Weisfeiler and Leman Go Loopy: A New Hierarchy for Graph Representational Learning

Raffaele Paolino [* 1 2] **Sohir Maskey** [* 1] **Pascal Welke** [3] **Gitta Kutyniok** [1 2]

Abstract

We introduce r-loopy Weisfeiler-Leman (r-ℓWL), a novel hierarchy of graph isomorphism tests and a corresponding GNN framework, r-ℓMPNN, that can count cycles up to length $r+2$. Most notably, we show that r-ℓWL can count homomorphisms of cactus graphs. This strictly extends classical 1-WL, which can only count homomorphisms of trees and, in fact, is incomparable to k-WL for any fixed k. We empirically validate the expressive and counting power of the proposed r-ℓMPNN on several synthetic datasets and present state-of-the-art predictive performance on various real-world datasets. The code is available online.

1. Introduction

Graph Neural Networks (GNNs) (Scarselli et al., 2009; Bronstein et al., 2017) have become a prevalent architecture for processing graph-structured data, contributing significantly to various applied sciences. Notable applications include the discovery of new antibiotics (Stokes et al., 2020), advancements in social recommendation systems (Fan et al., 2019), and the improvement of fake news detection (Monti et al., 2019). Among the various types of GNNs, Message Passing Neural Networks (MPNNs) (Gilmer et al., 2017) are widely used in practice. Based on the message-passing paradigm, MPNNs utilize local neighborhood aggregations to compute graph representations.

Despite their widespread success, the representational power of MPNNs is bounded by the Weisfeiler-Leman (WL) test, a classical algorithm for graph isomorphism testing (Xu et al., 2019; Morris et al., 2019). This limitation hinders MPNNs from recognizing even basic substructures such as cycles (Chen et al., 2020). However, specific substructures can be crucial in many applications. For example, in organic chemistry or bioinformatics, different types of cycles can impact various chemical properties of the underlying molecules (Deshpande et al., 2002; Koyutürk et al., 2004). Therefore, it is crucial to investigate whether GNNs can count certain substructures and to design architectures that surpass the limited power of MPNNs.

Many models have been proposed to match or surpass the expressive power of WL. Several draw inspiration from higher-order variants of the WL algorithm (Morris et al., 2019), enabling them to count a broader range of substructures. For instance, GNNs designed to emulate the 3-WL algorithm can count cycles up to length 7. However, this enhanced expressive power comes at a computational cost, limiting their range of applicability. Notably, the 3-WL algorithm already constructs a large computational graph, leading to cubical forward complexity. Hence, there is a critical need to design expressive GNNs that respect the inherent sparsity of real-world graphs.

In response to the urge for more expressive and scalable neural architectures (Morris et al., 2023), we introduce a novel class of color refinement algorithms called r-loopy Weisfeiler-Leman test (r-ℓWL), and construct a corresponding class of GNNs, termed r-loopy Graph Isomorphism Networks (r-ℓGIN). The fundamental idea is to not only collect messages from neighboring nodes but also from the paths connecting any two distinct neighboring nodes. This slight modification boosts the capabilities of the architecture to count cycles up to length $r+2$, surpassing the classical k-WL hierarchy. Specifically, for every k, there exists an r such that r-ℓWL is not less powerful than k-WL. We establish a hierarchical structure within the r-ℓWL tests, demonstrating that increasing r strictly enhances expressive power. Further, we establish a connection between our proposed algorithm and cactus graphs (a strict generalization of trees), proving that r-ℓWL can homomorphism-count any cactus graph. To corroborate our theoretical results, we conduct a comprehensive evaluation on synthetic datasets. Finally, we apply the proposed model to real-world tasks, showing its competitive performance on benchmarks datasets.

[*]Equal contribution [1]Department of Mathematics, Ludwig-Maximilians-Universität München, Munich, Germany [2]Munich Center for Machine Learning (MCML), Munich, Germany [3]TU Wien, Vienna, Austria. Correspondence to: Raffaele Paolino <paolino@math.lmu.de>, Sohir Maskey <maskey@math.lmu.de>.

2. Related Work

In early works on expressivity, Xu et al. (2019) and Morris et al. (2019) proved that the expressive power of MPNNs is bounded by 1-WL. Subsequent works (Maron et al., 2018; Morris et al., 2019) introduced higher-order GNNs that have the same expressive power as k-WL (Geerts et al., 2022). Although these networks are universal (Maron et al., 2019b; Keriven et al., 2019), their exponential time and space complexity in k renders them impractical. To address these limitations, local variants of k-WL and corresponding local k-GNNs were introduced (Morris et al., 2020). Additionally, k-hop GNNs (Abboud et al., 2022) were proposed, enhancing expressivity beyond 1-WL but within 3-WL (Feng et al., 2022). Another line of work leverages positional encodings through unique node identifiers (Vignac et al., 2020), random features (Abboud et al., 2021; Sato et al., 2021) or eigenvectors (Lim et al., 2022; Maskey et al., 2022) to augment the expressive power of standard MPNNs.

Subgraph GNNs (Bevilacqua et al., 2021; You et al., 2021; Frasca et al., 2022; Huang et al., 2022) compute graph representations by applying standard MPNNs separately to a bag of subgraphs selected from the initial input graph. Subgraph GNNs are known to be more expressive than 1-WL but upper-bounded by 3-WL (Frasca et al., 2022). B. Zhang et al. (2022) demonstrate that ESAN (Bevilacqua et al., 2021) is capable of calculating the biconnectivity of graphs, a relatively simple-to-calculate graph statistic. Additionally, Michel et al. (2023) explore GNNs that process paths in graphs to enhance their expressive power.

Lovász (1967) showed that *homomorphism counts* (see Definition 7) serve as a *complete graph invariant*, meaning two graphs are isomorphic if and only if their homomorphism counts are identical. Building upon this completeness property, Nguyen et al. (2020) and Welke et al. (2023) exploited homomorphism counts to develop expressive GNNs. Theoretical contributions from Tinhofer (1986, 1991) established the equivalence between 1-WL and the capacity to count homomorphisms from graphs with tree-width one. Extending these results to k-WL, Dell et al. (2018) demonstrated the equivalence between k-WL and the ability to count homomorphisms from graphs with tree-width k. More recently, B. Zhang et al. (2024) have introduced a quantitative framework that fully characterizes the representational power of GNNs. Extending beyond the k-WL hierarchy, they advocate for homomorphism-count as a complete measure of expressivity, as GNN architectures are proven to homomorphism-count particular families of motifs.

In our approach, we first present results from a more conventional perspective by relating our architecture to the k-WL hierarchy. This sets the stage for a subsequent exploration into the substructures we can effectively homomorphism-count.

3. Preliminaries

Let G be a simple and undirected graph. We denote the set of nodes by $V(G) \coloneqq \{1, 2, \ldots, N\}$ and the set of edges by $E(G) \subset \left\{e \,|\, e \in 2^{V(G)}, |e| = 2\right\}$. For a given node $v \in V(G)$, the *direct neighborhood* is defined as

$$\mathcal{N}(v) \coloneqq \{u \in V(G) \mid \{v, u\} \in E(G)\}\,.$$

We denote the set of all graphs by $\mathcal{G}$.

Definition 1 (Homomorphism)**.** *Let F and G be two graphs. A* homomorphism *from F to G is a map $h : V(F) \to V(G)$ such that*

$$\{u, v\} \in E(F) \implies \{h(u), h(v)\} \in E(G).$$

The set of homomorphisms from F to G is denoted by $\mathrm{Hom}(F, G)$, and its cardinality by $\mathrm{hom}(F, G) \coloneqq |\mathrm{Hom}(F, G)|$.

Intuitively, a homomorphism is an edge-preserving map, i.e., it maps adjacent vertices of F to adjacent vertices of G.

Definition 2 (Subgraph Isomorphism)**.** *A* subgraph isomorphism *is an injective homomorphism. The set of subgraph isomorphisms from F to G is denoted by $\mathrm{Sub}(F, G)$, and its cardinality by $\mathrm{sub}(F, G) = |\mathrm{Sub}(F, G)|$.*

Loosely speaking, a subgraph isomorphism h maps distinct nodes to distinct nodes Consequently, it also maps distinct edges to distinct edges.

Definition 3 (Isomorphism)**.** *An* isomorphism *is a bijective homomorphism whose inverse is also a homomorphism. If F is isomorphic to G, we write $F \cong G$. The set of isomorphisms from F to G is denoted by $\mathrm{Ind}(F, G)$, and its cardinality by $\mathrm{ind}(F, G) = |\mathrm{Ind}(F, G)|$.*

An isomorphism is a one-to-one correspondence between nodes. The requirements on the inverse being a homomorphism also guarantees a one-to-one correspondence between edges. We refer to Figure 1 to illustrate the difference between such concepts. It is worth noting that a subgraph isomorphism exists from F to G if and only if F is isomorphic to a subgraph of G – hence the name.

3.1. Graph Invariants

In order to present a unified framework for different expressivity measures, we introduce the concepts of node and graph invariants (Dimitrov et al., 2023).

Definition 4 (Node and Graph Invariant)**.** *Let P be a designated set, referred to as the* palette.

i) A node invariant *$\zeta_{(\cdot)}$ is a mapping that assigns to each graph $G \in \mathcal{G}$ a function $\zeta_G : V(G) \to P$, which*

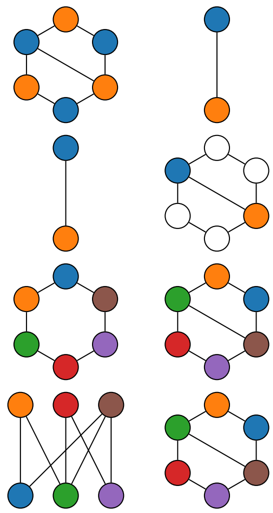


Figure 1: Examples of non-injective homomorphism (row 1), subgraph isomorphism (row 2), bijective homomorphism with non-homomorphic inverse (row 3), and isomorphism (row 4). For better clarity, the mappings $h : V(F) \to V(G)$ are visually represented with colors, where F is consistently on the left, and G is on the right in each row.

satisfies

$$\forall v \in V(G),\ \zeta_G(v) = \zeta_H(h(v)),$$

where H is any graph isomorphic to G and $h \in \mathrm{Ind}(G, H)$.

ii) A graph invariant *is a function $\zeta : \mathcal{G} \to P$ such that $\zeta(G) = \zeta(H)$ for all isomorphic pairs of graphs G, H.*

Note that every node invariant induces a graph invariant by collecting the multiset of node invariants for every node in the graph. For example, the degree of a node is a node invariant, and the degree sequence is a graph invariant.

Intuitively, a graph invariant does not change under isomorphic transformation, i.e., it does not depend on the order of nodes, but rather on the graph's structure. In addition to the already mentioned degree sequence, examples of graph invariants are the number of connected components, the diameter of the graph, and many more. An example of a function that is not a graph invariant is the number of edge intersections, as it depends on how the graph is drawn on the plane (see, e.g., last row of Figure 1).

