Medicinal Physical Chemistry - Machine Learning Module

0 What is machine learning 2h 18-19 marzo

- Myths and misconceptions about ML and AI

1 Python tutorial 6h 18-19 marzo

1. Introduction to python
2. Numpy and Scipy
3. OOP

Linear methods 3h and Nearest neighbours (remoto) 25 marzo

Linear regression - Logistic regression

1. Interpolation
2. linear regression cost function
3. gradient descent and other minimization methods
4. regularization - over fit - under fit
5. regression vs classification
6. Logistic regression cost function

nearest neighbours

- instance based methods
- model
- kNN classification

Dimensionality reduction 3h 1 aprile

1. distance and similarity
2. Principal component analysis
3. KPCA
4. TSNE

Clustering 3h 1 aprile

1. what is clustering
2. partition
3. validation
4. application
5. density based methods
6. DBSCAN
7. Density peaks

Case studies 2h remoto 28 aprile

- Force field training
- Conformer search

Metaheuristics 3h (presenza) 29 aprile

- Introduction to the problem and historical note
- genetic algortihms
- operators
- main loop
- minimization problem
- TSP problem
- N queen problem

SVM 2h (remoto) 19 maggio

- Maximum margin problem
- Linear SVM
- Kernel trick
- SVM as a constrained minimization problem

ANN 2h (remoto) 27 maggio

- motivation and biological inspiration
- perceptron
- ANN cost function
- simple ANN