Can graph neural networks count substructures?

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Abstract

The ability to detect and count certain substructures in graphs is important for solving many tasks on graph-structured data, especially in the contexts of computational chemistry and biology as well as social network analysis. Inspired by this, we propose to study the expressive power of graph neural networks (GNNs) via their ability to count attributed graph substructures, extending recent works that examine their power in graph isomorphism testing and function approximation. We distinguish between two types of substructure counting: matching-count and containment-count, and establish both positive and negative answers for popular GNN architectures. Specifically, we prove that Message Passing Neural Networks (MPNNs), 2-Weisfeiler-Lehman (2-WL) and 2-Invariant Graph Networks (2-IGNs) cannot perform matching-count of substructures consisting of 3 or more nodes, while they can perform containment-count of star-shaped substructures. We also prove positive results for \( k \)-WL and \( k \)-IGNs as well as negative results for \( k \)-WL with limited number of iterations. We then conduct experiments that support the theoretical results for MPNNs and 2-IGNs, and demonstrate that local relational pooling strategies inspired by Murphy et al. (2019) are more effective for substructure counting. In addition, as an intermediary step, we prove that 2-WL and 2-IGNs are equivalent in distinguishing non-isomorphic graphs, partly answering an open problem raised in Maron et al. (2019a).

1 Introduction

In recent years, graph neural networks (GNNs) have achieved empirical success on processing data from various fields such as social networks, quantum chemistry, particle physics, knowledge graphs and combinatorial optimization (Scarselli et al., 2008; Bruna et al., 2013; Duvenaud et al., 2015; Kipf and Welling, 2016; Defferrard et al., 2016; Bronstein et al., 2017; Dai et al., 2017; Nowak et al., 2017; Ying et al., 2018; Zhou et al., 2018; Choma et al., 2018; Zhang and Chen, 2018; You et al., 2018a,b, 2019; Yao et al., 2019; Ding et al., 2019; Stokes et al., 2020). Thanks to such progress, there have been growing interests in studying the expressive power of GNNs. One line of work does so by studying their ability to distinguish non-isomorphic graphs. In this regard, Xu et al. (2018a) and Morris et al. (2019) show that GNNs based on neighborhood-aggregation schemes are at most as powerful as the classical Weisfeiler-Lehman (WL) test (Weisfeiler and Leman, 1968) and propose GNN architectures that can achieve such level of power. While graph isomorphism testing is very interesting from a theoretical viewpoint, one may naturally wonder how relevant it is to real-world tasks on graph-structured data. Moreover, WL is powerful enough to distinguish almost all pairs of non-isomorphic graphs except for rare counterexamples (Babai et al., 1980). Hence, from the viewpoint of graph isomorphism testing, existing GNNs are in some sense already not far from being maximally powerful, which could make the pursuit of more powerful GNNs appear unnecessary.

Another perspective is the ability of GNNs to approximate permutation-invariant functions on graphs. For instance, Maron et al. (2019c) and Keriven and Peyré (2019) propose architectures that achieve universal
approximation of permutation-invariant functions on graphs, though such models involve tensors with order growing in the size of the graph and are therefore impractical. Importantly, Chen et al. (2019b) establishes an equivalence between the ability to distinguish any pair of non-isomorphic graphs and the ability to approximate arbitrary permutation-invariant functions on graphs. Nonetheless, for GNNs used in practice, which are not universally approximating, more efforts are needed to characterize what they can and cannot do. For example, Loukas (2019) shows that GNNs under assumptions are Turing universal but loses power when its depth and width are limited, though the arguments rely on the nodes all having distinct features and the focus is on the asymptotic depth-width tradeoff. Concurrently to our work, Garg et al. (2020) provide impossibility results of several classes of GNNs to decide graph properties including girth, circumference, diameter, radius, conjoint cycle, total number of cycles, and \( k \)-cliques. Despite these interesting results, we still need a perspective for understanding the expressive power of different classes of GNNs in a way that is intuitive, relevant to goals in practice, and potentially helpful in guiding the search for more powerful architectures.

Inspired by the relevance of detecting and counting \textit{graph substructures} in applications, we propose to understand the power of GNN architectures via the substructures that they can and cannot count. Also referred to by various names including \textit{graphlets}, \textit{motifs}, \textit{subgraphs} and \textit{graph fragments}, graph substructures are well-studied and relevant for graph-related tasks in computational chemistry (Deshpande et al., 2002; Murray and Rees, 2009; Duvenaud et al., 2015; Jin et al., 2018, 2019, 2020), computational biology (Koyutürk et al., 2004) and social network studies (Jiang et al., 2010). In organic chemistry, for example, certain patterns of atoms called functional groups are usually considered indicative of the molecules’ properties (Lemke, 2003; Pope et al., 2018). In the literature of molecular chemistry, substructure counts have been used to generate molecular fingerprints (Morgan, 1965; OBoyle and Sayle, 2016) and compute similarities between molecules (Akon et al., 2008; Rahman et al., 2009). In addition, for general graphs, substructure counts have been used to create graph kernels (Shervashidze et al., 2009) and compute spectral information (Preciado and Jadbabaie, 2010). The connection between GNNs and graph substructures is explored empirically by Ying et al. (2019) as a way to interpret the predictions made by GNNs. Thus, the ability of different GNN architectures to count graph substructures not only serves as an intuitive theoretical measure of their expressive power but also is highly relevant to real-world scenarios. While people have proposed variants of GNNs that take advantage of substructure information (Monti et al., 2018; Liu et al., 2018, 2019), often they rely on handcrafting rather than learning such information. More importantly, there is a lack of a systematic theoretical study of the ability of existing GNNs to count substructures.

In this work, we first build a theoretical framework for studying the ability of GNNs to count \textit{attributed substructures} based on both function approximation and graph discrimination. In particular, we distinguish between \textit{containment-count} and \textit{matching-count}, each corresponding to having \textit{subgraphs} and \textit{induced subgraphs} isomorphic to a given pattern, respectively. Next, we look at classical GNN architectures and prove the following results.

1. Focusing on matching-count, we establish that neither Message Passing Neural Networks (MPNNs) (Gilmer et al., 2017) nor 2nd-order Invariant Graph Networks (2-IGNs) (Maron et al., 2019c) can count any connected substructure of 3 or more nodes. For any such pattern, we prove this by constructing a pair of graphs that provably cannot be distinguished by any MPNN or 2-IGN but with different matching-counts of the given pattern. This result points at an important class of simple-looking tasks that are provably hard for classical GNN architectures.

2. We show positive results for containment-count of star-shaped patterns by MPNNs and 2-IGNs, generalizing results in Arvind et al. (2018), as well as for both matching- and containment-count of size-\( k \) patterns by \( k \)-WL and \( k \)-IGNs. The latter result hints at a hierarchy of the increasing power of \( k \)-WL’s in terms of counting substructures, which would be more intuitive than the hierarchy in terms distinguishing non-isomorphic graphs as shown in Cai et al. (1992), and therefore concretely motivates the search for GNNs with higher expressive power than 2-WL or MPNN.
3. While a tight negative result for general $k$-WL is difficult to obtain, we show that $T$ iterations of $k$-WL is unable to perform matching-count for the path pattern of $(k + 1)^2T$ or more nodes. It is relevant since real-life GNNs are often shallow, and also demonstrates an interplay between $k$ and depth.

We complement these theoretical results with synthetic experiments of counting triangles and stars in random graphs. In addition, while our negative theoretical results are worst-case in nature, the experiments illustrate an average-case difficulty for classical GNNs to count even the simplest graph substructures such as triangles. On the other hand, instead of performing iterative equivariant aggregations of information as is done in MPNNs and IGs, we propose a type of locally powerful models based on the observation that substructures present themselves in local neighborhoods known as egonets. One idea is to apply the Relational Pooling approach (Murphy et al., 2019) to egonets, resulting in a model we call Local Relational Pooling. We demonstrate that it can perform both matching- and containment-count in the experiments.

2 Framework

2.1 Attributed graphs, (induced) subgraphs and two types of counting

An unattributed graph $G$ with $n$ nodes is usually denoted by $G = (V, E)$, where typically $V = [n] := \{1, ..., n\}$ is the vertex set and $E \subseteq V^2 := V \times V$ is the edge set. We define an attributed graph or weighted graph as $G = (V, E, x, e)$, where in addition to $V$ and $E$, we let $x_i \in \mathcal{X}$ represent the node feature (or node attribute) of node $i$, and $e_{ij} \in \mathcal{Y}$ represent the edge feature of edge $(i, j)$ if $(i, j) \in E$. For simplicity, we only consider undirected graphs (i.e. if $(i, j) \in E$ then $(j, i) \in E$ and $e_{ij} = e_{ji}$), and we do not allow self-connections (i.e., $(i, i) \notin E$) or multi-edges (so that $E$ is a well-defined set). Note that an unattributed graph can be viewed as an attributed graph with identical node and edge features. If a graph has only node features and no edge features, we can also represent it as $G = (V, E, x)$.

Unlike the node and edge features, the indices of the nodes are not inherent properties of the graph. Rather, different ways of ordering the nodes result in different representations of the same underlying graph. This is characterized by the definition of graph isomorphism: Two attributed graphs $G^{[1]} = (V^{[1]}, E^{[1]}, x^{[1]}, e^{[1]})$ and $G^{[2]} = (V^{[2]}, E^{[2]}, x^{[2]}, e^{[2]})$ are isomorphic if there exists a bijection $\pi : V^{[1]} \rightarrow V^{[2]}$ such that (1) $(i, j) \in E^{[1]}$ if and only if $(\pi(i), \pi(j)) \in E^{[2]}$, (2) $x^{[1]}_i = x^{[2]}_{\pi(i)}$ for all $i \in V^{[1]}$, and (3) $e^{[1]}_{ij} = e^{[2]}_{\pi(i), \pi(j)}$ for all $(i, j) \in E^{[1]}$.

Before defining substructure counting, we first need to define subgraphs and induced subgraphs. For $G = (V, E, x, e)$, a subgraph of $G$ is any graph $G^\mathcal{S} = (V^\mathcal{S}, E^\mathcal{S}, x, e)$ with $V^\mathcal{S} \subseteq V$ and $E^\mathcal{S} \subseteq E$. An induced subgraphs of $G$ is any graph $G^\mathcal{S} = (V^\mathcal{S}, E^\mathcal{S}, x, e)$ with $V^\mathcal{S} \subseteq V$ and $E^\mathcal{S} = E \cap (V^\mathcal{S})^2$. In words, the edge set of an induced subgraph needs to include all edges in $E$ that have both end points belonging to $V^\mathcal{S}$. Thus, an induced subgraph of $G$ is also its subgraph, but the converse is not true.

We now define two types of counting attributed substructures: matching and containment, illustrated in Figure 1. Let $G^\mathcal{P} = (V^\mathcal{P}, E^\mathcal{P}, x^\mathcal{P}, e^\mathcal{P})$ be a (typically smaller) graph that we refer to as a pattern or substructure. We define $\mathcal{C}(G, G^\mathcal{P})$, called the containment-count of $G^\mathcal{P}$ in $G$, to be the number of subgraphs of $G$ that are isomorphic to $G^\mathcal{P}$. We define $\mathcal{M}(G; G^\mathcal{P})$, called the matching-count of $G^\mathcal{P}$ in $G$, to be the number of induced subgraphs of $G$ that are isomorphic to $G^\mathcal{P}$. Since all induced subgraphs are subgraphs, we always have $\mathcal{M}(G; G^\mathcal{P}) \leq \mathcal{C}(G; G^\mathcal{P})$.

Moreover, on a space of graphs $\mathcal{G}$, we call $\mathcal{M}(\cdot; G^\mathcal{P})$ the matching-count function of the pattern $G^\mathcal{P}$, and $\mathcal{C}(\cdot; G^\mathcal{P})$ the containment-count function of $G^\mathcal{P}$. To formalize the probe into whether certain GNN architectures can count different substructures, a natural question to study is whether they are able to approximate the matching-count and the containment-count functions arbitrarily well. Formally, given a target function $g : \mathcal{G} \rightarrow \mathbb{R}$, and family of functions, $\mathcal{F}$, which in our case is typically the family of functions that a GNN architecture can represent, we say $\mathcal{F}$ is able to approximate $g$ on $\mathcal{G}$ if for all $\epsilon > 0$ there exists $f \in \mathcal{F}$ such
Then, \( F \) where \( L \) and \( G \) are functions.

Thus, in the context of substructure counting, we have the following observation.

Suppose some neural network \( h \) is able to distinguish \( x \) such that, if we define the function \( f \) \( \forall x \in X \), we consider an augmented family of functions \( \mathcal{F} \) such that \( f(G) \neq f(G') \) (or \( C(G^{[1]}, G^{[2]}) \neq C(G^{[1]}, G^{[2]}) \)), they can be distinguished by \( F \).

What about the converse? When the space \( \mathcal{G} \) is finite, such as if the graphs have bounded numbers of nodes and the node as well as edge features belong to finite alphabets, we can show a slightly weaker statement than the exact converse. Following Chen et al. (2019b), we define an augmentation of families of functions using feed-forward neural networks as follows:

**Definition 1.** Given \( F \), a family of functions from a space \( X \) to \( \mathbb{R} \), we consider an augmented family of functions also from \( X \) to \( \mathbb{R} \) consisting of all functions of the following form

\[
x \mapsto h_{NN}([f_1(x), \ldots, f_d(x)]),
\]

where \( d \in \mathbb{N} \), \( h_1, \ldots, h_d \in F \), and \( h_{NN} \) is a feed-forward neural network / multi-layer perceptron. When \( NN \) is restricted to have \( L \) layers at most, we denote this augmented family by \( F^{+1} \).

**Lemma 1.** Suppose \( X \) is a finite space, \( g \) is a finite function on \( X \), and \( F \) is a family of functions on \( X \). Then, \( F^{+1} \) is able to approximate \( f \) on \( \mathcal{G} \) if \( \forall x_1, x_2 \in X \) with \( g(x_1) \neq g(x_2) \), \( \exists f \in F \) such that \( f(x_1) \neq f(x_2) \).

**Proof.** Since \( X \) is a finite space, for some large enough integer \( d \), \( \exists \) a collection of \( d \) functions, \( f_1, \ldots, f_d \in F \) such that, if we define the function \( f(x) = (f_1(x), \ldots, f_d(x)) \in \mathbb{R}^d \), then it holds that \( \forall x_1, x_2 \in X, f(x_1) = f(x_2) \Rightarrow g(x_1) = g(x_2) \). (In fact, we can choose \( d \leq \frac{|X|(|X|-1)}{2} \), since in the worst case we need one \( f_i \) per pair of \( x_1, x_2 \in X \) with \( x_1 \neq x_2 \).) Then, \( \exists \) a well-defined function \( h \) from \( \mathbb{R}^d \) to \( \mathbb{R} \) such that \( \forall x \in X, g(x) = h(f(x)) \). By the universal approximation power of neural networks, \( h \) can then be approximated arbitrarily well by some neural network \( h_{NN} \).

Thus, in the context of substructure counting, we have the following observation.
Observation 2. Suppose $\mathcal{G}$ is a finite space. If $\forall G^{[1]}, G^{[2]} \in \mathcal{G}$ with $M(G^{[1]}, G^{[P]}) \neq M(G^{[2]}, G^{[P]})$ (or $C(G^{[1]}, G^{[P]}) \neq C(G^{[2]}, G^{[P]})$), $\mathcal{F}$ is able to distinguish $G^{[1]}$ and $G^{[2]}$, then $\mathcal{F}^{t+1}$ is able to approximate the matching-count (or containment-count) function of the pattern $G^{[P]}$ on $\mathcal{G}$.

For many GNN families, $\mathcal{F}^{t+1}$ in fact has the same expressive power as $\mathcal{F}$. For example, consider $\mathcal{F}_{MPNN}$, the family of all Message Passing Neural Networks on $\mathcal{G}$. $\mathcal{F}_{MPNN}$ consists of functions that run several MPNNs on the input graph in parallel and stack their outputs to pass through an MLP. However, running several MPNNs in parallel is equivalent to running one MPNN with larger dimensions of hidden states and messages, and moreover the additional MLP at the end can be merged into the readout function. Similar holds for the family of all $k$-Invariant Graph Functions ($k$-IGNs). Hence, for such GNN families, we have an exact equivalence on finite graph spaces $\mathcal{G}$.