Definition 5 (Distinguishable Pair)**.** *Given two graphs G, H and a graph invariant $\zeta : \mathcal{G} \to P$, we say that ζ* distinguishes *G and H if $\zeta(G) \neq \zeta(H)$.*

While it is clear that if ζ distinguishes G and H then they are not isomorphic, the converse is not necessarily true: there could be pairs of non-isomorphic graphs that ζ cannot distinguish. For example, there are graphs with same degree sequence that are not isomorphic (see, e.g., Figure 2). If ζ can distinguish all non-isomorphic graphs, ζ is said to be a *complete graph invariant*. Complete graph invariants are important, as they have the maximal expressive power. However, no complete graph invariant is known to be solvable in polynomial time, forming the basis for long-standing research on one of the major mathematical problems–the graph isomorphism problem (Grohe et al., 2020).

To compare the expressive power of different graph invariants, we introduce the following definition.

Definition 6 (Power of Graph Invariants)**.** *Let γ, ζ be two graph invariants. We say that γ is* more powerful *than ζ (in symbols $\gamma \sqsubseteq \zeta$) if for every pair of graphs H, G*

$$\gamma(H) = \gamma(G) \implies \zeta(H) = \zeta(G).$$

We say that γ is strictly more powerful *than ζ if $\gamma \sqsubseteq \zeta$ and there exists a pair of graphs F, G such that $\gamma(H) \neq \gamma(G)$ and $\zeta(H) = \zeta(G)$.*

Loosely speaking, γ is more powerful than ζ if it can distinguish all pairs that ζ distinguishes, and it is strictly more powerful if it can distinguish more pairs than ζ. Definition 6 allows us to measure the expressive power of certain algorithms, particularly graph colorings and GNN architectures.

3.2. Weisfeiler-Leman and Graph Isomorphism Networks

The Weisfeiler-Leman (WL) algorithm, a well-established graph invariant (Weisfeiler et al., 1968), operates with linear complexity. Despite its efficiency, there are straightforward and common examples of pairs of graphs that 1-WL cannot distinguish. The algorithm iteratively updates the *colors* of each node $v \in V(G)$ by the following scheme:

$$c^{(t+1)}(v) \leftarrow \mathrm{HASH}\left(c^{(t)}(v), \left\{\left\{c^{(t)}(u) \mid u \in \mathcal{N}(v)\right\}\right\}\right), \tag{1}$$

where HASH is an injective function. The algorithm terminates when a stable coloring is achieved, meaning that the number of colors does not change in one iteration. The graph output after t iterations is given by

$$c^{(t)}(G) = \mathrm{HASH}\left(\left\{\left\{c^{(t)}(v) \mid v \in V(G)\right\}\right\}\right),$$

and the stable coloring is denoted by $c(G)$. In particular, the colorings $c^{(t)}$ and c are node (resp. graph) invariants, and, by a slight abuse of notation, referred to as 1-WL.

Xu et al. (2019) have proven that MPNNs updating node features via

$$m^{(t+1)}(v) = \mathrm{AGGR}^{(t+1)}\left(\left\{\left\{h^{(t)}(u) \mid u \in \mathcal{N}(v)\right\}\right\}\right),$$
$$h^{(t+1)}(v) = \mathrm{UPD}^{(t+1)}\left(h^{(t)}(u), m^{(t+1)}(u)\right),$$
$$h(G) = \mathrm{READ}\left(\left\{\left\{h^{(T)}(v) \mid v \in V(G)\right\}\right\}\right),$$

are as powerful as 1-WL if for every $t \in \{1, \dots, T\}$ the functions $\mathrm{AGGR}^{(t)}$, $\mathrm{UPD}^{(t)}$, and READ are injective functions on their respective domains.

3.3. Higher-Order Weisfeiler-Leman Tests

It is possible to uplift the expressive power of WL by considering higher-order interactions. The simplest higher-order variant of WL is the k-dimensional Weisfeiler-Leman test, denoted by k-WL. Given a graph G with nodes $V(G)$ and edges $E(G)$, the algorithm generates a new graph H where each node is a k-tuple of elements of $V(G)$

$$V(H) = \left\{\mathbf{v} = \{v_i\}_{i=1}^{k} \mid v_i \in V(G)\right\} = V(G)^k,$$

and edges $E(H)$ are built among those k-tuples that differ in one entry only

$$E(H) = \{\{\mathbf{v}, \mathbf{u}\} \mid d_H(\mathbf{v}, \mathbf{u}) = 1\,,\ \mathbf{u}, \mathbf{v} \in V(H)\}$$

where d_H is the Hamming distance. The algorithm assigns to each node $\mathbf{v} \in V(H)$ an initial color depending on the isomorphic type of the induced subgraph $G[\mathbf{v}]$. The color refinements scheme is exactly (1) applied to H. While H can be generated by a simple algorithm, the approach quickly becomes impractical as the number of nodes and edges grows exponentially in k.

3.4. Homomorphism and Subgraph Counting Expressivity

A more nuanced graph invariant can be built considering the occurrences of a motif F.

Definition 7 (Homomorphism and Subgraph Counts)**.** *Given a graph F, a graph invariant ζ can* homomorphism-count *F if for all pairs of graphs G, H*

$$\zeta(G) = \zeta(H) \implies \hom(F, G) = \hom(F, H).$$

By analogy, ζ can subgraph-count *F if for all pairs of graphs G, H*

$$\zeta(G) = \zeta(H) \implies \mathrm{sub}(F, G) = \mathrm{sub}(F, H).$$

If $\mathcal{F}$ is a family of graphs, we say that ζ can homomorphism- (resp. subgraph-) count $\mathcal{F}$ if ζ can homomorphism- (resp. subgraph-) count every $F \in \mathcal{F}$. We denote the (possibly infinite) vector of homomorphism counts by

$$\hom(\mathcal{F}, G) = (\hom(F, G))_{F \in \mathcal{F}}\,,$$

and the vector of subgraph counts by

$$\mathrm{sub}(\mathcal{F}, G) = (\mathrm{sub}(F, G))_{F \in \mathcal{F}}\,.$$

The ability of a graph invariant, such as a GNN architecture, to count homomorphisms is highly relevant because $\hom(\mathcal{G}, \cdot)$ is a complete graph invariant. Conversely, if ζ is a complete graph invariant, then ζ can homomorphism count all graphs (Lovász, 1967).

4. Loopy Weisfeiler-Leman Algorithm

In this section, we introduce a new graph invariant by enhancing the usual neighborhood of nodes with *simple paths* between neighbors.

Definition 8 (Simple Path)**.** *Given a graph G, a* simple path *of length r is a collection $\mathbf{p} = \{p_i\}_{i=1}^{r+1}$ of $r+1$ nodes such that consecutive nodes are adjacent, i.e.,*

$$\{p_i, p_{i+1}\} \in E(G),\ \forall i \in \{1, \dots, r\}\,,$$

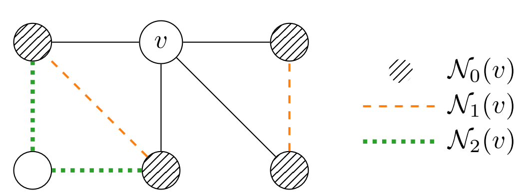
and there are no repeated nodes, i.e., $i \neq j \implies p_i \neq p_j$.

Simple paths are the building blocks of r-neighborhoods, which in turn are the backbone of the proposed graph invariant. The definition is inspired by (Cantwell et al., 2019; Kirkley et al., 2021).

Definition 9 (r-Neighborhood)**.** *Given a graph G and an integer $r \geq 1$, we define the* r-neighborhood *$\mathcal{N}_r(v)$ of $v \in V(G)$ as the set of all simple paths of length r between distinct direct neighbors of v which do not contain v, i.e.,*

$$\mathcal{N}_r(v) \coloneqq \{\mathbf{p} \mid \mathbf{p}\ r\text{-path},\ p_1, p_{r+1} \in \mathcal{N}(v), v \notin \mathbf{p}\}\,.$$

For consistency, we set $\mathcal{N}_0(v) = \mathcal{N}(v)$. An example of the construction of r-neighborhood is shown in the sketch below, where different r-neighborhoods of node v are represented with different colors.



We generalize the Weisfeiler-Leman algorithm in (1) as follows.

Definition 10 (Loopy Weisfeiler-Leman)**.** *We define the*

r-ℓWL test *by the following vertex coloring update*

$$c_r^{(t+1)}(v) \leftarrow \mathrm{HASH}_r\Bigg(c_r^{(t)}(v), \left\{\left\{c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_0(v)\right\}\right\}, \\ \vdots \\ \left\{\left\{c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_r(v)\right\}\right\}\Bigg), \tag{2}$$

where $c_r^{(t)}(\mathbf{p})$ *is the sequence of colors of every node in the path, i.e.,*

$$c_r^{(t)}(\mathbf{p}) = \left(c_r^{(t)}(p_1), c_r^{(t)}(p_2), \ldots, c_r^{(t)}(p_{r+1})\right).$$

We denote as $c_r^{(t)}(G)$ the final graph output after t iterations of r-ℓWL, i.e.,

$$c_r^{(t)}(G) = \mathrm{HASH}_r\left(\left\{\left\{c_r^{(t)}(v) \mid v \in V(G)\right\}\right\}\right),$$

and we denote the stable coloring after convergence as $c_r(G)$. The stable coloring c_r serves as graph invariant and will be referred to as r-ℓWL.

5. Expressivity of r-ℓWL

In this section, we analyze the expressivity of r-ℓWL in terms of its ability to distinguish non-isomorphic graphs, subgraph-count, and homomorphism-count motifs. We present the proofs for all statements in Appendix C.

5.1. Isomorphism Expressivity

It is straightforward to check that 0-ℓWL corresponds to 1-WL, since $\mathcal{N}_0(v) = \mathcal{N}(v)$ for all nodes v. However, increasing r leads to a strict increase in expressivity.

Proposition 1 (Hierarchy of r-ℓWL)**.** *Let $0 \leq q < r$. Then, r-ℓWL is strictly more powerful than q-ℓWL. In particular, every r-ℓWL is strictly more powerful than 1-WL.*

This shows that the number of graphs we can distinguish monotonically increases with r. We empirically verify this fact on several synthetic datasets in Section 7.

5.2. Subgraph Expressivity

It is known that 1-WL cannot subgraph-count cycles (Chen et al., 2020, Theorem 3.3). Similarly, 3-WL can only subgraph-count cycles of length up to 7 (Arvind et al., 2020, Theorem 3.5). Subgraph GNNs are also proven to have limited cycle-counting ability (Huang et al., 2022, Proposition 3.1). On the other hand, r-ℓWL can count cycles of arbitrary length, as shown in the following statement.

