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 for the purpose of obtaining the academic degree of Bachelor of Sciences.

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Contents

1 Definition

Definition 1. For any graphs G, H we will denote $G \simeq_{1\text{WL}} H$ if the 1-WL isomorphism test can not distinguish both graphs. Note that due to the soundness of this algorithm, if $G \not\simeq_{1\text{WL}} H$, we always can conclude that $G \not\simeq H$.

Definition 2. Let $\mathcal{C}$ be a collection of permutation invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$. We say $\mathcal{C}$ is **1-WL-Discriminating** if for all graphs $G_1, G_2 \in \mathcal{X}$ for which the 1-WL isomorphism test concludes non-isomorphic, there exists a function $h \in \mathcal{C}$ such that $f(G_1) \neq f(G_2)$.

Definition 3. Let $\mathcal{C}$ be a collection of permutation invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$. We say $\mathcal{C}$ is **GNN-Approximating** if for all permutation-invariant functions $\mathcal{A}$ computed by a GNN, and for all $\epsilon \in \mathbb{R}$ with $\epsilon > 0$, there exists $h_{\mathcal{A},\epsilon} \in \mathcal{C}$ such that $\|\mathcal{A} - h_{\mathcal{A},\epsilon}\|_\infty := \sup_{G\in\mathcal{X}} |f(G) - h_{\mathcal{A},\epsilon}(G)| < \epsilon$

2 Theorems

In this thesis we concentrate on finite graphs. We therefore, let $\mathcal{X}$ be $\mathcal{X} := \{1, \ldots, k\}$ for an arbitrary $k \in \mathbb{N}$.

Theorem 4. Let $\mathcal{C}$ be a collection of functions computed by 1-WL+NN models, then C is **1-WL-Discriminating**.

Theorem 5. Let $\mathcal{C}$ be a collection of functions that is **1-WL-Discriminating**, than $\mathcal{C}$ is also **GNN-Approximating**.

3 Proofs

Since we concentrate in this thesis on finite graphs, let $\mathcal{X}$ be $\mathcal{X} := \{1, \ldots, k\}$ for an arbitrary $k \in \mathbb{N}$.

3.1 1-WL+NN is 1-WL-Discriminating

Proof. We consider the collection $\mathfrak{B}_k$ of permutation invariant functions, where every $\mathcal{B} \in \mathfrak{B}_k$ is of the form $\mathcal{B} = \text{MLP} \circ f$. Here MLP is an arbitrary multilayer perceptron mapping vectors from $\mathbb{N}^K$ to $\mathbb{R}$ and f the *counting-encoding* function. Further, let $G_1, G_2 \in \mathcal{X}^{n\times n}$ such that the 1-WL isomorphism test concludes non-isomorphic ($G_1 \not\simeq G_2$). We denote with $(C_\infty)_G$ the final coloring computed by the 1-WL algorithm when applied on G.

Due to the 1-WL isomorphism test concluding $G_1 \not\simeq G_2$, there exists a color $c \in \mathbb{N}$ such that $(C_\infty)_{G_1}(c) \neq (C_\infty)_{G_2}(c)$. If we now consider as MLP the following function $\text{MLP} : \mathbb{N}^K \to \mathbb{R}, v \mapsto W \cdot v$ with $W \in \mathbb{N}^{1\times K}$ such that $W_{1,c} := 1$ and $W_{1,i} := 0$ for all $i \in [K] \setminus \{c\}$. Then we can conclude that $\mathcal{B}(G_1) \neq \mathcal{B}(G_2)$. Since G_1, G_2 are arbitrary, we can conclude the proof. $\square$

3.2 1-WL-Discriminating is also GNN-Approximating

Lemma 6.

Lemma 7 (My Lemma)**.** Test

Lemma 8. Let $\mathcal{C}$ be a class of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all $G \in \mathcal{X}^{n\times n}$, there exists $h_G \in \mathcal{C}$ satisfying $h_G(G^*) = 0$ if and only if $G \simeq G^*$ for all $G^* \in \mathcal{X}^{n\times n}$. Then for every $G \in \mathcal{X}^{n\times n}$, there exists a function $\phi_G \in \mathcal{C}$ such that for all $G^* \in \mathcal{X}^{n\times n}$: $\varphi_G(G^*) = \mathbb{1}_{G\simeq_{1\text{WL}}G^*}$.

