



清華大學
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Syllabus and Reading Materials for Machine Learning Theory



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Course Description (中文 / English)

中文: 你对机器学习 (ML) 感兴趣吗? 本课程为理解机器学习理论与实践基础的入门课程, 旨在为深度学习等更的研究奠定基础。通过学习本课程, 您将探索支撑该领域的核心原理, 包括数据学习所需的数学框架和算法。你将学到什么? 这门课程不仅教你如何使用机器学习, 还将为你提供分析工具, 帮助您理解其工作原理及其方法的局限性。对于有志于深入学习高级机器学习主题 (如深度学习) 的学生来说, 这是一个不可或缺的基础, 这些主题直接建立在课程涵盖的概念之上。这是一门不可或缺的基础课程, 适合希望深入学习高级机器学习主题 (如深度学习) 的学生, 因为这些内容直接建立在本课程所涵盖的概念之上。为什么要上这门课? — 培养批判性思维能力, 使用可靠的机器学习技术应对现实数据挑战。— 为机器学习和人工智能的进一步学习奠定基础。— 通过理论与实践相结合加深对机器学习的理解。我能上这门课吗? 当然可以! 本课程旨在自成体系, 对所有学习者开放, 无论是本科生还是研究生均可参与。无论你是刚刚开始机器学习, 还是希望在已有知识的基础上更进一步, 本课程都将为你提供所需的理论和实践工具。本课程是为即将进行机器学习理论研究工作的低年级研究生和有扎实数学基础且对机器学习有浓厚兴趣的高年级本科生设计, 将以原则性的方式介绍机器学习的数学基础和算法框架。从形式化的统计学习模型开始, 我们将讨论机器学习中的核心概念, 例如可学习性、学习的样本复杂性和计算复杂性、假设类及其复杂性度量、学习的稳定性和凸学习问题。基于这些概念并通过大量的数学推导, 我们将设计和分析机器学习中的重要算法框架, 包括线性回归、随机梯度下降、支持向量机、决策树、神经网络、聚类、在线学习和强化学习。在本课程中, 我们还将涉及机器学习领域的一些最先进的研究方向。完成本课程学习后, 同学们将系统的理解机器学习理论的历史和近期发展, 同时也可以为机器学习理论研究做好准备。

English: Are you fascinated by the potential of Machine Learning (ML)? This course is your gateway to understanding the theoretical and practical foundations of ML, designed to set the stage for more advanced studies like deep learning. By enrolling, you will explore the core principles that underpin the discipline, including the mathematical frameworks and algorithms that make learning from data possible. What will you



learn? This course doesn't just teach you to use machine learning; it equips you with the analytical tools to understand why it works and the limitations of its methods. It's an indispensable foundation for students aiming to delve into advanced ML topics, such as deep learning, which build directly on the concepts covered here. Why take this course? —Develop the critical thinking skills to tackle real-world data challenges with robust ML techniques. — Lay the groundwork for advanced studies in ML and AI, making this course a must-have stepping stone for your academic and professional journey. — Benefit from a blend of theory and practical insight. Can I Take This Course? Absolutely! This course is designed to be self-contained and accessible to learners of all levels, including both undergraduate and graduate students. Whether you're starting your journey in Machine Learning or building upon prior knowledge, this course will equip you with the theoretical and practical tools needed for this course. Are you fascinated by the potential of Machine Learning (ML)?



Course Syllabus

This course provides a rigorous, mathematically grounded exploration of the theory behind machine learning. Moving beyond implementation, students will study the formal principles that govern algorithmic learning, enabling a deep understanding of *why* algorithms work, under what conditions they succeed, and where their limitations lie. Topics include PAC learning, empirical risk minimisation, VC-dimension, Rademacher complexity, optimisation theory, kernel methods, generalisation in neural networks, and more. This course is especially suited for students interested in research or advanced applications of machine learning.

Prerequisites

The course is designed to be **self-contained**, enabling students from various backgrounds to engage with the material. However, familiarity with the following subjects will enhance learning:

- **Linear Algebra** (vector spaces, eigenvalues/eigenvectors, matrix decompositions)
- **Probability and Statistics** (distributions, expectation, variance, concentration inequalities)
- **Calculus** (differentiation, gradients, partial derivatives)

Students aiming to fully engage with the theoretical aspects are encouraged to have some exposure to: **Real Analysis:** Foundations for understanding convergence, limits, continuity, and rigorous proofs — essential in statistical learning theory. **Optimisation:** Especially convex optimisation, duality, and convergence analysis, which are central to machine learning. **Functional Analysis:** Critical for kernel methods and understanding infinite-dimensional hypothesis spaces.