Theorem 1 (Subgraph Counting Power of r-ℓWL)**.** *For any $r \geq 1$, r-ℓWL can subgraph-count all cycles with at most $r+2$ nodes.*

Since 3-WL cannot subgraph-count any cycle with more than 7 nodes, Theorem 1 implies that 6-ℓWL is not less powerful than 3-WL. This observation holds true for $k \geq 3$; the correct statement is presented next.

Corollary 1. *Let $k \in \mathbb{N}$. There exists $r \in \mathbb{N}$, such that r-ℓWL is not less powerful than k-WL.*

5.3. Homomorphism Expressivity

To establish our main results, we consider the class of *cactus graphs*, also referred to as Husimi trees (Harary et al., 1953).

Definition 11 (Cactus Graph)**.** *A* cactus graph *is a graph where every edge lies on at most one simple cycle. For $r \geq 2$, an* r-cactus *graph is a cactus where every simple cycle has at most r vertices. We denote by $\mathcal{M}$ the set of all cactus graphs, and by $\mathcal{M}^r$ the set comprising all q-cactus graphs for $q \leq r$.*

We refer to Figure 2 for illustrations of two small cactus graphs. We are now ready to present our main result.[1]

Theorem 2 (Homomorphism Counting Power of r-ℓWL)**.** *Let $r \geq 0$. Then, r-ℓWL can homomorphism-count $\mathcal{M}^{r+2}$.*

We refer to Appendix D for a detailed proof of Theorem 2, which is fairly involved and requires defining canonical tree decompositions of cactus graphs and unfolding trees of r-ℓWL. Demonstrating their strong connection, we then follow the approach in (Dell et al., 2018; B. Zhang et al., 2024) to decompose homomorphism counts of cactus graphs.

The class $\mathcal{M}^2$ contains only forests; hence, Theorem 2 implies the standard results on 1-WL ability to count forests. Since forests are the only class of graphs 1-WL can count, Theorem 2 implies that r-ℓWL is always strictly more powerful than 1-WL, corroborating the claim in Proposition 1.

The implications of Theorem 2 are profound: it establishes that r-ℓWL can homomorphism-count a large class of graphs. This result shows that even the simplest variant, 1-ℓWL, is not less powerful than Subgraph GNNs, which are limited to homomorphism-count graphs with end-point shared NED (B. Zhang et al., 2024). Importantly, Theorem 2 states a loose lower bound on the homomorphism expressivity of r-ℓWL. This observation opens the avenue for future research to explore tight lower bounds, or upper bounds, on the homomorphism expressivity of r-ℓWL.

[1] For technical reasons, in the remainder of this subsection, we augment node features of $\mathbf{p} \in \mathcal{N}_r(v)$ by adding atomic types. This indicates for every $p \in \mathbf{p}$ if $\{p, v\} \in E(G)$, see Definition 15 and (8). Note that this does not increase the computational complexity while being more powerful than the r-ℓWL given in Definition 10.

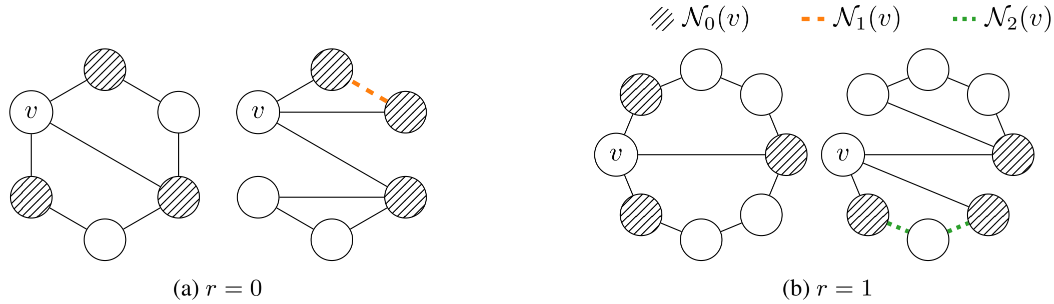


Figure 2: Example of two non-isomorphic graphs that are r-ℓWL equivalent but not $(r+1)$-ℓWL equivalent: a chordal cycle (left) and a cactus graph (right).

6. Loopy Message Passing

In this section, we construct a *neural* version of r-ℓWL.

Definition 12 (r-ℓMPNN)**.** *For $t \in \{0, \ldots, T-1\}$ and $k \in \{0, \ldots, r\}$, r-ℓMPNN applies the following message, update and readout functions*

$$
\begin{aligned}
m_k^{(t+1)}(v) &= \mathrm{AGGR}_k^{(t+1)}\left(\left\{\left\{h_k^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_k(v)\right\}\right\}\right) \\
h_r^{(t+1)}(v) &= \mathrm{UPD}^{(t+1)}\Big(h_r^{(t)}(v), m_0^{(t+1)}(v) \\
&\qquad \vdots \\
&\qquad m_r^{(t+1)}(v)\Big), \\
h_r^{(T)}(G) &= \mathrm{READ}\left(\left\{\left\{h_r^{(T)}(v) \mid v \in V(G)\right\}\right\}\right).
\end{aligned}
\tag{3}
$$

The function $h_r^{(t)} : V(G) \to C$ mapping $v \mapsto h_r^{(t)}(v)$ is a node invarant. In the following result we establish the relation beween $h_r^{(t)}$ and $c_r^{(t)}$, defined in (2).

Theorem 3 (GNN emulating r-ℓWL)**.** *For fixed $t, r \geq 0$, we have $c_r^{(t)} \sqsubseteq h_r^{(t)}$. Moreover, $h_r^{(t)} \sqsubseteq c_r^{(t)}$ if the message and update functions in Definition 12 are injective. In particular, t iterations of r-ℓWL are equally expressive as a t-layered r-ℓMPNN.*

Similarly to the 1-WL case (Xu et al., 2019; Morris et al., 2019), the previous result derives conditions under which r-ℓMPNN is as expressive as r-ℓWL.

To implement r-ℓMPNN in practice, we choose suitable neural layers for $\mathrm{AGGR}_k^{(t)}$, $\mathrm{UPD}^{(t)}$, and READ in (3). As a consequence of (Xu et al., 2019, Lemma 5), the aggregation function can be written as

$$
\mathrm{AGGR}_k^{(t+1)}(\mathcal{N}_k(v)) = f\left(\sum_{\mathbf{p} \in \mathcal{N}_k(v)} g(\mathbf{p})\right)
$$

for suitable functions f, g. Since 1-WL is injective on forests, hence on paths (Arvind et al., 2015), and since GIN can approximate 1-WL (Xu et al., 2019), we choose

$$
\mathrm{AGGR}_k^{(t+1)}(\mathcal{N}_k(v)) = \mathrm{MLP}\left(\sum_{\mathbf{p} \in \mathcal{N}_k(v)} \mathrm{GIN}(\mathbf{p})\right).
$$

Hence, r-ℓGIN is defined as an r-ℓMPNN that updates node features via

$$
\begin{aligned}
x_r^{(t+1)}(v) = \mathrm{MLP}\Bigg(& x_r^{(t)}(v) + (1+\varepsilon_0) \sum_{u \in \mathcal{N}_0(v)} x_r^{(t)}(u) \\
&+ \sum_{k=1}^{r} (1+\varepsilon_k) \sum_{\mathbf{p} \in \mathcal{N}_k(v)} \mathrm{GIN}_k(\mathbf{p})\Bigg).
\end{aligned}
\tag{4}
$$

To reduce the number of learnable parameters in (4), the GIN_k can be shared among all $k \in \{1, \ldots, r\}$, dropping the dependency on k. Nothing prevents from choosing a different path-processing layer; we opted for GIN because it is simple yet maximally expressive on paths.

Comparison with (Michel et al., 2023) Michel et al. (2023) introduce an approach that updates node features by computing all possible paths starting from each node. In contrast, our approach selects paths between distinct neighbors, potentially resulting in fewer paths. For instance, a tree's r-neighborhoods ($r \geq 1$) are empty, while counts of paths between nodes are quadratic. Notably, Michel et al. (2023) do not explore the impact of increasing the path length on architecture expressiveness, a consideration we address (see, e.g., Proposition 1 and Corollary 1).

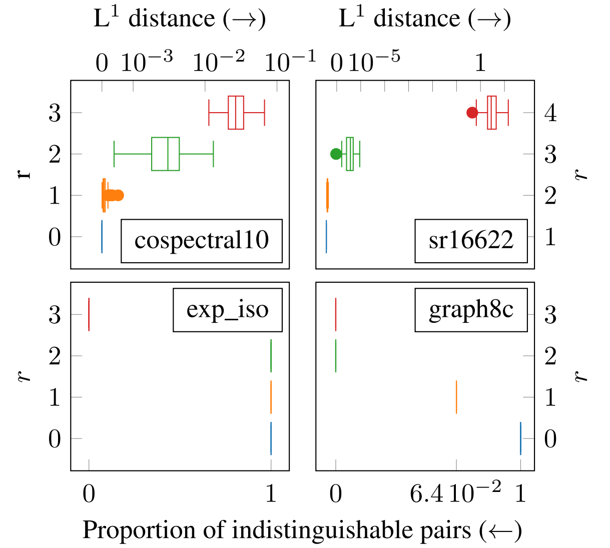
Another significant contribution of our work, which we assert does not hold (at least not trivially) for the architecture proposed by Michel et al. (2023), is the provable ability to subgraph-count cycle graphs (see, e.g., Theorem 1) and homomorphism-count cactus graphs (see, e.g., Theorem 2).

7. Experiments

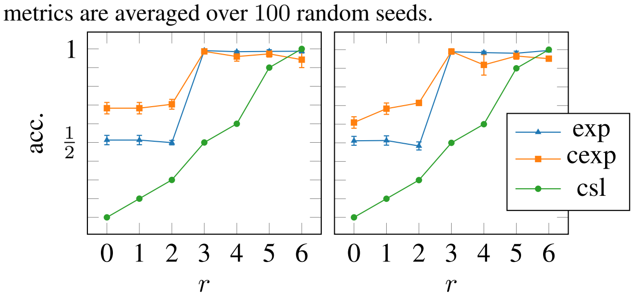
We demonstrate the expressive power of r-ℓGIN on synthetic datasets and its performance on real-world datasets.

Table 1: Num. of indistinguished pairs (↓). OOM stands for out of memory, - for no improvement.

BREC	#pairs	r = 1	2	3	4
Basic	60	8	0	-	-
Extension	100	95	16	6	5
Regular	50	2	1	0	-
4-Vertex Condition	20	20	OOM	-	-
Distance Regular	20	20	20	20	OOM
Strongly Regular	50	50	4	1	0
CFI	100	100	98	98	OOM



(a) Undistinguishable pairs at initialization, symlog scale. The metrics are averaged over 100 random seeds.



(b) Test accuracy on classification task, average of 5 random splits; (left) shared and (right) non-shared GIN's per r-ℓGIN layer in (4).

Figure 3: Results on the expressive power of r-ℓMPNN.