Therefore, we define substructure counting alternatively as follows, which are equivalent thanks to the results above and easier to work with when we study particular GNN architectures:

Definition 2. We say $\mathcal{F}$ is able to perform matching-count (or containment-count) of a pattern $G^{[P]}$ on $\mathcal{G}$ if $\forall G^{[1]}, G^{[2]} \in \mathcal{G}$ such that $M(G^{[1]}, G^{[P]}) \neq M(G^{[2]}, G^{[P]})$ (or $C(G^{[1]}, G^{[P]}) \neq C(G^{[2]}, G^{[P]})$), $\mathcal{F}$ is able to distinguish $G^{[1]}$ and $G^{[2]}$.

Another benefit of this definition is that it naturally allows us to also define the ability of graph isomorphism tests to count substructures. A graph isomorphism test, such as the Weisfeiler-Lehman (WL) test, takes as input a pair of graphs and returns whether or not they are believed to be isomorphic. Typically, the test will return true if the two graphs are indeed isomorphic but does not necessarily return false for every pair of non-isomorphic graphs. Given such a graph isomorphism test, we say it is able to perform matching-count (or containment-count) of a pattern $G^{[P]}$ on $\mathcal{G}$ if $\forall G^{[1]}, G^{[2]} \in \mathcal{G}$ such that $M(G^{[1]}, G^{[P]}) \neq M(G^{[2]}, G^{[P]})$ (or $C(G^{[1]}, G^{[P]}) \neq C(G^{[2]}, G^{[P]})$), the test can tell these two graphs apart.

Additional notations used in the proofs are given in Appendix A.

3 Message Passing Neural Networks and $k$-Weisfeiler-Lehman tests

Message Passing Neural Network (MPNN) is a generic model that incorporates many popular architectures, and it is based on learning local aggregations of information in the graph (Gilmer et al., 2017). When applied to an undirected graph $G = (V, E, x, e)$, an MPNN with $T$ layers is defined iteratively as follows. For $t < T$, to compute the message $m_{i}^{(t+1)}$ and the hidden state $h_{i}^{(t+1)}$ for each node $i \in V$ at the $(t + 1)$th layer, we apply the following update rule:

$m_{i}^{(t+1)} = \sum_{N(i)} M_{i}(h_{i}^{(t)}, h_{j}^{(t)}), e_{i,j}$

$h_{i}^{(t+1)} = U_{t}(h_{i}^{(t)}, m_{i}^{(t+1)})$

where $N(i)$ is the neighborhood of node $i$ in $G$, $M_{i}$ is the message function at layer $t$ and $U_{t}$ is the vertex update function at layer $t$. Finally, a graph-level prediction is computed as

$\hat{y} = R(\{h_{i}^{(T)} : i \in V\})$,

where $R$ is the readout function. Typically, the hidden states at the first layer are set as $h_{i}^{(0)} = x_{i}$. Learnable parameters can appear in the functions $M_{i}$, $U_{t}$ (for all $t \leq T$) and $R$.

Xu et al. (2018a) and Morris et al. (2019) show that, when the graphs’ edges are unweighted, such models are at most as powerful as the Weisfeiler-Lehman (WL) test in distinguishing non-isomorphic graphs. We will prove an extension of this result that incorporates edge features, which MPNNs naturally accommodate, so that by examining the ability of 2-WL to count substructures, we can draw conclusions for MPNNs. Before that, we will first introduce the hierarchy of $k$-WL tests.
3.1 The hierarchy of \( k \)-Weisfeiler-Lehman (\( k \)-WL) tests

We will introduce the general \( k \)-WL test for \( k \in \mathbb{N}^* \) applied to a pair of graphs, \( G^{[1]} \) and \( G^{[2]} \). Assume that the two graphs have the same number of vertices, since otherwise they can be told apart easily. Without loss of generality, we assume that they share the same set of vertex indices, \( V \) (but can differ in \( E, x \) or \( e \)).

For each of the graphs, at iteration 0, the test assigns an initial color in some color space to every \( k \)-tuple in \( V^k \) according to its isomorphism type\(^1\), and then updates the coloring in every iteration. For any \( k \)-tuple \( s = (i_1, ..., i_k) \in V^k \), we let \( c_k^{(t)}(s) \) denote the color of \( s \) in \( G^{[k]} \) assigned at \( t \)th iteration, and let \( c_k^{(t)}(s) \) denote the color it receives in \( G^{[2]} \). \( c_k^{(t)}(s) \) and \( c_k^{(t)}(s) \) are updated iteratively as follows. For each \( w \in [k] \), define the neighborhood
\[
N_w(s) = \{(i_1, ..., i_{w-1}, j, i_{j+1}, ..., i_k) : j \in V\}
\]
Given \( c_k^{(t-1)} \) and \( c_k^{(t-1)} \), define
\[
C_k^{(t)}(s) = \text{HASH}_{t,1}\left(\left\{c_k^{(t-1)}(\tilde{s}) : \tilde{s} \in N_w(s)\right\}\right)
\]
\[
C_k^{(t)}(s) = \text{HASH}_{t,1}\left(\left\{c_k^{(t-1)}(\tilde{s}) : \tilde{s} \in N_w(s)\right\}\right)
\]
with \( \{\} \) representing a multiset, and \( \text{HASH}_{t,1} \) being some hash function that maps injectively from the space of multisets of colors to some intermediate space. Then let
\[
c_k^{(t)}(s) = \text{HASH}_{t,2}\left(\left(c_k^{(t-1)}(s), \left(\left(C_k^{(t)}(s), ..., C_k^{(t)}(s)\right)\right)\right)\right)
\]
\[
c_k^{(t)}(s) = \text{HASH}_{t,2}\left(\left(c_k^{(t-1)}(s), \left(\left(C_k^{(t)}(s), ..., C_k^{(t)}(s)\right)\right)\right)\right)
\]
where \( \text{HASH}_{t,2} \) maps injectively from its input space to the space of colors. The test will terminate and return the result that the two graphs are not isomorphic if at some iteration \( t \), the following two multisets differ:
\[
\{c_k^{(t)}(s) : s \in V^k\} \neq \{c_k^{(t)}(s) : s \in V^k\}
\]

Some properties of \( k \)-WL For graphs with unweighted edges, 1-WL and 2-WL are known to have the same discriminative power (Maron et al., 2019b). For \( k \geq 2 \), it is known that \( (k+1) \)-WL is strictly more powerful than \( k \)-WL, in the sense that there exist pairs of graph distinguishable by the former but not the latter (Cai et al., 1992). Thus, with growing \( k \), the set of \( k \)-WL tests forms a hierarchy with increasing discriminative power. Note that there has been an different definition of WL in the literature, sometimes known as Folklore Weisfeiler-Lehman (FWL), with different properties (Maron et al., 2019b; Morris et al., 2019). When people use the term “Weisfeiler-Lehman test” without specifying “\( k \)”, it usually refers to 1-WL, 2-WL or 1-FWL.

Extending the aforementioned results by Xu et al. (2018a); Morris et al. (2019) in a nontrivial way to incorporate edge features, we present the following theorem, to be proved in Appendix C.

**Theorem 1.** Say two graphs \( G^{[1]} \) and \( G^{[2]} \) cannot be distinguished by 2-WL. Then there is no MPNN that can distinguish them.

**Proof intuition:** If 2-WL cannot distinguish the two graphs, then at any iteration \( t \), \( \{c_k^{(t)}(s) : s \in V^2\} = \{c_k^{(t)}(s) : s \in V^2\} \). This guarantees the existence of a bijective map from pairs of nodes in \( G^{[1]} \) to pairs of nodes in \( G^{[2]} \) that preserve the coloring. Through examining the update rules of 2-WL and MPNNs, we will show by induction that for any MPNN, at the \( t \)th layer, such a map will also preserve the hidden states of the nodes involved in the pair as well as the edge feature. This implies that any MPNN with \( t \) layers will

\(^1\)We define isomorphism types rigorously in Appendix B.
Figure 2: Illustration of the construction in the proof of Theorem 2 for the pattern from Figure 1 (left). Note that $M(G^{[1]}; G^{[P]}) = 0$ whereas $M(G^{[2]}; G^{[P]}) = 2$. The graphs $G^{[1]}$ and $G^{[2]}$ are not distinguishable by MPNNs, 2-WL, or 2-IGNs.

return identical outputs when applied to the two graphs.

This result motivates us to study what patterns 2-WL can and cannot count in the next subsection.

### 3.2 Substructure counting by 2-WL and MPNNs

Whether or not 2-WL can perform matching-count of a pattern is completely characterized by the number of nodes in the pattern. Any connected pattern with 1 or 2 nodes (i.e., representing a node or an edge) can be easily counted by an MPNN with 0 and 1 layer of message-passing, respectively, or by 2-WL with 0 iteration\(^2\). In contrast, for all other patterns, we provide the following negative result, to be proved in Appendix D.

**Theorem 2.** 2-WL cannot perform matching-count of any connected pattern with 3 or more nodes.

**Proof Intuition.** Given any connected pattern of at least 3 nodes, we can construct a pair of graphs that have different matching-counts of the pattern but cannot be distinguished from each other by 2-WL. For instance, if we run 2-WL on the pair of graphs in Figure 2, then there will be $c_2^{(t)}((1,3)) = c_2^{(t)}((1,3))$, $c_2^{(t)}((1,2)) = c_2^{(t)}((1,6))$, $c_2^{(t)}((1,6)) = c_2^{(t)}((1,2))$, and so on. We can in fact show that $\{c_2^{(t)}(s) : s \in V^2\} = \{c_2^{(t)}(s) : s \in V^2\}$, $\forall t$, which implies that 2-WL cannot distinguish the two graphs.

Thus, together with Theorem 1, we have

**Corollary 1.** MPNNs cannot perform matching-count of any connected pattern with 3 or more nodes.

For containment-count, if both nodes and edges are unweighted, Arvind et al. (2018) show that the only patterns 1-WL (and equivalently 2-WL) can count are either star-shaped patterns and pairs of disjoint edges. We prove the positive result that MPNNs can count star-shaped patterns even when node and edge features are allowed, utilizing a result in Xu et al. (2018a) that the message functions are able to approximate any function on multisets.

**Theorem 3.** MPNNs can perform containment-count of star-shaped patterns.

By Theorem 1, this implies that

**Corollary 2.** 2-WL can perform containment-count of star-shaped patterns.

\(^2\)Rigorously, this is a special case of Theorem 4.
3.3 Substructure counting by $k$-WL

There have been efforts to extend the power of GNNs by going after $k$-WL for higher $k$, such as Morris et al. (2019). Thus, it is also interesting to study the patterns that $k$-WL can and cannot count. Firstly, since $k$-tuples are assigned initial colors based on their isomorphism types, the following is easily seen, and we provide a proof in Appendix F.

**Theorem 4.** $k$-WL, at initialization, is able to perform both matching-count and containment-count of patterns consisting of at most $k$ nodes.

This establishes a potential hierarchy of increasing power in terms of substructure counting by $k$-WL. However, tighter results can be much harder to achieve. For example, to show that 2-FWL (and therefore 3-WL) cannot count cycles of length 8, Fürer (2017) has to rely on performing computer counting on the classical Cai-Fürer-Immerman counterexamples to $k$-WL (Cai et al., 1992). We leave the pursuit of general and tighter characterizations of $k$-WL’s substructure counting power for future research, but we are nevertheless able to provide a partial negative result concerning finite iterations of $k$-WL.

**Definition 3.** A path pattern of size $m$, denoted by $H_m$, is an unattributed graph, $H_m = (V_{[k]}, E_{[k]})$, where $V_{[k]} = [n]$, and $E_{[k]} = \{(i, i + 1) : 1 \leq i < m\} \cup \{(i + 1, i) : 1 \leq i < m\}$.

**Theorem 5.** Running $T$ iterations of $k$-WL cannot perform matching-count of any path pattern of $(k + 1)2^T$ or more nodes.

The proof is given in Appendix G. This bound grows quickly when $T$ becomes large. However, since in practice, many if not most GNN models are designed to be shallow (Zhou et al., 2018; Wu et al., 2019), we believe this result is still relevant for studying finite-depth GNNs that are based on $k$-WL.

4 Invariant Graph Networks

Recently, diverging from the strategy of local aggregation of information as adopted by MPNNs and $k$-WLs, an alternative family of GNN models called Invariant Graph Networks (IGNs) was introduced in Maron et al. (2018, 2019c,b). Here we restate its definition.

**Definition 4.** A $k$th-order Invariant Graph Network (k-IGN) is a function $F : \mathbb{R}^{n^k \times d_0} \rightarrow \mathbb{R}$ that can be decomposed in the following way:

$$F = m \circ h \circ L^{(T)} \circ \sigma \circ \cdots \circ \sigma \circ L^{(1)},$$

where each $L^{(l)}$ is a linear equivariant layer from $\mathbb{R}^{n^k \times d_{l-1}}$ to $\mathbb{R}^{n^k \times d_l}$, $\sigma$ is a pointwise activation function, $h$ is a linear invariant layer from $\mathbb{R}^{n^k \times d_T}$ to $\mathbb{R}$, and $m$ is an MLP.

Maron et al. (2019c) show that if $k$ is allowed to grow as a function of the size of the graphs, then $k$-IGNs can achieve universal approximation of permutation-invariant functions on graphs. Nonetheless, due to the quick growth of computational complexity and implementation difficulty as $k$ increases, in practice it is hard to have $k > 2$, while if $k = 2$, it is proven to lose the universal approximation power (Chen et al., 2019b). However, it remains interesting to study what are the things that 2-IGNs are capable of doing, especially from the perspective of substructure counting. Note that the 2-IGN takes as input a third-order tensor, $B^{(0)}$, defined for a given graph $G = (V = [n], E, x, e)$ in the following way. Supposing without loss of generality that the node and edge features both have dimension $d$, we have $B^{(0)} \in \mathbb{R}^{n \times n \times (d+1)}$, such that: $\forall i \in [n], B_{i,i,2:(d+1)}^{(0)} = x_i$; $\forall i, j \in [n]$ with $i \neq j$, $B_{i,j,1}^{(0)} = A_{i,j}$ and $B_{i,j,2:(d+1)}^{(0)} = e_{i,j}$. If we use $B^{(t)}$ to denote the output of the $t$th layer of the 2-IGN, then they are obtained iteratively by

$$B^{(t+1)} = \sigma(L^{(t)}(B^{(t)}))$$

(1)
4.1 2-IGNs equivalent to 2-WL

Before studying how well 2-IGNs count substructures, we first relate it to 2-WL. It is known that 2-IGNs are at least as powerful as 2-WL, while the other direction remains an open problem (Maron et al., 2019c,a). Here we answer the question by proving the converse, that 2-IGNs are no more powerful than 2-WL. The full argument can be found in Appendix H.

Theorem 6. If two graphs \( G^{[1]} \) and \( G^{[2]} \) cannot be distinguished by the 2-WL test, then there is no 2-IGN that can distinguish them either.

Proof intuition: Given two nodes \( i, j \in V \) with \( i \neq j \), we can partition \( V^2 \) as the union of nine disjoint subsets:

- \( A_1 = \{(i, j)\} \)
- \( A_2 = \{(i, i)\} \)
- \( A_3 = \{(j, j)\} \)
- \( A_4 = \{(i, k) : k \neq i \text{ or } j\} \)
- \( A_5 = \{(k, i) : k \neq i \text{ or } j\} \)
- \( A_6 = \{(j, k) : k \neq i \text{ or } j\} \)
- \( A_7 = \{(k, j) : k \neq i \text{ or } j\} \)
- \( A_8 = \{(k, l) : k \neq l \text{ and } \{k, l\} \cap \{i, j\} = \emptyset\} \)
- \( A_9 = \{(k, k) : k \notin \{i, j\}\} \).

If 2-WL cannot distinguish the two graphs in \( t \) iterations, then there exists not only a color-preserving bijective map from pairs of nodes in \( G^{[1]} \) to pairs of nodes in \( G^{[2]} \), mapping \((i, j)\) to some \((i', j')\), but also a color-preserving bijective map from \( A_w \) to \( A'_w \) for each \( w \in [9] \), where \( A'_w \) is the corresponding subset of \( V^2 \) associated with \((i', j')\). By the update rule of 2-IGNs, this allows us to show that \( B_{i,j}^{(t)} = B'_{i',j'}^{(t)} \), and hence a \( t \)-layer 2-IGN cannot return distinct outputs when applied to the two graphs.

