The expressive power of $k$th-order invariant graph networks

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ABSTRACT

The expressive power of graph neural network formalisms is commonly measured by their ability to distinguish graphs. For many formalisms, the $k$-dimensional Weisfeiler-Leman ($k$-WL) graph isomorphism test is used as a yardstick. In this paper we consider the expressive power of $k$th-order invariant (linear) graph networks ($k$-IGNs). It is known that $k$-IGNs are expressive enough to simulate $k$-WL. This means that for any two graphs that can be distinguished by $k$-WL, one can find a $k$-IGN which also distinguishes those graphs. The question remains whether $k$-IGNs can distinguish more graphs than $k$-WL. This was recently shown to be false for $k = 2$. Here, we generalise this result to arbitrary $k$. In other words, we show that $k$-IGNs are bounded in expressive power by $k$-WL. This implies that $k$-IGNs and $k$-WL are equally powerful in distinguishing graphs.

1 Introduction

Graph neural networks (GNNs) have become a standard means to analyse graph data. One of the most widely adopted GNN formalisms are the so-called message-passing neural networks (MPNNs) (Scarselli et al., 2009; Gilmer et al., 2017). In MPNNs, features of vertices are iteratively updated based on the features of neighbouring vertices, and the current feature of the vertex itself. In their simplest form, when only the features of vertices are taken into account, the capability of MPNNs to distinguish vertices and graphs is rather limited. Indeed, Xu et al. (2019) and Morris et al. (2019) show that the expressive power of MPNNs is bounded by the 1-dimensional (Folklore) Weisfeiler-Leman (1-FWL) graph isomorphism test (Cai et al., 1992), or equivalently, the 2-dimensional Weisfeiler-Leman (2-WL) test (Grohe & Otto, 2015; Grohe, 2017)1. That is, when two graphs cannot be distinguished by 2-WL, then neither can they be distinguished by any MPNN. The expressive power of 2-WL is well-understood. For example, when two graphs cannot be distinguished by 2-WL then they can also not be distinguished by sentences in the two-variable fragment, $C_2$, of first-order logic with counting. More relevant in the context of GNNs is the complete characterisation of 2-WL in terms of invariant graph properties (Fürer, 2017; Arvind et al., 2020). For example, 2-WL is unable to detect cycles of length greater than four or triangles in graphs. We also like to point out connections between 2-WL and homomorphism profiles. More specifically, two graphs are indistinguishable by 2-WL if and only if they have the same number of homomorphisms from graphs of treewidth at most one (Dell et al., 2018). Finally, one can rephrase indistinguishability by 2-WL in terms of agreement of functions defined in terms of linear algebra operators (Geerts, 2019).

The limited expressive power of MPNNs is primarily due to the fact that vertices are anonymous, i.e., two vertices with the same feature are regarded as equivalent, and that only neighbouring vertices

1In works related to Weisfeiler-Leman one has to carefully consider whether or not the Folklore WL test is used. That is, in some papers, 1-WL refers to 1-FWL. For general $k$, $k$-FWL is equivalent to $(k + 1)$-WL (Grohe & Otto, 2015).
are considered. When, for example, MPNNs are degree-aware, meaning that they can distinguish vertices based on both their features and degrees, MPNNs get a slight jump start when compared to 2-WL and can potentially distinguish graphs in one iteration earlier than 2-WL (Geerts et al., 2020). Notable examples of degree-aware MPNNs are the graph convolutional networks by Kipf & Welling (2017). More powerful variants of MPNNs can be obtained by incorporating port numbering, which allows to treat features from different neighbours differently (Sato et al., 2019), assigning random initial features (Sato et al., 2020), and having static vertex identifiers (Loukas, 2020). We refer Sato (2020) for a more detailed overview of these and other variations of MPNNs.

Instead of considering 2-WL or variations of standard MPNNs, this paper concerns GNNs inspired by the $k$-dimensional Weisfeiler-Leman ($k$-WL) graph isomorphism test, for $k \geq 2$. These tests iteratively update features of $k$-tuples of vertices, based on the features of neighbouring $k$-tuples of vertices. It is known that the expressive power of $k$-WL grows with increasing $k$ (Cai et al., 1992). As such, they provide a promising basis for the development of more expressive GNNs. Of particular interest is the ability of $k$-WL, for $k \geq 2$, to distinguish graphs based on the presence or absence of specific graph patterns, such as cycles and cliques. For example, 3-WL can distinguish graphs based on their number of cycles up to 7 and triangles (Fürer, 2017; Geerts, 2019; Arvind et al., 2020). Furthermore, graphs that are indistinguishable by $k$-WL satisfy the same sentences in $C_k$, the $k$-variable fragment of first-order logic with counting (Cai et al., 1992), and this in turn is equivalent to the two graphs having the same number of homomorphisms from graphs of treewidth at most $k - 1$ (Dell et al., 2018). The latter correspondence has led NT & Maehara (2020) to define GNNs based on graph homomorphism convolutions. We refer to Grohe (2020) for other interesting interpretations of $k$-WL and relationships to embeddings of graph, and more generally, structured data.

Given the promise of an increase in expressive power, Morris et al. (2019) propose $k$-GNNs based a set-variant of $k$-WL. We will not consider this set-variant of $k$-WL in this paper and only mention that $k$-GNNs match the set-variant of $k$-WL in expressive power. More relevant to this paper is the work by Maron et al. (2019b) in which it is shown that the class of $k$th-order invariant graph networks ($k$-IGNs) is as powerful as $k$-WL in expressive power, for each $k \geq 2$. In other words, when two graphs can be distinguished by $k$-WL, then there exists a $k$-IGN which also distinguishes those graphs. Invariant graph networks ($k$-IGN) are built-up from equivariant layers defined over $k$th-order tensors (Kondor et al., 2018; Maron et al., 2019c). By contrast to $k$-WL, $k$-IGNs update features of $k$-tuples of vertices based on the features of all $k$-tuples, i.e., not only those that are neighbours as in $k$-WL. As a consequence, it is not immediately clear that $k$-IGNs are bounded by $k$-WL in expressive power. We remark, however, that in a $k$-IGN, not all (features of) $k$-tuples are treated the same due to the equivariance of its layers. More precisely, given a $k$-tuple $\bar{v}$ of vertices, the space of all $k$-tuples of vertices is partitioned according to which equality and inequality conditions are satisfied together with $\bar{v}$. Then, during the feature update process of $\bar{v}$, two $k$-tuples of vertices with the same feature may be treated differently by a $k$-IGN if the two $k$-tuples belong to different parts of the partition relative to $\bar{v}$.

Maron et al. (2019a) raise the natural question whether, despite that $k$-IGNs use more information than $k$-WL, the expressive power of $k$-IGNs is still limited to that of $k$-WL. In other words, can there be graphs that can be distinguished by a $k$-IGN which cannot be distinguished by $k$-WL. This question was recently answered by Chen et al. (2020) for $k = 2$. More precisely, they show that, for undirected graphs, the expressive power of 2-IGNs is indeed bounded by 2-WL. Furthermore, there is a one-to-one correspondence between the layers in a 2-IGN and iterations in 2-WL. That is, when two graphs cannot by distinguished by 2-WL in $t$ iterations, then neither can they be distinguished by a 2-IGN using $t$ equivariant layers.

In this paper, we generalise this result to arbitrary $k$. More precisely, we show that the expressive power of $k$-IGNs is indeed bounded by $k$-WL. What is interesting to note is that the one-to-one correspondence between iterations of $k$-WL and layers in $k$-IGNs needs to be revisited. As it turns out, for general $k$, each layer of a $k$-IGN can be seen to correspond to $k - 1$ iterations by $k$-WL. We remark that when $k = 2$, the one-to-one correspondence from Chen et al. (2020) is recovered. This implies that, in principle, a $k$-IGN can distinguish graphs a factor of $k - 1$ faster compared to $k$-WL. Of course, this comes at a cost of a more intensive feature update process involving all $k$-tuples of vertices. Chen et al. (2020) establish their result for $k = 2$ in a pure combinatorial way and by means of a case analysis, which is feasible for a fixed $k$. For general $k$, we borrow ideas from Chen et al. (2020) but additionally rely on the known connection between $k$-WL and the logic $C_k$ mentioned earlier. We remark that connections with logic, MPNNs and 2-WL have been used before to assess the logical expressiveness of MPNNs (Barceló et al., 2020).
We also remark that k-IGNs incur a large cost in memory and computation. Alternatives to k-IGNs are put forward based on the folklore k-dimensional Weisfeiler-Leman (k-FWL) test, which is known to be more efficient to implement. For example, Maron et al. (2019b) propose provably powerful graph networks (k-PPGNs) that are able to simulate k-FWL (and thus (k + 1)-WL) by using kth-order tensors only but in which the layers are allowed to use tensor multiplication. For 2-FWL, a single matrix multiplication suffices. The impact of matrix multiplication in layers has been further investigated in Geerts (2020). In that work, inspired by the work of Lichter et al. (2019), walk MPNNs are proposed as a general formalism for 2-PPGNs. It is readily verified that walk MPNNs are bounded in expressive power by 2-FWL, and since 2-PPGNs can be seen as instances of walk MPNNs, they are bounded in expressive power by 2-FWL as well (Geerts, 2020). This has been generalised by Azizian & Lelarge (2020) who show that k-PPGNs are bounded by k-FWL, for arbitrary k. We also note that allowing more than one matrix multiplication in 2-PPGNs does not increase their expressive power. Instead, multiple matrix multiplications may result in that 2-PPGNs can distinguish graphs faster than 2-FWL (Geerts, 2020). In this paper, we only consider k-IGNs and k-WL.

**Structure of the paper.** We start by describing k-WL, C_k and k-IGNs in Section 2. Then, in Section 2 we prove that k-IGNs are bounded by k-WL in expressive power. We conclude in Section 4.

2 Background

We first describe k-WL and its connections to logic, followed by the definition of k-IGNs. We use \{ \} to denote sets and \{ \} to denote multisets. The sets of natural and real numbers are denoted by \( \mathbb{N} \) and \( \mathbb{R} \), respectively. For \( n \in \mathbb{N} \) with \( n > 0 \), we define \( [n] := \{1, \ldots, n\} \). A (directed) graph \( G = (V(G), E(G)) \) consists of a vertex set \( V(G) \) and edge set \( E(G) \subseteq V^2 \). A (vertex-)coloured graph \( G = (V(G), E(G), \chi_G) \) is a graph in which every vertex \( v \in V(G) \) is assigned a colour \( \chi_G(v) \) in some set \( C \) of colours. In the following, when we refer to graphs we always mean coloured graphs. Without loss of generality we assume that \( V(G) = [n] \) for some \( n \in \mathbb{N} \). Furthermore, if \( A \in \mathbb{R}^{n \times p} \) is a kth-order tensor, then we denote by \( A_{\bar{v},s} \in \mathbb{R} \) with \( \bar{v} \in [n]^k \) and \( s \in [p] \) the value of \( A \) in entry \( (\bar{v}, s) \), and \( A_{\bar{v}, \bullet} \in \mathbb{R}^p \) denotes the vector \( (A_{\bar{v}, s} \mid s \in [p]) \) in \( \mathbb{R}^p \).