Expressive Power. The COSPECTRAL10 dataset (van Dam et al., 2003) comprises two cospectral 4-regular non-isomorphic graphs on 10 nodes, 1-WL equivalent (Figure 4a). The SR16622 dataset (Figure 4c) comprises 2 strongly regular graphs on 16 nodes, namely the Shrikhande and the $4{\times}4$ rook graph, which are 3-WL equivalent. The GRAPH8C dataset (Balcilar et al., 2021) comprises all the 11 117 possible connected non-isomorphic simple graphs on 8 nodes; 312 pairs are 1-WL equivalent but none of them are 3-WL equivalent. The EXP_ISO dataset (Abboud et al., 2022) comprises 600 pairs of 1-WL equivalent graphs. The goal is to check whether the model is able to distinguish non-isomorphic pairs at initialization, i.e., with no training. The results are shown in Figure 3a. For COSPECTRAL10 and SR16622, we report the L^1 distance between graph embeddings. For GRAPH8C and EXP_ISO, we report the proportion of indistinguished pairs: 2 graphs are deemed indistinguishable if the L^1 distance of their embeddings is less than 10^{-3}. The results are shown in Figure 3a.

The EXP and CEXP datasets (Abboud et al., 2021), come with a classification task that requires expressive power beyond 1-WL. The CSL dataset (Murphy et al., 2019) comprises 150 cycle graphs equipped with skip links (see, e.g., Figure 4b). The task is to classify them based on the length of the skip link. The results are shown in Figure 3b

The BREC dataset (Wang et al., 2023) includes 400 pairs of non-isomorphic graphs ranging from 1-WL to 4-WL equivalent. The aim is to train the model on non-isomorphic pairs for few epochs and test whether they are deemed equivalent via a T^2 statistic. We feed into $(r+1)$-ℓGIN only those pairs that were not distinguished by r-ℓGIN. The results are reported in Table 1.

Counting Power. The subgraphcount dataset (Chen et al., 2020) comprises 5000 graphs. The task is to predict the number of cycles of fixed length $L \in \{3,4,5,6\}$. The results, reported in Table 2, again further substantiates our theory, as r-ℓWL can effectively count cycles of length $r+2$ (see, e.g., Theorem 1).

Real-World Datasets. We experimented with three benchmark datasets: ZINC250K (Irwin et al., 2012), ZINC12K (Dwivedi et al., 2022), and QM9 (Wu et al., 2018).

The ZINC250K dataset comprises approximately 250 000 molecules, while ZINC12K consists of 12 000 molecules. As baseline models, we selected standard MPNNs (GIN, GCN, GAT), Subgraph GNNs (NestedGNN, GNNAK+, SUN), domain-agnostic GNNs fed with substructure counts (GSN, CIN), a GNN processing paths (PathNN), and expressive GNNs with provable cycle counting power (HIMP, SignNet, I2-GNN, DRFWL GNN). Following the standard procedure, we kept the number of parameters under 500K (Dwivedi et al., 2022) for ZINC12K. Additional experimental details can be found in Appendix B. The results are detailed in Table 3.

Table 2: Count of subgraphs: top three models as 1st, 2nd, 3rd. S stands for shared GIN, N for non-shared.

Model		Test MAE (↓) Triangle	4-Cycle	5-Cycle	6-Cycle
0-ℓ		$(3.95 \pm 0.01)\ 10^{-1}$	$(2.48 \pm 0.01)\ 10^{-1}$	$(1.83 \pm 0.003)\ 10^{-1}$	$(1.44 \pm 0.01)\ 10^{-1}$
1-ℓ		$(2.67 \pm 0.59)\ 10^{-4}$	$(1.91 \pm 0.03)\ 10^{-1}$	$(1.40 \pm 0.03)\ 10^{-1}$	$(1.10 \pm 0.01)\ 10^{-1}$
2-ℓ	S	$(2.98 \pm 1.05)\ 10^{-4}$	$(3.30 \pm 0.77)\ 10^{-3}$	$(1.33 \pm 0.04)\ 10^{-1}$	$(1.12 \pm 0.05)\ 10^{-1}$
	N	$(4.58 \pm 1.28)\ 10^{-4}$	$(2.56 \pm 0.49)\ 10^{-4}$	$(1.39 \pm 0.04)\ 10^{-1}$	$(1.19 \pm 0.04)\ 10^{-1}$
3-ℓ	S	$(1.21 \pm 0.84)\ 10^{-3}$	$(4.70 \pm 3.39)\ 10^{-3}$	$(1.21 \pm 0.19)\ 10^{-3}$	$(1.01 \pm 0.02)\ 10^{-1}$
	N	$(2.93 \pm 0.94)\ 10^{-3}$	$(1.56 \pm 1.03)\ 10^{-3}$	$(1.51 \pm 1.06)\ 10^{-3}$	$(8.73 \pm 0.08)\ 10^{-2}$
4-ℓ	S	$(1.64 \pm 1.20)\ 10^{-2}$	$(1.95 \pm 2.01)\ 10^{-2}$	$(5.71 \pm 1.37)\ 10^{-3}$	$(1.12 \pm 0.61)\ 10^{-2}$
	N	$(9.87 \pm 5.06)\ 10^{-3}$	$(1.36 \pm 0.56)\ 10^{-2}$	$(3.94 \pm 2.02)\ 10^{-3}$	$(3.67 \pm 2.41)\ 10^{-3}$

Table 3: Test MAE (↓) on graph regression, ZINC dataset. Top three models as 1st, 2nd, 3rd.

Model	ZINC12K	ZINC250K
GIN	0.163 ± 0.004	0.088 ± 0.002
GCN	0.321 ± 0.009	-
GAT	0.384 ± 0.007	-
GSN	0.115 ± 0.012	-
CIN	0.079 ± 0.006	0.022 ± 0.002
NestedGNN	0.111 ± 0.003	0.029 ± 0.001
SUN	0.083 ± 0.003	-
GNNAK+	0.080 ± 0.001	-
I2-GNN	0.083 ± 0.001	0.023 ± 0.001
DRFWL GNN	0.077 ± 0.002	0.025 ± 0.003
SignNet	0.084 ± 0.004	0.024 ± 0.003
HIMP	0.151 ± 0.006	0.036 ± 0.002
PathNN	0.090 ± 0.004	-
5-ℓGIN	0.072 ± 0.002	0.022 ± 0.001

Table 4: Normalized test MAE (↓) on graph regression, QM9 dataset. Top three models as 1st, 2nd, 3rd.

Model	μ	α	$\varepsilon_{\text{homo}}$
1-GNN	0.493	0.78	0.00321
1-2-3-GNN	0.476	0.27	0.00337
DTNN	0.244	0.95	0.00388
Deep LRP	0.364	0.298	0.00254
PPGN	0.231	0.382	0.00276
NestedGNN	0.428	0.290	0.00265
I2-GNN	0.428	0.230	0.00261
DRFWL GNN	0.346	0.222	0.00226
5-ℓGIN	0.350 ± 0.011	0.217 ± 0.025	0.00205 ± 0.00005

For the QM9 dataset, consisting of approximately 130 000 molecules with 19 regression targets, we focused on the first three regression targets and followed the setup of (Huang et al., 2022; Zhou et al., 2023). Specifically, the test MAE is multiplied by the standard deviation of the target and divided by the corresponding conversion unit. The baseline results and models were obtained from (Zhou et al., 2023), including expressive GNNs with provable (but bounded) cycle counting power. The results are presented in Table 4.

Discussion of Experiments The results in Figure 3 and Table 1 constitute a strong empirical validation of our theory: increasing r leads to more expressive r-ℓMPNN. Albeit only 6-ℓWL is not less powerful than 3-WL (see, e.g., Section 5.2), in practice smaller values of r can already distinguish pair of graphs that are 3-WL equivalent, such as the Shrikhande and the 4×4 rook graphs.

In the BREC dataset, 4-ℓGIN distinguishes all pairs of strongly regular graphs, significantly outperforming 3-WL (0/50 graphs). Notably, 4-ℓGIN can already distinguish 257 out of 400 total pairs of graphs, surpassing other expressive GNNs like PPGN (233/400), theoretically equivalent to 3-WL, and NestedGNN (166/400). For detailed baseline results, refer to Table 2 in (Wang et al., 2023).

On real-world molecular datasets, we observe that r-ℓGIN, although designed for subgraph-counting cycles and homomorphism-counting cactus graphs, is highly competitive. Notably, we outperform the baseline 0-ℓGIN by 226% on ZINC12K and 400% on ZINC250K, and even surpass domain-agnostic methods such as CIN or GSN. We conjecture that this is attributed to straightforward optimization, driven by the simplicity of the architecture (see Figure 6 for visualization) and its inductive bias towards counting cycles.

Finally, we note that our architecture is not designed for dense graphs, making path calculations, although a preprocessing step, infeasible due to $\mathcal{O}(n\, d^r)$ complexity, where d is the average node degree. However, for sparse graphs, the runtime remains reasonably low. For instance, preprocessing ZINC12K for $r = 5$ takes just over a minute.

8. Conclusion

In this paper, we introduced a novel hierarchy of color refinement algorithms, denoted as r-ℓWL, which incorporates an augmented neighborhood mechanism accounting for nearby paths. Additionally, we presented a GNN, r-ℓMPNN, designed to emulate and match the expressive power of r-ℓWL. Theoretical and empirical evidence supported the claim that r-ℓMPNN can effectively subgraph-count cycles and homomorphism-count cactus graphs. Moreover, we established connections between r-ℓWL and k-WL.

Future research could focus on identifying the exact class of graphs that r-ℓWL can and cannot homomorphism-count.

References

Abboud, R., Ceylan, I. I., Grohe, M., and Lukasiewicz, T. (2021). "The Surprising Power of Graph Neural Networks with Random Node Initialization". In: *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence*. Montreal, Canada: International Joint Conferences on Artificial Intelligence Organization, pp. 2112–2118.

Abboud, R., Dimitrov, R., and Ceylan, I. I. (2022). "Shortest Path Networks for Graph Property Prediction". In: *Proceedings of the First Learning on Graphs Conference*. PMLR, 5:1–5:25.

Arvind, V., Fuhlbrück, F., Köbler, J., and Verbitsky, O. (2020). "On Weisfeiler-Leman Invariance: Subgraph Counts and Related Graph Properties". In: *Journal of Computer and System Sciences* 113, pp. 42–59.

Arvind, V., Köbler, J., Rattan, G., and Verbitsky, O. (2015). "On the Power of Color Refinement". In: *Fundamentals of Computation Theory - 20th International Symposium, FCT 2015, Gdansk, Poland, August 17-19, 2015, Proceedings*. Vol. 9210. Lecture Notes in Computer Science. Springer, pp. 339–350.

Balcilar, M., Heroux, P., Gauzere, B., Vasseur, P., Adam, S., and Honeine, P. (2021). "Breaking the Limits of Message Passing Graph Neural Networks". In: *Proceedings of the 38th International Conference on Machine Learning*. PMLR, pp. 599–608.