Corollary 3. 2-IGNs are exactly as powerful as 2-WL.

4.2 Substructure counting by 2-IGNs

Thanks to the equivalence shown above, the two following theorems are direct consequences of Theorem 2 and Corollary 2, though we also provide a direct proof of Corollary 4 in Appendix I.

Corollary 4. 2-IGNs cannot perform matching-count of any connected pattern with 3 or more nodes.

Corollary 5. 2-IGNs can perform containment-count of star-shaped patterns.

4.3 Substructure counting by \( k \)-IGNs

Since \( k \)-IGNs are no less powerful than \( k \)-WL (Maron et al., 2019b), we have as a corollary of Theorem 4 that

Corollary 6. \( k \)-IGNs can perform both matching-count and containment-count of patterns consisting of at most \( k \) nodes.

5 Local Relational Pooling

Though MPNNs and 2-IGNs are able to aggregate information from multi-hop neighborhoods, we have seen above that they are unable to preserve information such as the matching-counts of nontrivial patterns. To bypass such limitations, we suggest going beyond the strategy of iteratively aggregating information in an equivariant way, which underlies both MPNNs and IGNs. One helpful observation is that, if a pattern is present in the graph, it can always be found in a sufficiently large local neighborhood, or egonet, of some node in the graph (Preciado et al., 2012). An egonet of depth \( l \) centered at a node \( i \) is the induced subgraph consisting of \( i \) and all nodes within distance \( l \) from it. Note that any pattern with radius \( r \) is a subgraph of some egonet of depth \( l = r \). Hence, by applying a powerful local model to each egonet separately and then aggregating the outputs, we could potentially obtain a model capable of counting patterns.

For such a local model, we adopt the Relational Pooling (RP) idea from Murphy et al. (2019). In summary, it creates a powerful permutation-invariant model by symmetrizing a powerful model that is not necessarily permutation-invariant, where the symmetrization is performed by averaging or summing over all permutations.
of the nodes’ ordering. Formally, if $\mathbf{B} \in \mathbb{R}^{n \times n \times d}$ is a node-ordering-dependent representation of the graph $G$, such as the adjacency matrix or the $\mathbf{B}^{(0)}$ defined above for 2-IGNs, then define

$$f_{\text{RP}}(G) = \sum_{\pi \in S_n} \bar{f}(\pi \circ \mathbf{B}),$$

where $\bar{f}$ can be some non-permutation-invariant function, $S_n$ is the set of permutations on $n$ nodes, and $\pi \circ \mathbf{B}$ is $\mathbf{B}$ transformed by permuting its first two dimensions according to $\pi$. Such $\bar{f}$’s are shown to be an universal approximators of permutation-invariant functions (Murphy et al., 2019). The summation quickly becomes intractable once $n$ is large, and hence approximation methods have been introduced. In our case, however, since we apply this model to egonets that are usually smaller than the entire graph, the tractability issue is greatly alleviated. Moreover, since egonets are rooted graphs, we can reduce the symmetrization over all permutations in $S_n$ to the subset $S_n^{\text{BFS}} \subseteq S_n$ of permutations compatible with breath-first-search (BFS) to further reduce the complexity, as suggested in Murphy et al. (2019).

Concretely, we define $\mathbf{C}_{i,l}^{[\text{ego}]}$ as the egonet centered at node $i$ of depth $l$, $\mathbf{B}_{i,l}^{[\text{ego}]}$ as the corresponding representation and $n_{i,l}$ as the number of nodes in $\mathbf{C}_{i,l}^{[\text{ego}]}$. For computational efficiency, every tensor representation of egonet $\mathbf{B}$ is cropped into a fixed-sized subtensor $\mathbf{C}_k(\mathbf{B}) = \mathbf{B}_{[k],[k]} : \in \mathbb{R}^{k\times k \times d}$. Then our model over the entire graph $G$ is expressed as

$$f_{\text{LRP}}^{l,k}(G) = \sum_{i \in V} \sum_{\pi \in S_{n_{i,l}}^{\text{BFS}}} \bar{f}(\mathbf{C}_k(\pi \circ \mathbf{B}_{i,l}^{[\text{ego}]})),$$

We call it depth-$l$ size-$k$ Local Relational Pooling (LRP-$l$-$k$). If node degrees are upper-bounded by $D$, the time complexity is $O(n \cdot (D!)^{D'} \cdot k^2)$, and hence linear in $n$ if $D$, $k$ and $l$ are fixed. In the experiments below, we implement a variant of LRP-1-4 designed as, with bias terms ignored,

$$f_{\text{LRP}}^{1,4}(G) = W_1 \sum_{i \in V} \sigma \left[ \frac{\text{MLP}(D_i)}{|S_{n_{i,l}}^{\text{BFS}}|} \circ \sum_{\pi \in S_{n_{i,l}}^{\text{BFS}}} f_{\sigma}(\pi \circ \mathbf{B}_{i,l}^{[\text{ego}]} \right],$$

where $D_i$ is the degree of node $i$, $\sigma$ is ReLU, MLP maps from $\mathbb{R}$ to $\mathbb{R}^H$, where $H$ is the hidden dimension, $W_1 \in \mathbb{R}^{1 \times H}$ and $\forall j \in [H], (f_{\sigma}(\mathbf{X}))_j = \tanh(\sum W_{2,j} \circ C_d(\mathbf{X})) \in \mathbb{R}$ with $W_{2,j} \in \mathbb{R}^{4 \times 4 \times d}$. The motivation of MLP($D_i$) is to adaptively learn an invariant function over permutation, such as summing and averaging.

6 Experiments

Tasks. In this section, we verify our theoretical results on two graph-level regression tasks: matching-counting triangles and containment-counting 3-stars, with both patterns unattributed, as illustrated in Figure 3. By Theorem 2 and Corollary 1, MPNNs and 2-IGNs can perform matching-count of triangles. Note that since a triangle is a clique, its matching-count and containment-count are equal. We generate the ground-truth counts of triangles in each graph with an counting algorithm proposed by Shervashidze et al. (2009). By Theorem 3 and Corollary 2, MPNNs and 2-IGNs can perform containment-count though not matching-count of 3-stars. For its ground-truth count, we compute the number of stars centered at each node as $d^3$, where $d$ is the degree of each node, and then sum over all nodes in the graph.

Synthetic datasets. We generate two synthetic datasets of random unattributed graphs. The first one is a set of 5000 Erdős-Rényi random graphs denoted as $ER(m,p)$, where $m = 10$ is the number of nodes in each graph and $p = 0.3$ is the probability that an edge exists. The second one is a set of 5000 random regular graphs (Steger and Wormald, 1999) denoted as $RG(m,d)$, where $m$ is the number of nodes in each
Figure 3: Substructures to be counted in the experiments. Left: A triangle. Right: A 3-star.

graph and \( d \) is the node degree. We uniformly sample \((m, d)\) from \((\{10, 6\}, \{15, 6\}, \{20, 5\}, \{30, 5\})\). We also randomly delete \( m \) edges in each graph from the second dataset. For both datasets, we randomly split them into training-validation-test sets with percentages 30%-20%-50%.

**Models.** We consider LRP, GIN (Xu et al., 2018a), GCN (Kipf and Welling, 2016), 2-IGN (Maron et al., 2018) and spectral GNN (sGNN) (Chen et al., 2019a), with GIN and GCN belonging to the category of MPNNs. Details of GNN architectures are provided in Appendix J. We use mean squared error (MSE) for regression loss. Each model is trained on 1080ti five times with different random seeds.

**Results.** The results on the two tasks are shown in Table 1, measured by the MSE on the test set divided by the variance of the ground truth counts of the pattern computed over all graphs in the dataset. Firstly, the almost-negligible errors of LRP on all the tasks supports our theory that depth-1 LRP is powerful enough for counting triangles and 3-stars, both of which are patterns with radius 1. GIN, 2-IGN and sGNN produce much smaller test error than the variance of the ground truth counts for the 3-star tasks, consistent with their theoretical power to perform containment-count of stars. Relative to the variance of the ground truth counts, GIN and 2-IGN have worse top performance on the triangle task than on the 3-star task, also as expected from the theory. Moreover, the experiment results provide interesting insights into the average-case performance in the substructure counting tasks, which are beyond what our theory can predict at this point.

| Erdős-Renyi | Random Regular |
|-------------|----------------|
| Triangle (M) | 3-Star (C) | Triangle (M) | 3-Star (C) |
| top 1 | top 3 | top 1 | top 3 | top 1 | top 3 | top 1 | top 3 |
| LRP-1-4 | 1.56E-4 | 2.49E-4 | 2.17E-5 | 5.23E-5 | 2.47E-4 | 3.83E-4 | 1.88E-6 | 2.81E-6 |
| 2-IGN | 9.83E-2 | 9.85E-1 | 5.40E-4 | 5.12E-2 | 2.62E-1 | 5.96E-1 | 1.19E-2 | 3.28E-1 |
| GIN | 1.23E-1 | 1.25E-1 | 1.62E-4 | 3.44E-4 | 4.70E-1 | 4.74E-1 | 3.73E-4 | 4.65E-4 |
| GCN | 6.78E-1 | 8.27E-1 | 4.36E-1 | 4.55E-1 | 1.82 | 2.05 | 2.63 | 2.80 |
| sGNN | 9.25E-2 | 1.13E-1 | 2.36E-3 | 7.73E-3 | 3.92E-1 | 4.43E-1 | 2.37E-2 | 1.41E-1 |

**Table 1: Performance of different GNNs on matching-counting triangles and containment-counting 3-stars on the two datasets, measured by test MSE divided by variance of the ground truth counts. Shown here are the best and the median performances of each model over five runs. Note that we select the best out of four variants for each of GCN, GIN and sGNN, and the better out of two variants for 2-IGN. Details of the GNN architectures and raw results can be found in Appendices J, K.**

**7 Conclusions**

We propose a theoretical framework to study the expressive power of classes of GNNs based on their ability to count substructures. We distinguish two kinds of counting: containment-count (counting subgraphs) and matching-count (counting induced subgraphs). We prove that neither MPNNs nor 2-IGNs can matching-count any connected structure with 3 or more nodes; \( k \)-IGNs and \( k \)-WL can containment-count and matching-count...
any pattern of size \( k \). We also provide an upper bound on the size of “path-shaped” substructures that finite iterations of \( k \)-WL can matching-count. To establish these results, we prove an equivalence between approximating graph functions and discriminating graphs. Also, as intermediary results, we prove that MPNNs are no more powerful than 2-WL on attributed graphs, and that 2-IGNs are equivalent to 2-WL in distinguishing non-isomorphic graphs, which partly answers an open problem raised in Maron et al. (2019a). In addition, we perform numerical experiments that support our theoretical results and show that the Local Relational Pooling approach inspired by Murphy et al. (2019) can successfully count certain substructures. In summary, we build the foundation for using substructure counting as an intuitive and relevant measure of the expressive power of GNNs, and our concrete results for existing GNNs motivate the search for more powerful designs of GNNs.

One limitation of our theory is that it only pertains to the expressive power of GNNs and does not speak about optimization or generalization. In addition, our theoretical results are worse-case in nature and cannot predict average-case performance, which is interesting to study as well. Nonetheless, even within this new framework, many interesting questions remain, including better characterizing the ability to count substructures of general \( k \)-WL and \( k \)-IGNs as well as other architectures such as spectral GNNs (Chen et al., 2019a) and polynomial IGNs (Maron et al., 2019a). Another interesting future direction is to study the relevance of substructure counting in empirical tasks, following the work of Ying et al. (2019). Finally, we hope our framework can help guide the search for more powerful GNNs by having substructure counting as a criterion.

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A Additional notations

For two positive integers $a$ and $b$, we define $\text{MOD}_a(b)$ to be $a$ if $a$ divides $b$ and the number $c$ such that $b \equiv c \pmod{a}$ otherwise. Hence the value ranges from 1 to $a$ as we vary $b \in \mathbb{N}^*$.

For a positive integer $c$, let $[c]$ denote the set $\{1, \ldots, c\}$.

Two $k$-tuples, $(i_1, \ldots, i_k), (j_1, \ldots, j_k) \in V^k$ are said to be in the same equivalent class if $\exists \pi$ a permutation $\pi$ on $V$ such that $(\pi(i_1), \ldots, \pi(i_k)) = (j_1, \ldots, j_k)$. Note that belonging to the same equivalence class is a weaker condition than having the same isomorphism type, as will be defined in Appendix B, which has to do with what the graphs look like.

For any $k$-tuple, $s = (i_1, \ldots, i_k)$, and for $w \in [k]$, use $s_i$ to denote the $i$th entry of $s$.

B Isomorphism types of $k$-tuples in $k$-WL for attributed graphs

Say $G^{[1]} = (V^{[1]}, E^{[1]}, x^{[1]}, e^{[1]})$, $G^{[2]} = (V^{[2]}, E^{[2]}, x^{[2]}, e^{[2]})$.

a) $\forall s = (i_1, \ldots, i_k), s' = (i'_1, \ldots, i'_k) \in (V^{[1]})^k$, $s$ and $s'$ are said to have the same isomorphism type if
   1. $\forall \alpha, \beta \in [k], i_\alpha = i_\beta \Leftrightarrow i'_\alpha = i'_\beta$
   2. $\forall \alpha \in [k], x^{[1]}_{i_\alpha} = x^{[1]}_{i'_\alpha}$
   3. $\forall \alpha, \beta \in [k], (i_\alpha, i_\beta) \in E^{[1]} \Leftrightarrow (i'_\alpha, i'_\beta) \in E^{[1]}$, and moreover, if either side is true, then $e^{[1]}_{i_\alpha, i_\beta} = e^{[1]}_{i'_\alpha, i'_\beta}$

b) Similar if both $s, s' \in (V^{[2]})^k$.

c) $\forall s = (i_1, \ldots, i_k) \in (V^{[1]})^k$, $s' = (i'_1, \ldots, i'_k) \in (V^{[2]})^k$, $s$ and $s'$ are said to have the same isomorphism type if
   1. $\forall \alpha, \beta \in [k], i_\alpha = i_\beta \Leftrightarrow i'_\alpha = i'_\beta$
   2. $\forall \alpha \in [k], x^{[2]}_{i_\alpha} = x^{[2]}_{i'_\alpha}$
   3. $\forall \alpha, \beta \in [k], (i_\alpha, i_\beta) \in E^{[1]} \Leftrightarrow (i'_\alpha, i'_\beta) \in E^{[2]}$, and moreover, if either side is true, then $e^{[1]}_{i_\alpha, i_\beta} = e^{[2]}_{i'_\alpha, i'_\beta}$

In $k$-WL tests, two $k$-tuples $s$ and $s'$ in either $(V^{[1]})^k$ or $(V^{[2]})^k$ are assigned the same color at iteration 0 if and only if they have the same isomorphism type.

For a reference, see Maron et al. (2019b).

C Proof of Theorem 1 (MPNNs are no more powerful than 2-WL)

Proof. Suppose for contradiction that there exists an MPNN with $T_0$ layers that can distinguish the two graphs. Let $m^{(t)}$ and $h^{(t)}$, $m'^{(t)}$ and $h'^{(t)}$ be the messages and hidden states at layer $t$ obtained by applying the MPNN on the two graphs, respectively. Define

$$
\tilde{h}^{(t)}_{i,j} = \begin{cases} 
    h^{(t)}_{i,j} & \text{if } i = j \\
    h^{(t)}_{i,j}, a_{i,j}, e_{i,j} & \text{otherwise}
\end{cases}
$$

$$
\tilde{h}'^{(t)}_{i,j} = \begin{cases} 
    h'^{(t)}_{i,j} & \text{if } i = j \\
    h'^{(t)}_{i,j}, a'_{i,j}, e'_{i,j} & \text{otherwise}
\end{cases}
$$

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where \( a_{i,j} = 1 \) if \((i, j) \in E^{(1)}\) and 0 otherwise, \( e_{i,j} = e^{(1)}_{i,j} \) is the edge feature of the first graph, and \( a', e' \) are defined similarly for the second graph.

