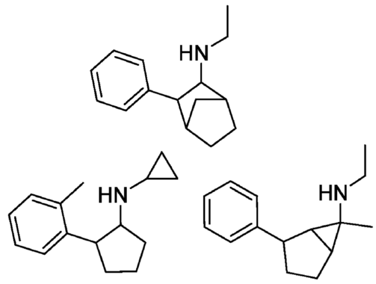
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Distributed Computing

Prof. R. Wattenhofer

Generative Adversarial Networks for Graphs



Graph generation is an interesting problem which is encountered when trying to generate novel molecules or proteins with desired properties or variations of social graphs that used to test hypotheses in social sciences. However, graph generation is very a challenging problem due to the non-uniqueness of graphs and the complex non-local dependencies between their edges. Deep learning based generators have shown promising initial results, but they are still quite limited as they are either restricted to generating very small graphs with only ten or twenty nodes or they use sequential generation, which results in low novelty of the generated graphs as the model largely re-creates graphs from the training set.

In this thesis we will build a novel Generative Adversarial Network (GAN) which is able to generate larger graphs, such as proteins with high sample novelty. GANs are particularly suited for novel graph generation, as they implicitly model the true graph distribution, but so far no-one was able to make them work for anything but tiny graphs. We will borrow some ideas from spectral graph theory, high-resolution image GANs and novel expressive graph neural networks to achieve our goals.

Requirements: Strong motivation, knowledge in deep learning, or a solid background in machine learning. Experience with Python and PyTorch or TensorFlow is an advantage as well as knowledge in graph theory, generative models and graph neural networks.

Interested? Please contact us for more details!

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