Bevilacqua, B., Frasca, F., Lim, D., Srinivasan, B., Cai, C., Balamurugan, G., Bronstein, M. M., and Maron, H. (2021). "Equivariant Subgraph Aggregation Networks". In: *International Conference on Learning Representations*.

Bodnar, C., Frasca, F., Otter, N., Wang, Y., Liò, P., Montufar, G. F., and Bronstein, M. (2021). "Weisfeiler and Lehman Go Cellular: CW Networks". In: *Advances in Neural Information Processing Systems*. Vol. 34. Curran Associates, Inc., pp. 2625–2640.

Bouritsas, G., Frasca, F., Zafeiriou, S., and Bronstein, M. M. (2023). "Improving Graph Neural Network Expressivity via Subgraph Isomorphism Counting". In: *IEEE Transactions on Pattern Analysis and Machine Intelligence* 45.1, pp. 657–668.

Bronstein, M. M., Bruna, J., LeCun, Y., Szlam, A., and Vandergheynst, P. (2017). "Geometric Deep Learning: Going beyond Euclidean Data". In: *IEEE Signal Processing Magazine* 34.4, pp. 18–42.

Cantwell, G. T. and Newman, M. E. J. (2019). "Message Passing on Networks with Loops". In: *Proceedings of the National Academy of Sciences* 116.47, pp. 23398–23403.

Chen, Z., Chen, L., Villar, S., and Bruna, J. (2020). "Can Graph Neural Networks Count Substructures?" In: *Advances in Neural Information Processing Systems*. Vol. 33. Curran Associates, Inc., pp. 10383–10395.

Colbourn, C. J. and Booth, K. S. (1981). "Linear Time Automorphism Algorithms for Trees, Interval Graphs, and Planar Graphs". In: *SIAM Journal on Computing* 10.1, pp. 203–225.

Dell, H., Grohe, M., and Rattan, G. (2018). "Lovász Meets Weisfeiler and Leman". In: *45th International Colloquium on Automata, Languages, and Programming, ICALP 2018, July 9-13, 2018, Prague, Czech Republic*. Vol. 107. LIPIcs. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 40:1–40:14.

Deshpande, M., Kuramochi, M., and Karypis, G. (2002). "Automated Approaches for Classifying Structures". In: *Proceedings of the 2nd ACM SIGKDD Workshop on Data Mining in Bioinformatics (BIOKDD 2002), July 23rd, 2002, Edmonton, Alberta, Canada*, pp. 11–18.

Dimitrov, R., Zhao, Z., Abboud, R., and Ceylan, I. I. (2023). "PlanE: Representation Learning over Planar Graphs". In: *Thirty-seventh Conference on Neural Information Processing Systems*.

Dwivedi, V. P., Joshi, C. K., Luu, A. T., Laurent, T., Bengio, Y., and Bresson, X. (2022). "Benchmarking Graph Neural Networks". In: *Journal of Machine Learning Research* 24.43, pp. 1–48.

Fan, W., Ma, Y., Li, Q., He, Y., Zhao, Y. E., Tang, J., and Yin, D. (2019). "Graph Neural Networks for Social Recommendation". In: *The World Wide Web Conference, WWW 2019, San Francisco, CA, USA, May 13-17, 2019*. ACM, pp. 417–426.

Feng, J., Chen, Y., Li, F., Sarkar, A., and Zhang, M. (2022). "How Powerful are K-hop Message Passing Graph Neural Networks". In: *Advances in Neural Information Processing Systems 35: Annual Conference on Neural Information Processing Systems 2022, NeurIPS 2022, New Orleans, LA, USA, November 28 - December 9, 2022*.

Fey, M., Yuen, J. G., and Weichert, F. (2020). "Hierarchical Inter-Message Passing for Learning on Molecular Graphs". In: *ICML Graph Representation Learning and Beyond (GRL+) Workhop*.

Fey, M. and Lenssen, J. E. (2019). *Fast Graph Representation Learning with PyTorch Geometric*. arXiv: 1903.02428.

Frasca, F., Bevilacqua, B., Bronstein, M., and Maron, H. (2022). "Understanding and Extending Subgraph GNNs by Rethinking Their Symmetries". In: *Advances in Neural Information Processing Systems* 35, pp. 31376–31390.

Geerts, F. and Reutter, J. L. (2022). "Expressiveness and Approximation Properties of Graph Neural Networks". In: *International Conference on Learning Representations*.

Gilmer, J., Schoenholz, S. S., Riley, P. F., Vinyals, O., and Dahl, G. E. (2017). "Neural Message Passing for Quantum Chemistry". In: *Proceedings of the 34th International Conference on Machine Learning*. Vol. 70. Proceedings of Machine Learning Research. PMLR, pp. 1263–1272.

Grohe, M. and Schweitzer, P. (2020). "The graph isomorphism problem". In: *Communications of the ACM* 63.11, pp. 128–134.

Hagberg, A. A., Schult, D. A., Swart, P., and Hagberg, J. (2008). "Exploring Network Structure, Dynamics, and Function using NetworkX". In.

Harary, F. and Uhlenbeck, G. E. (1953). "On the Number of Husimi Trees, I". In: *Proceedings of the National Academy of Sciences of the United States of America* 39.4, pp. 315–322.

Hu*, W., Liu*, B., Gomes, J., Zitnik, M., Liang, P., Pande, V., and Leskovec, J. (2020). "Strategies for Pre-training Graph Neural Networks". In: *International Conference on Learning Representations*.

Huang, Y., Peng, X., Ma, J., and Zhang, M. (2022). "Boosting the Cycle Counting Power of Graph Neural Networks with I^2-GNNs". In: *The Eleventh International Conference on Learning Representations*.

Ioffe, S. and Szegedy, C. (2015). "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift". In: *ArXiv* abs/1502.03167.

Irwin, J. J., Sterling, T., Mysinger, M. M., Bolstad, E. S., and Coleman, R. G. (2012). "ZINC: A Free Tool to Discover Chemistry for Biology". In: *Journal of Chemical Information and Modeling* 52, pp. 1757–1768.

Keriven, N. and Peyré, G. (2019). "Universal invariant and equivariant graph neural networks". In: *Advances in Neural Information Processing Systems* 32.

Kingma, D. P. and Ba, J. (2014). "Adam: A Method for Stochastic Optimization". In: *CoRR* abs/1412.6980.

Kipf, T. N. and Welling, M. (2017). "Semi-Supervised Classification with Graph Convolutional Networks". In: *International Conference on Learning Representations*.

Kirkley, A., Cantwell, G. T., and Newman, M. E. J. (2021). "Belief Propagation for Networks with Loops". In: *Science Advances* 7.17, eabf1211.

Koyutürk, M., Grama, A. Y., and Szpankowski, W. (2004). "An efficient algorithm for detecting frequent subgraphs in biological networks". In: *Bioinformatics* 20 Suppl 1, pp. i200–7.

Lim, D., Robinson, J. D., Zhao, L., Smidt, T., Sra, S., Maron, H., and Jegelka, S. (2022). "Sign and Basis Invariant Networks for Spectral Graph Representation Learning". In: *The Eleventh International Conference on Learning Representations*.

Lovász, L. M. (1967). "Operations with structures". In: *Acta Mathematica Academiae Scientiarum Hungarica* 18, pp. 321–328.

Maron, H., Ben-Hamu, H., Serviansky, H., and Lipman, Y. (2019a). "Provably Powerful Graph Networks". In: *Advances in Neural Information Processing Systems*. Vol. 32. Curran Associates, Inc.

Maron, H., Ben-Hamu, H., Shamir, N., and Lipman, Y. (2018). "Invariant and Equivariant Graph Networks". In: *International Conference on Learning Representations*.

Maron, H., Fetaya, E., Segol, N., and Lipman, Y. (2019b). "On the Universality of Invariant Networks". In: *Proceedings of the 36th International Conference on Machine Learning*. Vol. 97. Proceedings of Machine Learning Research. PMLR, pp. 4363–4371.

Maskey, S., Parviz, A., Thiessen, M., Stärk, H., Sadikaj, Y., and Maron, H. (2022). "Generalized Laplacian Positional Encoding for Graph Representation Learning". In: *NeurIPS 2022 Workshop on Symmetry and Geometry in Neural Representations*.

Michel, G., Nikolentzos, G., Lutzeyer, J. F., and Vazirgiannis, M. (2023). "Path Neural Networks: Expressive and Accurate Graph Neural Networks". In: *Proceedings of the 40th International Conference on Machine Learning*. PMLR, pp. 24737–24755.

Monti, F., Frasca, F., Eynard, D., Mannion, D., and Bronstein, M. M. (2019). *Fake News Detection on Social Media using Geometric Deep Learning*. arXiv: 1902.06673.

Morris, C., Lipman, Y., Maron, H., Rieck, B., Kriege, N. M., Grohe, M., Fey, M., and Borgwardt, K. (2023). *Weisfeiler and Leman Go Machine Learning: The Story so Far*. arXiv: 2112.09992.

Morris, C., Rattan, G., and Mutzel, P. (2020). "Weisfeiler and Leman go sparse: Towards scalable higher-order graph embeddings". In: *Advances in Neural Information Processing Systems* 33, pp. 21824–21840.

Morris, C., Ritzert, M., Fey, M., Hamilton, W. L., Lenssen, J. E., Rattan, G., and Grohe, M. (July 2019). "Weisfeiler and Leman Go Neural: Higher-Order Graph Neural Networks". In: *Proceedings of the AAAI Conference on Artificial Intelligence* 33.01, pp. 4602–4609.

Murphy, R., Srinivasan, B., Rao, V., and Ribeiro, B. (2019). "Relational Pooling for Graph Representations". In: *Proceedings of the 36th International Conference on Machine Learning*. PMLR, pp. 4663–4673.

Neuen, D. (2023). *Homomorphism-Distinguishing Closedness for Graphs of Bounded Tree-Width*. arXiv: 2304.07011.

Nguyen, H. and Maehara, T. (2020). "Graph Homomorphism Convolution". In: *Proceedings of the 37th International Conference on Machine Learning*. Vol. 119. Proceedings of Machine Learning Research. PMLR, pp. 7306–7316.

Paszke, A. et al. (2019). "PyTorch: An Imperative Style, High-Performance Deep Learning Library". In: *Neural Information Processing Systems*.

Sato, R., Yamada, M., and Kashima, H. (2021). "Random Features Strengthen Graph Neural Networks". In: *Proceedings of the 2021 SIAM International Conference on Data Mining, SDM 2021, Virtual Event, April 29 - May 1, 2021*. SIAM, pp. 333–341.

Scarselli, F., Gori, M., Tsoi, A. C., Hagenbuchner, M., and Monfardini, G. (2009). "The Graph Neural Network Model". In: *IEEE Transactions on Neural Networks* 20.1, pp. 61–80.

Stokes, J. M. et al. (2020). "A deep learning approach to antibiotic discovery". In: *Cell* 180.4, 688–702.e13.