2.1 Weisfeiler-Leman

The k-dimensional Weisfeiler-Leman (k-WL) graph isomorphism test iteratively produces colourings of k-tuples of vertices, starting from a given graph \( G = (V(G), E(G), \chi_G) \). We follow here the presentation as given in Morris et al. (2019). Given \( G = (V(G), E(G), \chi_G) \), we denote by \( \chi_{G,k}^{(t)} : [n]^k \to C \) the colouring of k-tuples generated by k-WL after \( t \) rounds. For \( t = 0 \), \( \chi_{G,k}^{(0)} : [n]^k \to C \) is a colouring in which each k-tuple \( \bar{v} \in [n]^k \) is coloured with the isomorphism type of its induced subgraph. More specifically, \( \chi_{G,k}^{(0)}(v_1, \ldots, v_k) = \chi_{G,k}^{(0)}(v'_1, \ldots, v'_k) \) if and only if for all \( i \in [k] \) we have that \( \chi_G(v_i) = \chi_G(v'_i) \) and for all \( i, j \in [k] \), it holds that \( v_i = v_j \) if and only if \( v'_i = v'_j \) and \( (v_i, v_j) \in E(G) \) if and only if \( (v'_i, v'_j) \in E(G) \). Then, for \( t > 0 \), we define the colouring \( \chi_{G,k}^{(t)} : [n]^k \to C \) as

\[
\chi_{G,k}^{(t)}(\bar{v}) := \text{Hash}\left(\chi_{G,k}^{(t-1)}(\bar{v}), (C_1^{(t)}(\bar{v}), \ldots, C_k^{(t)}(\bar{v}))\right),
\]

in which for \( i \in [k] \),

\[
C_i^{(t)}(\bar{v}) := \text{Hash}\left(\{\chi_{G,k}^{(t-1)}(\bar{v}[v_i/v']) \mid v' \in [n]\}\right),
\]

where \( \bar{v}[v_i/v'] := (v_1, \ldots, v_{i-1}, v', v_{i+1}, \ldots, v_k) \) and \( \text{Hash}(\cdot) \) is a hash function that maps its input in an injective manner to a colour in \( C \).

Let \( \chi_1, \chi_2 : [n]^k \to C \) be colourings of k-tuples of vertices in \( G \). We say that \( \chi_1 \) refines \( \chi_2 \), denoted by \( \chi_1 \preceq \chi_2 \), if for all \( \bar{v}, \bar{v}' \in [n]^k \) we have \( \chi_1(\bar{v}) = \chi_1(\bar{v}') \Rightarrow \chi_2(\bar{v}) = \chi_2(\bar{v}') \). Then \( \chi_1 \preceq \chi_2 \) hold, we say that \( \chi_1 \) and \( \chi_2 \) are equivalent and we denote this by \( \chi_1 \equiv \chi_2 \).

We note that, by definition, \( \chi_{G,k}^{(t)} \preceq \chi_{G,k}^{(t-1)} \) for all \( t \geq 1 \). We define \( \chi_{G,k} \) as \( \chi_{G,k}^{(t)} \) for which \( \chi_{G,k}^{(t)} = \chi_{G,k}^{(t+1)} \) holds. It is known that this “stable” colouring is obtained in a most \( n^{O(k)} \) rounds. For
two graphs \( G = (V(G), E(G), \chi_G) \) and \( H = (V(H), E(H), \chi_H) \), one says that k-WL distinguishes \( G \) and \( H \) in round \( t \) if
\[
\{ \chi_{G,k}^{(t)}(\bar{v}) \mid \bar{v} \in (V(G))^k \} \neq \{ \chi_{H,k}^{(t)}(\bar{w}) \mid \bar{w} \in (V(H))^k \}.
\]
We write \( G \equiv_{k-WL}^t H \) if k-WL does not distinguish \( G \) and \( H \) in round \( t \). When \( G \equiv_{k-WL}^t H \) for all \( t \geq 0 \), we write \( G \equiv_{k-WL} H \) and say that \( G \) and \( H \) cannot be distinguished by k-WL.

2.2 Counting logics

The \( k \)-dimensional Weisfeiler-Leman graph isomorphism test is closely tied to the \( k \)-variable fragment of first-order logic with counting, denoted by \( C_k \), on graphs. This logic is defined over a finite set of \( k \) variables, \( x_1, \ldots, x_k \), and a formula \( \varphi \) in \( C_k \) is formed according to the following grammar:
\[
\varphi ::= x_i = x_j \mid \text{Col}_c(x_i) \mid \text{Edge}(x_i, x_j) \mid \neg \varphi \mid \varphi_1 \land \varphi_2 \mid \exists^2\tau x_i \varphi,
\]
for \( i, j \in [k] \), \( c \in C \), \( r \in \mathbb{N} \) with \( r > 0 \). The first three cases in the grammar correspond to so-called atomic formulas. For a formula \( \varphi \), we define its free variables \( \text{free}(\varphi) \) in an inductive way, i.e., \( \text{free}(x_i = x_j) := \{ x_i, x_j \} \), \( \text{free}(\text{Col}_c(x_i)) := \{ x_i \} \), \( \text{free}(\text{Edge}(x_i, x_j)) := \{ x_i, x_j \} \), \( \text{free}(\neg \varphi) := \text{free}(\varphi) \), \( \text{free}(\varphi_1 \land \varphi_2) := \text{free}(\varphi_1) \cup \text{free}(\varphi_2) \), and \( \text{free}(\exists^2\tau x_i \varphi) := \text{free}(\varphi) \setminus \{ x_i \} \). We write \( \varphi(x_1, \ldots, x_k) \) to indicate that all free variables of \( \varphi \) are among \( x_1, \ldots, x_k \). A sentence is formula without free variables. We further need the quantifier rank of a formula \( \varphi \), denoted by \( \text{qr}(\varphi) \). It is defined as follows: \( \text{qr}(\varphi) := 0 \) if \( \varphi \) is atomic, \( \text{qr}(\neg \varphi) := \text{qr}(\varphi) \), \( \text{qr}(\varphi_1 \land \varphi_2) := \max\{\text{qr}(\varphi_1), \text{qr}(\varphi_2)\} \), and \( \text{qr}(\exists^2\tau x_i \varphi) := \text{qr}(\varphi) + 1 \).

Let \( G = (V(G), E(G), \chi_G) \) be a graph and let \( \varphi(x_1, \ldots, x_k) \) be a formula in \( C_k \). Consider an assignment \( \alpha \) from the variables \( \{x_1, \ldots, x_k\} \) to vertices in \( V(G) \). We denote by \( \alpha(x_i) = v \) for \( v \in V(G) \) the assignment which is equal to \( \alpha \) except that \( \alpha(x_i) := v \). We define the satisfaction of a formula by a graph, relative to an assignment \( \alpha \), denoted by \( G \models \varphi[\alpha] \), in an inductive manner. That is, \( G \models (x_i = x_j)[\alpha] \) if and only if \( \alpha(x_i) = \alpha(x_j) \), \( G \models \text{Col}_c(x_i)[\alpha] \) if and only if \( \chi_H(\alpha(x_i)) = c \), \( G \models \text{Edge}(x_i, x_j)[\alpha] \) if and only if \( \alpha(x_i), \alpha(x_j) \in E, G \models \neg \varphi[\alpha] \) if and only if not \( G \models \varphi[\alpha] \), \( G \models (\varphi_1 \land \varphi_2)[\alpha] \) if and only if \( G \models \varphi_1[\alpha] \) and \( G \models \varphi_2[\alpha] \), and finally, \( G \models \exists^2\tau x_i \varphi[\alpha] \) if and only if there are at least \( \tau \) distinct vertices \( v_1, \ldots, v_{\tau} \) in \( V(G) \) such that \( G \models \varphi[\alpha(x_i/v_j)] \) holds for all \( j \in [\tau] \).

When \( G \) and \( H \) satisfy the same sentences in \( C_k \) of quantifier rank at most \( t \), we denote this by \( G \equiv_{C_k}^t H \). If \( G \equiv_{C_k}^t H \) holds for all \( t \geq 0 \), then we write \( G \equiv_{C_k} H \) and say that \( G \) and \( H \) are indistinguishable by \( C_k \). The connection to k-WL is as follows.

**Theorem 1** (Cai et al., 1992). Let \( G \) and \( H \) be two graphs. Then, \( G \equiv_{k-WL}^t H \) if and only if \( G \equiv_{C_k}^t H \). As a consequence, \( G \equiv_{k-WL} H \) if and only if \( G \equiv_{C_k} H \). \( \square \)

Of particular interest is that the proof of this theorem shows that, for \( c \in C \), there exists a formula \( \psi^{(t)}_c(x_1, \ldots, x_k) \) in \( C_k \) of quantifier rank at most \( t \) such \( \chi_{G,k}^{(t)}(v_1, \ldots, v_k) = c \) if and only if \( G \models \psi^{(t)}_c[\alpha] \) with \( \alpha \) defined as \( x_i \mapsto v_i \).

Later in the paper we also use the shorthand notation \( \exists^2\tau(x_1, \ldots, x_{\ell}) \varphi \) to indicate that are at least \( \ell \) distinct \( \tau \)-tuples satisfying \( \varphi \). It is readily verified\(^2\) that if \( \varphi \) is a formula in \( C_k \) of quantifier rank \( t \), then \( \exists^2\tau(x_1, \ldots, x_{\ell}) \varphi \) is equivalent to a formula in \( C_k \) of quantifier rank at most \( t + \ell \). Here, two formulas \( \varphi \) and \( \psi \) are equivalent if \( G \models \varphi[\alpha] \) if and only if \( G \models \psi[\alpha] \) for all assignments \( \alpha \) and graphs \( G \). As a consequence, quantifiers of the form \( \exists^2\tau(x_1, \ldots, x_{\ell}) \varphi \) for \( \ell > 1 \) do not add expressive power to \( C_k \). In what follows, for a formula \( \varphi(x_1, \ldots, x_k) \) and assignment \( \alpha \), we write \( \varphi[v_1, \ldots, v_k] \) instead of \( \psi^{(t)}_c[\alpha] \) with \( \alpha \) such that \( x_i \mapsto v_i \).

2.3 Invariant graph neural networks

Let \( S_n \) denote the symmetric group over \( [n] \), i.e., \( S_n \) consists of all permutation \( \pi \) of \( [n] \). Let \( \pi \in S_n \) and \( A \) a tensor in \( \mathbb{R}^{n^k \times p} \). We define \( \pi \ast A \in \mathbb{R}^{n^k \times p} \) such that \( \pi \ast A)_{\bar{v}(\pi)} = A_{\bar{v}} \) for all \( \bar{v} \in [n]^k \). A \( k \)-th order equivariant linear layer is a mapping \( L : \mathbb{R}^{n^k \times p} \rightarrow \mathbb{R}^{n^q \times q} \) such that \( L(\pi \ast A) = \pi \ast L(A) \) for all \( A \in \mathbb{R}^{n^k \times p} \). When \( \ell = 0 \), and thus \( L(\pi \ast A) = L(A) \) for all

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\(^2\)I would like to acknowledge Jan Van den Bussche for pointing this out.
We next use the \( \chi \) described by a partition \( n \). The colour \( F \) of \( \chi \) can be distinguished by a pointwise non-linear activation function such as the ReLU function, \( I \) is a linear invariant layer from \( R^{n \times s_0} \rightarrow R^{s_0} \), and \( M \) is a multi layer perceptron (MLP) from \( R^{s_0+1} \rightarrow R^s \).

