
ml-ms

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- **Aims:**

The NYU-ECNU Center for Computational Chemistry at [New York University Shanghai](#) (a.k.a, NYU Shanghai) announced a summer school dedicated to machine learning and its applications in the molecular sciences to be held June, 2017 at the NYU Shanghai Pudong Campus. Using a combination of technical lectures and hands-on exercises, the school aimed to instruct attendees in both the fundamentals of modern machine learning techniques and to demonstrate how these approaches can be applied to solve complex computational problems in chemistry, biology, and materials science. In order to promote the idea of free to code, this project is built to help you understand some basic machine learning models mentioned below.

- **Topics:**

Fundamental topics to be covered include basic machine learning models such as *kernel methods* and *neural networks optimization schemes*, *parameter learning* and *delta learning paradigms*, *clustering*, and *decision trees*. Application areas will feature machine learning models for representing and predicting properties of individual molecules and condensed phases, learning algorithms for bypassing explicit quantum chemical and statistical mechanical calculations, and techniques applicable to biomolecular structure prediction, bioinformatics, protein-ligand binding, materials and molecular design and various others.

CHAPTER 1

Introduction to Machine Learning

CHAPTER 2

External Links

- [genindex](#)
- [search](#)