Tinhofer, G. (1986). "Graph isomorphism and theorems of Birkhoff type". In: *Computing* 36, pp. 285–300.

– (1991). "A note on compact graphs". In: *Discret. Appl. Math.* 30, pp. 253–264.

van Dam, E. R. and Haemers, W. H. (2003). "Which Graphs Are Determined by Their Spectrum?" In: *Linear Algebra and its Applications*. Combinatorial Matrix Theory Conference (Pohang, 2002) 373, pp. 241–272.

Velickovic, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., and Bengio, Y. (2018). "Graph Attention Networks". In: *International Conference on Learning Representations*.

Vignac, C., Loukas, A., and Frossard, P. (2020). "Building powerful and equivariant graph neural networks with structural message-passing". In: *Advances in Neural Information Processing Systems* 33, pp. 14143–14155.

Wang, Y. and Zhang, M. (2023). *Towards Better Evaluation of GNN Expressiveness with BREC Dataset*. arXiv: 2304.07702.

Weisfeiler, B. and Lehman., A. (1968). "The reduction of a graph to canonical form and the algebra which appears therein". In: *Nauchno-Technicheskaya Informatsia* 9.

Welke, P., Thiessen, M., Jogl, F., and Gärtner, T. (2023). "Expectation-Complete Graph Representations with Homomorphisms". In: *Proceedings of the 40th International Conference on Machine Learning*. Vol. 202. Proceedings of Machine Learning Research. PMLR, pp. 36910–36925.

Wu, Z., Ramsundar, B., Feinberg, E. N., Gomes, J., Geniesse, C., Pappu, A. S., Leswing, K., and Pande, V. (2018). *MoleculeNet: A Benchmark for Molecular Machine Learning*. arXiv: 1703.00564.

Xu, K., Hu, W., Leskovec, J., and Jegelka, S. (2019). "How Powerful Are Graph Neural Networks?" In: *International Conference on Learning Representations*.

You, J., Gomes-Selman, J. M., Ying, R., and Leskovec, J. (2021). "Identity-Aware Graph Neural Networks". In: *Proceedings of the AAAI Conference on Artificial Intelligence* 35.12, pp. 10737–10745.

Zhang, B., Gai, J., Du, Y., Ye, Q., He, D., and Wang, L. (2024). *Beyond Weisfeiler-Lehman: A Quantitative Framework for GNN Expressiveness*. arXiv: 2401.08514.

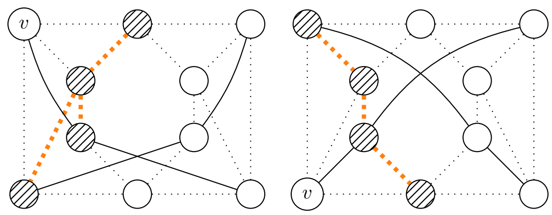
Zhang, B., Luo, S., Wang, L., and He, D. (2022). "Rethinking the Expressive Power of GNNs via Graph Biconnectivity". In: *The Eleventh International Conference on Learning Representations*.

Zhang, M. and Li, P. (2021). "Nested Graph Neural Networks". In: *Advances in Neural Information Processing Systems*. Vol. 34. Curran Associates, Inc., pp. 15734–15747.

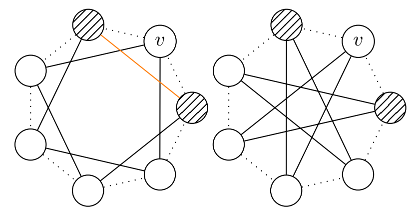
Zhao, L., Jin, W., Akoglu, L., and Shah, N. (2021). "From Stars to Subgraphs: Uplifting Any GNN with Local Structure Awareness". In: *International Conference on Learning Representations*.

Zhou, J., Feng, J., Wang, X., and Zhang, M. (2023). "Distance-Restricted Folklore Weisfeiler-Leman GNNs with Provable Cycle Counting Power". In: *Thirty-seventh Conference on Neural Information Processing Systems*.

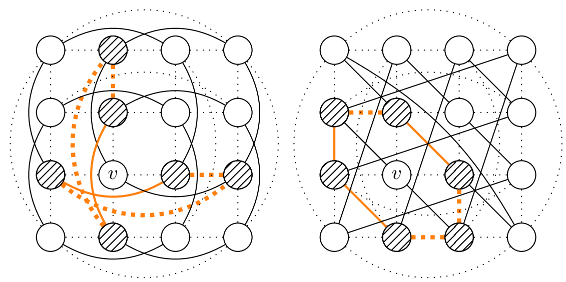
A. Additional Figures



(a) cospectral10.



(b) csl example, skip length 2 (left) and 3 (right).



(c) sr16622.

Figure 4: Some synthetic datasets. The dotted lines are the common edges. The orange edges identifies $\mathcal{N}_1(v)$.

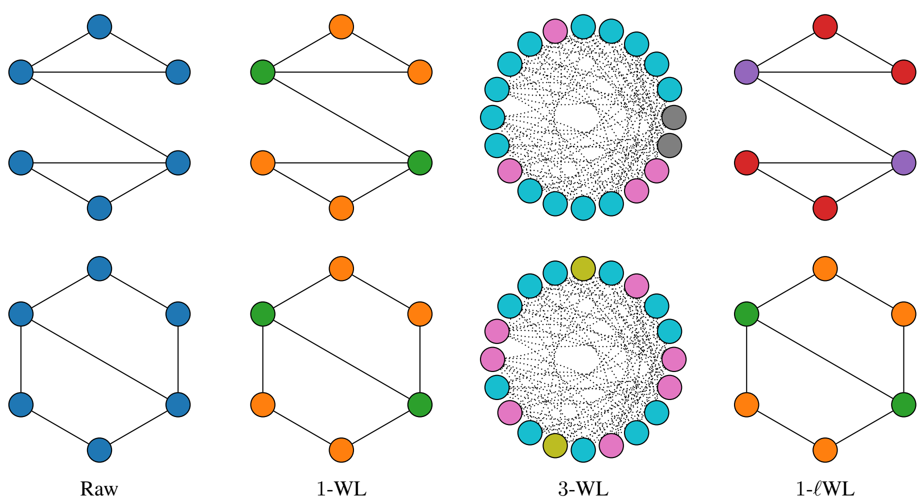


Figure 5: The pair of raw graphs on the left cannot be distinguished by 1-WL, since the color distribution after convergence of the algorithm is equal. 3-WL can distinguish them at the cost of creating new dense graphs. Our proposed 1-ℓWL can distinguish the two graphs heeding the original graph sparsity.

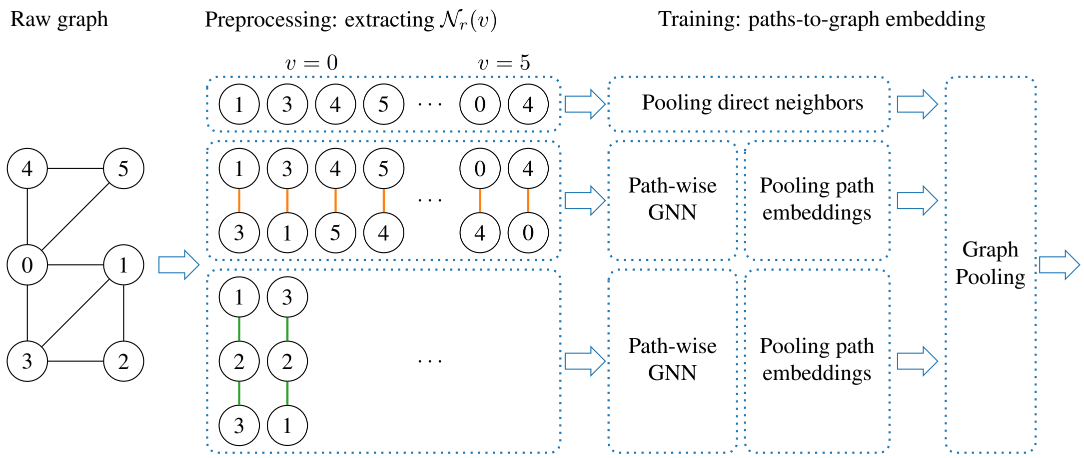


Figure 6: Visual depiction of the architecture.

B. Experimental Details

In the following, we describe our experimental setup.

General experimental details Our model is implemented in `PyTorch` (Paszke et al., 2019), using `PyTorch Geometric` (Fey et al., 2019). The r-neighborhoods are computed with `NetworkX` (Hagberg et al., 2008) as preprocessing. All instructions to reproduce the experiments are available on GitHub. Hyperparameters on real-world datasets were tuned using grid search; for synthetic experiments, we fixed one configuration of hyperparameters. All experiments were run on an internal cluster with NVIDIA RTX 3090 and NVIDIA RTX A6000 GPUs with 24 GB and 48 GB of memory, respectively. All models are trained with Adam optimizer (Kingma et al., 2014).

B.1. Synthetic Datasets

The SR16622 dataset is retrieved from the official PATHNN repository (Michel et al., 2023). The GRAPH8C dataset is downloaded from Australian National University webpage. The EXP, EXP_ISO, and CEXP datasets are downloaded from GNN-RNI official repository (Abboud et al., 2021), while the corresponding splits are generated via Stratified 5-fold cross-validation. The CSL dataset is provided by `torch_geometric`, while the corresponding splits are taken from PathNN official repository. The SUBGRAPHCOUNT dataset is downloaded from GNNAK official repository (Zhao et al., 2021). The BREC dataset is downloaded from its official repository (Wang et al., 2023). The configuration of hyperparameters can be found in Table 5. For the synthetic datasets, we fixed one configuration and studied the effect of increasing r on the expressive and counting power of the architecture.

B.2. Real-World Datasets

All real-world datasets are provided by `torch_geometric`. The splits for both ZINC datasets are also provided by `torch_geometric`. For QM9, we follow the set-up of (Zhou et al., 2023) and use random $80/10/10$ splits. Details for the datasets are provided in Table 6.

Hyperparameters were tuned using grid search. For ZINC12K, the grid was defined by Hidden Size $\in \{64, 128\}$ and Num. Layers $\in \{3, 4, 5\}$. For ZINC250K, the grid was defined by Hidden Size $\in \{128, 256\}$ and Num. Layers $\in \{4\}$. For the QM9 tasks, the grid was defined by Hidden Size $\in \{64, 128\}$ and Num. Layers $\in \{3, 4, 5\}$. For the QM9 tasks, we followed the training set-up of (Zhou et al., 2023), training for 400 epochs with a `ReduceLROnPlateau` scheduler, reducing the learning rate by a factor of 0.9 if the validation metric did not decrease for 10 epochs. The exact hyperparameters are given in Table 7.

All real-world datasets come with edge features. We use an encoder layer, followed by a linear layer to encode node, edge features, and atomic types before passing them to the r-ℓGIN. Within the r-ℓGIN layers, we process the edge features via a 2-layered learnable MLP, and replace the GIN in (4) by GINE layers (Hu* et al., 2020). After t rounds of r-ℓGIN layer,

Table 5: Hyperparameter configuration for synthetic experiments.

