** is aimed at describing the full probability distribution of inputs x or input/output pairs (x, y) .

$$p(x, y) = p(x)p(y|x)$$

- **Discriminative Learning** aims at describing the conditional probability of output given the input, or a statistics/function of such probability

$$p(y|x) \quad \text{or} \quad y = f(x)$$

[to fix:]

- **Supervised Learning**: The algorithm learns from labeled data by mapping inputs to outputs.
- **Unsupervised Learning**: The algorithm identifies patterns or structures in unlabeled data.
- **Data Generation**: The algorithm generates new data points.

Inference and Estimation

Two central concepts for probabilistic machine learning are:

- **Inference:** Compute marginals and conditional probability distributions applying the laws of probability.
- **Estimation:** Given data and a family of models, find the best parameters/models that explain the data.

In the Bayesian world: estimation \approx inference.

Probability

Probability is a mathematical theory that deals with **uncertainty**

When a certain problem has to face practical difficulties due to its complexity, we can use probability to model the *aleatorical uncertainty*, which is the uncertainty due to the randomness of the system.

More often, we have a limited knowledge of the system, and we can use probability to model the *epistemic uncertainty*, which is the uncertainty due to the lack of knowledge.

💡 **Tip:** *Everything is a probability distribution*

In machine learning **everything is a probability distribution**, even if not explicitly stated.

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