Since the two graphs cannot be distinguished by 2-WL, then for the \( T_0 \)th iteration, there is

\[
\{ c^{(T_0)}_2(s) : s \in V^2 \} = \{ c'^{(T_0)}_2(s) : s \in V^2 \},
\]

which implies that there exists a permutation on \( V^2 \), which we can call \( \eta_0 \), such that \( \forall s \in V^2 \), there is \( c^{(T_0)}_2(s) = c'^{(T_0)}_2(\eta_0(s)) \). To take advantage of this condition, we introduce the following lemma, which is central to the proof.

**Lemma 2.** \( \forall t \leq T_0, \forall i, j, i', j' \in V, \) if \( c^{(t)}_2((i, j)) = c'^{(t)}_2((i', j')) \), then

1. \( i = j \iff i' = j' \).
2. \( \tilde{h}^{(t)}_{i,j} = \tilde{h}^{(t)}_{i',j'} \).

**Proof of Lemma 2:** First, we state the following simple observation without proof, which is immediate given the update rule of k-WL:

**Lemma 3.** For k-WL, \( \forall s, s' \in V^k \), if for some \( t_0 \), \( c^{(t_0)}_k(s) = c^{(t_0)}_k(s') \), then \( \forall t \in [0, t_0], c^{(t)}_k(s) = c^{(t)}_k(s') \).

For the first condition, assuming \( c^{(t)}_2((i, j)) = c'^{(t)}_2((i', j')) \), Lemma 3 then tells us that \( c^{(0)}_2((i, j)) = c'^{(0)}_2((i', j')) \). Since the colors in 2-WL are initialized by the isomorphism type of the node pair, it has to be that \( i = j \iff i' = j' \).

We will prove the second condition by induction on \( t \). For the base case, \( t = 0 \), we want to show that \( \forall i, j, i', j' \in V \), if \( c^{(0)}_2((i, j)) = c'^{(0)}_2((i', j')) \) then \( \tilde{h}^{(0)}_{i,j} = \tilde{h}^{(0)}_{i',j'} \). If \( i = j \), then \( c^{(0)}_2((i, i)) = c'^{(0)}_2((i', i')) \) if and only if \( x_i = x'_i \), which is equivalent to \( h^{(0)}_{i,j} = h^{(0)}_{i',j'} \), and hence \( \tilde{h}^{(0)}_{i,j} = \tilde{h}^{(0)}_{i',j'} \). If \( i \neq j \), then by the definition of isomorphism types given in Appendix B, \( c^{(0)}_2((i, j)) = c'^{(0)}_2((i', j')) \) implies that

- \( x_i = x'_i \Rightarrow h^{(0)}_{i,j} = h^{(0)}_{i',j'} \)
- \( x_j = x'_j \Rightarrow h^{(0)}_{i,j} = h^{(0)}_{i',j'} \)
- \( a_{i,j} = a'_{i',j'} \)
- \( e_{i,j} = e'_{i',j'} \)

which yields \( \tilde{h}^{(0)}_{i,j} = \tilde{h}^{(0)}_{i',j'} \).

Next, to prove the inductive step, assume that for some \( T \in [T_0] \), the statement in Lemma 2 holds for all \( t \leq T - 1 \), and consider \( \forall i, j, i', j' \in V \) such that \( c^{(T)}_2((i, j)) = c'^{(T)}_2((i', j')) \). By the update rule of 2-WL, this implies that

\[
\begin{align*}
\{ c^{(T-1)}_2((i, j)) : i \in V \} & = \{ c'^{(T-1)}_2((i', j')) : i \in V \} \\
\{ c^{(T-1)}_2((k, j)) : k \in V \} & = \{ c'^{(T-1)}_2((k, j')) : k \in V \} \\
\{ c^{(T-1)}_2((i, k)) : k \in V \} & = \{ c'^{(T-1)}_2((i', k)) : k \in V \}
\end{align*}
\]

The first condition, thanks to the inductive hypothesis, implies that \( \tilde{h}^{(T-1)}_{i,j} = \tilde{h}^{(T-1)}_{i',j'} \). In particular, if \( i \neq j \), then we have

\[
\begin{align*}
a_{i,j} &= a'_{i',j'} \\
e_{i,j} &= e'_{i',j'}
\end{align*}
\]
The third condition implies that \( \exists \) a permutation on \( V \), which we can call \( \xi_{i,i'} \), such that \( \forall k \in V, \)
\[
e_2^{(T-1)}((i,k)) = e_2^{(T-1)}((i',\xi_{i,i'}(k)))
\]
By the inductive hypothesis, there is \( \forall k \in V, \)
\[
\hat{h}_{i,k}^{(T-1)} = \hat{h}_{i',\xi_{i,i'}(k)}^{(T-1)}
\]
and moreover, \( \xi_{i,i'}(k) = i' \) if and only if \( k = i \). For \( k \neq i \), we thus have
\[
h_{i}^{(T-1)} = h_{i'}^{(T-1)}
\]
\[
h_{k}^{(T-1)} = h_{\xi_{i,i'}(k)}^{(T-1)}
\]
\[
a_{i,k} = a_{i',\xi_{i,i'}(k)}
\]
\[
e_{i,k} = e_{i',\xi_{i,i'}(k)}
\]
Now, looking at the update rule at the \( T \)th layer of the MPNN,
\[
m_i^{(T)} = \sum_{k \in N(i)} M_T(h_i^{(T-1)}, h_k^{(T-1)}, e_{i,k})
\]
\[
= \sum_{k \in V} a_{i,k} \cdot M_T(h_i^{(T-1)}, h_k^{(T-1)}, e_{i,k})
\]
\[
= \sum_{k \in V} a_{i',\xi_{i,i'}(k)} \cdot M_T(h_{i'}^{(T-1)}, h_k^{(T-1)}, e_{i',\xi_{i,i'}(k)})
\]
\[
= \sum_{k' \in V} a_{i',k'} \cdot M_T(h_{i'}^{(T-1)}, h_k^{(T-1)}, e_{i',k'})
\]
\[
= m_{i'}^{(T)}
\]
where between the third and the fourth line we made the substitution \( k' = \xi_{i,i'}(k) \). Therefore,
\[
h_i^{(T)} = U_t(h_i^{(T-1)}, m_i^{(T)})
\]
\[
= U_t(h_{i'}^{(T-1)}, m_{i'}^{(T)})
\]
\[
= h_{i'}^{(T)}
\]
By the symmetry between \( i \) and \( j \), we can also show that \( h_j^{(T)} = h_{j'}^{(T)} \). Hence, together with 3, we can conclude that
\[
\hat{h}_{i,j}^{(T)} = \hat{h}_{i',j'}^{(T)}
\]
which proves the lemma. \( \square \)

Thus, the second result of this lemma tells us that \( \forall i,j \in V^2, \hat{\hat{h}}_{i,j}^{(T_{h_{0}})} = \hat{\hat{h}}_{\tau_{0}(i,j)}^{(T_{h_{0}})} \). Moreover, by the first result, \( \exists \) a permutation on \( V \), which we can call \( \tau_0 \), such that \( \forall i \in V, \eta((i,i)) = (\tau_0(i),\tau_0(i)) \). Combining the two, we have that \( \forall i \in V, h_i^{(T_{h_{0}})} = h_{\tau_{0}(i)}^{(T_{h_{0}})} \), and hence
\[
\{h_i^{(T_{h_{0}})} : i \in V \} = \{h_{i'}^{(T_{h_{0}})} : i' \in V \}
\]
Therefore, \( \hat{\hat{g}} = \hat{\hat{g}}' \), meaning that the MPNN returns identical outputs on the two graphs. \( \square \)
Proof of Theorem 2 (2-WL is unable to matching-count patterns of 3 or more nodes)

Proof. Say $G^{[p]} = (V^{[p]}, E^{[p]}, x^{[p]}, e^{[p]})$ is a connected pattern of $m$ nodes, where $m > 2$, and thus $V^{[p]} = [m]$. If $G^{[p]}$ is not a clique, then by definition, there exists two distinct nodes $i, j \in V^{[p]}$ such that $i$ and $j$ are not connected by an edge. Assume without loss of generality that $i = 1$ and $j = 2$. Now, construct two graphs $G^{[1]} = (V = [2m], E^{[1]}, x^{[1]}, e^{[1]})$, $G^{[2]} = (V = [2m], E^{[2]}, x^{[2]}, e^{[2]})$ both with $2m$ nodes. For $G^{[1]}$, let $E^{[1]} = \{(i, j) : i, j \leq m, (i, j) \in E^{[p]} \} \cup \{(i + m, j + m) : i, j \leq m, (i, j) \in E^{[p]} \} \cup \{(1, 2), (2, 1), (1 + m, 2 + m), (2 + m, 1 + m)\}$; $\forall i \leq m, x^{[1]}_i = x^{[p]}_i; \forall (i, j) \in E^{[p]}, e^{[1]}_{ij} = e^{[p]}_{ij}$, and moreover we can randomly choose a value of edge feature for $e^{[1]}_{1,2} = e^{[1]}_{2,1} = e^{[1]}_{1+m,2+m} = e^{[1]}_{2+m,1+m}$. For $G^{[2]}$, let $E^{[2]} = \{(i, j) : i, j \leq m, (i, j) \in E^{[p]} \} \cup \{(i + m, j + m) : i, j \leq m, (i, j) \in E^{[p]} \} \cup \{(1, 2 + m), (2 + m, 1), (1 + m, 2), (2, 1 + m)\}$; $\forall i \leq m, x^{[2]}_i = x^{[p]}_i; \forall (i, j) \in E^{[p]}, e^{[2]}_{ij} = e^{[2]}_{i+j+m} = e^{[p]}_{ij}$, and moreover we let $e^{[2]}_{1,2} = e^{[2]}_{1,2+m} = e^{[2]}_{2,1+m} = e^{[2]}_{1,2+m}$. In words, both $G^{[1]}$ and $G^{[2]}$ are constructed based on two copies of $G^{[p]}$, and the difference is that, $G^{[1]}$ adds the edges $\{(1, 2), (2, 1), (1 + m, 2 + m), (2 + m, 1 + m)\}$, whereas $G^{[2]}$ adds the edges $\{(1, 2), (1, 2 + m), (2 + m, 1), (1 + m, 2), (2, 1 + m)\}$, all with the same edge feature.

On one hand, by construction, 2-WL will not be able to distinguish $G^{[1]}$ from $G^{[2]}$. This is intuitive if we compare the rooted subtrees in the two graphs, as there exists a bijection from $V^{[1]}$ to $V^{[2]}$ that preserves the rooted subtree structure. A rigorous proof is given at the end of this section. In addition, we note that this is also consequence of the direct proof of Corollary 4 given in Appendix I, in which we will show that the same pair of graphs cannot be distinguished by 2-IGNs. Since 2-IGNs are no less powerful than 2-WL (Maron et al., 2019b), this implies that 2-WL cannot distinguish them either.

On the other hand, $G^{[1]}$ and $G^{[2]}$ has different matching-count of the pattern. $G^{[1]}$ contains no subgraph isomorphic to $G^{[p]}$. Intuitively this is obvious; to be rigorous, note that firstly, neither the subgraph induced by the nodes $\{1, \ldots, m\}$ nor the subgraph induced by the nodes $\{1 + m, \ldots, 2m\}$ is isomorphic to $G^{[p]}$, and secondly, the subgraph induced by any other set of $m$ nodes is not connected, whereas $G^{[p]}$ is connected. $G^{[2]}$, however, has at least two induced subgraphs isomorphic to $G^{[p]}$, one induced by the nodes $\{1, \ldots, m\}$, and the other induced by the nodes $\{1 + m, \ldots, 2m\}$.

If $G^{[p]}$ is a clique, then we also first construct $G^{[1]}$, $G^{[2]}$ from $G^{[p]}$ as two copies of $G^{[p]}$. Then, for $G^{[1]}$, we pick two distinct nodes $1, 2 \in V^{[p]}$ and remove the edges $(1, 2), (2, 1), (1 + m, 2 + m)$ and $(2 + m, 1 + m)$ from $V^{[1]}$, while adding edges $(1, 2 + m), (2 + m, 1), (1 + m, 2), (2, 1 + m)$ with the same edge features. Then, $G^{[1]}$ contains no subgraph isomorphic to $G^{[p]}$, while $G^{[2]}$ contains two. Note that the pair of graphs is the same as the counterexample pair of graphs that could have been constructed in the non-clique case for the pattern that is a clique with one edge deleted. Hence 2-WL still cant distinguish $G^{[1]}$ from $G^{[2]}$.

Proof of 2-WL failing to distinguish $G^{[1]}$ and $G^{[2]}$:

To show that 2-WL cannot distinguish $G^{[1]}$ from $G^{[2]}$, we need to show that if we run 2-WL on the two graphs, then $V T, \{e^{(T)}(i, j) : i, j \in V \} = \{e^{(T)}(i, j) : i, j \in V \}$. For this to hold, it is sufficient to find a bijective map $\eta : V^2 \rightarrow V^2$ such that $e^{(T)}(i, j) = e^{(T)}(\eta(i, j))$, $\forall i, j \in V$. First, we define a set $S = \{(1, 2), (2, 1), (1 + m, 2 + m), (2 + m, 1 + m), (1, 2 + m), (2 + m, 1), (1 + m, 2), (2, 1 + m)\}$, which represents the “special” pairs of nodes that capture the difference between $G^{[1]}$ and $G^{[2]}$. Then we can define $\eta : V^2 \rightarrow V^2$ as

$\eta(i, j) = \begin{cases} (i, j), & \text{if } (i, j) \notin S \\ (i, \text{MOD}_{2m}(j + m)), & \text{if } (i, j) \in S \end{cases}$
Note that \( \eta \) is a bijective. It is easy to verify that \( \eta \) is a color-preserving map between node pairs in \( G^{[1]} \) and node pairs in \( G^{[2]} \) at initialization, i.e. \( c^{(0)}((i,j)) = c^{(0)}(\eta((i,j))), \forall i, j \in V \). We will prove by induction that in fact it remains such a color-preserving map at any iteration \( T \). The inductive step that we need to prove is,

**Lemma 4.** For any positive integer \( t \), supposing that \( c^{(t-1)}((i,j)) = c^{(t-1)}(\eta((i,j))), \forall i,j \in V \), then we also have \( c^{(t)}((i,j)) = c^{(t)}(\eta((i,j))), \forall i,j \in V \).

**Proof of Lemma 4:** By the update rule of 2-WL, \( \forall i,j \in V \), to show that \( c^{(t)}((i,j)) = c^{(t)}(\eta((i,j))) \), we need to establish three conditions:

\[
eq c^{(t-1)}((i,j)) = c^{(t-1)}(\eta((i,j)))
\]

\[
\{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i,j))\} = \{c^{(t-1)}(\eta(\tilde{s})) : \tilde{s} \in N_1(\eta((i,j)))\}
\]

\[
\{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i,j))\} = \{c^{(t-1)}(\eta(\tilde{s})) : \tilde{s} \in N_2(\eta((i,j)))\}
\]

The first condition is already guaranteed by the inductive hypothesis. Now we prove the last two conditions by examining different cases separately below.

**Case 1** \( i,j \notin \{1,2,1+m,2+m\} \)

Then \( \eta((i,j)) = (i,j) \), and \( N_1((i,j)) \cap S = \emptyset, N_2((i,j)) \cap S = \emptyset \). Therefore, \( \eta \) restricted to \( N_1((i,j)) \) or \( N_2((i,j)) \) is the identity map, and thus

\[
\{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i,j))\} = \{c^{(t-1)}(\eta(\tilde{s})) : \tilde{s} \in N_1(\eta((i,j)))\}
\]

\[
= \{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2(\eta((i,j)))\},
\]

thanks to the inductive hypothesis. Similar for the condition (7).

**Case 2** \( i \in \{1,1+m\}, j \notin \{1,2,1+m,2+m\} \)

Then \( \eta((i,j)) = (i,j) \), \( N_2((i,j)) \cap S = \{(i,2),(i,2+m)\} \), and \( N_1((i,j)) \cap S = \emptyset \). To show condition (7), note that \( \eta \) is the identity map when restricted to \( N_2((i,j)) \) \( \backslash \{(i,2),(i,2+m)\} \), and hence

\[
\{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i,j)) \backslash \{(i,2),(i,2+m)\}\} = \{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2(\eta((i,j))) \backslash \{(i,2),(i,2+m)\}\}
\]

Moreover, \( \eta((i,2)) = (i,2+m) \) and \( \eta((i,2+m)) = (i,2) \). Hence, by the inductive hypothesis, \( c^{(t-1)}((i,2)) = c^{(t-1)}((i,2+m)) \) and \( c^{(t-1)}((i,2+m)) = c^{(t-1)}((i,2)) \). Therefore,

\[
\{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i,j))\} = \{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2(\eta((i,j)))\}
\]

\[
= \{c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2(\eta((i,j)))\},
\]

which shows condition (7). Condition (6) is easily seen as \( \eta \) restricted to \( N_1((i,j)) \) is the identity map.