	COSPECTRA10	GRAPH8C	SR16622	EXP_ISO	EXP	CEXP	CSL	SUBGRAPHCOUNT	BREC
Epochs	-	-	-	-	10^3	10^3	10^3	10^3	40
Learning Rate	-	-	-	-	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-4}
Early Stopping	-	-	-	-	lr $< 10^{-5}$	lr $< 10^{-5}$	lr $< 10^{-5}$	lr $< 10^{-5}$	lr $< 10^{-5}$
Scheduler	-	-	-	-	$\{50, 0.5\}$	$\{50, 0.5\}$	$\{50, 0.5\}$	$\{50, 0.5\}$	$\{50, 0.5\}$
Hidden Size	64	64	64	64	64	64	64	64	32
Num. Layers	3	3	3	3	3	3	3	3	5
Num. Encoder Layers	2	2	2	2	2	2	2	2	2
Num. Decoder Layers	2	2	2	2	2	2	2	2	2
Batch Size	64	64	64	64	64	64	64	64	64
Dropout	0	0	0	0	0	0	0	0	0
Readout	sum	sum	sum	sum	sum	sum	sum	sum	sum

we apply a two-layered MLP as decoder layer. In all experiments, `BatchNorm1D` (Ioffe et al., 2015) is used in the MLP layers. We refer to Figure 6 for a depiction of the architecture.

Table 6: Statistics of real-world datasets.

Dataset	**Number of graphs**	**Average number of nodes**	**Average number of edges**
QM9	130 831	18.0	18.7
ZINC12K	12 000	23.2	24.9
ZINC250K	249 456	23.2	24.9

C. Proofs

C.1. Appendix for Section 5.1

We begin by recalling some core concepts.

Definition 13 (Node Invariant Refinement)**.** *Given two node invariants γ and ζ. We say that ζ refines γ if for every fixed graph G and nodes $u, v \in V(G)$, it holds $\zeta_G(u) = \zeta_G(v) \Rightarrow \gamma_G(u) = \gamma_G(v)$. We write $\zeta \sqsubseteq \gamma$.*

We emphasize that every node invariant ζ induces a graph invariant $\mathcal{A}[\gamma]$ by collecting the multiset, i.e., $G \mapsto \{\{\zeta_G(v)\}\}_{v \in V(G)}$. We denote the induced graph invariant of a node invariant γ as $\mathcal{A}[\gamma]$.

The following lemma establishes a connection between the expressive power of two node invariants (see Definition 13) and that of their induced graph invariants (see Definition 6).

Lemma 1. *Let ζ, γ be node invariant. If $\zeta \sqsubseteq \gamma$, then $\mathcal{A}[\zeta]$ is more powerful than $\mathcal{A}[\gamma]$.*

Proof. Let G, H be two graphs, and let P be the underlying palette of ζ, γ. Consider the function

$$\phi : P \longrightarrow P,\ \zeta(u) \mapsto \gamma(u)\ \forall u \in V(G) \cup V(H).$$

Table 7: Hyperparameters configuration for real-world experiments. Results are aggregated across 4 seeds.

	ZINC12K	**ZINC250K**	**QM9 (μ)**	**QM9 (α)**	**QM9 ($\varepsilon_{\text{homo}}$)**
Epochs	1000	2000	400	400	400
Learning Rate	0.001	0.001	0.001	0.001	0.001
Early Stopping	lr $< 10^{-5}$	lr $< 10^{-6}$	lr $< 10^{-5}$	lr $< 10^{-5}$	lr $< 10^{-5}$
Scheduler	$\{50, 0.5\}$	$\{50, 0.5\}$	$\{10, 0.9\}$	$\{10, 0.9\}$	$\{10, 0.9\}$
r	5	5	5	5	5
Hidden Size	64	256	64	64	64
Depth	3	4	4	5	5
Batch Size	64	128	64	64	64
Dropout	0	0	0	0	0
Readout	sum	sum	sum	sum	sum
# Parameters	452 633	2 379 041	418 481	519 677	519 677
Preprocessing Time [sec]	77.4	1278.5	427.5	425.9	517.4

As a consequence of $\zeta \sqsubseteq \gamma$, ϕ is well-defined, since

$$\zeta(u) = \zeta(v) \implies (\phi \circ \zeta)(u) = \gamma(u) = \gamma(v) = (\phi \circ \zeta)(v).$$

Assume that $\mathcal{A}[\zeta](G) = \mathcal{A}[\zeta](H)$, i.e,

$$\{\{\zeta(u) \mid u \in V(G)\}\} = \{\{\zeta(v) \mid v \in V(H)\}\}.$$

As ϕ is well-defined, we have

$$\{\{\phi \circ \zeta(u) \mid u \in V(G)\}\} = \{\{\phi \circ \zeta(x) \mid v \in V(H)\}\},$$

which leads to $\mathcal{A}[\gamma](G) = \mathcal{A}[\gamma](H)$. $\square$

We proceed with the proof of Proposition 1 from the main paper.

Proposition 1 (Hierarchy of r-ℓWL)**.** *Let $0 \leq q < r$. Then, r-ℓWL is strictly more powerful than q-ℓWL. In particular, every r-ℓWL is strictly more powerful than 1-WL.*

Proof of Proposition 1. Let $r \geq 0$. We aim to prove that $(r+1)$-ℓWL is strictly more powerful than r-ℓWL. We begin by demonstrating that $(r+1)$-ℓWL is more powerful than r-ℓWL.

To establish this, we rely on Lemma 1. Specifically, we demonstrate that the underlying $(r+1)$-ℓWL node invariant c_{r+1} refines c_r. Moreover, we go beyond and show that the node invariant $c_{r+1}^{(t)}$ refines $c_r^{(t)}$ at every iteration $t \geq 0$, which shows that t iterations of $(r+1)$-ℓWL are more powerful than t iterations of r-ℓWL.

For this purpose, let G be a graph with node set $V(G)$. For $t = 0$, $c_{r+1}^{(0)} \sqsubseteq c_r^{(0)}$ since both algorithms start with the same labels. By induction, we assume that

$$c_{r+1}^{(t)}(u) = c_{r+1}^{(t)}(v) \implies c_r^{(t)}(u) = c_r^{(t)}(v) \tag{5}$$

holds; we need to prove that (5) implies

$$c_{r+1}^{(t+1)}(u) = c_{r+1}^{(t+1)}(v) \implies c_r^{(t+1)}(u) = c_r^{(t+1)}(v). \tag{6}$$

Since HASH in Definition 10 is injective, $c_{r+1}^{(t)}(u) = c_{r+1}^{(t)}(v)$ in (5) leads to

$$\left\{\left\{c_{r+1}^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_q(u)\right\}\right\} = \left\{\left\{c_{r+1}^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_q(v)\right\}\right\}$$

for all $q \in \{0, \ldots, r\}$. The assumption $c_r^{(t)}(u_{l,k}^q) = c_r^{(t)}(v_{l,k}^q)$ in (5) is satisfied for every path $\mathbf{u}_l^q = \left\{u_{l,k}^q\right\} \in \mathcal{N}_q(u)$ and $\mathbf{v}_l^q = \left\{v_{l,k}^q\right\} \in \mathcal{N}_q(v)$ for $q = 0, \ldots, r$, $l = 1, \ldots, |\mathcal{N}_v|$ and $k = 1, \ldots, q+1$. Hence,

$$\left\{\left\{c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_k(u)\right\}\right\} = \left\{\left\{c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_k(v)\right\}\right\}$$

Inputting this into Definition 10, we get (6), i.e, $c_{r+1}^{(t+1)} \sqsubseteq c_r^{(t+1)}$.

The "strictly" can be deduced as follows. The cycle graph on $(2r+6)$ nodes equipped with a chord between nodes 1 and $r+4$ is r-ℓWL equivalent to the graph consisting of two $(r+3)$-cycles connected by one edge; however, they are not $(r+1)$-ℓWL equivalent (see, e.g., Figure 2). ☐

C.2. Appendix for Section 5.2

The goal of this subsection is to provide a proof for Theorem 1. In fact, we present and prove a more general statement. Specifically, for a graph G and $v \in V(G)$, we introduce the node invariant $\mathrm{sub}(F^x, G^v)$, defined as the count of subgraph isomorphisms from F to G that are rooted, meaning that x is mapped to v. Let us denote this node invariant as $\mathrm{sub}(F^x, \cdot)$. Our result establishes that $c_r^{(1)}(\cdot)$ refines $\mathrm{sub}(C^x, \cdot)$ for every cycle graph C with at most r nodes. In simpler terms, this $c_r^{(1)}$ can count how often node y appears in a cycle C.

Theorem 4. *Let $r \geq 1$. For every cycle graph C with at most $r+2$ nodes and $x \in V(C)$, it holds $c_r^{(1)}(\cdot) \sqsubseteq \mathrm{sub}(C^x, \cdot)$.*

Proof of Theorem 4. Let G be any graph, $u, v \in V(G)$, and $q = 1, \ldots, r+2$. Let C be a cycle graph with q nodes. It is important to note that for every $x_1, x_2 \in C$, we have $\mathrm{sub}(C^{x_1}, G^v) = \mathrm{sub}(C^{x_2}, G^v)$ since every node in C is automorphic to each other. Therefore, we can arbitrarily choose any $x \in V(C)$.

We show that

$$\mathrm{sub}\left(C^x, G^u\right) \neq \mathrm{sub}\left(C^x, G^v\right) \implies c_r^{(1)}(u) \neq c_r^{(1)}(v)$$

The number of injective homomorphisms from the q-long cycles C^x to G^v, i.e., $\mathrm{sub}(C_q^a, G^v)$, is equal to the number of paths of length $(q-2)$ between distinct neighbors of v.

The neighborhood $\mathcal{N}_{(q-2)}(v)$ comprises exactly all paths of length $(q-2)$ between any two distinct neighbors of v. Therefore,

$$\mathrm{sub}\left(C^x, G^v\right) = \left|\mathcal{N}_{(q-2)}(v)\right|.$$

Thus

$$\mathrm{sub}\left(C^x, G^u\right) \neq \mathrm{sub}\left(C^x, G^v\right) \implies \left|\mathcal{N}_{(q-2)}(u)\right| \neq \left|\mathcal{N}_{(q-2)}(v)\right|,$$

which implies

$$\left\{\left\{c_{q-2}^{(0)}(\mathbf{p}) : \mathbf{p} \in \mathcal{N}_{(q-2)}(u)\right\}\right\} \neq \left\{\left\{c_{q-2}^{(0)}(\mathbf{p}) : \mathbf{p} \in \mathcal{N}_{(q-2)}(v)\right\}\right\}.$$

Finally, as HASH in Definition 10 is injective, we get the thesis $c_{q-2}^{(1)}(u) \neq c_{q-2}^{(1)}(v)$. ☐

Now, Theorem 1 from the main paper is a simple corollary of Theorem 4.

