Junior Professor for Machine Learning on Graphs

RWTH AACHEN UNIVERSITY

The present work was submitted to the Machine Learning on Graphs Group at the Chair of Computer Science 6, RWTH Aachen University

A Theoretical and Empirical Investigation into the Equivalence of Graph Neural Networks and the Weisfeiler-Leman Algorithm

From the Faculty of Mathematics, Physics, and Computer Science approved for the purpose of obtaining the academic degree of Bachelor of Sciences.

Eric Tillmann Bill

Supervisor:
Prof. Dr. rer. nat. Christopher Morris

Machine Learning on Graphs Group
RWTH Aachen University

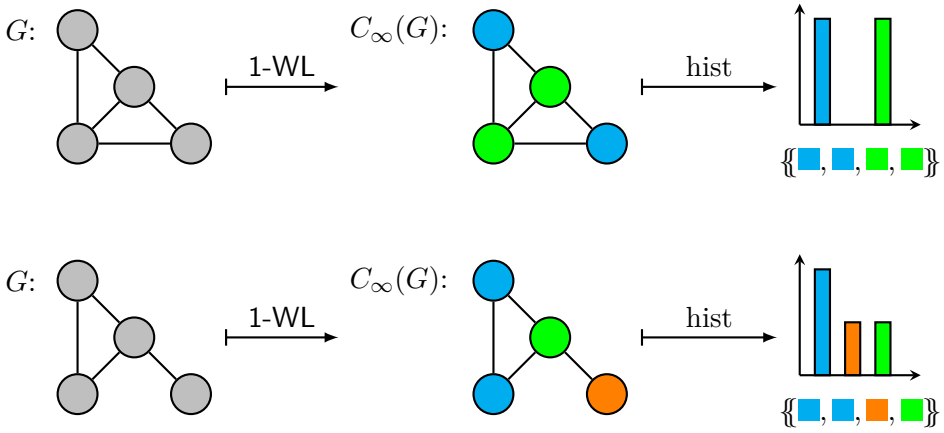
August, 2023

Table 1: Overview of the mean absolute error and the standard deviation (logMAE) on large-scale (multi-target) molecular regression tasks. We highlighted the lowest error for the 1-WL+NN and GNN models for each dataset.

Method	**Dataset**			
	ALCHEMY	ALCHEMY (10K)	ZINC	ZINC (10K)
1-WL+NN	0.600 ±0.004 -0.625 ±0.032	0.305 ±0.001 -1.740 ±0.042	0.229 ±0.003	0.465 ±0.009
GNN	0.523 ±0.016 -0.705 ±0.035	0.282 ±0.002 -1.890 ±0.031	0.104 ±0.005	0.298 ±0.034

Table 2: Accuracy and standard deviation in percent achieved by the best-performing 1-WL+NN, 1-WL:GNN, and GNN model on each classification dataset.

Model	**Dataset**					
	ENZYMES	IMDB-BINARY	MUTAG	NCI1	PROTEINS	REDDIT-BINARY
1-WL+NN	48.3 ±8.1	72.4 ±4.1	85.1 ±8.6	83.6 ±2.2	75.2 ±3.9	78.4 ±2.7
GNN	34.4 ±7.0	74.7 ±3.8	84.6 ±8.7	79.9 ±2.2	74.3 ±5.1	86.9 ±3.2



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