**Case 3** \( j \in \{1,1+m\}, i \notin \{1,2,1+m,2+m\} \)

There is \( \eta((i,j)) = (i,j) \), \( N_1((i,j)) \cap S = \{(2,j),(2+m,j)\} \), and \( N_2((i,j)) \cap S = \emptyset \). Hence the proof can be carried out analogously to case 2.

**Case 4** \( i \in \{2,2+m\}, j \notin \{1,2,1+m,2+m\} \)

There is \( \eta((i,j)) = (i,j) \), \( N_2((i,j)) \cap S = \{(i,1),(i,1+m)\} \), and \( N_1((i,j)) \cap S = \emptyset \). Hence the proof can be carried out analogously to case 2.

**Case 5** \( j \in \{2,2+m\}, i \notin \{1,2,1+m,2+m\} \)

There is \( \eta((i,j)) = (i,j) \), \( N_1((i,j)) \cap S = \{(1,j),(1+m,j)\} \), and \( N_2((i,j)) \cap S = \emptyset \). Hence the proof can be carried out analogously to case 2.
Case 6 \((i, j) \in S\)

There is \(\eta((i, j)) = (i, \text{MOD}_2m(j)), N_1((i, j)) \cap S = \{(i, j), (\text{MOD}_2m(i), j)\}, N_2((i, j)) \cap S = \{(i, j), (i, \text{MOD}_2m(j))\}\).

Thus, \(N_1(\eta((i, j))) = N_1((i, \text{MOD}_2m(j))), N_2(\eta((i, j))) = N_2((i, \text{MOD}_2m(j))) = N_2((i, j))\). Once again, \(\eta\) is the identity map when restricted to \(N_1((i, j)) \setminus S\) or \(N_2((i, j)) \setminus S\). Hence, by the inductive hypothesis, there is

\[
\{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i, j)) \setminus \{(i, j), (\text{MOD}_2m(i), j)\} \}
\]

\[
\{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i, j)) \setminus \{(i, j), (i, \text{MOD}_2m(j))\} \}
\]

Also from the inductive hypothesis, we have

\[
c^{(t-1)}((i, j)) = c^{(t-1)}(\eta((i, j))) = c^{(t-1)}((i, \text{MOD}_2m(j))), \tag{8}
\]

\[
c^{(t-1)}((i, j)) = c^{(t-1)}((j, i)) = c^{(t-1)}(\eta((j, i))) = c^{(t-1)}((j, \text{MOD}_2m(i))) = c^{(t-1)}((\text{MOD}_2m(i), j)), \tag{9}
\]

\[
c^{(t-1)}((i, \text{MOD}_2m(j))) = c^{(t-1)}(\eta((i, \text{MOD}_2m(j)))) = c^{(t-1)}((i, \text{MOD}_2m(\text{MOD}_2m(j)))) = c^{(t-1)}((i, j)), \tag{10}
\]

\[
c^{(t-1)}((\text{MOD}_2m(i), j)) = c^{(t-1)}((j, \text{MOD}_2m(i))) = c^{(t-1)}(\eta((j, \text{MOD}_2m(i)))) = c^{(t-1)}((j, \text{MOD}_2m(\text{MOD}_2m(i)))) = c^{(t-1)}((j, i)) = c^{(t-1)}((i, j)), \tag{11}
\]

where in (9) and (11), the first and the last equalities are thanks to the symmetry of the coloring between any pair of nodes \((i', j')\) and its “reversed” version \((j', i')\), which persists throughout all iterations, as well as the fact that if \((i', j') \in S\), then \((j', i') \in S\). Therefore, we now have

\[
\{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i, j)) \} = \{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i, j)) \} \tag{12}
\]

\[
\{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i, j)) \} = \{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_2((i, j)) \} \tag{13}
\]

Since \(\eta((i, j)) = (i, \text{MOD}_2m(j))\), we have

\[
N_1(\eta((i, j))) = \{(k, \text{MOD}_2m(j)) : k \in V\}
\]

\[
= \{(k, \text{MOD}_2m(j)) : (\text{MOD}_2m(k), j) \in N_1((i, j))\}
\]

\[
= \{(\text{MOD}_2m(k), \text{MOD}_2m(j)) : (k, j) \in N_1((i, j))\}
\]

Thanks to the symmetry of the coloring under the map \((i', j') \mapsto (\text{MOD}_2m(i'), \text{MOD}_2m(j'))\), we then have

\[
\{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1(\eta((i, j))) \} = \{ c^{(t-1)}((\text{MOD}_2m(k), \text{MOD}_2m(j))) : (k, j) \in N_1((i, j)) \}
\]

\[
= \{ c^{(t-1)}((k, j)) : (k, j) \in N_1((i, j)) \}
\]

\[
= \{ c^{(t-1)}(\tilde{s}) : \tilde{s} \in N_1((i, j)) \}
\]

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Therefore, combined with (12), we see that (6) is proved. (7) is a straightforward consequence of (13), since \( N_2((i, j)) = N_2(\eta((i, j))) \).

Case 7 \( i, j \in [1, 1 + m] \)

There is \( \eta((i, j)) = (i, j) \), \( N_2((i, j)) \cap S = \{(i, 2), (i, 2 + m)\} \), and \( N_1((i, j)) \cap S = \{(2, j), (2 + m, j)\} \). Thus, both (6) and (7) can be proved analogously to how (7) is proved for case 2.

Case 8 \( i, j \in \{2, 2 + m\} \)

There is \( \eta((i, j)) = (i, j) \), \( N_2((i, j)) \cap S = \{(i, 1), (i, 1 + m)\} \), and \( N_1((i, j)) \cap S = \{(1, j), (1 + m, j)\} \). Thus, both (6) and (7) can be proved analogously to how (7) is proved for case 2.

With conditions (6) and (7) shown for all pairs of \((i, j)\) \(\in V^2\), we know that by the update rules of 2-WL, there is \( c^{(t)}((i, j)) = c^{(t)}(\eta((i, j))), \forall i, j \in V \).

With Lemma 4 justifying the inductive step, we see that for any positive integer \( T \), there is \( c^{(T)}((i, j)) = c^{(T)}(\eta((i, j))), \forall i, j \in V \). Hence, we can conclude that \( \forall T, \{c^{(T)}((i, j)) : i, j \in V\} = \{c^{(T)}((i, j)) : i, j \in V\} \), which implies that the two graphs cannot be distinguished by 2-WL.

\( \square \)

E Proof of Theorem 3 (MPNNs are able to containment-count star-shaped patterns)

(See Section 2.1 of Arvind et al. (2018) for a proof for the case where all nodes have identical features.)

\( \textbf{Proof.} \) Without loss of generality, we represent a star-shaped pattern by \( G^{[p]} = (V^{[p]}, E^{[p]}, x^{[p]}, e^{[p]}) \), where \( V^{[p]} = [m] \) (with node 1 representing the center) and \( E^{[p]} = \{(1, i) : 2 \leq i \leq m\} \cup \{(i, 1) : 2 \leq i \leq m\} \).

Given a graph \( G \), for each of its node \( j \), we define \( N(j) \) as the set of its neighbors in the graph. Then the neighborhood centered at \( j \) contributes to \( C_C(G, G^{[p]}) \) if and only if \( x_j = x_1^{[p]} \) and \( \exists S \subseteq N(j) \) such that the multiset \( \{(x_k, e_{jk}) : k \in S\} \) equals the multiset \( \{(x_k^{[p]}, e_{1k}^{[p]}) : 2 \leq k \leq m\} \). Moreover, the contribution to the number \( C_C(G, G^{[p]}) \) equals the number of all such subsets \( S \subseteq N(j) \). Hence, we have the following decomposition

\[
C_C(G, G^{[p]}) = \sum_{j \in V} f^{[p]}(x_j, \{(x_k, e_{jk}) : k \in N(j)\}),
\]

where \( f^{[p]} \), is defined for every 2-tuple consisting of a node feature and a multiset of pairs of node feature and edge feature (i.e., objects of the form \( \{(x_\alpha, e_\alpha) : \alpha \in K\} \)) as

\[
f^{[p]}(x, M) = \begin{cases} 0 & \text{if } x \neq x_1^{[p]} \#[p]_M \\
\#[p]_M & \text{if } x = x_1^{[p]} \#[p]_M \end{cases}
\]

where \( \#[p]_M \) denotes the number of sub-multisets of \( M \) that equals the multiset \( \{(x_k^{[p]}, e_{1k}^{[p]}) : 2 \leq k \leq m\} \).

Thanks to Corollary 6 of Xu et al. (2018a) based on Zaheer et al. (2017), we know that \( f^{[p]} \) can be expressed by some message-passing function in an MPNN. Thus, together with summation as the readout function, MPNN is able to express \( C_C(G, G^{[p]}) \).

\( \square \)
F  Proof of Theorem 4 (k-WL is able to count patterns of k or fewer nodes)

Proof. Suppose we run k-WL on two graphs, $G^{[1]}$ and $G^{[2]}$. In k-WL, the colorings of the k-tuples are initialized according to their isomorphism types as defined in Appendix B. Thus, if for some pattern of no more than k nodes, $G^{[1]}$ and $G^{[2]}$ have different matching-count or containment-count, then there exists an isomorphism type of k-tuples such that $G^{[1]}$ and $G^{[2]}$ differ in the number of k-tuples under this type. This implies that \( \{c_k^{(0)}(s) : s \in (V^{[1]})^k\} \neq \{c_k^{(0)}(s') : s' \in (V^{[2]})^k\} \), and hence the two graphs can be distinguished at the 0th iteration of k-WL.

G  Proof of Theorem 5 (T iterations of k-WL cannot matching-count path patterns of size \((k+1)^2 \) or more)

Proof. For any integer $m \geq (k+1)^2$, we will construct two graphs $G^{[1]} = (V^{[1]} = [2m], E^{[1]}, x^{[1]}, e^{[1]})$ and $G^{[2]} = (V^{[2]} = [2m], E^{[2]}, x^{[2]}, e^{[2]})$, both with $2m$ nodes but with different matching-counts of $H_m$, and show that k-WL cannot distinguish them. Define $E_{\text{double}} = \{(i, i+1) : 1 \leq i < m\} \cup \{(i+1, i) : 1 \leq i < m\}$, which is the edge set of a graph that is exactly two disconnected copies of $H_m$. For $G^{[1]}$, let $E^{[1]} = E_{\text{double}} \cup \{(1, m), (m, 1), (1 + m, 2m), (2m, 1 + m)\}$; $\forall i \leq m, x^{[1]}_i = x^{[1]}_{i+m} = x^{[1]}_i$; $\forall (i, j) \in E^{[1]}, e^{[1]}_{i,j} = e^{[1]}_{i+m,j+m} = e^{[1]}_{i,j}$. For $G^{[2]}$, let $E^{[2]} = E_{\text{double}} \cup \{(1, 2m), (2m, 1), (1 + m, 2m), (2m, 1 + m)\}$; $\forall i \leq m, x^{[2]}_i = x^{[2]}_{i+m} = x^{[2]}_i$; $\forall (i, j) \in E^{[2]}, e^{[2]}_{i,j} = e^{[2]}_{i+m,j+m} = e^{[2]}_{i,j}$. In words, both $G^{[1]}$ and $G^{[2]}$ are constructed based on two copies of $H_m$, and the difference is that, $G^{[1]}$ adds the edges $\{(1, m), (m, 1), (1 + m, 2m), (2m, 1 + m)\}$, whereas $G^{[2]}$ adds the edges $\{(1, 2m), (2m, 1), (1 + m, 2m), (2m, 1 + m)\}$, all with the same edge feature. For the case $k = 3, m = 8, T = 1$, for example, the constructed graphs are illustrated in Figure 4.

Can $G^{[1]}$ and $G^{[2]}$ be distinguished by k-WL? Let $c_k^{(t)}$ be the coloring functions of k-tuples for $G^{[1]}$ and $G^{[2]}$, respectively, obtained after running k-WL on the two graphs simultaneously for $t$ iterations. To show that the answer is negative, we want to prove that

$$\{c_k^{(T)}(s) : s \in [2m]^k\} = \{c_k^{(T)}(s) : s \in [2m]^k\}$$

To show this, if is sufficient to find a permutation $\eta : [2m]^k \rightarrow [2m]^k$ such that $\forall k$-tuple $s \in [2m]^k, c_k^{(T)}(s) = c_k^{(T)}(\eta(s))$. Before defining such an $\eta$, we need the following lemma.

Lemma 5. Let $p$ be a positive integer. If $m \geq (k+1)p$, then $\forall s \in [2m]^k, \exists i \in [m]$ such that $\{i, i+1, \ldots, i+p-1\} \cap \{\text{Mod}_m(j) : j \in s\} = \emptyset$.

Proof of Lemma 5: We can use a simple counting argument to show this. For $u \in [k+1]$, define $A_u = \{up, up+1, \ldots, (u+1)p-1\} \cup \{up + m, up + m + 1, \ldots, (u+1)p-1+m\}$. Then $|A_u| = 2p, A_u \cap A_{u'} = \emptyset$ if $u \neq u'$, and

$$[2m] \supseteq \bigcup_{u \in [k+1]} A_u$$

since $m \geq (k+1)p$. Suppose that the claim is not true, then each $A_i$ contains at least one node in $s$, and therefore

$$s \supseteq (s \cap [2m]) \supseteq \bigcup_{u \in [k+1]} (s \cap A_u)$$
With this lemma, we see that \( \forall \sigma \in [2m]^k \), \( \exists i \in [m] \) such that \( \forall j \in s, \text{MOD}_m(j) \) either \( < i \) or \( \geq i + 2^{T+1} - 1 \). Thus, we can first define the mapping \( \chi : [2m]^k \to [m] \) from a \( k \)-tuple \( s \) to the smallest such node index \( i \in [m] \). Next, \( \forall i \in [m] \), we define a mapping \( \tau_i \) from \([2m]\) to \([2m]\) as

\[
\tau_i(j) = \begin{cases} 
  j, & \text{if } \text{MOD}_m(j) \leq i \\
  \text{MOD}_m(j + m), & \text{otherwise}
\end{cases}
\]  

(16)\]

\( \tau_i \) is a permutation on \([2m]\). For \( \forall i \in [m] \), this allows us to define a mapping \( \zeta_i \) from \([2m]^k \to [2m]^k \) as, \( \forall s = (i_1, ..., i_k) \in [2m]^k \),

\[
\zeta_i(s) = (\tau_i(i_1), ..., \tau_i(i_k)).
\]  

(17)\]

Finally, we define a mapping \( \eta \) from \([2m]^k \to [2m]^k \) as,

\[
\eta(s) = \zeta_{\chi(s)}(s).
\]  

(18)\]

The maps \( \chi, \tau \) and \( \eta \) are illustrated in Figure 4.

To fulfill the proof, there are two things we need to show about \( \eta \). First, we want it to be a permutation on \([2m]^k \). To see this, observe that \( \chi(s) = \chi(\eta(s)) \), and hence \( \forall s \in [2m]^k \), \( (\eta \circ \eta)(s) = (\zeta_{\chi(\eta(s))} \circ \zeta_{\chi(s)})(s) = s \), since \( \forall i \in [m], \tau_i \circ \tau_i \) is the identity map on \([2m]\).

Second, we need to show that \( \forall s \in [2m]^k, c_k^{(T)}(s) = c_k^{(T)}(\eta(s)) \). This will be a consequence of the following lemma.

