Neural networks for generation of graphs

Supervisors

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Description

A large class of problems can be formalized with graphs. In these problems entities (vertices) are connected with relationships (edges). Such structures naturally occur in chemistry (molecules), logistics (road networks), power control (energy grids), sociology (social networks) and economics (financial networks). Specific problems handled with graphs include optimization of a path between entities, entity classification, whole graph classification and others.

The goal of this project is to design neural architectures whose goal is to generate graphs based on their functional requirements. These architectures could be applied to automatically synthesize structures in a variety of areas. Examples include generation of molecules compatible, in a specified sense, to given molecules, or generation of designs (e.g., hydraulic installations) complementary to given structures (e.g., architectural designs).

There has been great progress in generative models in the field of machine learning in recent years. Examples include the transformer and the stable diffusion. There have been some approaches to graph synthesis such as GraphRNN [1], the graph transformer [2], or attempts to adjust the diffusion model to graphs [3,4]. All of the already existing approaches are limited to generating graphs similar to those present in the training set. However, graph synthesis based on functional requirements has not been explored sufficiently. The project is intended to fill this gap.

Requirements

- MSc degree in computer science or related field,
- Good knowledge of deep learning, including practical experience with programming in Python and relevant libraries (PyTorch, TensorFlow, Keras)
- Advanced skills in written and spoken English
- Outstanding academic or professional achievements in computer science or mathematics

References

[1] J. You, R. Ying, X. Ren, W. L. Hamilton, J. Leskovec, “GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models”, 2018, arXiv:1802.08773

[2] V.P. Dwivedi, X. Bresson, "A Generalization of Transformer Networks to Graphs," 2021, arXiv:2012.09699

[3] M. Thorpe, T. M. Nguyen, H. Xia, T. Strohmer, A. Bertozzi, S. Osher, B. Wang, "GRAND++: Graph Neural Diffusion with A Source Term," ICLR 2022

[4] L. Kong, J. Cui, H. Sun, Y. Zhuang, B. A. Prakash, C. Zhang, “Autoregressive Diffusion Model for Graph Generation,” 2023, arXiv: 2307.08849