Reinforcement Learning for Spatial Graph Design

Scope

This project may be instantiated as a Master's project or thesis. Prior knowledge in Reinforcement Learning and Deep Learning is strongly recommended.

Problem Setting

Graphs can be used to represent a variety of information ranging from networks of friends to spatial information such as 3D positions of atoms in a molecule.
Being able to automatically design graphs fulfilling a desired property would thus be useful in a variety of setting. We want to use Reinforcement Learning (RL) to tackle this task.

Method

In this project we want to utilize a Graph Neural Network (GNN), specifically the Permutation-Invariant Variational Autoencoder for Graph-Level Representation Learning to learn a latent representation for given graphs. Starting from the latent representation of an initial graph we want to modify the latent representation such that it corresponds to a graph with desirable properties. The modification process will be done by an RL agent which maximizes a reward corresponding to the "quality" of the resulting graph.

Roadmap

We want to design graphs representing points in a 2D or 3D space.
Therefore we represent each point as a node in a graph and encode their relative positions in the edges. To show that we can use an RL agent to modify/optimize such graphs we suggest the following roadmap for this project:

1. Create a dataset of graphs representing N nodes and E edges in 2D/3D space
2. Train the GNN to successfully encode and decode the given graphs
3. Confirm that we can linearly interpolate between two graphs in the latent space (see Figure 3 in the corresponding paper)
4. Define a suited reward function for the RL agent. For example if we want to design equilateral triangles in 2D we could use the negative deviation from 60° angles.
5. Train an RL agent maximize the reward function, thus transforming a given graph into a target graph fulfilling a desired property

Organization

If you are interested in this project, write an email to nrprojects@informatik.uni-freiburg.de with a clear reference to this project proposal or contact vogty@cs.uni-freiburg.de.