**Lemma 6.** At iteration \( t \), \( \forall s \in [2m]^k \), \( \forall i \) such that \( \forall j \in s \), either \( \text{MOD}_m(j) < i \) or \( \text{MOD}_m(j) \geq i + 2^t \), there is

\[
c_k^{(t)}(s) = c_k^{(t)}(\zeta_i(s)).
\]  

(19)\]

\[\text{G}^{[1]}\]

\[\text{G}^{[2]}\]

Figure 4: Illustration of the construction in the proof of Theorem 5 in Appendix G. In this particular case, \( k = 3, m = 8, T = 1 \). If we consider \( s = (1, 12, 8) \) as an example, where the corresponding nodes are marked by blue squares in \( \text{G}^{[1]} \), there is \( \chi(s) = 2 \), and thus \( \eta(s) = \zeta_2(s) = (1, 4, 16) \), which are marked by blue squares in \( \text{G}^{[2]} \). Similarly, if we consider \( s = (3, 14, 15) \), then \( \chi(s) = 4 \), and thus \( \eta(s) = \zeta_4(s) = (3, 6, 7) \). In both cases, we see that the isomorphism type of \( s \) in \( \text{G}^{[1]} \) equals the isomorphism type of \( \eta(s) \) in \( \text{G}^{[2]} \). In the end, we will show that \( c_k^{(T)}(s) = c_k^{(T)}(\eta(s)) \).
Remark: This statement allows \( i \) to depend on \( s \), as will be the case when we apply this lemma to \( \eta(s) = \zeta_k(s)(s) \), where we set \( i \) to be \( \chi(s) \).

**Proof of Lemma 6:** Notation-wise, for any \( k \)-tuple, \( s = (i_1, \ldots, i_k) \), and for \( w \in [k] \), use \( I_w(s) \) to denote the \( w \)th entry of \( s \), \( i_w \).

The lemma can be shown by using induction on \( t \). Before looking at the base case \( t = 0 \), we will first show the inductive step, which is:

\[
\forall \bar{T}, \text{ suppose the lemma holds for all } t \leq \bar{T} - 1,
\]

then it also holds for \( t = \bar{T} \).

**Inductive step:**
Fix a \( \bar{T} \) and suppose the lemma holds for all \( t \leq \bar{T} - 1 \). Under the condition that \( \forall j \in s \), either \( \text{MOD}_m(j) < i \) or \( \text{MOD}_m(j) \geq i + 2^T \), to show \( c_k^{(T)}(s) = c_k^{(T)}(\zeta_i(s)) \), we need two things to hold:

1. \( c_k^{(T-1)}(s) = c_k^{(T-1)}(\zeta_i(s)) \)

2. \( \forall w \in [k], \{ c_k^{(T-1)}(\bar{s}) : \bar{s} \in N_w(s) \} = \{ c_k^{(T-1)}(\bar{s}) : \bar{s} \in N_w(\zeta_i(s)) \} \)

The first condition is a consequence of the inductive hypothesis, as \( i + 2^T > i + 2^{(T-1)} \). For the second condition, it is sufficient to find for all \( w \in [k] \), a bijective mapping \( \xi \) from \( N_w(s) \) to \( N_w(\zeta_i(s)) \) such that \( \forall \bar{s} \in N_w(s), c_k^{(T-1)}(\bar{s}) = c_k^{(T-1)}(\zeta_i(\bar{s})) \).

We then define \( \beta(i, \bar{s}) = \begin{cases} 
\text{MOD}_m(I_w(\bar{s})) + 1, & \text{if } i \leq \text{MOD}_m(I_w(\bar{s})) < i + 2^{T-1} \\
i, & \text{otherwise}
\end{cases} \)

(21)

Now, consider any \( \bar{s} \in N_w(s) \). Note that \( \bar{s} \) and \( s \) differ only in the \( w \)th entry of the \( k \)-tuple.

- If \( i \leq \text{MOD}_m(I_w(\bar{s})) < i + 2^{T-1} \), then \( \forall j \in \bar{s} \),
  - either \( j \in s \), in which case either \( \text{MOD}_m(j) < i < \text{MOD}_m(I_w(\bar{s})) + 1 = \beta(i, \bar{s}) \) or \( \text{MOD}_m(j) \geq i + 2^T \geq \text{MOD}_m(I_w(\bar{s})) + 1 + 2^{T-1} = \beta(i, \bar{s}) + 2^{T-1} \),
  - or \( j = I_w(\bar{s}) \), in which case \( \text{MOD}_m(j) < \text{MOD}_m(I_w(\bar{s})) + 1 = \beta(i, \bar{s}) \).

- If \( \text{MOD}_m(I_w(\bar{s})) < i \) or \( \text{MOD}_m(I_w(\bar{s})) \geq i + 2^{T-1} \), then \( \forall j \in \bar{s} \),
  - either \( j \in s \), in which case either \( \text{MOD}_m(j) < i = \beta(i, \bar{s}) \) or \( \text{MOD}_m(j) \geq i + 2^T \geq \beta(i, \bar{s}) + 2^{T-1} \),
  - or \( j = I_w(\bar{s}) \), in which case either \( \text{MOD}_m(j) < i = \beta(i, \bar{s}) \) or \( \text{MOD}_m(j) \geq i + 2^{T-1} \geq \beta(i, \bar{s}) + 2^{T-1} \).

Thus, in all cases, there is \( \forall j \in \bar{s} \), either \( \text{MOD}_m(j) < \beta(i, \bar{s}) \), or \( \text{MOD}_m(j) \geq i + 2^{T-1} \). Hence, by the inductive hypothesis, we have \( c_k^{(T-1)}(\bar{s}) = c_k^{(T-1)}(\beta(\xi(\bar{s})) \). This inspires us to define, for \( \forall w \in [k], \forall \bar{s} \in N_w(s) \),

\[
\xi(\bar{s}) = \zeta_{\beta(\xi(\bar{s}))}(\bar{s})
\]

(22)

Additionally, we still need to prove that, firstly, \( \xi \) maps \( N_w(s) \) to \( N_w(\zeta_i(s)) \), and secondly, \( \xi \) is a bijection. For the first statement, note that \( \forall \bar{s} \in N_w(s), \zeta_{\beta(\xi(\bar{s}))}(\bar{s}) = \zeta_i(s) \) because \( s \) contains no entry between \( i \) and \( \beta(i, \bar{s}) \), with the latter being less than \( i + 2^T \). Hence, if \( \bar{s} \in N_w(s) \), then \( \forall w' \in [k] \) with \( w' \neq w \), there is \( I_{w'}(\bar{s}) = I_{w'}(s) \), and therefore \( \text{I}_{w'}(\zeta_i(s)) = \text{I}_{w'}(\zeta_{\beta(\xi(\bar{s}))}(\bar{s})) = \beta(\xi(\bar{s}))(\text{I}_{w'}(\bar{s}) = \text{I}_{w'}(\zeta_{\beta(\xi(\bar{s}))}(\bar{s})) = \text{I}_{w'}(\zeta_{\beta(\xi(\bar{s}))}(\bar{s})) = \text{I}_{w'}(\zeta_i(s)) \), which ultimately implies that \( \xi(\bar{s}) \in N_w(\zeta_i(s)) \).
Base case:
We need to show that
\[ \forall s \in [2m]^{k}, \forall i^{*} \text{ such that } \forall j \in s, \text{ either } \text{MOD}_{m}(j) < i^{*} \]
or \[ \text{MOD}_{m}(j) \geq i^{*} + 1, \text{ there is } c_{k}^{(i^{*})}(s) = c_{k}^{(0)}(\zeta_{s}(s)) \]  
(23)
Due to the way in which the colorings of the \( N \) known that \((\text{Mod}_{i}^{(i)}(s)) \) to \( N \)

Lemma 7. Say \( s = (i_{1}, ..., i_{k}) \), in which case \( \zeta_{s}(s) = (\tau_{s}(i_{1}), ..., \tau_{s}(i_{k})) \). Then

1. \( \forall \alpha, \beta \in s, \alpha = \beta \Leftrightarrow \tau_{s}(\alpha) = \tau_{s}(\beta) \)
2. \( \forall \alpha \in s, x_{i}^{[1]} = x_{i}^{[2]} \), and moreover \( x_{i}^{[1]} = x_{i}^{[2]} \) if \( i \leq m \).
3. Define \( S = \{(1, m), (m, 1), (1 + m, 2m), (2m, 1 + m), (2m, 1), (m, 1 + m), (1 + m, 2m)\} \), which is the set of “special” pairs of nodes in which \( G^{[1]} \) and \( G^{[2]} \) differ. Note that \( \forall (i_{a}, i_{b}) \in [2m]^{2}, (i_{a}, i_{b}) \in S \) if and only if the sets \( \{\text{MOD}_{m}(i_{a}), \text{MOD}_{m}(i_{b})\} = \{1, m\} \).

By the assumption on \( i^{*} \) in (23), we know that \( i_{a}, i_{b} \not\in \{i^{*}, i^{*} + m\} \). Now we look at 16 different cases separately, which comes from \( 4 \) possibilities for each of \( i_{a} \) and \( i_{b} \): \( i_{a} \) (or \( i_{b} \)) belonging to \( \{1, ..., i^{*} - 1\}, \{i^{*} + 1, ..., m\}, \{1 + m, ..., i^{*} - 1 + m\} \), or \( \{i^{*} + 1 + m, ..., 2m\} \)

Case 1 \( 1 \leq i_{a}, i_{b} < i^{*} \)
Then \( \tau_{s}(i_{a}) = i_{a}, \tau_{s}(i_{b}) = i_{b} \). In addition, as \( \text{MOD}_{m}(i_{a}), \text{MOD}_{m}(i_{b}) \neq m \), there is \( (i_{a}, i_{b}) \not\in S \).
Thus, if \( (i_{a}, i_{b}) \in E^{[1]} \), then \( (i_{a}, i_{b}) \in E_{\text{double}} \subset E^{[2]} \), and moreover, \( e_{i_{a}, i_{b}}^{[1]} = e_{i_{a}, i_{b}}^{[2]} = e_{\tau_{s}(i_{a}), \tau_{s}(i_{b})}^{[2]} \).

Case 2 \( 1 + m \leq i_{a}, i_{b} < i^{*} + m \)
Similar to case 1.

Case 3 \( i^{*} + 1 \leq i_{a}, i_{b} \leq m \)
Then \( \tau_{s}(i_{a}) = i_{a} + m, \tau_{s}(i_{b}) = i_{b} + m \). In addition, as \( \text{MOD}_{m}(i_{a}), \text{MOD}_{m}(i_{b}) \neq 1 \), there is \( (i_{a}, i_{b}) \not\in S \). Thus, if \( (i_{a}, i_{b}) \in E^{[1]} \), then \( (i_{a}, i_{b}) \in E_{\text{double}} \), and hence \( (i_{a} + m, i_{b} + m) \in E_{\text{double}} \subset E^{[2]} \), and moreover, \( e_{i_{a}, i_{b}}^{[1]} = e_{i_{a} + m, i_{b} + m}^{[2]} = e_{e_{\tau_{s}(i_{a}), \tau_{s}(i_{b})}^{[2]}}^{[2]} \).

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Case 4 \( i^* + 1 + m \leq i_\alpha, i_\beta \leq 2m \)
Similar to case 3.

Case 5 \( 1 \leq i_\alpha < i^*, i^* + 1 \leq i_\beta \leq m \)
If \( i_\alpha \neq 1 \) or \( i_\beta \neq m \), then since \( H_m \) is a path and \( i_\alpha < i^* \leq i_\beta - 1 \), \((i_\alpha, i_\beta) \notin E[1] \) or \( E[2] \). Now we consider the case where \( i_\alpha = 1, i_\beta = m \). As \( 1 \leq i^* < m \), by the definition of \( \tau \), there is \( \tau^*(1) = 1 \), and \( \tau^*(m) = 2m \). Note that both \((1, m) \in E[1] \) and \((1, 2m) \in E[2] \) are true, and moreover, \( e_1[1] = e_2[2] \).

Case 6 \( 1 \leq i_\beta < i^*, i^* + 1 \leq i_\alpha \leq m \)
Similar to case 5.

Case 7 \( 1 + m \leq i_\alpha < i^* + m, i^* + 1 + m \leq i_\beta \leq 2m \)
Similar to case 5.

Case 8 \( 1 + m \leq i_\beta < i^* + m, i^* + 1 + m \leq i_\alpha \leq 2m \)
Similar to case 5.

Case 9 \( 1 \leq i_\alpha < i^* \) and \( 1 + m \leq i_\beta < i^* + m \)
Then \( \tau_s(i_\alpha) = i_\alpha, \tau_s(i_\beta) = i_\beta \), and \((i_\alpha, i_\beta) \notin E[1] \) or \( E[2] \).

Case 10 \( 1 \leq i_\beta < i^* \) and \( 1 + m \leq i_\alpha < i^* + m \)
Similar to case 9.

Case 11 \( i^* + 1 \leq i_\alpha < m \) and \( i^* + 1 + m \leq i_\beta \leq 2m \)
\((i_\alpha, i_\beta) \notin E[1] \), \( \tau_s(i_\alpha) = i_\alpha + m, \tau_s(i_\beta) = i_\beta - m \). Hence \((\tau_s(i_\alpha), \tau_s(i_\beta)) \notin E[2] \) either.

Case 12 \( i^* + 1 \leq i_\beta \leq m \) and \( i^* + 1 + m \leq i_\alpha \leq 2m \)
Similar to case 11.

Case 13 \( 1 \leq i_\alpha < i^* \) and \( i^* + 1 + m \leq i_\beta \leq 2m \)
\((i_\alpha, i_\beta) \notin E[1] \) obviously. We also have \( \tau_s(i_\alpha) = i_\alpha \in [1, i^*], \tau_s(i_\beta) = i_\beta - 1 \notin [i^* + 1, m], \) and hence \((\tau_s(i_\alpha), \tau_s(i_\beta)) \notin E[2] \).

Case 14 \( 1 \leq i_\beta < i^* \) and \( i^* + 1 + m \leq i_\alpha \leq 2m \)
Similar to case 13.

Case 15 \( 1 + m \leq i_\alpha < i^* + m \) and \( i^* + 1 \leq i_\beta \leq m \)
Similar to case 13.

Case 16 \( 1 + m \leq i_\beta < i^* + m \) and \( i^* + 1 \leq i_\alpha \leq m \)
Similar to case 13.

This concludes the proof of Lemma 7.

Lemma 7 completes the proof of the base case, and hence the induction argument for Lemma 6.

\[ \forall s \in [2m]^k, \text{ since } \eta(s) = \zeta_{\chi(s)}(s), \text{ and } \chi(s) \text{ satisfies } \forall j \in s, \text{ either } \text{MOD}_m(j) < i \text{ or } \text{MOD}_m(j) \geq i + 2^T, \]
Lemma 6 implies that at iteration \( T \), we have \( c_k^{(T)}(s) = c_k^{(T)}(\zeta_{\chi(s)}(s)) = c_k^{(T)}(\eta(s)) \). Since we have shown that \( \eta \) is a permutation on \([2m]^k \), this let’s us conclude that
\[ \{c_k^{(T)}(s) : s \in [2m]^k\} = \{c_k^{(T)}(s) : s \in [2m]^k\}, \]
and therefore \( k \)-WL cannot distinguish between the two graphs in \( T \) iterations.
H Proof of Theorem 6 (2-IGNs are no more powerful than 2-WL)

Proof. For simplicity of notations, we assume $d_t = 1$ in every layer of a 2-IGN. The general case can be proved by adding more subscripts. For 2-WL, we use the definition in section 3.1 except for omitting the subscript $k$ in $c_k^{(t)}$.

To prove the consequent, we assume that for some $T$

This lemma can be shown by induction. To see this, first note that the lemma is equivalent to the statement

To start, it is straightforward to show (and we will prove it at the end) that the theorem can be deduced from the following lemma:

Lemma 8. Say $G^{[4]}$ and $G^{[2]}$ cannot be distinguished by the 2-WL. Then $\forall t \in \mathbb{N}$, it holds that

This lemma can be shown by induction. To see this, first note that the lemma is equivalent to the statement that

This allows us to carry out an induction in $T \in \mathbb{N}$. For the base case $t = T = 0$, this is true because $c^{(0)}$ and $c^{(0)}$ in WL and $B^{(0)}$ and $B^{(0)}$ in 2-IGN are both initialized in the same way according to the subgraph isomorphism. To be precise, $c^{(0)}(s) = c^{(0)}(s')$ if and only if the subgraph in $G^{[1]}$ induced by the pair of nodes $s$ is isomorphic to the subgraph in $G^{[2]}$ induced by the pair of nodes $s'$, which is also true if and only if $B^{(0)} = B^{(0)}$.