We next use k-IGNs \( F \) to define an equivalence relation on graphs. To do so, we first turn a graph \( G = (V(G),E(G),\chi_G) \) into a tensor \( A_G \in R^{n \times s_0} \). More precisely, we consider the initial k-WL colouring \( \chi_{G,k}^{(0)} : [n]^k \rightarrow C \) (recall that we identified \( V(G) \) with \( [n] \)). Then, suppose that \( \chi_{G,k}^{(0)} \) assigns \( s_0 \) distinct colours \( c_1, \ldots, c_{s_0} \) to the \( k \)-tuples in \( [n]^k \). We identify each colour \( c_s \) with the \( s \)-th basis vector \( b_s \) in \( R^{s_0} \) and define for \( \bar{v} \in [n]^k \) and \( s \in [s_0] \), \( (A_G)_{\bar{v},s} := 1 \) if \( \chi_{G,k}^{(0)}(\bar{v}) = c_s \) and \( (A_G)_{\bar{v},s} := 0 \) otherwise. Given this, we say that two graphs \( G \) and \( H \) are indistinguishable by a k-IGN \( F \), denoted by \( G \equiv_f H \), if and only if \( F(A_G) = F(A_H) \). We also consider another equivalence relation defined in terms the \( F \)-ignorant part of an k-IGN \( F \). More precisely, for \( t > 0 \), let \( F^{(t)} : R^{n \times s_0} \rightarrow R^{n \times s_t} \) defined by \( F^{(t)} := \sigma \circ L^{(t)} \circ \cdots \circ \sigma \circ L^{(1)} \). We let \( F^{(0)} \) be the identity mapping from \( R^{n \times s_0} \rightarrow R^{n \times s_0} \). We then denote by \( G \equiv^{(t)}_F H \) that

\[
\{ (F^{(t)}(A_G))_{\bar{v},s} : \bar{v} \in (V(G))^k \} = \{ (F^{(t)}(A_H))_{\bar{w},s} : \bar{w} \in (V(H))^k \}.
\]

In other words, when viewing the tensors \( F^{(t)}(A_G) \) and \( F^{(t)}(A_H) \) in \( R^{n \times s_t} \) as colouring of \( k \)-tuples, i.e., \( \bar{v} \in (V(G))^k \) is assigned the “colour” \( F^{(t)}(A_G)_{\bar{v},s} \in R^{s_t} \) and similarly, \( \bar{w} \in (V(H))^k \) is assigned the “colour” \( F^{(t)}(A_H)_{\bar{w},s} \in R^{s_t} \), then \( G \equiv^{(t)}_F H \) just says these labelings are equivalent. In the remainder of the paper we establish correspondences between \( \equiv^{(t)}_F \) and \( \equiv^d_F \), and the equivalence relations \( \equiv^{(t)}_{k-WL} \) and \( \equiv_k-WL \).

3 The expressive power of k-IGNs

Let us start by recalling what is known about the relationship between the equivalence relations \( \equiv^{(t)}_{k-WL} \) and \( \equiv^d_F \). For every \( k \geq 2 \) and any two graphs \( G \) and \( H \), it is known that there exists a k-IGN \( F \) such that \( G \equiv^d F H \Rightarrow G \equiv^{(k-1)}_{k-WL} H \) (Maron et al., 2019b). In other words, if \( G \) and \( H \) can be distinguished by k-WL, then the k-IGN \( F \) distinguishes them as well. Hence, the class of k-IGNs is powerful enough to match k-WL in expressive power. The k-IGN \( F \) used by Maron et al. (2019b) consists of \( d \) equivariant layers, where \( d \) is such that k-WL reaches the stable colourings \( \chi_{G,k} \) and \( \chi_{H,k} \) of \( G \) and \( H \), respectively, in \( d \) rounds. In fact, Maron et al. (2019b) show that \( G \equiv^{(t)}_F H \Rightarrow G \equiv^{(t)}_{k-WL} H \) holds as well, for \( t \in [d] \), so the rounds of k-WL and the layers of \( F \) are
in one-to-one correspondence. It was posed as an open problem in Maron et al. (2019a) whether or not k-IGNs can distinguish more graphs than k-WL. More specifically, the question is whether the implication \( G \equiv_{k\text{-WL}} H \Rightarrow G \equiv_F H \) also holds, and this for any k-IGN \( F \). This question was recently answered for \( k = 2 \). Indeed, Chen et al. (2020) show that \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_F H \) holds for any 2-IGN \( F \). As a consequence, 2-WL and 2-IGNs have equal distinguishing power. In proving \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_F H \), Chen et al. (2020) show first that, when \( F \) consists of \( d \) equivariant layers, then for each \( t \in \mathbb{N} \) \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_{2t\text{-WL}} H \). By leveraging this, they then verify \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_F H \). Since \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_{2t\text{-WL}} H \) for all \( t \geq 0 \), the implication \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_F H \) follows. We remark that Chen et al. (2020) consider undirected graphs only. We next generalise this result to arbitrary \( k \geq 2 \) and to directed graphs. In other words, our main result is:

**Theorem 2.** For any two graphs \( G \) and \( H \), \( G \equiv_{k\text{-WL}} H \Rightarrow G \equiv_F H \) for any k-IGN \( F \).

This theorem will be proved, in analogy with the proof by Chen et al. (2020), by using Lemmas 3 and 4 below. The first lemma is the counterpart, for general \( k \), of the implication \( G \equiv_{2\text{-WL}} H \Rightarrow G \equiv_F H \) by Chen et al. (2020). We see, however, that the correspondence between rounds of k-WL and layers in k-IGNs is slightly more involved.

**Lemma 3.** Let \( F \) be a k-IGN consisting of \( d \) equivariant layers and consider graphs \( G \) and \( H \). Then for any \( t \geq 0 \),

\[
G \equiv_{t\text{-WL}} H \Rightarrow G \equiv_{\frac{t}{k}\text{-WL}} H.
\]

(\dagger)

Note that when \( k = 2 \), \( \frac{t}{k} = t \) and hence the known implication for \( k = 2 \) from Chen et al. (2020) is recovered. Since \( F \) consists of \( d \) layers, we limit \( t \) to be in the range of \((d+1)(k-1)-1\) such that \( \frac{t}{k} \leq d \). As part of the proof of Lemma 3 we show a stronger implication. More precisely, we show that if \( G \equiv_{t\text{-WL}} H \) holds, then

\[
\chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \Rightarrow (F^{(1\times\frac{t}{k}-1)}(A_G))_{\bar{v},\bar{w}} = (F^{(1\times\frac{t}{k}-1)}(A_H))_{\bar{w},\bar{w}}.
\]

for any \( \bar{v}, \bar{w} \in (V(G))^k \). We use this property in the next lemma.

**Lemma 4.** Let \( F \) be a k-IGN consisting of \( d \) equivariant layers and consider graphs \( G \) and \( H \). Let \( t = d(k-1) \) and assume that the following implication holds for \( \bar{v}, \bar{w} \in (V(G))^k \):

\[
\chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \Rightarrow (F^{(d)}(A_G))_{\bar{v},\bar{w}} = (F^{(d)}(A_H))_{\bar{w},\bar{w}}.
\]

Then \( G \equiv_{t\text{-WL}} H \Rightarrow G \equiv_{t\text{-WL}} H \).

These two lemmas suffice to prove Theorem 2:

**Proof.** Indeed, suppose that \( G \equiv_{t\text{-WL}} H \) holds. By definition, this implies \( G \equiv_{t\text{-WL}} H \) for all \( t \geq 0 \). In particular, this holds for \( t = d(k-1) \). As mentioned above, as part of proving Lemma 3 we obtain for \( \bar{v}, \bar{w} \in (V(G))^k \), the implication \( \chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \Rightarrow (F^{(d)}(A_G))_{\bar{v},\bar{w}} = (F^{(d)}(A_H))_{\bar{w},\bar{w}} \). Then, Lemma 4 implies \( G \equiv_F H \), as desired.

Before showing the lemmas, we provide some intuition behind the implication (\dagger) in Lemma 3. In a nutshell, it reflects that a single (equivariant) layer of a k-IGN corresponds to \( k-1 \) rounds of k-WL. This is because k-IGNs propagate information to \( k \)-tuples from all other \( k \)-tuples, whereas k-WL only propagates information from neighbouring \( k \)-tuples.

To see this, consider \( k = 3 \) and let \( \bar{v} = (v_1, v_2, v_3) \) be a triple in \((V(G))^3 \). When a 3-IGN \( F \) applies a layer \( L^{(t)} \), the vector \( (L^{(t)}(F^{(t-1)}(A_G)))_{\bar{v},\bar{w}} \) is computed based on all vectors \( (F^{(t-1)}(A_G))_{\bar{v}',\bar{w}} \) with \( \bar{v}' = (v_1', v_2', v_3') \) with \( v_i' \) and \( v_i'' \) being different from \( v_i \), \( v_2 \), and \( v_3 \). By contrast, in round 3, 3-WL updates the label of \( \bar{v} \) only based on the labels, computed in round \( t-1 \), of triples of the form \((v_1', v_2, v_3), (v_1, v_2', v_3), (v_1, v_2, v_3') \) and \((v_1, v_2, v_3')\) for \( v_1', v_2', v_3' \in V(G) \). We observe that the triple \( \bar{v}' \) is not included here and hence the label \( \bar{v} \) is not updated in round \( t \) based on the label, computed in round \( t-1 \), of \( \bar{v}' \). We note, however, that in round \( t \), 3-WL also updates the label of the triple \((v_1, v_2, v_3')\).
based on the label, computed in round $t - 1$, of $\bar{v}' = (v_1, v_2, v_3)$ as $\bar{v}'$ is now one of the neighbours of $(v_1, v_2, v_3)$. As a consequence, in round $t + 1$, 3-WL will update the label of $\bar{v}$ based on the label, computed in round $t$, of $(v_1, v_2, v_3)$. The latter now depends on the label, computed in round $t - 1$, of $\bar{v}'$. Hence, only in round $t + 1$ the label of $\bar{v}$ includes information about the label, computed in round $t - 1$, of $\bar{v}'$. By contrast, as we have seen earlier, \( L^{(t)}(F^{(t-1)}(A_G)) \) immediately takes into account information from $\bar{v}' = (v_1, v_2, v_3)$. We thus see that 3-WL needs two rounds for a single application of an equivariant layer in a 3-IGN. In other words, $t$ rounds of 3-WL correspond to application of $\frac{t}{2}$ equivariant layers in an 3-IGN. This holds more generally for any $k \geq 2$.

Furthermore, it is thanks to the invariance and equivariance of the layers in k-IGNs that the information propagation happens in a controlled way. More specifically, a k-IGN propagates information from triples with the same equality pattern in the same way. As we will see shortly, this is crucial for showing Lemmas 3 and 4.

3.1 Proof of Lemma 3

We show $G \equiv^t \text{WL}_k H \Rightarrow G \equiv^t F^{(t)} H$ by induction on $t$. The proof strategy is similar to the one used by Chen et al. (2020) except that we rely on a more general key lemma in the inductive step. As mentioned earlier, we will show a stronger induction hypothesis. More specifically, we show that for any $t$ and $k$-tuples $\bar{v} \in (V(G))^k$ and $\bar{w} \in (V(H))^k$, if $G \equiv^t H$, then

\[
\chi_{G,k}((\bar{v})) = \chi_{H,k}((\bar{w})) \Rightarrow (F^{(1)}(\bar{v}))(A_G) = (F^{(1)}(\bar{w}))(A_H). \tag{\dagger}
\]

It is an easy observation that the implication (\dagger) implies $G \equiv^t H \Rightarrow G \equiv^t F H$. Indeed, suppose that $G \equiv^t H$ holds. By definition, this is equivalent to

\[
\left\{ \chi_{G,k}(\bar{v}) \mid \bar{v} \in (V(G))^k \right\} = \left\{ \chi_{H,k}(\bar{w}) \mid \bar{w} \in (V(H))^k \right\}.
\]

In other words, with every $\bar{v} \in (V(G))^k$ one can associate a corresponding $\bar{w} \in (V(H))^k$ such that $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$. Then, (\dagger) implies $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$, (\dagger) holds. Since this holds for any $\bar{v} \in (V(G))^k$ and its corresponding $\bar{w} \in (V(H))^k$, we have

\[
\left\{ (F^{(1)}(\bar{v}))(A_G) \mid \bar{v} \in (V(G))^k \right\} = \left\{ (F^{(1)}(\bar{w}))(A_H) \mid \bar{w} \in (V(H))^k \right\}.
\]

This in turn is equivalent to $G \equiv^t F H$, by definition.

