



## Topics in Graph Machine Learning

Graphs are interesting data structures for many complex real-world data: chemical molecules, proteins, road networks, social interactions, . . . . Graph Neural Networks (GNNs) are an adoption of deep learning to work on graph structured data. There are some interesting results but the whole GNN field is very new and we see many interesting paths for improvement. The general way these GNNs work is having an internal state/embedding, exchange messages with their neighbors and update these embeddings. These kinds of GNNs are referred to as message passing GNNs. They perform well on some tasks, but we are also aware of several limitations. This thesis advertisement is kind of a wrapper for a plethora of ideas we think about exploring, such as:

- We want to look into inherently explainable GNN architectures (keyword: explainable AI). Exactly like other Deep Learning Architectures, current GNNs are black boxes, but can we build other architectures that are more explainable.
- GNN explainability methods: If we have a GNN that is not inherently explainable, can we have methods to explain their predictions. In previous work, we did first investigations and examined how to properly test such methods but there is more to be done.
- Closely related to explanations are adversarial attacks. How can I create a fake input that can mess with the GNN to make a wrong prediction? If we have an explanation, we know an angle to attack and vice versa.
- How can we create GNNs with better performance? We have some ideas using different frameworks than message passing or ensembling that we want to try out.
- Are there new interesting ideas, problems or datasets that we can try GNNs on?

**Requirements:** Prior experience or a strong interest in Machine Learning is recommended. Knowledge about graphs in the form of graph algorithms or graph mining is advantageous as well. Depending on the topic such knowledge is not recommended but strongly recommended ;) In the projects we will have weekly meetings to discuss questions and progress and think about new directions.

**Interested? Please contact us for more details!**

### Contact

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