Proof. Following **??**, for every $G \in \mathcal{X}^{n\times n}$ there exists $\tilde{h_G} \in \mathcal{C}$ such that for all $G^* \in \mathcal{X}^{n\times n}$: $h_G(G^*) = 0$ if and only if $G \simeq_{1\text{WL}} G^*$. Due to $\mathcal{X}$ being finite, we can define for every graph G the constant:

$$\delta_G := \frac{1}{2} \min_{G^*\in\mathcal{X}^{n\times n}, G\not\simeq_{1\text{WL}}G^*} |h_G(G^*)| > 0.$$

With this constant, we can use a so-called "bump" function working from $\mathbb{R}$ to $\mathbb{R}$ that will be similar to the indicator function. For parameter $a \in \mathbb{R}$ with $a > 0$ let:

$$\psi_a(x) := \max(\frac{x}{a} - 1, 0) + \max(\frac{x}{a} + 1, 0) - 2 \cdot \max(\frac{x}{a}, 0).$$

The interesting property of ψ_a is that it maps every value x to 0, except for x being drawn from the interval $(-a, a)$. We use this property to define for every graph $G \in \mathcal{X}^{n\times n}$ the function $\varphi_G(G^*) := \psi_{\delta_G}(h_G(G^*))$. We will quickly demonstrate that this function is equal to the indicator function, let G be fixed and G^* an arbitrary graph from $\mathcal{X}^{n\times n}$:

1. If $G \simeq_{1\text{WL}} G^*$, then $h_G(G^*) = 0$ resulting in $\varphi_G(G^*) = \psi_{\delta_G}(0) = 1$.
2. If $G \not\simeq_{1\text{WL}} G^*$ then $h_G(G^*) > 0$, such that $|h_G(G^*)| > \delta_G$ resulting in $\varphi_G(G^*) = 0$.

Note we can encode each φ_G via a single MLP layer, where δ_G is a constant and the max operator is replaced by the non-linear activation function ReLU of the layer. □

Lemma 9. Let $\mathcal{C}$ be a class of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all $G \in \mathcal{X}^{n\times n}$, there exists $\varphi_G \in \mathcal{C}$ satisfying $\varphi_G(G^*) = \mathbb{1}_{G\simeq_{1\text{WL}}G^*}$ for all $G^* \in \mathcal{X}^{n\times n}$, then C^{+1} is universally approximating.

Proof. Let $\mathcal{C}$ be a collection of permutation invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$. For any function $\mathcal{A}$ computed by an GNN, we want to show that we can decompose it as follows for any $G^* \in \mathcal{X}^{n\times n}$:

$$\begin{aligned}
\mathcal{A}(G^*) &= \Big(\frac{1}{|\mathcal{X}^{n\times n}/\!\simeq_{1\text{WL}}(G^*)|} \sum_{G\in\mathcal{X}^{n\times n}} \mathbb{1}_{G\simeq_{1\text{WL}}G^*} \Big) \cdot \mathcal{A}(G^*) \\
&= \frac{1}{|\mathcal{X}^{n\times n}/\!\simeq_{1\text{WL}}(G^*)|} \sum_{G\in\mathcal{X}^{n\times n}} \mathcal{A}(G) \cdot \mathbb{1}_{G\simeq G^*} \\
&= \sum_{G\in\mathcal{X}^{n\times n}} \frac{\mathcal{A}(G)}{|\mathcal{X}^{n\times n}/\!\simeq_{1\text{WL}}(G^*)|} \cdot \varphi_G(G^*) \qquad (0.1)
\end{aligned}$$

with $\mathcal{X}^{n\times n}/\!\simeq_{1\text{WL}}(G^*)$ denoting the set of all graphs G over $\mathcal{X}^{n\times n}$ that are equivalent to G^* according to the $\simeq_{1\text{WL}}$ relation.

Since $\mathcal{A}$ is permutation-invariant, and GNNs are at most as good as the 1-WL algorithm in distinguishing non-isomorphic graphs, we can use the fact that for every graph $G, H \in \mathcal{X}^{n\times n}$ with $G \simeq_{1\text{WL}} H$: $\mathcal{A}(G) = \mathcal{A}(H)$. Therefore, we can decompose $\mathcal{A}$ as outlined above. We can encode this decomposition in a single MLP layer with $\frac{\mathcal{A}(G)}{|\mathcal{X}^{n\times n}/\simeq_{1\text{WL}}(G^*)|}$ being and $\varphi_G \in \mathcal{C}$ encoding the indicator function. Important to note, we can only do this since $\mathcal{X}$ is finite, making the overall sum finite and the size of $\mathcal{X}^{n\times n}/\!\simeq_{1\text{WL}}(G^*)$ well-defined.

□

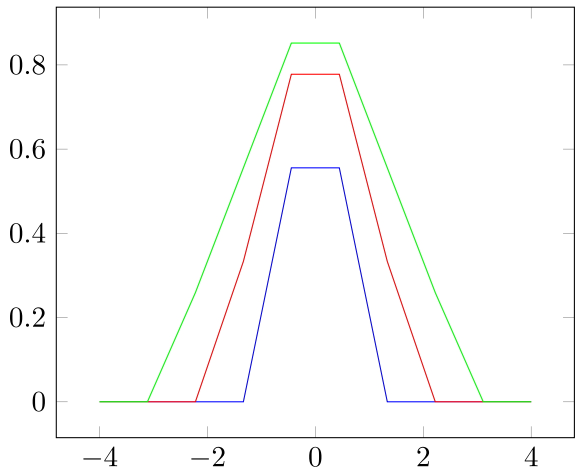

Figure 1: Illustration of the so-called “bump” function $\psi_a(x)$ with $a = 1$ in blue, $a = 2$ in red and $a = 3$ in green.