# Project: Graph Separation

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A famous result in the theory of message passing networks (MPNs) states that their expressive power is equal to the 1-WL isomorphism test. More accurately, MPNs is a general framework for graph neural networks that can be instatiated in many ways. While any realization of an MPN cannot separate graphs unless they are separable by the WL isomorphism test, the converse claim can be showed to be true for specific MPN constructions. The two classical constructions of MPNs which are equivalent to WL are by Xu [2] and by Morris [1].

In this project we will focus on the construction by Xu and a disadvantage of this construction. A follow up project (e.g., for thesis) would aim to fix these disadvantage, for example by using a sorting based MPN construction.

1. Read [2]. Reading or at least glancing at thre proofs is recommended.

2. A key result for the proof of separation of GINs in Lemma 5. The lemma states that if $\mathcal{X}$ is a countable set and $N$ is a fixed natural number, there exists a function $f : \mathcal{X} \to \mathbb{R}$ such that, for every $X_1, X_2 \subseteq \mathcal{X}$ of size $< N$,

$$\sum_{x \in X_1} f(x) \neq \sum_{x \in X_2} f(x).$$

   In GINs, this $f$ is replaced with an MLP $m$ which can approximate $f$ arbitrarily well due to the universality of MLP. Note however that it is not clear how large the MLP must be in order to be a good approximation of $f$. In fact, we will show that an MLP of fixed size can never enjoy the same separation properties that $f$ has. For simplicity we will focus on univariate functions.

   (a) Set $\mathcal{X} = \mathbb{Z}$. Show that for any affine function $m(x) = ax + b$ there exist finite sub-multisets $X_1 \neq X_2 \subseteq \mathcal{X}$ such that

$$\sum_{x \in X_1} m(x) = \sum_{x \in X_2} m(x)$$

   (hint: consider $X_1, X_2$ which sum to the same number)

(b) Any MLP from $m : \mathbb{R} \to \mathbb{R}$ is a continuous piecewise linear function. Show that for any continuous piecewise linear functions there exist multi-sets $X_1 \neq X_2 \subseteq \mathcal{X} = \mathbb{Z}$ such that

$$\sum_{x \in X_1} m(x) = \sum_{x \in X_2} m(x)$$

(Hint: use the fact that there is a partition of the line into a finite number of segments, such that $m$ is affine on each segment.).

3. Conduct an empirical study of the separation power of GINs. Take a GIN with randomly generated weights and apply it to a collection of Erdos-Reyni graphs. Are there different graphs which get the same value? How frequent is this? How does this depend on the size of the MLPs in GIN and on the parameters of the Erdos-Reyni generation process?

4. Suggest a loss to train GINs to be 'as separating as possible'. Does the trained GIN separate better than the randomly initialized GIN? Does it separate 'perfectly'?

# References


[1] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and leman go neural: Higher-order graph neural networks. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 4602–4609, 2019.

[2] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *International Conference on Learning Representations*, 2018.