

Utility of Minimal DFS Codes

I currently investigate the utility of using minimal DFS codes to improve the prediction performance of message passing neural networks and transformers in graph learning tasks.

Chris Wendler

▸ Message Passing Neural Networks

In this experiment I compared a message passing neural network with an attention based readout function to an identical one but the input graphs are augmented by the DFS indices corresponding to their minimal DFS codes. Pink is without and cyan is with DFS codes.

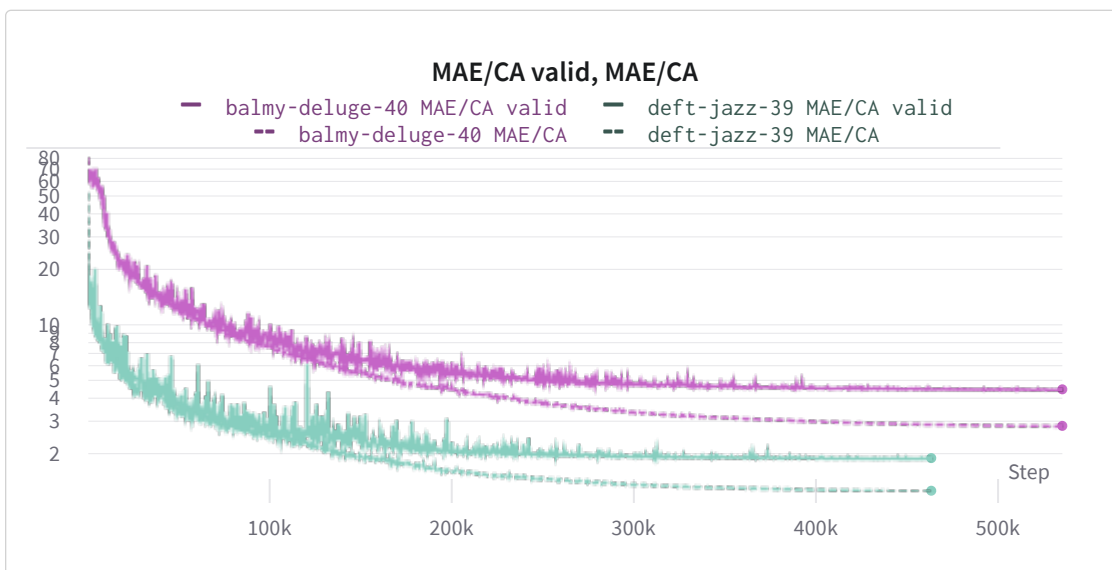
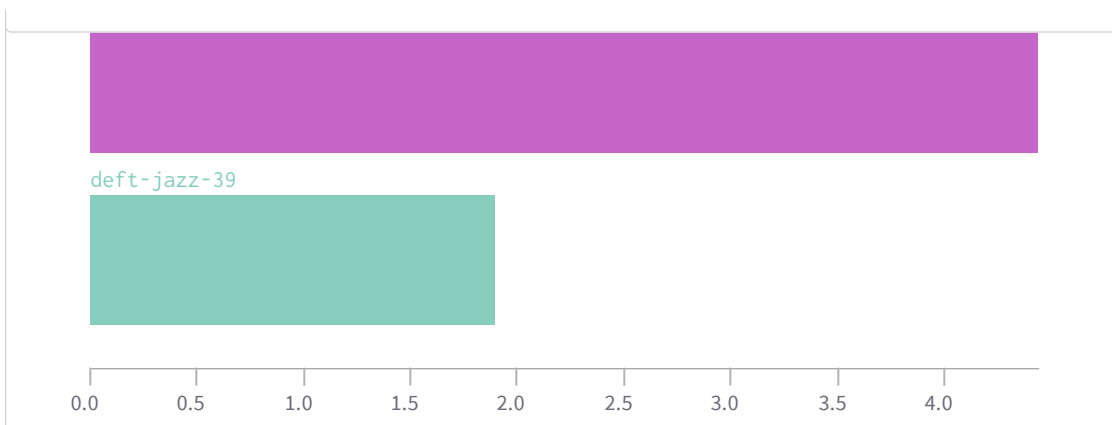
The task is a molecular property prediction task. To be precise, I fit the U0 column of the QM9 dataset. U0 is the atomization energy at 0 Kelvin, it is the energy required to break up the molecule into all of its atoms at 0 K.

State-of-the-art methods achieve scores that are smaller than 0.5 in the reported metric. These results are for an message passing neural network that I defined myself in the process of learning pytorch geometric. Next, I will have a look whether I observe similar results by augmenting State-of-the-art message passing neural networks.

TEST MAE/CA

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<https://wandb.ai/chrisxx/QM9-GAT/reports/Utility-of-Minimal-DFS-Codes---VmIldzo4NzI1NTA>

