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., classification 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 learing 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 & Kriegel, 2005; Kriege et al., 2017), as well as the Weisfeiler-Lehman subtree kernel (Shervashidze et al., 2011; 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 a 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) evalute 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 evalution procudures, and baseline methods. Moreover, we report results on a experimental study comparing graph kernels and GNNs on a subset of the TUD DATASET.

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2. Overview of the datasets

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

3. Installation, usage, and evaluation tools

4. Experimental evaluation

4.1. Experimental protocol

5. Conclusion

References

Borgwardt, K. M. and Kriegel, H.-P. Shortest-path kernels on graphs. In *IEEE International Conference on Data Mining*, pp. 74–81, 2005.

Bruna, J., Zaremba, W., Szlam, A., and LeCun, Y. Spectral networks and deep locally connected networks on graphs. In *International Conference on Learning Representation*, 2014.

Defferrard, M., X., B., and Vandergheynst, P. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in Neural Information Processing Systems*, pp. 3844–3852, 2016.

Duvenaud, D. K., Maclaurin, D., Iparraguirre, J., Bombarell, R., Hirzel, T., Aspuru-Guzik, A., and Adams, R. P. Convolutional networks on graphs for learning molecular fingerprints. In *Advances in Neural Information Processing Systems*, pp. 2224–2232, 2015.

Dwivedi, V. P., Joshi, C. K., Laurent, T., Bengio, Y., and Bresson, X. Benchmarking graph neural networks. *CoRR*, abs/2003.00982, 2020.

Errica, F., Podda, M., Bacciu, D., and Micheli, A. A fair comparison of graph neural networks for graph classification. *CoRR*, abs/1912.09893, 2019.

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

Gärtner, T., Flach, P., and Wrobel, S. On graph kernels: Hardness results and efficient alternatives. In *Learning Theory and Kernel Machines*, volume 2777 of *Lecture Notes in Computer Science*, pp. 129–143. 2003.

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. Inductive representation learning on large graphs. In *Advances in Neural Information Processing Systems*, pp. 1025–1035, 2017.

Kipf, T. N. and Welling, M. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations*, 2017.

Kireev, D. B. Chemnet: A novel neural network based method for graph/property mapping. *Journal of Chemical Information and Computer Sciences*, 35(2):175–180, 1995. ACS.

Kondor, R. and Pan, H. The multiscale laplacian graph kernel. In *Advances in Neural Information Processing Systems*, pp. 2982–2990. NIPS, 2016.

Kriege, N. M., Giscard, P.-L., and Wilson, R. C. On valid optimal assignment kernels and applications to graph classification. In *Advances in Neural Information Processing Systems*, pp. 1615–1623. NIPS, 2016.

Kriege, N. M., Neumann, M., Morris, C., Kersting, K., and Mutzel, P. A unifying view of explicit and implicit feature maps for structured data: Systematic studies of graph kernels. *CoRR*, abs/1703.00676, 2017. Accepted for publication in *Data Mining and Knowledge Discovery*.

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*.

Li, W., Saidi, H., Sanchez, H., Schäf, M., and Schweitzer, P. Detecting similar programs via the Weisfeiler-Leman graph kernel. In *International Conference on Software Reuse*, pp. 315–330, 2016.

Merkwirth, C. and Lengauer, T. Automatic generation of complementary descriptors with molecular graph networks. *Journal of Chemical Information and Modeling*, 45(5):1159–1168, 2005.

Morris, C., Kersting, K., and Mutzel, P. Glocalized Weisfeiler-Lehman kernels: Global-local feature maps of graphs. In *IEEE International Conference on Data Mining*, pp. 327–336, 2017.

Nikolentzos, G., Meladianos, P., and Vazirgiannis, M. Matching node embeddings for graph similarity. In *AAAI Conference on Artificial Intelligence*, pp. 2429–2435, 2017.

Nikolentzos, G., Meladianos, P., Limnios, S., and Vazirgiannis, M. A degeneracy framework for graph similarity. In *International Joint Conference on Artificial Intelligence*, pp. 2595–2601, 2018.

Scarselli, F., Gori, M., Tsoi, A. C., Hagenbuchner, M., and Monfardini, G. The graph neural network model. *IEEE Transactions on Neural Networks*, 20(1):61–80, 2009.

Shervashidze, N., Schweitzer, P., van Leeuwen, E. J., Mehlhorn, K., and Borgwardt, K. M. Weisfeiler-Lehman

graph kernels. *Journal of Machine Learning Research*, 12:2539–2561, 2011.

Sugiyama, M. and Borgwardt, K. M. Halting in random walk kernels. In *Advances in Neural Information Processing Systems*, pp. 1639–1647, 2015.

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.

Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., and Yu, P. S. A comprehensive survey on graph neural networks. *arXiv preprint arXiv:1901.00596*, 2019.

Zhou, J., Cui, G., Zhang, Z., Yang, C., Liu, Z., Wang, L., Li, C., and Sun, M. Graph neural networks: A review of methods and applications. *arXiv preprint arXiv:1812.08434*, 2018.