Furthermore, we observe that it suffices to show (\dagger) for $t$ being a multiple of $k - 1$. Indeed, suppose that $t$ is not a multiple of $k - 1$. That is, $t = m(k - 1) + r$ for some $m, r \in \mathbb{N}$ satisfying $0 < r < k - 1$. Let us consider $t' = m(k - 1)$ and note that $\frac{t'}{k-1} = \frac{m(k-1)}{k-1} = m$. Suppose that we already have shown (\dagger) for $t'$. It now suffices to observe that $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$ implies $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$ since k-WL produces refinements of colourings and $t' \leq t$. Because, by assumption, $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$ implies $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w})$, and $\frac{t'}{k-1} = \frac{m(k-1)+r}{k-1} = m$, we may conclude that (\dagger) holds for $t$ as well. In the following we therefore assume that $t = m(k - 1)$ for some $m \in \mathbb{N}$ with $0 \leq m \leq d$. We next show the implication (\dagger).

**Base case.** In this case, $t = 0$ and the induction hypothesis is $\chi_{G,k}^{(0)}(\bar{v}) = \chi_{H,k}^{(0)}(\bar{w}) \Rightarrow (F^{(0)}(\bar{v}))(A_G) = (F^{(0)}(\bar{w}))(A_H)$. Since $F^{(0)}$ is defined as the identity mapping, we need to verify $(A_G)_{\bar{v}} = (A_H)_{\bar{w}}$. We note, however, that $A_G$ and $A_H$ are defined by hot-one encoding $\chi_{G,k}$ and $\chi_{H,k}$, respectively. In particular, if $\chi_{G,k}(\bar{v}) = \chi_{H,k}(\bar{w}) = s$ for $s \in [s_0]$ and $s_0 \in C$ (recall that $s_0$ denotes the number of colours assigned by the initial k-WL colouring), then

\[
(A_G)_{\bar{v}} = b_s = (A_H)_{\bar{w}},
\]

where $b_s$ is the $s$th basis vector in $\mathbb{R}^{s_0}$. In other words, the base case holds.
Inductive case. Let \( t = m(k - 1) \) for some \( m \in [d] \) and assume that (\( \dagger \)) holds for \( t' = (m - 1)(k - 1) \). We claim that (\( \dagger \)) holds for \( t \), provided that we can show the key lemma below. The lemma is shown by a different proof technique than used by Chen et al. (2020) for \( k = 2 \). More specifically, we leverage the connection between \( k \)-WL and counting logics. By contrast, Chen et al. (2020) use a case analysis and combinatorical arguments which do not easily generalise to arbitrary \( k \). We defer the proof the lemma to Section 3.3.

Key Lemma. Let \( t = m(k - 1) \) and \( t' = (m - 1)(k - 1) \) for \( m \in \mathbb{N} \) and \( m \geq 1 \). Let \( G \) and \( H \) be such that \( G \equiv_{k \text{-WL}}^t H \) holds and let \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \) be \( k \)-tuples satisfying \( \chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \). Then,

\[
\left\{ (\chi_{G,k}^{(t')}(\bar{v}'), \bar{v}' \in \mu) \right\} = \left\{ (\chi_{H,k}^{(t')}(\bar{w}'), \bar{w}' \in \mu) \right\}
\]

(\( \ddagger \ddagger \)) for every equality pattern \( \mu \in [n]^{2k}/\sim \).

Intuitively, this lemma allows us to reason over multisets of colours of \( k \)-tuples grouped together according to an equality pattern. Since each equivariant layer in a \( k \)-IGNs treats tuples satisfying the same equality pattern in the same way, the lemma suffices to show the implication (\( \dagger \)). In the remainder of this section, we formally verify that the Key Lemma indeed implies the implication (\( \dagger \)) for \( t = m(k - 1) \).

Let us assume \( G \equiv_{k \text{-WL}}^t H \) and consider \( k \)-tuples \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \) satisfying \( \chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \). We need to show \( (F^{(m)}(A_G))_{\bar{v},*} = (F^{(m)}(A_H))_{\bar{w},*} \). We observe that \( G \equiv_{k \text{-WL}}^t H \) implies \( G \equiv_{k \text{-WL}}^{t'} H \) since \( t' \leq t \) and \( k \)-WL produces refinements of colourings. As a consequence, the Key Lemma applies. Furthermore, by induction, for any \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \), if \( G \equiv_{k \text{-WL}}^{t'} H \), then \( \chi_{G,k}^{(t')}(\bar{v}) = \chi_{H,k}^{(t')}(\bar{w}) \Rightarrow (F^{(m-1)}(A_G))_{\bar{v}',*} = (F^{(m-1)}(A_H))_{\bar{w}',*} \). From the equality (\( \ddagger \ddagger \)) we can now infer

\[
\left\{ (F^{(m-1)}(A_G))_{\bar{v}',*} \left| (\bar{v}, \bar{v}' \in \mu) \right\} = \left\{ (F^{(m-1)}(A_H))_{\bar{w}',*} \left| (\bar{w}, \bar{w}' \in \mu) \right\},
\]

(1)

for any \( \mu \in [n]^{2k}/\sim \). We recall that \( F^{(m)} = \sigma \circ L^{(m)} \circ F^{(m-1)} \). We next use that \( L^{(m)} : \mathbb{R}^{n^k × s_{m-1}} \to \mathbb{R}^{n^k × s_m} \) is an equivariant layer and hence can be decomposed according to equality types \( \mu \in [n]^{2k}/\sim \), as shown in Section 2. More specifically, we next show that the equality (1) implies

\[
(L^{(m)}(F^{(m-1)}(A_G)))_{\bar{v},*} = (L^{(m)}(F^{(m-1)}(A_H)))_{\bar{w},*},
\]

(2)

for every \( \mu \in [n]^{2k}/\sim \). Indeed, let us first recall that for \( a \in [s_m] \) and equality pattern \( \mu \in [n]^{2k}/\sim \):

\[
(L^{(m)}(F^{(m-1)}(A_G)))_{\bar{v},a} = \sum_{\bar{v}' \in [n]^k} \sum_{b \in [s_{m-1}]} c_{\mu,a,b} (F^{(m-1)}(A_G))_{\bar{v}',b},
\]

\[
(L^{(m)}(F^{(m-1)}(A_H)))_{\bar{w},a} = \sum_{\bar{w}' \in [n]^k} \sum_{b \in [s_{m-1}]} c_{\mu,a,b} (F^{(m-1)}(A_H))_{\bar{w}',b}.
\]

It now suffices to observe that the coefficients \( c_{\mu,a,b} \) only depend on the equality pattern \( \mu \), \( a \in [s_m] \) and \( b \in [s_{m-1}] \). From equality (1) we know that with each \( \bar{v}' \) satisfying \( (\bar{v}, \bar{v}') \in \mu \) we can associate a unique \( \bar{w}' \) satisfying \( (\bar{w}, \bar{w}') \in \mu \) such that for each \( b \in [s_{m-1}] \),

\[
(F^{(m-1)}(A_G))_{\bar{v}',b} = (F^{(m-1)}(A_H))_{\bar{w}',b},
\]

and thus also

\[
c_{\mu,a,b} (F^{(m-1)}(A_G))_{\bar{v}',b} = c_{\mu,a,b} (F^{(m-1)}(A_H))_{\bar{w}',b}
\]

holds. Given that \( (L^{(m)}(F^{(m-1)}(A_G)))_{\bar{v},*} \) and \( (L^{(m)}(F^{(m-1)}(A_H)))_{\bar{w},*} \) are defined as the sums over elements \( \bar{v}' \) and \( \bar{w}' \) satisfying \( (\bar{v}, \bar{v}') \in \mu \) and \( (\bar{w}, \bar{w}') \in \mu \), respectively, we may conclude that \( (L^{(m)}(F^{(m-1)}(A_G)))_{\bar{v},*} = (L^{(m)}(F^{(m-1)}(A_H)))_{\bar{w},*} \), as desired.
We next show that equality (2) implies
\[
\left( L^{(m)}(F^{(m-1)}(A_G)) \right)_{\bar{e}, \bullet} = \left( L^{(m)}(F^{(m-1)}(A_H)) \right)_{\bar{w}, \bullet}.
\] (3)
Indeed, we recall that for \( a \in [s_m] \):
\[
\left( L^{(m)}(F^{(m-1)}(A_G)) \right)_{\bar{e}, a} = \sum_{\mu \in [n]^{2k}/\sim} \left( L^{(m)}(F^{(m-1)}(A_G)) \right)_{\bar{e}, a} + c_{\tau, a}
\]
\[
\left( L^{(m)}(F^{(m-1)}(A_H)) \right)_{\bar{w}, a} = \sum_{\mu \in [n]^{2k}/\sim} \left( L^{(m)}(F^{(m-1)}(A_H)) \right)_{\bar{w}, a} + c_{\tau', a}
\]
where \( \tau, \tau' \in [n]^{k}/\sim \) and \( \bar{v} \in \tau \) and \( \bar{w} \in \tau' \). Clearly, (2) implies (3) if we can show that \( \tau = \tau' \) and thus \( c_{\tau, a} = c_{\tau', a} \) for all \( a \in [s_m] \). Stated differently, we need to show that \( \bar{v} \sim \bar{w} \). This is, however, a direct consequence of the assumption \( \chi^{(t)}_{G,K}(\bar{v}) = \chi^{(t)}_{H,K}(\bar{w}) \). Indeed, \( \chi^{(t)}_{G,K}(\bar{v}) = \chi^{(t)}_{H,K}(\bar{w}) \) implies
\[
\chi^{(0)}_{G,K} = \chi^{(0)}_{H,K}(\bar{w}),
\]
which in turn implies that \( \bar{v} \) and \( \bar{w} \) have the same isomorphism type.

To conclude the proof, it remains to show \( F^{(m)}(A_G)_{v, \bullet} = F^{(m)}(A_H)_{\bar{w}, \bullet} \). We recall again that \( F^{(m)} = \sigma \circ L^{(m)} \circ F^{(m-1)} \) and hence, due to the equality (3) it suffices to observe that (3) remains to true after applying the activation function \( \sigma \). We recall that such an activation function \( \sigma \) is defined in a pointwise manner. That is, for a vector \( \bar{a} \in \mathbb{R}^{q} \), \( \sigma(\bar{a}) = (\sigma(a_1), \ldots, \sigma(a_q)) \). More generally, for a tensor \( A \in \mathbb{R}^{n^k \times q} \) and \( \bar{v} \in [n]^k \), \( \sigma(A)_{v, \bullet} = \sigma(A_{v, \bullet}) \). Hence, the equality (3) indeed implies
\[
\left( \sigma \left( L^{(m)}(F^{(m-1)}(A_G)) \right) \right)_{\bar{e}, \bullet} = \left( \sigma \left( L^{(m)}(F^{(m-1)}(A_H)) \right) \right)_{\bar{w}, \bullet},
\]
from which \( F^{(m)}(A_G)_{v, \bullet} = F^{(m)}(A_H)_{\bar{w}, \bullet} \) follows, as desired. 

\[ \square \]

3.2 Proof of Lemma 4

Let \( t = d(k - 1) \). We show that if for any two \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \), we have \( \chi^{(t)}_{G,K}(\bar{v}) = \chi^{(t)}_{H,K}(\bar{w}) \Rightarrow (F^{(d)}(A_G))_{v, \bullet} = (F^{(d)}(A_H))_{\bar{w}, \bullet} \), then \( G \equiv_L H \Rightarrow G \equiv_F H \) holds.

