

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 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 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) (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 of *Tud datasets*. The benchmark collection consists of over 150 datasets from a wide range of domains for supervised learning with graphs, i.e., classifi-

ation and regression. All datasets are provided in a common dataset format at graphlearning.io, and easily be accessed from popular graph learning frameworks such as *Pytorch Geometric* (Fey & Lenssen, 2019) and *DGL* (Wang et al., 2019).

Related work. There exists two approaches to supervised learning with graphs, graph kernels and graph neural networks (GNNs). Graph kernels have been studied extensively in the past 15 years, see (Kriege et al., 2019) for a thorough overview. Important approaches include random-walk and shortest paths based kernels (Gärtner et al., 2003; Sugiyama & Borgwardt, 2015; Borgwardt & Krieger, 2005; Kriege et al., 2017), as well as the Weisfeiler-Lehman subtree kernel (Shervashidze et al., 2011a; Morris et al., 2017). Further recent works focus on assignment-based approaches (Kriege et al., 2016; Nikolentzos et al., 2017), spectral approaches (Kondor & Pan, 2016), and graph decomposition approaches (Nikolentzos et al., 2018).

Recently, GNNs (Gilmer et al., 2017) emerged as an alternative to graph kernels. Notable instances of this model include (Duvenaud et al., 2015), (Li et al., 2016), (Hamilton et al., 2017) and the spectral approaches proposed in (Bruna et al., 2014; Defferrard et al., 2016; Kipf & Welling, 2017)—all of which descend from early work in (Kireev, 1995; Merkwirth & Lengauer, 2005; Scarselli et al., 2009). A unifying message passing architecture can be found in (Gilmer et al., 2017). Two recent surveys (Wu et al., 2019; Zhou et al., 2018) provide a thorough overview of graph neural networks

The papers (Fey & Lenssen, 2019; Errica et al., 2019; Dwivedi et al., 2020) evaluate GNNs using a unified evaluation procedure, however, both only use small scale datasets. Recently, ogb.stanford.edu launchend, however the provided datasets for graph classification focus on chemistry applications, and the number is quite limited at this point.

Contributions We give an overview of TUD DATASET, its unified evaluation procedures, and baseline methods. Moreover, we report results on an experimental study comparing graph kernels and GNNs on a subset of the TUD DATASET.

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

2. Overview of the datasets

The TUD DATASET contain over 150 datasets provided at graphlearning.io.

3. Installation, baseline, and evaluation tools

The data loader, baseline methods, experimental evaluation tool can be installed by running `pip install tud-datasets`, see XXX for further details.

3.1. Baselines

In order to provide meaningful baselines, we provide implementation of common graph kernels as well as GNNs baselines. We have implemented the *Weisfeiler-Lehman Subtree* (Shervashidze et al., 2011b), *Shortest-path* (Borgwardt & Kriegel, 2005), *Graphket* (Shervashidze et al., 2009), *Weisfeiler-Lehman Optimal Assignment* (Kriege et al., 2016) kernel, as well as the higher-order WL kernels (Morris & Mutzel, 2019), in C++ and made them accessible through the Python interface of TUD DATASET, see XXX for further details. Moreover, all GNN architectures implemented in PyTorch Geometric can be used as baseline as well.

Vertex kernel and edge kernel?

3.2. Evaluation tools

In order to insure a fair and meaningful comparison between methods, we propose the following evaluation procedures, and software tools for kernels and GNN approaches. All proposed methods can be conveniently accessed from the Python interface, see XXX for further details. First, for kernels we propose the established *C-SVM* implementation LIBSVM (Chang & Lin, 2011) for kernels that compute a Gram matrix, and the linear *C-SVM* implementation LIBLINEAR (Fan et al., 2008) for kernels that can be computed based on explicit feature maps. We optimize GNNs end-to-end using ADAM (). To compute accuracies and other metrics for evaluation, we propose to use 10-fold cross validation, where we select a validation set uniformly at random from each training fold (10% of the training fold), to select hyperparameters, e.g., number of iterations, *C* parameter, number of layers, learning rate, feature dimension, etc.

4. Experimental evaluation

4.1. Experimental protocol

5. Conclusion

We gave an overview of the TUD DATASET, and reported on the results of an experimental study comparing graph kernels and GNNs on a subset of the data. We believe that our dataset collection will spark further progress in the area

of graph representation learning. We are looking forward to adding more dataset to our collection, and are excited about contributions from the community, and researchers and practitioners from other areas.

6. Acknowledgement

We thank everybody who provided datasets for TUD DATASET.

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