TUD Datasets: A collection of benchmark datasets for learning with graphs

Anonymous Authors[1]

Abstract

Recently, there has been an increasing interest in learning with graph data, especially using graph neural networks. However, the development of meaningful benchmark datasets and standardized evaluation procedures is lagging behind. That is, most paper papers evaluate their methods on small-scale datasets leading to high standard deviations and hard to interpret results, consequently hindering advancements in this area. To address this, we introduce the TUD BENCHMARK DATASET for graph classification and regression. The dataset consists of over 150 datasets from a wide range of applications and varying sizes. We provide Python-based data loaders, baseline implementations, and evaluation tools. Here, we give an overview of the datasets, evaluation tools, and provide baseline experiments.

1. Introduction

Graph-structured data is ubiquitous across application domains ranging from chemo- and bioinformatics to image and social network analysis. To develop successful machine learning models in these domains, we need techniques that can exploit the rich information inherent in the graph structure, as well as the feature information contained within nodes and edges. In recent years, numerous approaches have been proposed for machine learning with graphs—most notably, approaches based on graph *kernels* (Kriege et al., 2019) or using *graph neural networks* (GNNs) (Hamilton et al., 2017; Gilmer et al., 2017). However, most papers, even recent ones, evaluate newly proposed architectures or methods on a fixed set of small-scale benchmark datasets leading to high standard deviations and hard to interpret results.

Here, we give an overview *TUD benchn* The bencharmk consists of over 150 datasets from a wide range of domains and can be accessed via mark dataset for supervised learning with graphs, i.e., classificiation and regression. All datasets can conviently be downloaded from `graphlearning.io`, and easily be accessed form popoluar graph learning frameworks such as Pytorch Geoeotric (Fey & Lenssen, 2019) and DGL (Wang et al., 2019).

Related work. Give short over view of GNNs and other benchmarks and expermental studies.

Contributions/

2. Overview of the datasets

3. Installation, usage, and evaluation tools

4. Experimental evaluation

4.1. Experimental protocol

5. Conclusion

References

Fey, M. and Lenssen, J. E. Fast graph representation learning with pytorch geometric. *CoRR*, abs/1903.02428, 2019.

Gilmer, J., Schoenholz, S. S., Riley, P. F., Vinyals, O., and Dahl, G. E. Neural message passing for quantum chemistry. In *International Conference on Machine Learning*, 2017.

Hamilton, W. L., Ying, R., and Leskovec, J. Representation learning on graphs: Methods and applications. *IEEE Data Engineering Bulletin*, 40(3):52–74, 2017.

Kriege, N. M., Johansson, F. D., and Morris, C. A survey on graph kernels. *CoRR*, abs/1903.11835, 2019. Accepted for publication in *Applied Network Science*.

Wang, M., Yu, L., Zheng, D., Gan, Q., Gai, Y., Ye, Z., Li, M., Zhou, J., Huang, Q., Ma, C., Huang, Z., Guo, Q., Zhang, H., Lin, H., Zhao, J., Li, J., Smola, A. J., and Zhang, Z. Deep graph library: Towards efficient and scalable deep learning on graphs. *ICLR Workshop on Representation Learning on Graphs and Manifolds*, 2019. URL `https://arxiv.org/abs/1909.01315`.

[1]Anonymous Institution, Anonymous City, Anonymous Region, Anonymous Country. Correspondence to: Anonymous Author <anon.email@domain.com>.

Preliminary work. Under review by the International Conference on Machine Learning (ICML). Do not distribute.