We assume that \( G \equiv_L H \) holds for \( t = d(k - 1) \). By definition, this implies
\[
\left\{ \chi^{(t)}_{G,K}(\bar{v}) \mid \bar{v} \in (V(G))^k \right\} = \left\{ \chi^{(t)}_{H,K}(\bar{w}) \mid \bar{w} \in (V(H))^k \right\}.
\] (4)

Furthermore, we observe that \( \chi^{(t)}_{G,K}(\bar{v}) = \chi^{(t)}_{H,K}(\bar{w}) \Rightarrow \chi^{(0)}_{G,K}(\bar{v}) = \chi^{(0)}_{H,K}(\bar{w}) \). As observed earlier, this implies that \( \bar{v} \sim \bar{w} \). In other words, \( \bar{v} \) and \( \bar{w} \) have the same equality pattern \( \tau \in [n]^k/\sim \). As a consequence, together with (4) this implies that for every \( \tau \in [n]^k/\sim \),
\[
\left\{ \chi^{(t)}_{G,K}(\bar{v}) \mid \bar{v} \in \tau, \bar{v} \in (V(G))^k \right\} = \left\{ \chi^{(t)}_{H,K}(\bar{w}) \mid \bar{w} \in \tau, \bar{w} \in (V(H))^k \right\}.
\] (5)

We further assume that for \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \), \( \chi^{(t)}_{G,K}(\bar{v}) = \chi^{(t)}_{H,K}(\bar{w}) \Rightarrow (F^{(d)}(A_G))_{v, \bullet} = (F^{(d)}(A_H))_{\bar{w}, \bullet} \). Hence, (5) implies
\[
\left\{ (F^{(m)}(A_G))_{v, \bullet} \mid \bar{v} \in \tau \right\} = \left\{ (F^{(m)}(A_H))_{\bar{w}, \bullet} \mid \bar{w} \in \tau \right\}
\] (6)
for every equality pattern \( \tau \in [n]^k/\sim \).

We now recall that \( F = M \circ I \circ F^{(d)} \) and we need to show that \( F(A_G) = F(A_H) \). It suffices to show that \( I(F^{(d)}(A_G)) = I(F^{(d)}(A_H)) \) since \( M \) is an MLP which encodes a function from
We recall that $I$ is an invariant layer from $\mathbb{R}^{n \times s_{d+1}}$ to $\mathbb{R}^s$. Since invariant layers are a special case of equivariant layers, they can again be decomposed based on equality patterns. More specifically, for a tensor $A \in \mathbb{R}^{n \times s_{d+1}}$ and $a \in [s_{d+1}]$,

$$I(A)_a = \sum_{\tau \in [n]/\sim} I_\tau(A)_a + c_a \text{ with } I_\tau(A)_a = \sum_{\bar{\nu} \in [n]/\sim} \sum_{\bar{\nu}' \in \tau} c_{\tau,a,b} A_{\bar{\nu}',b}.$$ Then, just as in the proof of Lemma 3, when $I$ is applied to $F^{(m)}(A_G)$ and $F^{(m)}(A_H)$, and by observing that the constants $c_{\tau,a,b}$ only depend on $\tau$, $a$ and $b$, we can conclude from (6) that

$$(I(F^{(m)}(A_G))_a) = (I(F^{(m)}(A_H))_a) \text{ for all } a \in [s_{d+1}].$$ In other words, $I(F^{(d)}(A_G)) = I(F^{(d)}(A_H))$ and thus $G \equiv_F H$, as desired. \hfill $\Box$

### 3.3 Proof of the key lemma

Let $m = (k-1)$ and $\ell' = (m-1)(k-1)$. We recall that the Key Lemma requires us to show that if $\bar{v}$ and $\bar{w}$ satisfy $\chi^{(l)}_{G,k}(\bar{v}) = \chi^{(\ell)}_{H,k}(\bar{w})$ and if $G \equiv^{\ell'}_{k,\text{WL}} H$ holds, then

$$\{\chi^{(\ell')}_{G,k} (\bar{v}' ) \mid (\bar{v}, \bar{v}') \in \mu\} = \{\chi^{(\ell')}_{H,k} (\bar{w}' ) \mid (\bar{w}, \bar{w}') \in \mu\}$$

for any equality pattern $\mu \in [n]/\sim$.

We will show the equality (7) by assuming, for the sake of contradiction, that there exists an equality pattern $\mu$ for which equality (7) does not hold. For such a pattern $\mu$, and $k$-tuples $\bar{v} \in (V(G))^k$ and $\bar{w} \in (V(H))^k$, we then construct a formula $\varphi(x_1, \ldots, x_k)$ in $C_k$ of quantifier rank at most $t$, such that $G \models \varphi[\bar{v}]$ but $H \not\models \varphi[\bar{w}]$. This contradicts $\chi^{(l)}_{G,k}(\bar{v}) = \chi^{(\ell)}_{H,k}(\bar{w})$ as this implies that $\bar{v}$ and $\bar{w}$ satisfy the same formulas in $C_k$ of quantifier rank at most $t$ (cfr. Theorem 1). In other words, no equality pattern $\mu$ can exist that violates (7). There will be some special equality patterns for which no formula can be constructed. We treat these cases separately using the assumption $G \equiv^{\ell'}_{k,\text{WL}} H$ instead.

We start by introducing some concepts related to equality patterns. Let $\mu \in [n]/\sim$, and let $\bar{v} = (v_1, \ldots, v_k) \in (V(G))^k$ and $\bar{v}' = (v_1', \ldots, v_k') \in (V(G))^k$. We represent $\mu$ by its partition $[2k] = I_1 \cup \cdots \cup I_r$. For a class $I_s$, with $s \in [r]$, we define $\text{rep}(I_s)$ as the smallest index $i$ in $I_s$. We now distinguish between different kinds of classes. A class $I_s$ is called constant if $\text{rep}(I_s) \leq k$. When $\text{rep}(I_s) > k$ we call $I_s$ variable. Among constant classes, we further distinguish between constant classes that are used, and those that are not. A constant class $I_s$ is called used when it contains entries strictly larger than $k$. Intuitively, indexes $i > k$ in a used constant class $I_s$ indicate that for $(\bar{v}, \bar{v}')$ to be in $\mu$, $v_i' \neq v_s'$ if and only if $v_s' \neq v_s$.

For notational convenience we introduce $P_{\mu, \bar{v}} := \{\bar{v}' \in (V(G))^k \mid (\bar{v}, \bar{v}') \in \mu\}$ and similarly, $Q_{\mu, \bar{w}} := \{\bar{w}' \in (V(H))^k \mid (\bar{w}, \bar{w}') \in \mu\}$. It will be useful to rephrase $\bar{v}' \in P_{\mu, \bar{v}}$ in terms of equality and inequality conditions relative to the partition $[2k] = I_1 \cup \cdots \cup I_r$ of $\mu$. More specifically, $\bar{v}' \in P_{\mu, \bar{v}}$ if and only if:

(a) $v_i' = v_j'$ for $k + i, k + j \in I_s$, where $I_s$ is a variable or a used constant class;

(b) $v_i' \neq v_j'$ for $k + i \in I_s$, $k + j \in I_{s'}$, $s \neq s'$, where $I_s$ and $I_{s'}$ are either variable or used constant classes;

(c) $v_i' = v_{\text{rep}(I_s)}$ for $k + i \in I_s$, where $I_s$ is a used constant class; and

(d) $v_i' \neq v_{\text{rep}(I_s)}$ for $k + i \in I_s$, where $I_s$ is a variable class and $v_{\text{rep}(I_s)}$ is a constant but unused class.

That is, condition (a) simply states which entries in $\bar{v}'$ must be the same and condition (c) tells which entries in $\bar{v}'$ take values from entries in $\bar{v}$. Moreover, condition (b) states which entries in $\bar{v}'$ are distinct from each other. These conditions together imply that any entry in $\bar{v}'$ belonging to a variable class is necessarily distinct from entries in $\bar{v}$ belonging to a used constant class. Finally, condition (d) states that any entry in $\bar{v}'$ belonging to a variable class should also be distinct from entries in $\bar{v}$ belonging to an unused constant class. With this notation, we can rephrase equality (7) as:

$$\{\chi^{(\ell')}_{G,k}(\bar{v}') \mid \bar{v}' \in P_{\mu, \bar{v}}\} = \{\chi^{(\ell')}_{H,k}(\bar{w}') \mid \bar{w}' \in Q_{\mu, \bar{w}}\},$$

as follows.
where $\chi_{G, k}^{(t)}(\vec{\nu}) = \chi_{H, k, \nu}^{(t)}(\vec{\nu})$. Directly applying our proof strategy, using formulas in $C_k$ of quantifier rank at most $t$, to $k$-tuples in $P_{\mu, \nu}$ and $Q_{\mu, \bar{w}}$, is problematic, however, as is illustrated in the following example.

**Example 1.** Let $k = 3$ and consider the equality pattern $\mu \in [n]^{6/\sim}$ represented by $[6] = I_1 \uplus I_2 \uplus I_3 \uplus I_4 \uplus I_5$ with $I_1 := \{1, 4\}$, $I_2 := \{2\}$, $I_3 := \{3\}$, $I_4 := \{5\}$ and $I_5 := \{6\}$. We remark that $I_1$ is the only used constant class with $\text{rep}(I_1) = 1$. The unused constant classes are $I_2$ and $I_5$, and the variables classes are $I_3$ and $I_4$. For a six-tuple $(\vec{\nu}, \vec{\nu}')$ to be in $\mu$, all entries in $\vec{\nu} = (v_1, v_2, v_3)$ must be pairwise distinct and $\vec{\nu}' = (v_1', v_2', v_3')$ is of the form $(v_1, v_2, \nu_3')$ with $v_2' \neq v_3'$ and $v_2'$ and $v_3'$ distinct from $v_1$, $v_2$ and $v_3$. Suppose that the equality (7) does not hold for our example $\mu$. Assume, for example, that there are more than $m$ triples in $P_{\mu, \nu}$ of colour $c'$, assigned by 3-WL in round $t'$, whereas $Q_{\mu, \bar{w}}$ has less than $m$ such triples. By assumption, we have that $\chi_{G, 3}^{(t)}(\bar{w}) = \chi_{H, 3}^{(t)}(\bar{w})$ and let us assume that 3-WL assigns colour $c$ in round $t$ to both these triples. We now intend to use a formula in $C_3$ of quantifier rank at most $t$ that allows us to distinguish $\bar{w}$ from $\bar{w}'$. As previously mentioned, if we can find such a formula, then we obtain a contradiction to our assumption $\chi_{G, 3}^{(t)}(\bar{w}) = \chi_{H, 3}^{(t)}(\bar{w})$.

A candidate formula would be one that is satisfied for any triple $\bar{w}$ of colour $c$, assigned by 3-WL in round $t$, and for which there are more than $m$ triples in $P_{\mu, \nu}$ of colour $c'$, assigned by 3-WL in round $t'$. Indeed, by assumption, $\bar{w}$ would satisfy this formula whereas $\bar{w}'$ would not. To express this as a logical formula one can consider $\varphi(x_1, x_2, x_3)$ defined as

$$
\psi_c^{(t)}(x_1, x_2, x_3) \land (\exists \overline{\exists}^{m}(x_2', x_3') \psi_{c'}^{(t)}(x_1, x_2', x_3') \land x_2' \neq x_3') \land \bigwedge_{i \in [3]} (x_i \neq x_2' \land x_i \neq x_3')
$$

where $\psi_c^{(t)}$ and $\psi_{c'}^{(t)}$ are $C_3$ formulas expressing that a tuple is assigned colour $c$ and $c'$ by 3-WL in round $t$ and $t'$, respectively. We note, however, that we use five variables because we need to ensure that $x_2'$ and $x_3'$ are distinct from $x_1$, $x_2$ and $x_3$. What can easily be expressed using three variables, however, is the following:

$$
\varphi(x_1, x_2, x_3) := \psi_c^{(t)}(x_1, x_2, x_3) \land (\exists \overline{\exists}^{m}(x_2, x_3) \psi_{c'}^{(t)}(x_1, x_2, x_3) \land x_2 \neq x_3 \land x_1 \neq x_2 \land x_1 \neq x_3)
$$

Here, we reused the variables $x_2$ and $x_3$ and require them to be distinct from each other, as before, but now only require them to be distinct from $x_1$, the free variable in the second conjunct.