Learning Objectives

This course is designed to provide students with a rigorous and comprehensive understanding of the theoretical foundations of machine learning. Emphasis will be placed on mathematical analysis, formal proofs, and the conceptual frameworks that underpin learning algorithms. By the end of the course, students will have developed the theoretical tools and critical thinking skills necessary to:

- **Understand and apply the theoretical foundations of machine learning.** Students will gain a deep understanding of the mathematical principles that underpin machine learning algorithms, including concepts such as generalisation bounds, VC-dimension, and statistical learning frameworks.
- **Analyse learning algorithms through the lens of mathematics.** Learners will develop the ability to dissect and critically analyse algorithms using tools from probability theory, optimisation, and linear algebra, allowing for a principled assessment of algorithmic performance.
- **Critically assess when and why learning algorithms succeed or fail.** The course will enable students to identify the conditions under which algorithms generalise well, recognise scenarios that lead to overfitting or underfitting, and understand the theoretical trade-offs in model complexity and data.
- **Connect foundational theory with modern trends in machine learning research.** Students will explore how classical results inform current developments in machine learning, including deep learning, overparameterisation, and PAC-Bayesian analysis, preparing them to engage with advanced research or applications.

Course Syllabus

1. Introduction to Machine Learning Theory

- Introduction to Machine Learning
- Learning Paradigms and Theoretical Foundations

2. PAC Learning and Generalisation

- PAC Learning Framework
- Agnostic PAC Learning



3. Empirical Risk Minimisation

- Empirical Risk Minimisation (ERM)
- Overfitting and Regularisation in ERM

4. Complexity and Learnability

- VC-Dimension
- Growth Functions and Sauer's Lemma

5. Statistical Learning Theory

- Uniform Convergence
- The No-Free-Lunch Theorem

6. Rademacher Complexity

- Introduction to Rademacher Complexity
- Applications of Rademacher Complexity

7. Optimisation for Learning

- Convex Optimisation Problems (Gradient Descent)
- Stochastic Gradient Descent (SGD) and Variants

8. Kernel Methods

- Kernel Basics and Representer Theorem
- Kernel Ridge Regression

9. Neural Networks

- Training and Optimisation; Universal Approximation Theorem
- Generalisation in Neural Networks

10. Deep Neural Networks

- Foundations of Deep Neural Networks
- Challenges and Applications

11. Ensemble Learning



- Bagging and Random Forests
- Boosting Techniques

12. Probabilistic Methods

- Bayesian Inference
- PAC-Bayesian Analysis

13. Structured Prediction

- Structured Prediction Tasks
- Max-Margin Methods in Structured Prediction

14. Overparameterisation

- Implicit Bias in Gradient Descent
- Double Descent Phenomenon

15. Advanced Topics

- Lower Bounds on Learnability
- Emerging Trends in Machine Learning Theory



What to Read? Key Readings for Machine Learning Theory

Machine learning is the study of algorithms that allow machines to learn patterns and make predictions based on data. Formally, it explores how a system can generalise from observed samples to unseen instances, minimising error whilst balancing constraints such as computational complexity and data availability. In essence, **learning** is a mathematical process that seeks to identify a hypothesis function from a class of possible functions that performs well on unseen data.

The goal of machine learning is to **approximate an unknown function** that maps inputs to outputs, given a finite set of observations. For example, the task of predicting whether an email is spam can be described mathematically: we seek a function $h \in \mathcal{H}$, from a hypothesis class \mathcal{H} , such that $h(x) \approx y$ for input-output pairs (x, y) drawn from an unknown probability distribution D . The challenge is to identify a function that minimises error on new, unseen samples—not just the observed data. Central to the theory of learning is the concept of **generalisation**: how well a hypothesis learned from a training set applies to unseen instances. This requires us to formalise notions of risk, such as the expected error (or generalisation error), and develop algorithms that can efficiently search the hypothesis space to minimise it.

However, learning comes with fundamental limitations. **Overfitting**, for instance, occurs when a model performs well on the training data but poorly on unseen data. This leads us to trade-offs between model complexity and accuracy, captured mathematically through frameworks like Empirical Risk Minimisation (ERM), Structural Risk Minimisation (SRM), and regularisation techniques.

