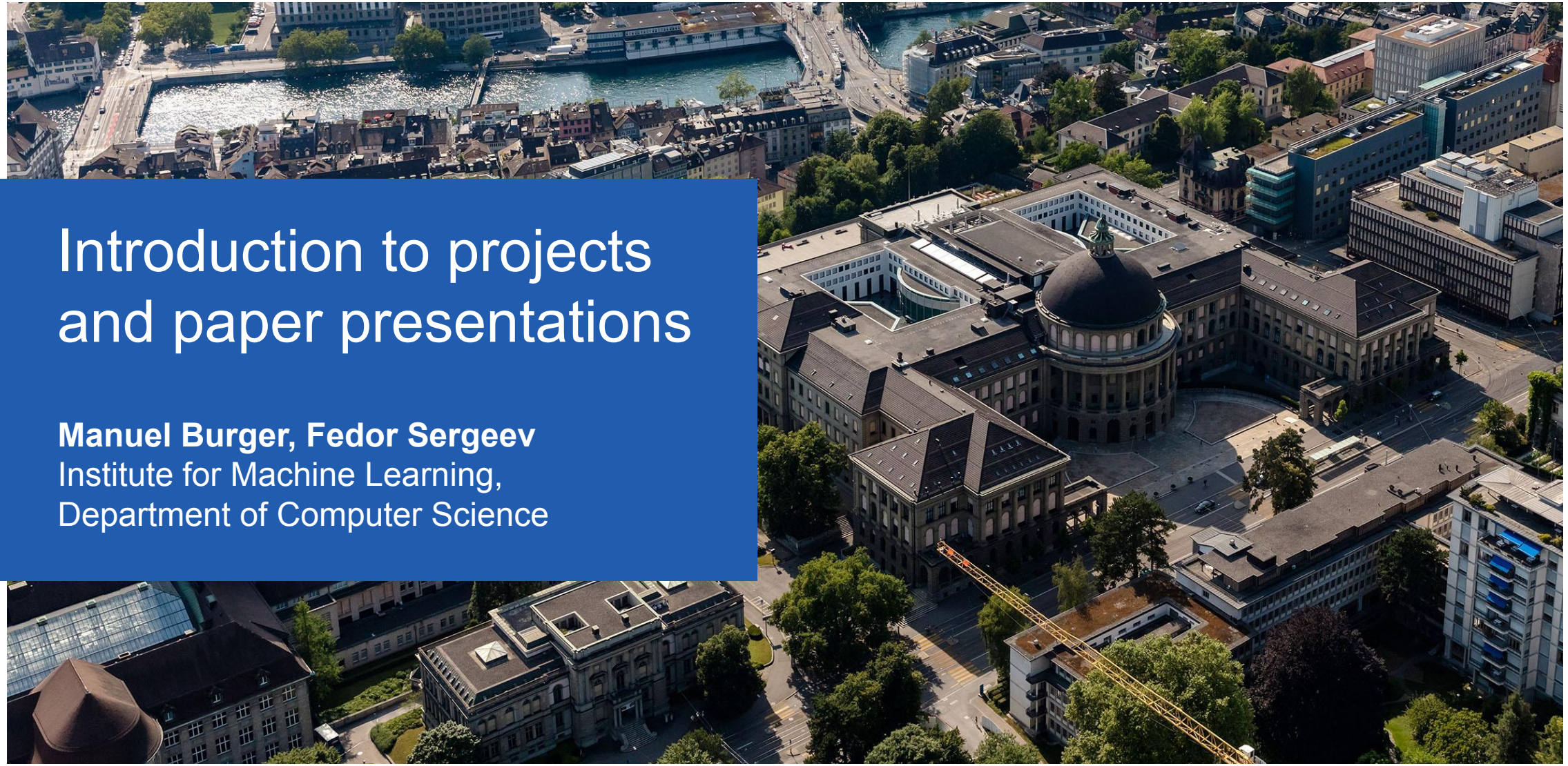
ETH zürich

BIOMEDICAL INFORMATICS



Introduction to projects and paper presentations

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Outline

1. TAs
2. Projects
3. Paper presentations
4. Exam and grading
5. Q&A
6. (Time to look for teammates)

TAs

Manuel Burger, Head TA

Fedor Sergeev, TA

Contact: **through moodle**
with a public or a private message

All course announcements:
through moodle

Projects

Projects

- **Format**
  - Team: 3 people
  - Assignment: Implement and apply deep learning on graphs
  - Coding: Python, PyTorch Geometric, Google Colab
  - Handouts (pdf) with point assignments will be provided
  - Deliverables
    - pdf report (background and results)
    - jupyter notebook (code and comments)
    - * presentation of notable projects
- **Project 1**
  - Duration: 3 weeks
  - Dates: out Oct 11 – due Nov 1
  - Topic
    - intro to GNNs and PyTorch geometric
    - node and graph level tasks
    - graph visualization and statistics
- **Project 2 (tentative)**
  - Duration: 4 weeks
  - Dates: out Nov 15 – due Dec 13
  - Topic
    - application of advanced GNNs to knowledge graphs
    - details will be announced later

