SoSe 2022 Syllabus of the MSc Course

Machine Learning for Complex Networks

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Lehrstuhl Informatik XV - Machine Learning for Complex Networks
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2 + 2 SWS (5 ECTS)

Executive Summary

Graph representations of relational data have become an important foundation to address data science and machine learning tasks across the sciences. Graph mining and learning techniques help us to detect functional modules in biological networks and communities in social networks, to find missing links in social networks, or to address node-, link-, or graph-level classification tasks. This course equips students with techniques to address supervised and unsupervised learning tasks in data on complex networks. We show how statistical learning techniques can be used to infer cluster patterns or predict links, introduce methods to learn low-dimensional vector-space representations of graph-structured data, and discuss applications of deep learning to complex networks. The course combines a series of lectures – which introduce theoretical concepts in statistical learning, representation learning, or graph neural networks – with practice sessions that show how we can apply them in practical graph learning tasks. The course material consists of annotated slides for lectures and a series of accompanying `jupyter` notebooks. Students can apply and deepen their knowledge through weekly exercise sheets. The successful completion of the course requires to pass a final written exam.

Chapter I: Foundations of Graph Learning

The first chapter of our course motivates the growing need for machine learning techniques for graph-shaped data in science, industry, and society. We introduce graph-theoretic and algorithmic foundations of network analysis and introduce probabilistic generative models that are the basis for statistical learning in networks.

L01 Motivation

We introduce our Chair and motivate challenges and opportunities of machine learning in data with a graph structure. We give an overview of topics covered in the course and discuss organizational issues.

- Introducing the Chair of Informatics XV
- Machine Learning for Graph-Structured Data
- Interdisciplinary Applications of Graph Learning
- Course Overview and Organizational Issues

L02 Graph Theory and Algorithms

We show how we can mathematically represent graphs and networks. We introduce the graph clustering problem and explain how it can be applied in general purpose machine learning.

- Graphs, networks, adjacency matrix
- Adjacency matrix and matrix powers
- Paths and Connected components
- Cluster detection with DBSCAN

L03 Statistical Ensembles and Inference

We introduce generative models of random graphs and explain how we can use them to define statistical ensembles of random graphs. We then illustrate how we can infer model parameters based on empirical data on complex networks.

- Generative models of random graphs
- Erdő-Rényi models
- Molloy-Reed Model
- Parameter Inference in Statistical Ensembles

Chapter II: Cluster Detection & Link Prediction

The second chapter of our course introduces techniques to detect cluster structures in networks. We show how we can use description length minimization and flow compression to find optimal parsimonious cluster structures. We further introduce the link prediction and discuss statistical, topological, and heuristic methods to address it.

L04 Stochastic Block Model

We illustrate ensemble-based statistical learning with the stochastic block model, a generative approach to detect clusters in networks.

- Statistical Inference of Community Structures
- Stochastic Block Model (SBM)
- Maximum Likelihood Estimation of SBM
- Likelihood Maximization and Overfitting

L05 Entropy and Description Length

We define entropy and evaluate the description length of a model. We show how we can use description length to infer parsimonious cluster structures.

- Entropy and Information Compression
- Entropy of Random Graphs
- Entropy of Stochastic Block Model
- Description Length Minimization

L06 Random Walks and InfoMap

We introduce an information-theoretic method to detect cluster structures based on the compression of random walks in networks.

- Markov Chains and Random Walks
- Huffman Code
- Compression Random Walks in Graphs
- The MapEquation and InfoMap

L07 Link Prediction

We introduce statistical and heuristic approaches for the supervised and unsupervised prediction of missing links in networks.

- Link Prediction in Networks
- Community-based Link Prediction
- Link Prediction with Topological Heuristics
- Similarity-based Link Prediction

Chapter III: Graph Representation Learning

The third chapter introduced techniques to learn low-dimensional vector space representations of networks, that can be used to address downstream graph learning tasks. We introduce matrix decomposition techniques for representation learning and show how neural networks and random walks can be used to position nodes in a vector space.

L08 Graph Representation Learning

We introduce basic techniques to learn low-dimensional representations of data. We then show how matrix decomposition can be applied to learn latent vector-space representations of graphs.

- Graphs vs. Euclidean Space
- Learning Low-Dimensional Representations
- Adjacency Matrix Factorization
- Laplacian Eigenmaps

L09 Neural Networks

Starting from logistic regression we show how we can use neural networks to address classification problems. We show how we can learn the parameters of deep neural networks using stochastic gradient descent.

- Logistic Regression
- Perceptron Classification
- Feed-Forward Neural Networks
- Backwards Propagation & Gradient Descent

L10 Walk-based Node Embedding

Building on the random walk model introduced in L06, we show how random walks and deep neural networks can be used to learn node embeddings for downstream graph learning tasks.

- Latent Semantic Analysis
- Neural Networks and Word Embedding
- DeepWalk
- node2vec

Chapter IV: Graph Neural Networks

In the final chapter, we show how deep learning techniques can be applied to graph-structured data. We introduce the concept of message passing and discuss how the graph Laplacian can be used to define graph convolutional networks. We introduce graph neural networks for node-, link-, and graph-level learning tasks.

L11 Graph Convolutional Networks

We explain how we can use message passing in neural networks to calculate graph convolutions, which provide a basis to apply deep learning to complex networks.

- Convolutional Neural Networks
- Laplace Filter and Nornmalized Graph Laplacian
- Message Passing and Graph Convolutions
- Graph Convolutional Networks (GCNs)

L12 Graph Neural Networks

We show how pooling can be used to coarsen graph representations. We introduce popular graph neural network architectures for link- and graph-level learning tasks.

- Node- vs. Graph-Level Learning Tasks
- Graph Neural Networks and Pooling
- GNN-based Graph Classification
- Link-level Learning in GNNs

L13 Graph Kernels

Educational Objective: We show how the kernel trick can be applied to graphstructured data. We show kernel function for graphs can be used to transform graphs into feature vectors that enable graph-level learning tasks.

- Kernel Methods in Machine Learning
- GraphKernels
- Graph2Vec
- Concluding Remarks

L14 Repetitorium

In the last week of our course, you have the chance to address open questions. We will repeat key sections of the course upon request.