What to Expect from This Course

In this course, we will delve deeply into the mathematical underpinnings of machine learning. Our goal is not just to implement algorithms but to rigorously understand **why**

they work and when they are expected to fail. You will engage with mathematical concepts such as probability theory, optimisation, and linear algebra, as they are essential tools for analysing learning algorithms. Here is an of what you can expect:

- **Introduction to Machine Learning Theory.** This part lays the groundwork by introducing what machine learning theory entails and why it is critical to modern science. We will discuss supervised and unsupervised learning paradigms, essential for understanding how models are trained and validated. Additionally, decision theory is introduced to frame predictions mathematically. This foundational knowledge helps clarify the scope and limitations of machine learning models and prepares students for deeper theoretical exploration.

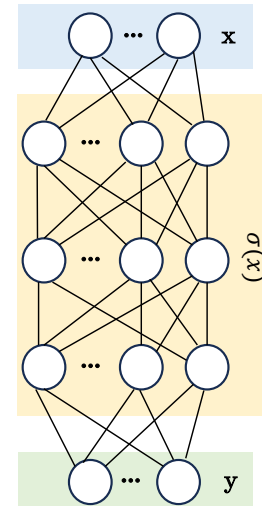
- **Formal Foundations of Learning.** This part focuses on formalising the process of learning using the PAC (Probably Approximately Correct) framework. The PAC framework provides the mathematical tools to reason about whether a machine can learn a given task. VC-dimension is introduced to quantify the capacity of hypothesis classes and their ability to generalise. Understanding these topics is critical for assessing whether a learning algorithm is well-suited for specific tasks and data.

- **Empirical Risk Minimisation and Regularisation.** ERM is a fundamental principle that underpins many learning algorithms. This week explores how ERM minimises errors on training data and highlights its shortcomings, particularly overfitting. Regularisation techniques like ridge regression are introduced to mitigate overfitting by balancing model complexity and performance. The bias-variance trade-off is discussed as a central framework for navigating the trade-offs inherent in model design. These concepts are key to building reliable and effective machine learning systems.

- **Complexity Measures and Learnability.** We delve into advanced measures of complexity such as Rademacher complexities and uniform convergence. These tools help assess the ability of a model to generalise to unseen data. We explore Sauer's lemma and growth functions, which provide theoretical insights into how complexity affects learnability. These topics are essential for selecting models that balance expressiveness with generalisation.

- **Computational Complexity and Generalisation.** Understanding the computational limits of learning is crucial for developing efficient algorithms. During this part of the course, we introduce the No-Free-Lunch theorem, which illustrates the trade-offs

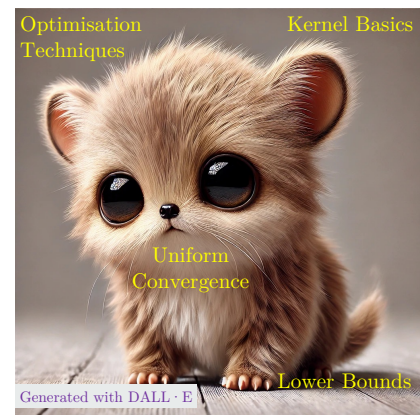
Activation Function — $\sigma(x)$



involved in making assumptions about learning tasks. PAC-Bayesian bounds are introduced to provide probabilistic guarantees for model generalisation. These insights are critical for understanding the practical feasibility of machine learning systems.

- **Advanced Generalisation Techniques.** This section expands on generalisation by introducing covering numbers, which refine our ability to bound generalisation errors. PAC-Bayesian analysis is revisited with a focus on applications to high-dimensional data, a critical challenge in modern machine learning. These techniques are vital for ensuring that models remain robust and reliable even in complex scenarios.

- **Optimisation Techniques.** Optimisation lies at the heart of training machine learning models. This part of the course introduces convex optimisation and stochastic gradient descent (SGD), focusing on their convergence properties in convex settings. Adaptive optimisation techniques, which are widely used in deep learning, are also discussed. Grasping these methods is crucial for implementing efficient and scalable machine learning algorithms.