Next, to show that the induction step holds, we need to prove the following statement:

Next, to show that the induction step holds, we need to prove the following statement:

To prove the consequent, we assume that for some $s, s' \in V^2$, there is $c^{(T)}(s) = c^{(T)}(s')$, and then attempt to show that $B^{(T)}_s = B^{(T)}_{s'}$. By the update rules of $k$-WL, the statement $c^{(T)}(s) = c^{(T)}(s')$ implies that

Case 1: $s = (i, j) \in V^2$ with $i \neq j$

Let’s first consider the case where $s = (i, j) \in V^2$ with $i \neq j$. In this case, we can also write $s' = (i', j') \in V^2$ with $i' \neq j'$, thanks to Lemma 2. Then, note that $V^2$ can be written as the union of 9 disjoint sets that are defined depending on $s$:

where we define $A_{s,1} = \{(i, j)\}$, $A_{s,2} = \{(i, i)\}$, $A_{s,3} = \{(j, j)\}$, $A_{s,4} = \{(i, k) : k \neq i \text{ or } j\}$, $A_{s,5} = \{(k, i) : k \neq i \text{ or } j\}$, $A_{s,6} = \{(j, k) : k \neq i \text{ or } j\}$, $A_{s,7} = \{(k, j) : k \neq i \text{ or } j\}$, $A_{s,8} = \{(k, l) : k \neq l \text{ and } \{k, l\} \cap \{i, j\} = \emptyset\}$, $A_{s,9} = \{(k, k) : k \notin \{i, j\}\}$. In this way, we partition $V^2$ into 9 different subsets, each of which consisting of pairs $(k, l)$ that yield a particular equivalence class of the 4-tuple $(i, j, k, l)$. Similarly, we can define $A_{s',w}$ for $w \in [9]$, which will also give us

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Moreover, note that

\[ N_1(s) = \bigcup_{w=1,3,7} A_{s,w} \]
\[ N_2(s) = \bigcup_{w=1,2,4} A_{s,w} \]
\[ N_1(s') = \bigcup_{w=1,3,7} A_{s',w} \]
\[ N_2(s') = \bigcup_{w=1,2,4} A_{s',w} \]

Before proceeding, we make the following definition to simplify notations:

\[ C_{s,w} = \{ c(T-1)(\tilde{s}) : \tilde{s} \in A_{s,w} \} \]
\[ C'_{s',w} = \{ c'(T-1)(\tilde{s}) : \tilde{s} \in A_{s',w} \} \]

This allows us to rewrite (26) as

\[ C_{s,1} = C'_{s',1} \] (27)

\[ \bigcup_{w=1,3,7} C_{s,w} = \bigcup_{w=1,3,7} C'_{s',w} \] (28)

\[ \bigcup_{w=1,2,4} C_{s,w} = \bigcup_{w=1,2,4} C'_{s',w} \] (29)

Combining (27) and (28), we obtain

\[ \bigcup_{w=3,7} C_{s,w} = \bigcup_{w=3,7} C'_{s',w} \] (30)

Combining (27) and (29), we obtain

\[ \bigcup_{w=2,4} C_{s,w} = \bigcup_{w=2,4} C'_{s',w} \] (31)

Note that \( V^2 \) can also be partitioned into two disjoint subsets:

\[ V^2 = \left( \bigcup_{w=1,4,5,6,7,8} A_{s,w} \right) \cap \left( \bigcup_{w=2,3,9} A_{s,w} \right), \]

where the first subset represent the edges: \( \{(i,j) : i \neq j \} \) and the second subset represent the nodes: \( \{(i,i) : i \in V \} \). Similarly,

\[ V^2 = \left( \bigcup_{w=1,4,5,6,7,8} A_{s',w} \right) \cap \left( \bigcup_{w=2,3,9} A_{s',w} \right), \]

As shown in Lemma 2, pairs of nodes that represent edges cannot share the same color with pairs of nodes the represent nodes in any iteration of 2-WL. Thus, we have

\[ \left( \bigcup_{w=1,4,5,6,7,8} C_{s,w} \right) \cap \left( \bigcup_{w=2,3,9} C'_{s',w} \right) = \emptyset \] (32)

\[ \left( \bigcup_{w=1,4,5,6,7,8} C'_{s',w} \right) \cap \left( \bigcup_{w=2,3,9} C_{s,w} \right) = \emptyset \] (33)
Combining (30) and (32) or (33), we get
\[ C_{s,3} = C'_{s',3} \]  
(34)
\[ C_{s,7} = C'_{s',7} \]  
(35)

Combining (31) and (32) or (33), we get
\[ C_{s,2} = C'_{s',2} \]  
(36)
\[ C_{s,4} = C'_{s',4} \]  
(37)

Thanks to symmetry between \((i,j)\) and \((j,i)\), as we work with undirected graphs, there is
\[ C_{s,5} = C_{s,4} = C'_{s',4} = C'_{s',5} \]  
(38)
\[ C_{s,6} = C_{s,7} = C'_{s',7} = C'_{s',6} \]  
(39)

In addition, since we assume that \(G^{[1]}\) and \(G^{[2]}\) cannot be distinguished by 2-WL, there has to be
\[ \bigcup_{w=1}^{9} C_{s,w} = \bigcup_{w=1}^{9} C'_{s',w} \]  
(40)

Combining this with (32) or (33), we get
\[ \bigcup_{w=1,4,5,6,7,8} C_{s,w} = \bigcup_{w=1,4,5,6,7,8} C'_{s',w} \]  
(41)

Combining (40) with (27), (37), (38), (39), (35), we get
\[ C_{s,8} = C'_{s',8} \]  
(42)

Combining (41) with (36) and (34), we get
\[ C_{s,9} = C'_{s',9} \]  
(43)

Hence, in conclusion, we have that \(\forall w \in [9]\),
\[ C_{s,w} = C'_{s',w} \]  
(44)

By the inductive hypothesis, this implies that \(\forall w \in [9]\),
\[ \{ B^{(T-1)}_{s} : \tilde{s} \in A_{s,w} \} = \{ B'^{(T-1)}_{s'} : \tilde{s} \in A_{s',w} \} \]  
(45)

Let us show how (45) may be leveraged. First, to prove that \(B^{(T)}_{s} = B'^{(T)}_{s'}\), recall that
\[ B^{(T)} = \sigma(L^{(T)}(B^{(T-1)})) \]
\[ B'^{(T)} = \sigma(L^{(T)}(B'^{(T-1)})) \]  
(46)

Therefore, it is sufficient to show that for all linear equivariant layer \(L\), we have
\[ L(B^{(T-1)})_{i,j} = L(B'^{(T-1)})_{i',j'} \]  
(47)
Also, recall that

\[
L(B^{(T-1)})_{i,j} = \sum_{(k,l) \in V^2} T_{i,j,k,l} B_{k,l} + Y_{i,j}
\]

By the definition of the \(A_{s,w}\)'s and \(A'_{s',w}\)'s, there is \(\forall \in [9], \forall (k, l) \in A_{s,w}, \forall (k', l') \in A'_{s',w}\), we have the 4-tuples \((i, j, k, l) \sim (i', j', k', l')\), i.e., \(\exists\) a permutation \(\pi\) on \(V\) such that \((i, j, k, l) = (\pi(i'), \pi(j'), \pi(k'), \pi(l'))\), which implies that \(T_{i,j,k,l} = T_{i',j',k',l'}\). Therefore, together with \((45)\), we have the following:

\[
L(B^{(T-1)})_{i,j} = \sum_{(k,l) \in V^2} T_{i,j,k,l} B_{k,l} + Y_{i,j}
= \sum_{w=1}^{9} \sum_{(k,l) \in A_{s,w}} T_{i,j,k,l} B_{k,l} + Y_{i,j}
= \sum_{w=1}^{9} \sum_{(k',l') \in A'_{s',w}} T_{i',j',k',l'} B'_{k',l'} + Y_{i',j'}
= L(B^{(T-1)})_{i',j'}
\]

and hence \(B^{(T)}_{i,j} = B'^{(T)}_{i',j'}\), which concludes the proof for the case that \(s = (i, j)\) for \(i \neq j\).

**Case 2:** \(s = (i, i) \in V^2\)

Next, consider the case \(s = (i, i) \in V^2\). In this case, \(s' = (i', i')\) for some \(i' \in V\). This time, we write \(V^2\) as the union of 5 disjoint sets that depend on \(s\) (or \(s'\)):

\[
V^2 = \bigcup_{w=1}^{5} A_{s,w},
\]

where we define \(A_{s,1} = \{(i, i)\}, A_{s,2} = \{(i, j) : j \neq i\}, A_{s,3} = \{(j, i) : j \neq i\}, A_{s,4} = \{(j, k) : j, k \neq i\} and A_{s,5} = \{(j, j) : j \neq i\}\). Similar for \(s'\). We can also define \(C_{s,w}\) and \(C'_{s',w}\) as above. Note that

\[
N_1(s) = \bigcup_{w=1}^{3} A_{s,w}
\]

\[
N_2(s) = \bigcup_{w=1}^{2} A_{s,w}
\]

\[
N_1(s') = \bigcup_{w=1}^{3} A'_{s',w}
\]

\[
N_2(s') = \bigcup_{w=1}^{2} A'_{s',w}
\]

Hence, we can rewrite \((26)\) as

\[
\bigcup_{w=1}^{3} C_{s,w} = C'_{s',1}
\]

\[
\bigcup_{w=1,3} C_{s,w} = \bigcup_{w=1,3} C'_{s',w}
\]

\[
\bigcup_{w=1,2} C_{s,w} = \bigcup_{w=1,2} C'_{s',w}
\]
Combining (50) with (51), we get
\[ C_{s,3} = C'_{s',3} \] (53)
Combining (50) with (52), we get
\[ C_{s,2} = C'_{s',2} \] (54)
Moreover, since we can decompose \( V^2 \) as
\[
V^2 = \left( \bigcup_{w=1,5} A_{s,w} \right) \cup \left( \bigcup_{w=2,3,4} A_{s,w} \right) = \left( \bigcup_{w=1,5} A'_{s',w} \right) \cup \left( \bigcup_{w=2,3,4} A'_{s',w} \right)
\]
with \( \bigcup_{w=1,5} A_{s,w} = \bigcup_{w=1,5} A'_{s',w} \) representing the nodes and \( \bigcup_{w=2,3,4} A_{s,w} = \bigcup_{w=2,3,4} A'_{s',w} \) representing the edges, we have
\[
\left( \bigcup_{w=1,5} C_{s,w} \right) \cap \left( \bigcup_{w=2,3,4} C'_{s',w} \right) = \emptyset \] (55)
\[
\left( \bigcup_{w=1,5} C'_{s',w} \right) \cap \left( \bigcup_{w=2,3,4} C_{s,w} \right) = \emptyset \] (56)
Since \( G^{(1)} \) and \( G^{(2)} \) cannot be distinguished by 2-WL, there is
\[
\bigcup_{w=1}^{5} C_{s,w} = \bigcup_{w=1}^{5} C'_{s',w}
\]
Therefore, combining this with (55) or (56), we obtain
\[
\bigcup_{w=1,5} C_{s,w} = \bigcup_{w=1,5} C'_{s',w} \] (57)
\[
\bigcup_{w=2,3,4} C_{s,w} = \bigcup_{w=2,3,4} C'_{s',w} \] (58)
Combining (57) with (50), we get
\[ C_{s,5} = C'_{s',5} \] (59)
Combining (58) with (54) and (53), we get
\[ C_{s,4} = C'_{s',4} \] (60)
Hence, in conclusion, we have that \( \forall w \in [5], \)
\[ C_{s,w} = C'_{s',w} \] (61)
By the inductive hypothesis, this implies that \( \forall w \in [5], \)
\[ \{ B^{(T-1)}_s : \tilde{s} \in A_{s,w} \} = \{ B'^{(T-1)}_{s'} : \tilde{s} \in A'_{s',w} \} \] (62)
Thus,
\[
L(B^{(T-1)})_{i,i} = \sum_{(k,l) \in V^2} T_{i,i,k,l} B_{k,l} + Y_{i,i}
\]
\[
= \sum_{w=1}^{5} \sum_{(k,l) \in A_{s,w}} T_{i,i,k,l} B_{k,l} + Y_{i,i}
\]
\[
= \sum_{w=1}^{5} \sum_{(k',l') \in A'_{s',w}} T'_{i',i',k',l'} B'_{k',l'} + Y'_{i',i'}
\]
\[ = L(B^{(T-1)})_{i',i'} \] (63)
and hence $B_{i,j}^{(T)} = B'_{i',j'}^{(T)}$, which concludes the proof for the case that $s = (i, i)$ for $i \in V$.

Now, suppose we are given any 2-IGN with $T$ layers. Since $G^{[1]}$ and $G^{[2]}$ cannot be distinguished by 2-WL, together with Lemma 2, there is

$$\{c^{(T)}((i,j)) : i,j \in V, i \neq j\} = \{c'^{(T)}((i',j')) : i',j' \in V, i' \neq j'\}$$

and

$$\{c^{(T)}((i,i)) : i \in V\} = \{c'^{(T)}((i',i')) : i' \in V\}$$

Hence, by the lemma, we have

$$\{B^{(T)}_{i,j} : i,j \in V, i \neq j\} = \{B'_{i',j'}^{(T)} : i',j' \in V, i' \neq j'\}$$

and

$$\{B^{(T)}_{i,i} : i \in V\} = \{B'_{i',i'}^{(T)} : i' \in V\}$$

Then, since the second-last layer $h$ in the 2-IGN can be written as

$$h(B) = \alpha \sum_{i,j \in V, i \neq j} B_{i,j} + \beta \sum_{i \in V} B_{i,i} \quad (63)$$

there is

$$h(B^{(T)}) = h(B'^{(T)}) \quad (64)$$

and finally

$$m \circ h(B^{(T)}) = m \circ h(B'^{(T)}) \quad (65)$$

which means the 2-IGN yields identical outputs on the two graphs.

I Direct proof of Corollary 4 (2-IGNs are unable to matching-count patterns of 3 or more nodes)

\textbf{Proof.} The same counterexample as in the proof of Theorem 2 given in Appendix D applies here, as we are going to show below. Note that we only need to consider the non-clique case, since the set of counterexample graphs for the non-clique case is a superset of the set of counterexample graphs for the clique case.

