AIM 5056-41: Homework 2

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(1) Good things about the paper

While most of the GNN studies focus on improving the performance of GNN model by adopting new algorithms or modules, the authors of “How powerful are Graph Neural Networks” deep dive into the theoretical background of GNN and wonder what GNN can and cannot do. By comparing GNN with Weisfeiler-Leham graph isomorphism test, they discovered what qualities of the WL test that makes it more expressive than GNN and theoretically figured out how to apply these qualities to GNN so that it can be as powerful as WL test. The appendix of this paper tells us how thoroughly the authors went through mathematically to prove their points. On top of that, they examined variant GNN models such as GCN and GraphSAGE with respect to neighborhood aggregation strategy, pooling, and readout function, and checked whether these functions could be seen as injective multiset function, and if not, they also mentioned the reasons for that. Furthermore, they did not finish the paper by just defining the conditions to make GNN more expressive, they proposed a novel model called Graph Isomorphism Network(GIN) that could maximize the expressive power of GNN, based on their studies. Thus, this paper not only discovered the theoretical qualities to make the model more expressive and developed a new model that brings only the strengths from both GNN and WL test.

(2) Your opinion to improve this paper or drawbacks

In section 4.2 Graph-level Readout of GIN, the author stresses that a sufficient number of iterations is needed to form good node representation and decides to concatenate all layers of GIN to preserve all the structural information across the layers. As author mentioned, as the number of hidden layers in GNN increases, the less distinguishable the node representation becomes, and this is called over-smoothing problem. GNN model still suffers from over-smoothing problem and many studies were done to mitigate this problem. I was wondering whether GIN model is free from over-smoothing problems since it concatenates graph representations across layers. If the author included an experiment result in the paper about the performance comparison between GIN and other GNN models as the number of layers increases, the paper would become more complete and could appeal to more researchers on how expressive and effective GIN model is even if the number of depths increases.