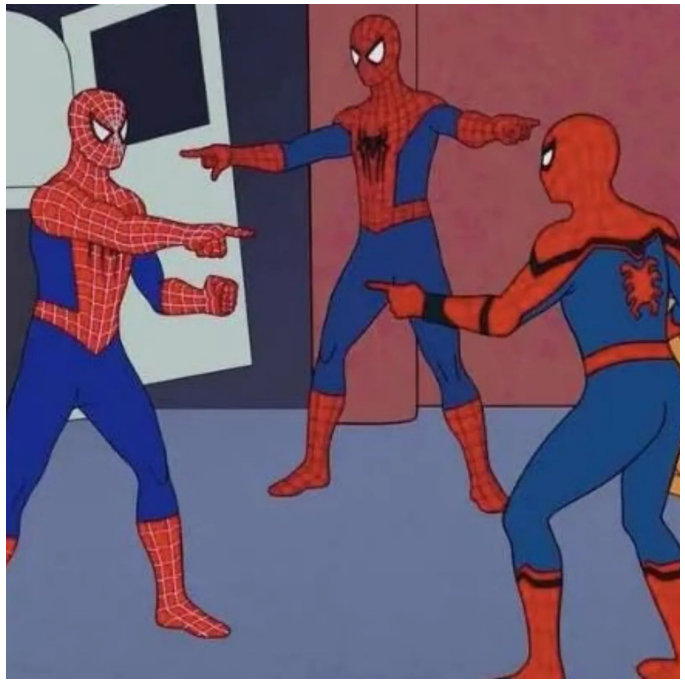

Fig.: Complete directed homogeneous graph with 3 vertices.

Sign up for projects

1. Find 2 team mates to build a group of 3
   - **The team is the same for both projects**
   - You can mingle after this presentation
   - You can also post on moodle if you are still looking for a team
   - There is a Forum on Moodle which you can use for team building
2. Register
   - You will be able to register your team on Moodle
   - Deadline and team lock is on the **5th of October**

Paper presentations

Paper presentations

- **Format**
  - Team: 2 people
  - Assignment: 1 paper on GNNs and applications
  - Deliverable: 10 min presentation + 5 min for questions
  - (3 presentations per session)
- **Motivation**
  - To learn about cutting-edge methods and applications of DL on graphs
  - To practice quick reading of lots of literature while capturing useful information
  - To practice presenting in a team to a large and qualified audience
- **Evaluation**
  - Covering the main points
  - Respecting the time limit
  - Preparing good slides
  - Answering the questions well
  - We will add a list of evaluation criteria to Moodle
- (see details on moodle)

Fig.: Group presentation of a recent paper on application of GNNs.

Evaluation Criterias for Paper Presentation

- Structural Aspects (e.g. Slides, Flow, Organization)
- Stylistic Aspects (e.g. Speaking, Explanations)
- Presentation Components:
  - Introduction and Motivation (Introduction, Related Work)
  - Technical Content (Methods, Results)
  - Conclusion (Summarizing)

Topics and papers

Date	Topic	Papers	Note
Oct 8	Applications of GNNs	A Deep Learning Approach to Antibiotic Discovery	
		Modeling Polypharmacy Side Effects with Graph Convolutional Networks	
		ETA Prediction with Graph Neural Networks in Google Maps	
Oct 25	Advanced GNNs	EIGNN: Efficient Infinite-Depth Graph Neural Networks	
		LightGCN: Simplifying and Powering Graph Convolution Network for Recommendation	
		Modeling Relational Data with Graph Convolutional Networks (R-GCN)	
Nov 1	Limits of GNNs	How does over-squashing affect the power of GNNs?	
		Expander Graph Propagation	
		Combining Label Propagation and Simple Models Out-performs Graph Neural Networks	
Nov 8	Misc (adversarial attack on graphs)	Adversarial Attacks on Neural Networks for Graph Data	
Nov 22	Clinical and genomics applications of GNNs	Learning the Graphical Structure of Electronic Health Records with Graph Convolutional Transformer	
		Graph-Guided Network for Irregularly Sampled Multivariate Time Series	
		Learning to Untangle Genome Assembly with Graph Convolutional Networks	
Nov 29	Development of GNNs	Design Space for Graph Neural Networks	
		Strategies for Pre-training Graph Neural Networks	
		Cluster-GCN: An Efficient Algorithm for Training Deep and Large Graph Convolutional Networks	
Dec 6	Knowledge graphs	Deep Bidirectional Language-Knowledge Graph Pretraining	students choose 3/4 papers
		Multimodal Analogical Reasoning over Knowledge Graphs	
		Neural-Symbolic Models for Logical Queries on Knowledge Graphs	
		Representation Learning on Graphs with Jumping Knowledge Networks	
Dec 13	Generative GNNs	CLEAR: Generative Counterfactual Explanations on Graphs	students choose 3/4 papers
		Efficient Graph Generation with Graph Recurrent Attention Networks	
		GeoDiff: a Geometric Diffusion Model for Molecular Conformation Generation	
		A Biologically Interpretable Graph Convolutional Network to Link Genetic Risk Pathways and Imaging Phenotypes of Disease	
Dec 13	Geometric GNNs and 3D graphs	Directional message passing for molecular graphs	
		Learning to Simulate Complex Physics with Graph Networks	
		HOOD: Hierarchical Graphs for Generalized Modelling of Clothing Dynamics	

- Recent works
- Cover a wide range of methods and applications
- Schedule approximately follows lectures

Sign up for paper presentations

1. Find a team mate
   - You can mingle after this presentation
   - We recommend picking a different partner from your project team
   - There is a Forum on Moodle which you can use for team building
2. Register
   - A link to a google form will be sent out later
   - You need to select **topics** you are interested in (you can select based on dates)
   - Registration deadline and team lock is on **5th of October**

Exam and grading

Exam and grading

- Exam
  - Lecture material
  - Written
  - Session Examination
  - 2 hours
  - 1 page (single side) of A4 paper is allowed for notes in the exam. The notes may be typed (font restriction: minimal font 10 pt) or handwritten.

- Final grade
  - Projects (30%, either a 15/15 split or a 10/20, it will say on the handout of the first project)
  - Paper presentation (10%)
  - Exam (60%)

Q&A

Time to look for teammates

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