Let $B$ be the input tensor corresponding to $G^{[1]}$, and $B'$ corresponding to $G^{[2]}$. For simplicity, we assume in the proof below that $d_0, ..., d_T = 1$. The general case can be proved in the same way but with more subscripts. (In particular, for our counterexamples, (69) can be shown to hold for each of the $d_0$ feature dimensions.) Define a set $S = \{(1, 2), (2, 1), (1 + m, 2 + m), (2 + m, 1 + m), (1, 2 + m), (2 + m, 1), (1 + m, 2), (2, 1 + m)\}$, which represents the “special” edges that capture the difference between $G^{[1]}$ and $G^{[2]}$. We aim to show something like this:
∀t,

\[
\begin{align*}
B_{i,j}^{(t)} &= B_{i,j}^{(t)}, \forall (i,j) \notin S \\
B_{1,2}^{(t)} &= B_{1+m,2}^{(t)} \\
B_{2,1}^{(t)} &= B_{2,1+m}^{(t)} \\
B_{1+m,2+m}^{(t)} &= B_{1,2+m}^{(t)} \\
B_{2+m,1+m}^{(t)} &= B_{2+m,1}^{(t)} \\
B_{1+m,2+m}^{(t)} &= B_{1,2+m}^{(t)} \\
B_{2+m,1+m}^{(t)} &= B_{2,1+m}^{(t)} \\
B_{2,1+m}^{(t)} &= B_{2,1}^{(t)}
\end{align*}
\]

Thus, (66) can be rewritten as

\[
(67)
\]

Thus, by symmetry, (66) can be rewritten as

\[
∀t, B_{i,j}^{(t)} = B_{\eta_1(i,j)}^{(t)}
\]

Next, define the permutation \( \tau_1 \) on \( V \times V \):

\[
\tau_1((i,j)) = (\kappa_1(i), \kappa_1(j))
\]

and then \( \eta_1 \) as the restriction of \( \tau_1 \) on the set \( S \subseteq V \times V \):

\[
\eta_1((i,j)) = \begin{cases} 
\tau_1((i,j)), & \text{if } (i,j) \in S \\
(i,j), & \text{otherwise}
\end{cases}
\]

Thus, (66) can be rewritten as

\[
∀t, B_{i,j}^{(t)} = B_{\eta_1(i,j)}^{(t)}
\]

Before trying to prove (67), let’s define \( \kappa_2, \tau_2 \) and \( \eta_2 \) analogously:

\[
\kappa_2(i) = \begin{cases} 
\text{MOD}_{2m}(2+m), & \text{if } i \in \{2, 2+m\} \\
i, & \text{otherwise}
\end{cases}
\]

\[
\tau_2((i,j)) = (\kappa_2(i), \kappa_2(j))
\]

\[
\eta_2((i,j)) = \begin{cases} 
\tau_2((i,j)), & \text{if } (i,j) \in S \\
(i,j), & \text{otherwise}
\end{cases}
\]

Thus, by symmetry, (67) is equivalent to

\[
∀t, B_{i,j}^{(t)} = B_{\eta_2(i,j)}^{(t)} = B_{\eta_2(i,j)}^{(t)}
\]

Because of the recursive relation (1), we will show (68) by induction on \( t \). For the base case, it can be verified that

\[
B_{i,j}^{(0)} = B_{\eta_1(i,j)}^{(0)} = B_{\eta_2(i,j)}^{(0)}
\]

thanks to the construction of \( G^{[1]} \) and \( G^{[2]} \). Moreover, if we define another permutation \( V \times V \), \( \zeta_1 \):

\[
\zeta_1((i,j)) = \begin{cases} 
(\text{MOD}_{2m}(i+m), \text{MOD}_{2m}(j+m)), & \text{if } j \in \{1, 1+m\} \text{ and } i \notin \{2, 2+m\} \\
or i \in \{1, 1+m\} \text{ and } j \notin \{2, 2+m\} & \text{if } j \notin \{1, 1+m\} \\
(i,j), & \text{otherwise}
\end{cases}
\]
then thanks to the symmetry between \((i, j)\) and \((i + m, j + m)\), there is

\[
B_{i,j}^{(0)} = B'_{\zeta_1(i,j)}^{(0)}, \quad B'_{i,j} = B'_{\zeta_1(i,j)}^{(0)}
\]

Thus, for the induction to hold, and since \(\sigma\) applies entry-wise, it is sufficient to show that

**Lemma 9.** If

\[
B_{i,j} = B_{\zeta_1(i,j)}, \quad B'_{i,j} = B'_{\zeta_1(i,j)}
\]

then

\[
B_{i,j} = B'_{\zeta_1(i,j)}, \quad B'_{i,j} = B'_{\eta_1(i,j)}
\]

(71)

(72)

(73)

(74)

**Proof of Lemma 9:** Again, by symmetry between \((i, j)\) and \((i + m, j + m)\), (73) can be easily shown.

For (74), because of the symmetry between \(\eta_1\) and \(\eta_2\), we will only prove the first equality. By Maron et al. (2018), we can express the linear equivariant layer \(L\) by

\[
L(B)_{i,j} = \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,k,l} B_{k,l} + Y_{i,j}
\]

where crucially, \(T_{i,j,k,l}\) depends only on the equivalence class of the 4-tuple \((i, j, k, l)\).

We consider eight different cases separately.

**Case 1** \(i, j \notin \{1, 2, 1 + m, 2 + m\}\)

There is \(\eta_1((i, j)) = (i, j)\), and \((i, j, k, l) \sim (i, j, \eta_1((k, l)))\), and thus \(T_{i,j,k,l} = T_{i,j,\eta_1((k, l))}\). Therefore,

\[
L(B')_{\eta_1((i, j))} = L(B')_{i,j}
\]

\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,k,l} B'_{k,l} + Y_{i,j}
\]

\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,\eta_1((k, l))} B'_{\eta_1((k, l))} + Y_{i,j}
\]

\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,\eta_1((k, l))} B'_{\eta_1((k, l))} + Y_{i,j}
\]

\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,k,l} B'_{\eta_1((k, l))} + Y_{i,j}
\]

\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,k,l} B_{k,l} + Y_{i,j}
\]

\[
= B_{i,j}
\]

**Case 2** \(i \in \{1, 1 + m\}, \ j \notin \{1, 2, 1 + m, 2 + m\}\)

There is \(\eta_1((i, j)) = (i, j)\), and \((i, j, k, l) \sim (i, j, \eta_2((k, l)))\), because \(\eta_2\) only involves permutation between

\[
\]

35
nodes 2 and 2 + m, while i and j ∉ \{2, 2 + m\}. Thus, \(T_{i,j,k,l} = T_{i,j,\eta_2((k,l))}\). Therefore,

\[
L(B')_{\eta_1((i,j))} = L(B')_{i,j} \\
= \sum_{(k,l) = (1,1)}^{(2m,2m)} T_{i,j,k,l} B'_{k,l} + Y_{i,j} \\
= \sum_{(k,l) = (1,1)}^{(2m,2m)} T_{i,j,\eta_2((k,l))} B'_{\eta_2((k,l))} + Y_{i,j} \\
= \sum_{(k,l) = (1,1)}^{(2m,2m)} T_{i,j,k,l} B'_{\eta_2((k,l))} + Y_{i,j} \\
= \sum_{(k,l) = (1,1)}^{(2m,2m)} T_{i,j,k,l} B_{k,l} + Y_{i,j} \\
= B_{i,j}
\]

**Case 3** \(j \in \{1,1 + m\}, i \notin \{1, 2, 1 + m, 2 + m\}\)
Analogous to case 2.

**Case 4** \(i \in \{2, 2 + m\}, j \notin \{1, 2, 1 + m, 2 + m\}\)
There is \(\eta_1((i,j)) = (i,j)\), and \((i,j,k,l) \sim (i,j,\eta_1((k,l)))\), because \(\eta_1\) only involves permutation between nodes 1 and 1 + m, while \(i\) and \(j\) ∉ \{1, 1 + m\}. Thus, \(T_{i,j,k,l} = T_{i,j,\eta_1((k,l))}\). Therefore, we can apply the same proof as for case 2 here except for changing \(\eta_2\)’s to \(\eta_1\)’s.

**Case 5** \(j \in \{2, 2 + m\}, i \notin \{1, 2, 1 + m, 2 + m\}\)
Analogous to case 4.

**Case 6** \((i,j) \in S\)
Define one other permutation on \(V \times V\), \(\xi_1\), as \(\xi_1((i,j)) = \)

\[
\begin{cases}
(M \bmod 2m(i + m), j), & \text{if } M \bmod m(j) = 1, M \bmod m(i) \neq 1 \text{ or } 2 \\
(i, M \bmod 2m(j + m)), & \text{if } M \bmod m(i) = 1, M \bmod m(j) \neq 1 \text{ or } 2 \\
i, j, & \text{otherwise}
\end{cases}
\]

It can be verified that

\(\xi_1 \circ \tau_1 = \eta_1 \circ \xi_1\)

Moreover, it has the property that if \((i,j) \in S\), then

\((i,j,k,l) \sim (i,j,\xi_1(k,l))\)

because \(\xi_1\) only involves permutations among nodes not in \{1, 2, 1 + m, 2 + m\} while \(i, j \in \{1, 2, 1 + m, 2 + m\}\). Thus, we have

\[
(i,j,k,l) \sim (\kappa_1(i), \kappa_1(j), \kappa_1(k), \kappa_1(l)) \\
= (\tau_1(i,j), \tau_1(k,l)) \\
= (\eta_1(i,j), \eta_1(k,l)) \\
= (\eta_1(i,j), \xi_1 \circ \tau_1(k,l)) \\
= (\eta_1(i,j), \eta_1 \circ \xi_1(k,l)).
\]
implying that \( T_{i,j,k,l} = T_{\eta_1(i,j),\eta_1(i,k,l)} \). In addition, as \( \eta_1((i,j)) \sim (i,j) \), there is \( Y_{\eta_1((i,j))} = Y_{i,j} \). Moreover, by (71),
\[
B'_{\eta_1((i,j))} = B'_{\eta_1((i,k,l))} = B_{k,l}
\]
Therefore,
\[
L(B')_{\eta_1((i,j))} = \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{\eta_1((i,j)),k,l}B'_{k,l} + Y_{\eta_1((i,j))}
\]
\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{\eta_1((i,j)),\eta_1((k,l))}B'_{\eta_1((k,l))} + Y_{\eta_1((i,j))}
\]
\[
= \sum_{(k,l)=(1,1)}^{(2m,2m)} T_{i,j,k,l}B_{k,l} + Y_{i,j}
\]
\[
= B_{i,j}
\]

Case 7 \( i,j \in \{1, 1 + m\} \)
There is \( \eta_1(i,j) = (i,j) \) and \( (i,j,k,l) \sim (i,j,\eta_2((k,l))) \). Thus, \( T_{i,j,k,l} = T_{i,j,\eta_2((k,l))} \), and the rest of the proof proceeds as for case 2.

Case 8 \( i,j \not\in \{1, 1 + m\} \)
There is \( \eta_1(i,j) = (i,j) \) and \( (i,j,k,l) \sim (i,j,\eta_1((k,l))) \). Thus, \( T_{i,j,k,l} = T_{i,j,\eta_1((k,l))} \), and the rest of the proof proceeds as for case 4.

With the lemma above, (67) can be shown by induction as a consequence. Thus, \( B^{(T)}_{i,j} = B^{(T)}_{\eta_1(i,j)} \),

Maron et al. (2018) show that the space of linear invariant functions on \( \mathbb{R}^{n \times n} \) is two-dimensional, and so for example, the second-last layer \( h \) in the 2-IGN can be written as
\[
h(B) = \alpha \sum_{i,j=(1,1)}^{(2m,2m)} B_{i,j} + \beta \sum_{i=1}^{2m} B_{i,i}
\]
for some \( \alpha, \beta \in \mathbb{R} \). Then since \( \eta_1 \) is a permutation on \( V \times V \) and also is the identity map when restricted to \( \{(i,i) : i \in V\} \), we have
\[
h(B^{(T)}) = \alpha \sum_{(i,j)=(1,1)}^{(2m,2m)} B^{(T)}_{i,j} + \beta \sum_{i=1}^{2m} B^{(T)}_{i,i}
\]
\[
= \alpha \sum_{(i,j)=(1,1)}^{(2m,2m)} B^{(T)}_{\eta_1((i,j))} + \beta \sum_{i=1}^{2m} B^{(T)}_{\eta_1((i,i))}
\]
\[
= \alpha \sum_{(i,j)=(1,1)}^{(2m,2m)} B^{(T)}_{i,j} + \beta \sum_{i=1}^{2m} B^{(T)}_{i,i}
\]
\[
= h(B^{(T)})
\]

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Therefore, finally,

\[ m \circ h(B^{(T)}) = m \circ h(B^{'(T)}) \]

\[ \square \]

### J Specific GNN architectures

In Section 6, we show experiments on synthetic datasets with several related architectures. Here are some explanation for them:

- **LRP-i-j**: Local Relational Pooling with egonet depth \( i \) and cropped subtensors of size \( j \), as described in the main text. In our experiments, we take \( i = 1 \), \( j = 4 \). Hence, the vectorized subtensor (or submatrix, as the graph is unattributed) is of size \( 4 \times 4 = 16 \). The nonlinear activation functions are chosen between ReLU and tanh by hand. The models are trained using the Adam optimizer Kingma and Ba (2014) with learning rate 0.1. The number of hidden dimensions is searched in \{1, 8, 16, 64, 128\}.

- **2-IGN**: 2nd-order Invariant Graph Networks proposed by Maron et al. (2018). In our experiments, we take 8 hidden dimensions for invariant layers and 16 hidden dimensions for output multi-layer perceptron. The models are trained using the Adam optimizer with learning rate 0.1. The numbers of hidden dimensions are searched in \{(16, 32), (8, 16), (64, 64)\}.

- **GCN**: Graph Convolutional Networks proposed by Kipf and Welling (2016). In our experiments, we adopt a 4-layer GCN with 128 hidden dimensions. The models are trained using the Adam optimizer with learning rate 0.01. The number of hidden dimensions is searched in \{8, 32, 128\}. Depth is searched in \{2, 3, 4, 5\}.

- **GIN**: Graph Isomorphism Networks proposed by Xu et al. (2018a). In our experiments, we adopt a 4-layer GIN with 32 hidden dimensions. The models are trained using the Adam optimizer with learning rate 0.01. The number of hidden dimensions is searched in \{8, 16, 32, 128\}.

- **sGNN**: Spectral GNN with operators from family \{\( I, A, \min(A^2, 1) \)\}. In our experiments, we adopt a 4-layer sGNN with 128 hidden dimensions. The models are trained using the Adam optimizer with learning rate 0.01. The number of hidden dimensions is searched in \{8, 128\}.

For GCN, GIN and sGNN, we train four variants for each architecture, depending on whether Jumping Knowledge (JK) (Xu et al., 2018b) and Instance Normalization (IN) / Spatial Batch Normalization (Ulyanov et al., 2016; Ioffe and Szegedy, 2015) are included or not. The use of IN in GNNs is seen in Chen et al. (2019a), in which normalization is applied to each dimension of the hidden states of all nodes in each graph. For 2-IGNs, as IN is not immediately well-defined, we only train two variants, one with JK and one without. All models are trained for 100 epochs. Learning rates are searched in \{1, 0.1, 0.05, 0.01\}. We pick the best model with the lowest MSE loss on validation set to generate the results.

### K Experiment results

The variances of the ground truth counts are: 311.1696 for the 3-star task on the Erdős-Renyi dataset, 7.3441 for the triangle task on the Erdős-Renyi dataset, 316.1284 for the 3-star task on the Random Regular dataset, and 9.4249 for the triangle task on the Random Regular dataset.
Table 2: Test MSE loss for all models with chosen parameters as specified in Appendix J. We run each model for five times and picked the best and the median (3rd best) results for Table 1. Note that each of GCN, GIN and sGNN has four variants while 2-IGN has two variants. The reported rows in Table 1 are bolded here.

| Dataset: Erdős-Rényi | 3-Star (C) | Triangle (M) |
|-----------------------|------------|--------------|
| LRP-1-4               | 6.74E-03   | 2.05E-02     |
| 2-IGN                 | 3.23E-01   | 7.23E-00     |
| 2-IGN + JK            | 1.08E-01   | 7.22E-01     |
| GCN                   | 1.42E-102  | 1.51E-02     |
| GCN + JK              | 2.59E-02   | 1.51E-02     |
| GCN + IN              | 5.67E-104  | 9.48E-01     |
| GCN + JK + IN         | 3.91E-01   | 2.18E-01     |
| GIN                   | 9.31E-01   | 2.18E-01     |
| GIN + JK              | 1.68E-01   | 2.18E-01     |
| GIN + IN              | 9.31E-01   | 2.18E-01     |
| sGNN                  | 3.10E+00   | 3.10E+00     |
| sGNN + JK             | 1.04E+02   | 1.04E+02     |
| sGNN + IN             | 1.17E+04   | 1.17E+04     |
| sGNN + JK + IN        | 3.04E+02   | 3.04E+02     |

| Dataset: Random Regular | 3-Star (C) | Triangle (M) |
|-------------------------|------------|--------------|
| LRP-1-4                 | 8.89E-04   | 2.33E-03     |
| 2-IGN                   | 1.04E+02   | 2.33E-03     |
| 2-IGN + JK              | 3.82E+02   | 2.33E-03     |
| GCN                     | 8.85E+02   | 2.33E-03     |
| GCN + JK                | 8.92E+02   | 2.33E-03     |
| GCN + IN                | 1.08E+05   | 2.33E-03     |
| GCN + JK + IN           | 1.49E+04   | 2.33E-03     |
| GIN                     | 3.38E+01   | 1.28E+01     |
| GIN + JK                | 4.32E-01   | 1.28E+01     |
| GIN + IN                | 4.32E-01   | 1.28E+01     |
| sGNN                    | 7.50E-00   | 1.28E+01     |
| sGNN + JK               | 7.50E-00   | 1.28E+01     |
| sGNN + IN               | 4.32E+04   | 4.32E+04     |
| sGNN + JK + IN          | 4.43E+04   | 4.43E+04     |

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