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

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Abstract

Recently, there has been an increasing interest in learning with graph data, especially in graph neural networks. However, the development of meaningful benchmark datasets and standarized evaluation prodecures are lagging behind. That is, most paper papers evaluate their methods on small-scale datasets leading to high standard deviations and coseuqntly hindering advancements in this area. To adress this, we intodruce the TUD BENCHMARK DATASET for graph classification and regression. The dataset consists of over 150 datasets from a wide range of applications and variying size. We provide Python based data loaders, baseline implementations, and evaluation tools. Here, we give an overview of the datasets, the evalution 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 convientlly 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

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