

Advanced Neural Networks in Chemistry

Course Workload		Assessment form (examination/ graded test/ ungraded test)
ECTS	Hours	
3	108	Exam

The course "Advanced Neural Networks in Chemistry" is designed to deepen students' understanding of neural network architectures and their advanced applications in the field of chemistry. This course will cover sophisticated techniques such as deep learning, convolutional neural networks (CNNs), recurrent neural networks (RNNs), and generative models. Students will explore cutting-edge applications in drug discovery, materials science, and chemical synthesis. By the end of the course, students will be equipped with the advanced skills necessary to design, implement, and analyze neural networks for complex chemical problems.Course structure:

1. Deep Learning Fundamentals

- 1.1. Review of Neural Network Basics and Deep Learning Introduction
- 1.2. Convolutional Neural Networks (CNNs) for Chemical Image Analysis
- 1.3. Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) Networks for Sequential Chemical Data

2. Advanced Neural Network Architectures

- 2.1. Generative Adversarial Networks (GANs) for Molecular Design
- 2.2. Graph Neural Networks (GNNs) for Molecular Representations
- 2.3. Autoencoders and Variational Autoencoders (VAEs) in Chemistry

3. Applications in Chemistry

- 3.1. Neural Networks in Drug Discovery: Target Identification and Lead Optimization
- 3.2. Neural Networks in Material Science: Designing New Materials
- 3.3. Predicting Reaction Outcomes Using Advanced Neural Networks

4. Practical Implementations and Challenges

- 4.1. Implementing Advanced Neural Networks with TensorFlow and PyTorch
- 4.2. Case Studies in High-Throughput Screening and Virtual Screening

4.3. Challenges and Ethical Considerations in AI Applications in Chemistry