- **Kernel Methods and High-Dimensional**

Data. Kernel methods provide a powerful framework for learning non-linear patterns in data. This week introduces the representer theorem and discusses common kernels such as polynomial and Gaussian kernels. Practical applications in high-dimensional data, including support vector machines (SVMs), are explored. These methods are particularly relevant for tasks requiring robust non-linear decision boundaries.

- **Neural Networks.** Neural networks are highly relevant to modern machine learning. This part of our course focuses on single-layer networks, exploring their ability to approximate functions through the universal approximation theorem. Challenges such as overparameterisation are discussed alongside neural tangent kernels, which provide theoretical insights into the success of deep learning. Understanding these topics is key to leveraging neural networks effectively in practice.

- **Ensemble Learning and Online Learning.** Ensemble methods such as bagging and boosting are introduced as strategies to improve model accuracy and robustness. Online learning algorithms, including weighted majority approaches, are explored for their ability to adapt to sequential data. These methods are essential for building flexible and adaptive systems that can handle dynamic environments.

- **Probabilistic Methods.** Probabilistic reasoning is important for modelling uncertainty in machine learning. This week covers Bayesian inference and Gaussian processes, which allow for robust uncertainty estimation. PAC-Bayesian analysis is revisited, with



practical examples in model selection and evaluation. These topics are particularly relevant for applications requiring reliable confidence measures.

- **Structured Prediction.** Many tasks involve predicting structured outputs, such as sequences or rankings. We will explore structured SVMs, loss functions for structured data, and decoding techniques. Mastering these methods is critical for tackling real-world tasks that extend beyond simple classification or regression.
- **Overparameterisation and Implicit Bias.** Modern deep learning systems often rely on overparameterised models. We examine the double descent phenomenon and the implicit bias of gradient descent, which explain why these models can generalise effectively despite their complexity. Understanding these phenomena is crucial for designing effective deep learning architectures.
- **Advanced Optimisation Techniques.** Non-convex optimisation presents significant challenges in machine learning. In this section, we explore strategies for navigating non-convex landscapes and introduces adaptive methods for large-scale problems. Techniques for handling sparse and high-dimensional data are also discussed, with applications to modern learning problems.
- **Causal Inference and Reinforcement Learning.** The course concludes with causal inference, focusing on causal models and counterfactual reasoning for decision-making. Reinforcement learning theory is introduced to address sequential decision-making problems. These topics are essential for building systems that make informed decisions based on cause-effect relationships.

Reading Materials

This course is supported by several core texts that provide the essential theoretical and practical knowledge required for this course on machine learning theory. In addition to the main readings, extra materials will be recommended throughout the course for those who are curious to explore advanced topics and gain deeper insights. Below is a brief description of the primary materials we will use, along with supplementary texts available for further study.

Main Materials

★ **Learning Theory from First Principles** by (Bach, 2024). This textbook offers a rigorous exploration of learning theory, emphasising derivation from first principles and linking theoretical insights to practical implementation. It covers essential topics in statistical learning, optimisation techniques, kernel methods, and overparameterised



models, while discussing challenges such as adaptivity, trade-offs in approximation, estimation, and optimisation errors. Special topics include ensemble learning, online learning, and structured prediction, enriched by illustrative experiments and exercises. The text is tailored for theory-oriented students and researchers who seek to understand the mathematical foundations and algorithmic innovations underpinning modern machine learning.

What Content Is Expected to Be Learned? A general overview of the foundational concepts can be found in Chapter 1, providing students with a structured introduction to machine learning fundamentals. For those already familiar with the subject matter, you may choose to jump directly into the core theoretical chapters. **The main theoretical fundamentals expected to be acquired in-depth are covered in Chapters 2, 4, 5, 6, 7, and 14.** These chapters encompass topics such as supervised learning paradigms, empirical risk minimisation, statistical learning theory, kernel methods, and probabilistic generalisation frameworks, all critical for understanding learning theory. In addition, we will examine specific algorithms and advanced theoretical discussions to gain a broad understanding of their purpose and implications. **While a detailed study isn't required for these, general familiarity with their definitions and motivations is encouraged.** These are found in Chapters 9, 10, 12, 13, and 15, which include neural networks, ensemble learning, overparameterisation, structured prediction, and theoretical lower bounds.

📖 The authors of that ([Bach, 2024](#)) provide a copy for personal use, as indicated by the authors, at the following [link](#).