As the example shows, we can easily encode (in-)equalities between reused variables and free variables. Intuitively, the free variables correspond to positions belonging to constant used classes. So, instead of considering $k$-tuples in $P_{\mu, \nu}$ and $Q_{\mu, \bar{w}}$, it seems feasible to detect differences in the number of occurrences of colours of multisets defined in terms if equality and inequality conditions unrelated to unused constant classes. That is, when the condition (d), part of the characterisation of tuples in $P_{\mu, \nu}$ and $Q_{\mu, \bar{w}}$ mentioned earlier, is ignored.

We thus define $\tilde{P}_{\mu, \nu}$ as $P_{\mu, \nu}$ but drop condition (d) from the conditions stated above. That is,

$$
\tilde{P}_{\mu, \nu} := \{ \vec{\nu}' \in (V(G))^k \mid \vec{\nu}' \text{ satisfies conditions (a), (b) and (c)} \}.
$$

We define $\tilde{Q}_{\mu, \bar{w}}$ in a similar way. We next show that we can use these sets of tuples to detect whether or not equality (7) holds. More precisely, we show that we can rewrite $P_{\mu, \nu}$ in terms of $\tilde{P}_{\mu, \nu}$ for some patterns $\mu$, as we will illustrate next.

**Example 2.** For our example $\mu$, consider the variable class $I_4$ and unused constant class $I_2$. Then, we consider $\mu(4 \mapsto 2)$ represented by $[6] = \{1, 4\} \uplus \{2, 5\} \uplus \{3\} \uplus \{6\}$, where $\{2, 5\}$ is the result of merging $I_4$ and $I_2$ of $\mu$. We note that

$$
\tilde{P}_{\mu(4 \mapsto 2), \nu} := \{(v_1, v_2, v_3') \in (V(G))^3 \mid v_3' \text{ is different from } v_1 \text{ and } v_2\}.
$$

We can similarly consider other pairs of variable and unused constant classes. More specifically, we can consider $\mu(4 \mapsto 3)$, $\mu(5 \mapsto 2)$ and $\mu(5 \mapsto 3)$ resulting in

$$
\tilde{P}_{\mu(4 \mapsto 3), \nu} := \{(v_1, v_3, v_3') \in (V(G))^3 \mid v_3' \text{ is different from } v_1 \text{ and } v_3\},
$$

$$
\tilde{P}_{\mu(5 \mapsto 2), \nu} := \{(v_1, v_2', v_2) \in (V(G))^3 \mid v_2' \text{ is different from } v_1 \text{ and } v_2\},
$$

$$
\tilde{P}_{\mu(5 \mapsto 3), \nu} := \{(v_1, v_2', v_3) \in (V(G))^3 \mid v_2' \text{ is different from } v_1 \text{ and } v_3\}.
$$

It is now readily verified that

$$
P_{\mu, \nu} = \tilde{P}_{\mu, \nu} \setminus (\tilde{P}_{\mu(4 \mapsto 2), \nu} \cup \tilde{P}_{\mu(4 \mapsto 3), \nu} \cup \tilde{P}_{\mu(5 \mapsto 2), \nu} \cup \tilde{P}_{\mu(5 \mapsto 3), \nu}).
$$
The rewriting of $P_{\mu,\tilde{v}}$ in terms of $\tilde{P}_{\mu,\tilde{v}}$ in the previous example holds in general.

**Observation 1.** Let $\mu \in [n]^{2k}/_{\sim}$ be an equality pattern and let $[2k] = I_1 \uplus \cdots \uplus I_r$ be its corresponding partition. Then,

$$P_{\mu,\tilde{v}} = \tilde{P}_{\mu,\tilde{v}} \setminus \left( \bigcup_{s,s'} \tilde{P}_{\mu[n-s'],\tilde{v}} \right)$$

where $s$ ranges over variables classes $I_s$ and $s'$ ranges over unused constant classes $I_{s'}$.

**Proof.** We first consider the inclusion $P_{\mu,\tilde{v}} \subseteq \tilde{P}_{\mu,\tilde{v}} \setminus \left( \bigcup_{s,s'} \tilde{P}_{\mu[n-s'],\tilde{v}} \right)$. Let $\tilde{v}' \in P_{\mu,\tilde{v}}$. This implies that $\tilde{v}'$ satisfies conditions (a), (b), (c) and (d) relative to $I_1 \uplus \cdots \uplus I_r$. We remark that this also shows that condition (c) is satisfied for the new used constant $I_{\text{rep}}$ for Example 3.

We remark that this also shows that condition (c) is satisfied for the new used constant $I_{\text{rep}}$. For the other direction, i.e., to show $\tilde{v}' \in P_{\mu,\tilde{v}}$, we argue in a similar way. Consider $\tilde{v}' \in \tilde{P}_{\mu,\tilde{v}} \setminus \left( \bigcup_{s,s'} \tilde{P}_{\mu[n-s'],\tilde{v}} \right)$. Since $\tilde{v}' \in \tilde{P}_{\mu,\tilde{v}}$, this implies that $\tilde{v}'$ satisfies conditions (a), (b) and (c) relative to $I_1 \uplus \cdots \uplus I_r$. If we can show that $\tilde{v}'$ also satisfies condition (d) then $\tilde{v}' \in P_{\mu,\tilde{v}}$, as desired. Suppose, for the sake of contradiction, that $\tilde{v}'$ does not satisfy condition (d) relative to $I_1 \uplus \cdots \uplus I_r$. This implies that there exists a variable class $I_s$ and an unused constant class $I_{s'}$ such that $k+i \in I_s$, $v'_i = v_{\text{rep}(I_s)}$. We now argue that $\tilde{v}' \in \tilde{P}_{\mu[n-s'],\tilde{v}}$, contradicting our assumption. It suffices to verify that $\tilde{v}'$ satisfies conditions (a), (b) and (c) relative to the partition $[2k] = I_1 \uplus \cdots \uplus I_{s'} \cup I_{s'+1} \uplus \cdots \uplus I_{k+i} \cup I_{k+i+1} \cup \cdots \cup I_r \cup (I_{s'} \cup I_s)$ corresponding to $\mu[s \mapsto s']$. For condition (a), we only need to consider the new used constant class $I_{s'} \cup I_s$ since all other used constant classes in $\mu[s \mapsto s']$ are used constant classes for $\mu$, for which condition (a) is already satisfied since $\tilde{v}' \in \tilde{P}_{\mu,\tilde{v}}$. Similarly, each variable class for $\mu[s \mapsto s']$ is equal to a variable class for $\mu$, so condition (a) holds for those already. Hence, we can focus on $I_{s'} \cup I_s$. Take elements $k+i$ and $k+j$ in $I_{s'} \cup I_s$. Since $I_{s'}$ only contains elements smaller or equal than $k$ (it is an unused constant class for $\mu$), $k+i, k+j \in I_s$. By assumption, $v'_i = v_{\text{rep}(I_s)} = v'_j$ and hence condition (a) is satisfied. We remark that this also shows that condition (c) is satisfied for the new used constant class $I_{s'} \cup I_s$. For condition (b), we need to compare $I_{s'} \cup I_s$ with used constant or variable classes $I_{s'}$. Assume that $I_{s'}$ is a used constant class. We need to show that for any $k+i \in I_{s'}$ and $k+j \in I_{s'} \cup I_s$, $v'_i \neq v'_j$. We note again that $k+j \in I_s$. Since $I_s$ is a variable class for $\mu$, $\tilde{v}' \in \tilde{P}_{\mu,\tilde{v}}$ and condition (c) is satisfied for $I_1 \uplus \cdots \uplus I_r$, $v'_i \neq v'_j$. Suppose next that $I_{s'}$ is a used constant class. Then, we know that $\text{rep}(I_{s'}) \neq \text{rep}(I_{s'})$ and, since for any $k+j \in I_s$, $v'_i = v_{\text{rep}(I_s)}$ and $v'_j = v_{\text{rep}(I_s)}$ for any $k+i \in I_{s'}$. Hence, $\tilde{v}' \in \tilde{P}_{\mu[n-s'],\tilde{v}}$, contradicting our assumption. In other words, $\tilde{v}' \in \tilde{P}_{\mu,\tilde{v}}$, as desired, and the inclusion follows. □

We note that all of the above holds for $Q_{\mu,\tilde{w}}$ as well.

We thus have reduced checking equality (7) to checking

$$\left\{ \left\{ (\lambda_{G,k}^{(t)}(\tilde{v})) \mid \tilde{v}' \in \tilde{P}_{\mu,\tilde{v}} \right\} \right\} = \left\{ \left\{ \lambda_{H,k}^{(t)}(\tilde{w}) \mid \tilde{v}' \in \tilde{Q}_{\mu,\tilde{w}} \right\} \right\},$$

(8)

for $\tilde{v} \in (V(G))^k$ and $\tilde{w} \in (V(H))^k$ satisfying $\lambda_{G,k}^{(t)}(\tilde{v}) = \lambda_{H,k}^{(t)}(\tilde{w})$, and for any equality pattern $\mu \in [n]^{2k}/_{\sim}$. To use our proof strategy to detect differences in the number of occurrences of colours of $k$-tuples in $\tilde{P}_{\mu,\tilde{v}}$ and $\tilde{Q}_{\mu,\tilde{w}}$ by means of formulas in $C_k$ of quantifier rank at most $t$, we need to overcome one last hurdle, as is illustrated next.

**Example 3.** Let $k = 3$ and consider the equality pattern $\mu$ represented by $[6] = I_1 \uplus I_2 \uplus I_3 \uplus I_4 \uplus I_5$ with $I_1 := \{1,5\}$, $I_2 := \{2\}$, $I_3 := \{3\}$, $I_4 := \{4\}$ and $I_5 := \{6\}$. Consider $\tilde{v} = (v_1, v_2, v_3)$ with
all its entries pairwise distinct. For $\vec{v}' = (v'_1, v'_2, v'_3)$ to be in $\vec{P}_{\mu,\vec{v}}$ it has to be of the form $(v_1, v_1, v_3')$ with $v_1'$ and $v_3'$ pairwise distinct and distinct from $v_1$. Similarly for $\vec{Q}_{\mu,\vec{w}}$, with $\vec{w} = (w_1, w_2, w_3)$ with all its entries pairwise distinct. Assume that $\vec{v}$ and $\vec{w}$ are assigned colour $c$ by $3$-WL in round $t$. Suppose that the equality (8) does not hold for the equality pattern $\mu$ and triples $\vec{v}$ and $\vec{w}$. In particular, we assume again that there are more than $m$ triples in $\vec{P}_{\mu,\vec{v}}$ of colour $c'$, assigned by $3$-WL in round $t'$, whereas there are less than $m$ such triples in $\vec{Q}_{\mu,\vec{w}}$. To express this as a logical formula, we can consider:

$$
\varphi(x_1, x_2, x_3) := \psi_c^{(t)}(x_1, x_2, x_3) \land \left( \exists x_m \geq m(x_1', x_2, x_3) \psi_c^{(t)}(x_1', x_2, x_3) \land x_3 \neq x_1' \land x_1' \neq x_1 \land x_3 \neq x_1 \land x_2 = x_1 \right).
$$

We note, however that we use four variables because we cannot reuse $x_1$ as it needs to be identified with the reused variable $x_2$.

In order to avoid having to introduce new variables, as in the previous example, we will replace $\vec{P}_{\mu,\vec{v}}$ by a permuted version. Let $\pi$ be a permutation of $[k]$. For an equality pattern $\mu \in [n]^{2k}/\sim$ represented by $I_1 \cup \cdots \cup I_r$ we define $\pi \ast \mu$ as the equality pattern in $[n]^{2k}/\sim$ represented by $\pi \ast I_1 \cup \cdots \cup \pi \ast I_r$, where $\pi \ast I_3 = \{ i \mid \pi(i) \in I_3, i \leq k \} \cup \{ i \in I_3 \mid i > k \}$. Furthermore, for a $k$-tuple $\vec{v} = (v_1, \ldots, v_k)$, we define $\pi \ast \vec{v} := (v_{\pi^{-1}(1)}, \ldots, v_{\pi^{-1}(k)})$ and similarly for $\vec{w}$ and $\pi \ast \vec{w}$.

We first observe that $\chi_{G,k}(\vec{v}) = \chi_{G,k}(\vec{w})$ implies $\chi_{G,k}^{(t)}(\pi \ast \vec{v}) = \chi_{G,k}^{(t)}(\pi \ast \vec{w})$ for any permutation $\pi$ of $[k]$. This is a direct consequence of the fact that $\vec{v}$ and $\vec{w}$ satisfy the same formulas in $C_k$ of quantifier rank at most $t$.

**Observation 2.** If $\chi_{G,k}(\vec{v}) = \chi_{G,k}(\vec{w})$, then also $\chi_{G,k}^{(t)}(\pi \ast \vec{v}) = \chi_{G,k}^{(t)}(\pi \ast \vec{w})$ for any permutation $\pi$ of $[k]$.

**Proof.** Consider a permutation $\pi : [k] \to [k]$ and suppose, for the sake of contradiction, that $\chi_{G,k}^{(t)}(\pi \ast \vec{v}) = c'$ and $\chi_{G,k}^{(t)}(\pi \ast \vec{w}) = c''$ with $c', c'' \in C$ and $c' \neq c''$. Let $\psi_c^{(t)}(x_1, \ldots, x_k)$ be the $C_k$ formula characterising that $k$-WL assigns colour $c'$ to $k$-tuples in round $t$. We have that $G \models \psi_c^{(t)}[\pi \ast \vec{v}]$ but $H \not\models \psi_c^{(t)}[\pi \ast \vec{w}]$. Consider now the formula

$$\pi \ast \psi_c^{(t)}(x_1, \ldots, x_k) := \psi_c^{(t)}[x_1/x_{\pi^{-1}(1)}, \ldots, x_k/x_{\pi^{-1}(k)}]$$

obtained from $\psi_c^{(t)}$ by renaming variable $x_i$ by $x_{\pi^{-1}(i)}$. This is again a formula in $C_k$ of quantifier rank at most $t$. Clearly, $G \models \pi \ast \psi_c^{(t)}[\vec{v}]$ if and only if $G \models \psi_c^{(t)}[\pi \ast \vec{v}]$. Similarly, $H \models \pi \ast \psi_c^{(t)}[\vec{w}]$ if and only if $H \models \psi_c^{(t)}[\pi \ast \vec{w}]$. We may thus conclude that $G \models \pi \ast \psi_c^{(t)}[\vec{w}]$ and $H \not\models \pi \ast \psi_c^{(t)}[\vec{w}]$, contradicting our assumption that $\chi_{G,k}^{(t)}(\vec{v}) = \chi_{G,k}^{(t)}(\vec{w})$ and thus $\vec{v}$ and $\vec{w}$ must satisfy the same formulas in $C_k$ of quantifier rank at most $t$.

**Remark 5.** For $k = 2$, the observation tells us that $\chi_{G,2}^{(t)}(v_1, v_2) = \chi_{H,2}^{(t)}(w_1, w_2)$ implies $\chi_{G,2}^{(t)}(v_2, v_1) = \chi_{H,2}^{(t)}(w_2, w_1)$. Chen et al. (2020) infer this by assuming that the graph is undirected. We see, however, that this assumption is not necessary.

We next illustrate how the permuted versions of $\mu$, $\vec{v}$ and $\vec{w}$ come in handy.

**Example 4.** Continuing with the previous example, let $\pi : [3] \to [3]$ be the permutation $1 \to 2$, $2 \to 1$ and $3 \to 3$. Note that $(v_2, v_1, v_3) = \pi \ast \vec{v}$ and $(w_2, w_1, w_3) = \pi \ast \vec{w}$. Consider the permuted equality pattern $\pi \ast \mu$ represented by $\pi \ast I_1 = \{ 2, 5 \}$, $\pi \ast I_2 = \{ 1 \}$, $\pi \ast I_3 = \{ 3 \}$, $\pi \ast I_4 = \{ 4 \}$ and $\pi \ast I_5 = \{ 6 \}$. Then, for $\vec{v}'$ to be in $\vec{P}_{\ast \mu,\pi \ast \vec{v}}$ it has to be of the form $(v_1', v_1, v_3')$ with $v_1'$ and $v_3'$ pairwise distinct and $v_1'$ and $v_3'$ different from $v_1$. We thus see that $\vec{P}_{\ast \mu,\pi \ast \vec{v}} = \vec{P}_{\ast \mu,\pi \ast \vec{w}}$ for $\vec{v}'$ from the previous example. Suppose that equality (8) does not hold for $\pi \ast \mu$ and triples $\pi \ast \vec{v}$ and $\pi \ast \vec{w}$. Since we assume that $\chi_{G,3}^{(t)}(\vec{v}) = \chi_{G,3}^{(t)}(\vec{w})$, Observation 2 implies that $\chi_{G,3}^{(t)}(\pi \ast \vec{v}) = \chi_{G,3}^{(t)}(\pi \ast \vec{w})$. Let us assume that $\pi \ast \vec{v}$ and $\pi \ast \vec{w}$ are assigned colour $c''$ by $3$-WL in round $t$. Furthermore, we suppose again that $\vec{P}_{\ast \mu,\pi \ast \vec{v}}$ has more than $m$ triples of colour $c'$, assigned by $3$-WL in round $t'$.
whereas \( \tilde{Q}_{\pi, \mu, \pi \ast \tilde{w}} \) has less than \( m \) such triples. We can now use the formula \( \varphi(x_1, x_2, x_3) \) defined as

\[
\psi^{(t)}(t_x(x_1, x_2, x_3) \land \left( 2^{\geq m}(x_1', x_2', x_3') \psi^{(t)}(t_x(x_1, x_2, x_3) \land x_3 \neq x_1' \land x_1' \neq x_2 \land x_3 \neq x_2) \right)
\]

to distinguish \( \pi \ast \tilde{v} \) from \( \pi \ast \tilde{w} \). Indeed, by moving to the permuted versions, we can simply use the variable \( x_2 \) to ensure that triples \( v' \) have \( v_1 \) as second entry, as this is now the second entry in \( \pi \ast \tilde{v} = (v_2, v_1, v_3) \). As a consequence, \( G \models \varphi[\pi \ast \tilde{v}] \) but \( H \not\models \varphi[\pi \ast \tilde{w}] \). Then, similarly as in the proof of Observation 2, we obtain that \( G \models \pi \ast \varphi(\tilde{v}) \) and \( H \not\models \pi \ast \varphi(\tilde{w}) \), contradicting \( \chi_{G,3}(\tilde{v}) = \chi_{H,3}(\tilde{w}) \) as well.

To carry out the strategy as outlined in the example, we need to find a good permutation \( \pi \) of \([k]\], show that \( P_{\mu, \tilde{v}} = \tilde{P}_{\pi, \mu, \pi \ast \tilde{v}} \) (and thus also \( Q_{\mu, \tilde{w}} = \tilde{Q}_{\pi, \mu, \pi \ast \tilde{w}} \)), and finally, construct a formula in \( C_k \) of quantifier rank at most \( t \) that allows us to distinguish \( \tilde{v} \) from \( \tilde{w} \).

We start by defining when a permutation is good in terms of a property of equality patterns. More specifically, we say that an equality pattern \( \mu \in [n]^{2k} / \sim \) is “good” if it satisfies the following condition, expressed in terms of the partition \([2k] = I_1 \cup \cdots \cup I_r\) of \( \mu \):

For every used constant class \( I_s \): If \( i \) is the smallest index satisfying \( k + i \in I_s \), then \( i \in I_s \) (e)

Intuitively, this condition corresponds to the requirement that when \( v' \in \tilde{P}_{\mu, \tilde{v}} \) and \( v'_i = v_{\text{rep}(I_s)} \) for a used constant class \( I_s \), then \( i \) is the smallest index such that \( k + i \in I_s \) and \( i \in I_s \). We then extend \( \pi \) to a permutation of \([k]\) in an arbitrary way.

Let us first show that \( \pi \ast \mu \) is good, i.e., that condition (e) is satisfied. Take a used constant class \( \pi \ast I_s \) in \( \pi \ast \mu \) and let \( j \) be the smallest index such that \( k + j \in \pi \ast I_s \). By definition of \( \pi \ast I_s \), \( k + j \) is also the smallest index in \( I_s \) larger than \( k \). As a consequence, for \( i = \text{rep}(I_s) \), \( \pi(i) \) is mapped to \( j \) by definition of \( \pi \). We note that \( \pi(i) = j \in \pi \ast I_s \), as desired.

Furthermore, to verify \( \tilde{P}_{\mu, \tilde{v}} = \tilde{P}_{\pi, \mu, \pi \ast \tilde{v}} \), it suffices to observe that \( k + i \in I_s \) if and only if \( k + i \in \pi \ast I_s \). In other words, classes in \( \pi \ast \mu \) and \( \pi \ast \mu \) agree on indexes larger than \( k \). This implies that \( k \)-tuples in \( \tilde{P}_{\mu, \tilde{v}} \) and \( \tilde{P}_{\pi, \mu, \pi \ast \tilde{v}} \) satisfy the same conditions (a) and (b). It remains to verify that they also satisfy the same conditions (c). That is, consider a used constant class \( I_s \) and \( k + i \in I_s \). For \( \tilde{v'} \) to be in \( \tilde{P}_{\pi, \mu, \pi \ast \tilde{v}} \), \( v'_{\text{rep}(I_s)} = (\pi \ast \mu)_{\text{rep}(\pi \ast I_s)} \). We show that \( v_{\text{rep}(I_s)} = (\pi \ast \mu)_{\text{rep}(\pi \ast I_s)} \). Indeed, we observe that \( (\pi \ast \mu)_{\text{rep}(\pi \ast I_s)} \) is equal to \( \tilde{v}_{\pi^{-1}(\text{rep}(\pi \ast I_s))} \). Let \( j = \text{rep}(\pi \ast I_s) \), i.e., \( j \) is the smallest index of the form \( \pi(j') \) for \( j' \in I_s \) with \( j' \leq k \). Hence, \( v_{\pi^{-1}(\text{rep}(\pi \ast I_s))} = v_{j'} \) for some \( j' \in I_s \) with \( j' \leq k \). As a consequence, \( v'_{j'} = v_{j'} = v_{\text{rep}(I_s)} \) since \( j' \) and \( \text{rep}(I_s) \) both belong to \( I_s \).

We are now finally ready to conclude the proof of the Key Lemma. Consider \( \tilde{v} \in (V(G))^k \) and \( \tilde{w} \in (V(H))^k \) satisfying \( \chi_{G,k}^{(t)}(\tilde{v}) = \chi_{H,k}^{(t)}(\tilde{w}) \). We have seen earlier, in Observation 1, that to ensure that equality (14) holds, it suffices to verify that equation (8) holds. Furthermore, Observation 3 tells us that we can find a permutation \( \pi \) such that \( \pi \ast \mu \) is good, and that it suffices to verify that \( \chi_{G,k}^{(t)}(\pi \ast \tilde{v}) = \chi_{H,k}^{(t)}(\pi \ast \tilde{w}) \) instead of \( \chi_{G,k}^{(t)}(\tilde{v}) = \chi_{H,k}^{(t)}(\tilde{w}) \).
All combined, it remains to show the following observations. Here, we restrict ourselves to equality patterns that have used constant classes. Equality patterns with only unused constant classes are dealt with afterwards.