★**Understanding Machine Learning: From Theory to Algorithms** by ([Shalev-Shwartz and Ben-David, 2014](#)). This book offers a well-rounded introduction to the theory and algorithms that form the foundation of modern machine learning. It begins by addressing fundamental questions about learning, including how learning can be formally defined and under what conditions it succeeds. The text delves into key concepts such as PAC learning, VC-dimension, and empirical risk minimisation, which underpin the theoretical side of the field. Alongside theory, the book introduces practical algorithms such as linear models, neural networks, and support vector machines, and explores optimisation methods like gradient descent and regularisation. Special attention is given to challenges such as overfitting, model selection, and evaluation strategies, equipping readers with the tools needed to build effective models.

What Content Is Expected to Be Learned? A general overview of the foundational concepts can be found in Chapter 1, offering students a structured introduction to machine learning fundamentals. For those already familiar with the subject matter,



you may choose to jump directly into the core chapters. **The main theoretical fundamentals expected to be acquired in-depth are covered in Chapters 2, 3, 5, 6, 13, and 14.** These chapters provide the mathematical and theoretical grounding essential for this course, covering topics such as PAC learning, VC-dimension, risk minimisation, and key algorithmic frameworks. In addition, we will explore several particular algorithms to establish a general understanding of their definitions and motivations. **While a detailed study isn't required for these, a general knowledge of their purpose and application is important.** These are found in Chapters 9, 15, 18-20, and 22-23.

📖 The authors of that ([Shalev-Shwartz and Ben-David, 2014](#)) provide a copy for personal use, as indicated by the authors, at the following [link](#).

★**Convex Optimisation: Algorithms and Complexity** by ([Bubeck et al., 2015](#)). This material offers a comprehensive introduction to convex optimisation with a particular focus on algorithms and their complexities. It begins by addressing fundamental aspects of convexity, such as the properties of convex functions and sets, and explains why convexity plays a central role in optimisation. The text also seeks to cover essential algorithms, including gradient descent, cutting plane methods, and stochastic optimisation, highlighting their convergence rates and computational feasibility. With a strong emphasis on both the theoretical underpinnings and practical implementation, this text is particularly valuable for optimisation and machine learning. The structured presentation makes it a great resource for the course, providing deeper insights into optimisation techniques critical for machine learning models.

What Content Is Expected to Be Learned? To gain a solid general understanding from this reading, students should focus on **Chapter 1 (a concise and very short overview) and Section 3.2.** These sections cover the foundational concepts and core methods sufficiently for a comprehensive introduction without delving into overly detailed analysis. This targeted reading is designed to equip students with essential insights into convex optimisation's role in machine learning and the main algorithms relevant to this course.

📖 The pre-print version of this material is available online in this [link](#).

★**Practical Implementation Resources.** Whilst this course focuses on machine learning theory, there will also be a practical component to reinforce your understanding. For this, homework exercises will primarily involve **Python-based implementations.** We encourage you to explore and become familiar with [Python's scikit-learn library](#), as it will be the main tool used for practical assignments.



🌐 For reference and guidance, please use the Scikit-learn project’s official documentation in [here](#).

Supplementary Materials

The following materials are supplementary and intended for students who are curious to gain deeper insights into the theory and practical aspects of machine learning. These resources are not part of the core curriculum but are provided to support those interested in exploring the subject further.

★ [Fit without fear: remarkable mathematical phenomena of deep learning through the prism of interpolation](#) by (Belkin, 2021). It explores foundational mathematical concepts related to deep learning, with particular focus on interpolation and over-parameterisation. The work is an attempt to bridge the gap between the theoretical underpinnings and practical success of deep learning models, which have outpaced traditional learning theory.

📖 The pre-print version of this material is available online in this [link](#).

★ [High-dimensional probability: An introduction with applications in data science](#) by Vershynin (2018). This supplementary material reading provides a rigorous exploration of probability theory specifically tailored for high-dimensional contexts, which are essential for understanding the theoretical foundations of machine learning. The book introduces essential concepts like concentration inequalities, random matrices, high-dimensional distributions, and random projections—all of which are central to the mathematical understanding of machine learning algorithms, particularly in high-dimensional and over-parameterised models. These topics align well with understanding how machine learning models generalise, optimise, and handle high-dimensional data, making it a valuable resource for students in this machine learning theory course.

📖 You can access a free draft of this material [here](#), *provided it is used only for personal and classroom needs as indicated by the author*.





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