**Observation 4.** Let \( \bar{v} \in (V(G))^k \) and \( \bar{w} \in (V(H))^k \) satisfying \( \chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \). Let \( \mu \in [n]^{2k} \) be a good equality pattern with at least one used constant class. Then,

\[
\left\{ \chi_{G,k}^{(t)}(\bar{v}') \mid \bar{v}' \in \bar{v} \right\} = \left\{ \chi_{H,k}^{(t)}(\bar{w}') \mid \bar{w}' \in \bar{w} \right\}.
\]

**Proof.** Suppose, for the sake of contradiction, that (9) does not hold. We assume that there are more than \( m \) \( k \)-tuples in \( \bar{P}_{\mu,\bar{v}} \) of colour \( c' \), assigned by \( k \)-WL in round \( t' \), but \( \bar{Q}_{\mu,\bar{w}} \) has less than \( m \) such \( k \)-tuples. We will express this property by means of a \( C_k \) formula of quantifier rank at most \( t \). Let \( \text{vidx} \) be the set of indexes \( i \) such that \( k + i \) is the smallest index (larger than \( k \)) in a used constant class \( I_s \) of \( \mu \). By our assumption that there is at least one used constant class for \( \mu \), \( \text{vidx} \) is non-empty. We denote by class\((i)\) the used constant class associated with \( i \). We remark that class\((i)\) \( \neq \) class\((j)\) for \( i, j \in \text{vidx} \) and \( i \neq j \). Indeed, otherwise \( I_s \) contains two smallest distinct entries \( k + i \) and \( k + j \). Let \( \text{vidx} = \{1, \ldots, k\} \setminus \text{vidx} \). We remark that when \( k + i \in I_s \) for a variable class \( I_s \), then \( i \in \text{vidx} \). Similarly, when \( k + i \in I_s \) is a used constant class and \( k + i \) is not the smallest such entry, \( i \in \text{vidx} \).

Consider now the formula \( \varphi(x_1, \ldots, x_k) \) defined as

\[
\psi_c^{(t)}(x_1, \ldots, x_k) \land \left( \exists^{\geq m}(x_1 \mid i \in \text{vidx}) \left( \psi_{c'}^{(t')}(x_1, \ldots, x_k) \land \bigwedge_{i \in \text{vidx}} \bigwedge_{k+j \in \text{class}(i)} x_j' = x_i ' \land \bigwedge_{I_s, I_{s'}, s \neq s', k+j \in I_{s'}} x_i' \neq x_j' \land \bigwedge_{I_s, k+j \in I_{s'}} x_j ' \neq x_i \right) \right).
\]

Before showing that this formula indeed expresses what we want, we observe that its quantifier rank is at most \( \max\{t, t' + |\text{vidx}|\} \). Indeed, recall from Section 2 that the sub-formula, using the quantifier \( \exists^{\geq m}(x_1 \mid i \in \text{vidx}) \), is equivalent to a formula in \( C_k \) of quantifier rank at most \( t' + |\text{vidx}| \). Since there is at least one used constant class for \( \mu \) and \( |\text{vidx}| \leq k - 1 \) and thus \( t' + |\text{vidx}| \leq t' + k - 1 = t \), as desired. We further observe that this is a formula only using variables \( x_1, \ldots, x_k \), and hence it is in \( C_k \).

We next show that \( \models G \models \varphi[\bar{v}] \) whereas \( H \models \varphi[\bar{w}] \), contradicting \( \chi_{G,k}^{(t)}(\bar{v}) = \chi_{H,k}^{(t)}(\bar{w}) \). To verify \( G \models \varphi[\bar{v}] \) we first observe that \( G \models \psi_c^{(t)}[\bar{v}] \) because \( \chi_{G,k}^{(t)}(\bar{v}) = c \). Conversely, \( G \models \varphi[\bar{v}] \) necessarily implies that \( G \models \psi_c^{(t)}[\bar{v}] \) and thus \( \chi_{G,k}^{(t)}(\bar{v}) = c \).

For the sub-formula under the quantifier \( \exists^{\geq m}(x_1 \mid i \in \text{vidx}) \), let \( \alpha : \{x_1, \ldots, x_k\} \to V(G) \) be the assignment corresponding to \( \bar{v} \), i.e., \( \alpha(x_i) = v_i \). Let \( \ell := |\text{vidx}| \). If \( G \models \varphi[\bar{v}] \) then this implies that there are more than \( m \ell \)-tuples \( (v_i' \mid i \in \text{vidx}) \) in \( (V(G))^\ell \) such that

\[
G \models \psi_{c'}^{(t')}[\alpha(x_i/v_i' \mid i \in \text{vidx})] \land \bigwedge_{I_s} \bigwedge_{k+i, k+j \in I_s} v_i' = v_j' \land \bigwedge_{i \in \text{vidx}} \bigwedge_{k+j \in \text{class}(i)} x_j ' \neq x_i ' \land \bigwedge_{I_s, I_{s'}, s \neq s', k+j \in I_{s'}} x_i ' \neq x_j' \land \bigwedge_{I_s, k+j \in I_{s'}} x_j ' \neq x_i \tag{i}
\]

holds. We verify that for each \( (v_i' \mid i \in \text{vidx}) \) defined above, the tuple \( \bar{v}'' := \alpha(x_i/v_i' \mid i \in \text{vidx}) \) is a tuple in \( \bar{P}_{\mu,\bar{v}} \) (here, we identify an assignment with its image). We verify that conditions (a), (b) and
(c) are satisfied for $v_i$. For condition (a), take $k+i$ and $k+j$ in a variable class $I_v$. We observed before that for such $i$ and $j$, $i,j \in I_v$ and thus $v_i^0 = v_j^0$ and $v_i^0 = v_j^0$. Hence, the equality conditions $v_i^0 = v_j^0$ in the sub-formula (i) ensure that condition (a) is satisfied for variable classes. Next, take $k+j$ in a used constant class $I_v$. Suppose that class $(i) = I_v$ and thus $i \in \text{idx}$. To satisfy conditions (a) and (c), we need $v_j^0 = v_{\text{rep}(i)}$. We now observe that $v_i = v_{\text{rep}(i)}$ and $v_i^0 = v_j^0$ for $j \neq i$. Hence the equalities $v_i^0 = v_j$ with $k+j \in I_v$ and $j \neq i$ in the sub-formula (ii) ensure that conditions (a) and (c) are satisfied for used constant classes. Finally, for condition (b) we argue in a similar way. More specifically, consider two distinct variable classes $I_v$ and $I_{v'}$, and let $k+i \in I_v$ and $k+j \in I_{v'}$. For $\bar{w}$ to satisfy condition (b), $v_i^0 \neq v_j^0$. Since $i$ and $j$ are in idx, the equalities $v_i^0 = v_j^0$ in the sub-formula (iii) ensure that condition (b) is satisfied for distinct variable classes. Similarly, let $I_v$ be a variable class and $I_{v'}$ are used constant class. Assume that $I_{v'} = \text{class}(i)$. We know from sub-formula (ii) that for all $k+j \in I_{v'}$, $j \neq i$, $v_i^0 = v_j = v_i$. To satisfy condition (b), we need $v_i^0 = v_j$ for $k+j \in I_v$ to be distinct from any $v_i^0$, for $k+j'' \in I_{v'}$. This is ensured by the inequalities $v_i^0 \neq v_i$ in the sub-formula (iv) since we have $v_i^0 = v_i$ for all $k+j'' \in I_{v'}$. Finally, let $I_v$ and $I_{v'}$ be two distinct used constant classes. Assume that $I_v = \text{class}(i)$ and $I_{v'} = \text{class}(j)$. Then the equalities in sub-formula (ii) ensure that for all $k+j \in I_v$, $j \neq i$, $v_i^0 = v_i' = v_i$ and $v_i^0 = v_j = v_j$. It now suffices to observe that $v_i \neq v_i$ since $i$ and $j$ belong to different used constant classes. Hence, $v_i^0 \neq v_j$ as desired by condition (b). As a consequence, $\bar{w}'' \in \bar{P}_{\mu,\bar{w}}$. Clearly, since $G \models \psi_{\bar{v}'}(\bar{w}'')$, $\bar{w}''$ has colour $c''$ assigned by $k$-WL in round $t$. We may thus conclude that when $G \models \varphi[\bar{w}]$ that there are more than $m$ $k$-tuples in $\bar{P}_{\mu,\bar{w}}$ of colour $c''$, assigned by $k$-WL in round $t$. Conversely, suppose that there are more than $m$ such tuples in $\bar{P}_{\mu,\bar{w}}$. Then clearly, $G \models \varphi[\bar{w}]$. The same holds for $H$ and $\bar{w}$. By assumption, $G \models \varphi[\bar{w}]$ but $H \not\models \varphi[\bar{w}]$, contradicting $\chi_{\varphi}(\bar{v}) = \chi_{\varphi}(\bar{w})$. In other words, the equality (9) must hold.

In the previous observation we assumed that $\mu$ has at least one used constant class. Indeed, otherwise, we need to existentially quantify over $k$ variables in the constructed formula $\varphi$. We note that when no used constant classes exist, this implies that $\bar{v}' \in \bar{P}_{\mu,\bar{w}}$ if and only if conditions (a) and (b) are satisfied for variables classes. In the following, we assume that $\mu$ has no used constant classes.

**Observation 5.** Let $\mu \in [n]^{3k}/\sim$ be an equality pattern without used constant classes. If $G \equiv_{k\text{-WL}} H$, then

$$\chi_{G,k}(\bar{v}') = \chi_{H,k}(\bar{w}')$$

for any $\bar{v} \in (V(G))^k$ and $\bar{w} \in (V(H))^k$.

**Proof.** As mentioned above, for $\bar{v}'$ to be in $\bar{P}_{\mu,\bar{w}}$ it simply needs to satisfy $v_i^0 = v_j^0$ whenever $k+i,j \in I_v$ with $I_v$ a variable class, and $v_i^0 \neq v_j^0$ whenever $k+i \in I_v$, $k+j \in I_{v'}$ with $s \neq s'$ and $I_v$ and $I_{v'}$ variables classes. In other words, due the absence of used constant classes, there is no relationship between $\bar{v}$ and $\bar{v}'$. This implies that we replace $\bar{v}' \in \bar{P}_{\mu,\bar{w}}$ by $\bar{v}' \in \tau$ with $\tau \in [n]^{3k}/\sim$ represented by $[k] = I_1 \sqcup \cdots \sqcup I_r$ with $I_i := \{k-i \mid i \in I_v\}$ and $I_v$ a variable class in $\mu$. As a consequence, instead of verifying the equality (10) it suffices to verify

$$\chi_{G,k}(\bar{v}') \equiv \chi_{H,k}(\bar{w}')$$

We have observed before, however, that $\chi_{G,k}(\bar{v}') = \chi_{H,k}(\bar{w}')$ implies that $\bar{v}' \sim \bar{w}'$ and thus both $\bar{v}$ and $\bar{w}$ belong to $\tau$. Given that $G \equiv_{k\text{-WL}} H$, or in other words,

$$\chi_{G,k}(\bar{v}') \equiv \chi_{H,k}(\bar{w}')$$

we can indeed infer that the equality (11) holds, as desired.

This concludes the proof of the Key Lemma.

4 Conclusion

We have shown that $k$-IGNs are equally expressive as $k$-WL in distinguishing graphs, hereby answering a question raised by Maron et al. (2019a). As part of the proof, we observe that a single layer of
a $k$-IGN corresponds to $k - 1$ iterations of $k$-WL. This may result in $k$-IGNs to quicker distinguish graphs than k-IGNs. The analysis of $k$-IGNs in terms of equality patterns hints towards equally powerful but less computationally intensive variants of $k$-IGNs in which certain equality patterns are disallowed. In this way, one can envisage $k$-IGN parameterised by a set of allowed equality patterns. In this way, one can obtain $k$-WL and $k$-IGNs as special cases, and tweak the correspondence between iterations of $k$-WL and layers of $k$-IGNs as one seems fit.

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