Theorem 1 (Subgraph Counting Power of r-ℓWL). *For any $r \geq 1$, r-ℓWL can subgraph-count all cycles with at most $r+2$ nodes.*

Proof of Theorem 1. Combining Theorem 4 and Lemma 1, we get that $c_r^{(1)}$ (as a graph invariant) is stronger than the induced graph invariant $\mathcal{A}\left[\mathrm{sub}(C^x, \cdot)\right]$. Now, consider graphs G, H, and assume without loss of generality that $|V(G)| = n = |V(H)|$.

If $c_r^{(1)}(G) = c_r^{(1)}(H)$, we have $\mathcal{A}\left[\mathrm{sub}(C^x, \cdot)\right](G) = \mathcal{A}\left[\mathrm{sub}(C^x, \cdot)\right](H)$. Hence, by definition of induced graph invariants,

$$\{\{\mathrm{sub}(C^x, G^v) \mid v \in V(G)\}\} = \{\{\mathrm{sub}(C^x, H^w) \mid w \in V(H)\}\}.$$

Hence,

$$\frac{1}{n}\sum_{v\in V(G)}\mathrm{sub}(C^x, G^v) = \frac{1}{n}\sum_{w\in V(H)}\mathrm{sub}(C^x, H^w),$$

which is equivalent to $\mathrm{sub}(C,G) = \mathrm{sub}(C,H)$. □

Corollary 1. *Let $k \in \mathbb{N}$. There exists $r \in \mathbb{N}$, such that r-ℓWL is not less powerful than k-WL.*

Proof of Corollary 1. Neuen (2023) shows that k-WL can subgraph count a graph F if and only if its *hereditary tree-width* is bounded by k. Since the hereditary tree-width of cycle graphs is not uniformly bounded, there always exists a cycle of length $c_k \in \mathbb{N}$ that k-WL can not subgraph-count. Set $r_k := c_k - 2$, and r_k-ℓWL is not less powerful than k-WL as it can subgraph-count any cycle of length c_k, see Theorem 1. □

C.3. Appendix for Section 6

Theorem 3 (GNN emulating r-ℓWL)**.** *For fixed $t, r \geq 0$, we have $c_r^{(t)} \sqsubseteq h_r^{(t)}$. Moreover, $h_r^{(t)} \sqsubseteq c_r^{(t)}$ if the message and update functions in Definition 12 are injective. In particular, t iterations of r-ℓWL are equally expressive as a t-layered r-ℓMPNN.*

Proof of Theorem 3. We begin by proving that $c_r^{(t)} \sqsubseteq h_r^{(t)}$. We argue by induction over t for any fixed $r \geq 0$.

Initially, $c_r^{(0)} = h_r^{(0)}$ as both labeling functions start with the same base labels. Now assume $c_r^{(t+1)}(u) = c_r^{(t+1)}(v)$ for some $u, v \in V(G)$. By definition,

$$\mathrm{HASH}\left(c_r^{(t)}(u), \left\{\left\{c_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_0(u)\right\}\right\}, \dots\right) = \mathrm{HASH}\left(c_r^{(t)}(v), \left\{\left\{c_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_0(v)\right\}\right\}, \dots\right).$$

This implies $c_r^{(t)}(u) = c_r^{(t)}(v)$ and

$$\left\{\left\{c_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_k(u)\right\}\right\} = \left\{\left\{c_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_k(v)\right\}\right\}, \quad \forall k \in \{0,\dots,r\},$$

as HASH is an injective function.

By induction hypothesis, we hence have $h_r^{(t)}(u) = h_r^{(t)}(v)$ and

$$\left\{\left\{h_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_k(u)\right\}\right\} = \left\{\left\{h_r^{(t)}(\mathbf{p})\,|\,\mathbf{p}\in\mathcal{N}_k(v)\right\}\right\}, \quad \forall k \in \{0,\dots,r\},$$

which implies that any function, in particular $\mathrm{AGGR}_k^{(t+1)}$ and $\mathrm{UPD}^{(t+1)}$ have to return the same result. Therefore, we have $h_r^{(t+1)}(u) = h_r^{(t+1)}(v)$.

We proceed to prove $h_r^{(t)} \sqsubseteq c_r^{(t)}$ if all message, update, and readout functions are injective in Definition 12. For this, we show that for each $t \geq 0$ there exists an injective function ϕ such that $h_r^{(t)} = \phi \circ c_r^{(t)}$. For $t = 0$, we can choose ϕ to be the identity function. Assume that for $t-1$ there exists an injective function ϕ such that $h_r^{(t-1)}(v) = \phi \circ c_r^{(t-1)}(v)$. Then, we can write

$$\begin{aligned} h_r^{(t)}(v) &= \mathrm{UPD}^{(t)}\left(h^{(t-1)}(v), m_0^{(t)}(v), \dots, m_r^{(t)}(v)\right) \\ &= \mathrm{UPD}^{(t)}\left(\phi\circ c_r^{(t-1)}(v), \phi\circ m_0^{(t)}(v), \dots, \phi\circ m_r^{(t)}(v)\right), \end{aligned}$$

where for every $q = 0,\dots,r$, we set $\phi\circ m_q^{(t)}(v) := \left\{\left\{(\phi\circ c_r^{(t-1)}(\mathbf{p}))\mid \mathbf{p}\in\mathcal{N}_q(v)\right\}\right\}$ and $(\phi\circ c_r^{(t-1)}(\mathbf{p})) = (\phi\circ c_r^{(t-1)}(p_1), \dots, \phi\circ c_r^{(t-1)}(p_{q+1}))$ for $\mathbf{p} = \{p_i\}_{i=1}^{q+1} \in \mathcal{N}_q(v)$. By assumption, all message, update, and readout functions are injective in Definition 12. Since the concatenation of injective functions is injective, there exists an injective function ψ

such that

$$\begin{aligned} h_r^{(t)}(v) = \psi\Bigg(c_r^{(t-1)}(v), &\left\{\!\!\left\{ c_r^{(t-1)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_0(v) \right\}\!\!\right\}, \\ &\left\{\!\!\left\{ c_r^{(t-1)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_1(v) \right\}\!\!\right\}, \\ &\vdots \\ &\left\{\!\!\left\{ c_r^{(t-1)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_r(v) \right\}\!\!\right\} \Bigg). \end{aligned}$$

As HASH in Definition 10 is injective, the inverse HASH^{-1} exists and is also injective. Hence,

$$\begin{aligned} h_r^{(t)}(v) &= \psi \circ \mathrm{HASH}^{-1} \circ \mathrm{HASH}\Bigg(c_r^{(t-1)}(v), \left\{\!\!\left\{ c_r^{(t-1)}(\mathbf{p}) \mid p \in \mathcal{N}_0(v) \right\}\!\!\right\}, \\ &\qquad\qquad \left\{\!\!\left\{ (c_r^{(t-1)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_1(v) \right\}\!\!\right\}, \\ &\qquad\qquad \vdots \\ &\qquad\qquad \left\{\!\!\left\{ (c_r^{(t-1)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_r(v) \right\}\!\!\right\} \Bigg) \\ &= \psi \circ \mathrm{HASH}^{-1}\left(c_r^{(t)}(v) \right). \end{aligned}$$

Choosing $\phi = \psi \circ \mathrm{HASH}^{-1}$ finishes the proof. $\square$

We conclude this section with the following lemma that justifies our architectural choice in (4).

Lemma 2. *Let $x \in \mathbb{Q}^r$. Then there exist $\varepsilon \in \mathbb{R}^r$ such that*

$$\varphi(x) = \sum_{k=0}^{r} \varepsilon_k x_k \tag{7}$$

is an injective function.

Proof. We prove this claim by induction. For $r = 0$, any $x \neq 0 \in \mathbb{R}$ fulfills the claim. Now, let $\varepsilon \in \mathbb{R}^r$ such that $\varphi(x) : \mathbb{Q}^r \to \mathbb{R}$ is injective. The set $\mathbb{Q}[\varepsilon_1, \ldots, \varepsilon_r] = \{\sum_{k=0}^{r} \varepsilon_k x_k \,|\, x \in \mathbb{Q}^r\}$ is countable and hence a proper subset of $\mathbb{R}$. It follows that there exists $\varepsilon_{r+1} \in \mathbb{R}$ with $\varepsilon_{r+1} \notin \mathbb{Q}[\varepsilon]$. Note that $0 \in \mathbb{Q}$ and hence $\varepsilon_{r+1} \neq 0$. We now prove our claim by contradiction.

Assume there exist $x \neq x' \in \mathbb{Q}^{r+1}$ with $\sum_{k=0}^{r+1} \varepsilon_k x_k = \sum_{k=0}^{r+1} \varepsilon_k x'_k$. We distinguish two cases:

$x_i = x'_i$ for all $i \leq r$ and $x_{r+1} \neq x'_{r+1}$: Then immediately

$$\begin{aligned} & x_{r+1} \neq x'_{r+1} \\ \Rightarrow\quad & \varepsilon_{r+1} x_{r+1} \neq \varepsilon_{r+1} x'_{r+1} \\ \Rightarrow\quad & \sum_{k=0}^{r} \varepsilon_k x_k + \varepsilon_{r+1} x_{r+1} \neq \sum_{k=0}^{r} \varepsilon_k x_k + \varepsilon_{r+1} x'_{r+1} \\ \Rightarrow\quad & \sum_{k=0}^{r+1} \varepsilon_k x_k \neq \sum_{k=0}^{r+1} \varepsilon_k x_k . \end{aligned}$$

$\sum_{k=0}^{r} \varepsilon_k x_k \neq \sum_{k=0}^{r} \varepsilon_k x'_k$: But then

$$\begin{aligned} & \sum_{k=0}^{r} \varepsilon_k x_k + \varepsilon_{r+1} x_{r+1} = \sum_{k=0}^{r} \varepsilon_k x'_k + \varepsilon_{r+1} x'_{r+1} \\ \Leftrightarrow \quad & \sum_{k=0}^{r} \varepsilon_k x_k - \sum_{k=0}^{r} \varepsilon_k x'_k = \varepsilon_{r+1}(x'_{r+1} - x_{r+1}) \end{aligned}$$

The left hand side is an element of $\mathbb{Q}[\varepsilon_1, \ldots, \varepsilon_r]$. However, $\varepsilon_{r+1}(x'_{r+1} - x_{r+1}) \notin \mathbb{Q}[\varepsilon_1, \ldots, \varepsilon_r]$ by choice of ε_{r+1}, leading to a contradiction. $\square$

D. Appendix on Homomorphism Counting and Section 5.3

In this section, we give background information and all proofs that are related to homomorphism counts. We begin by introducing additional definitions and notation.

Definition 14 (Induced Subgraph). *Let $G = (V(G), E(G))$ and $S \subset V(G)$. The* induced subgraph *$G[S]$ of G over S is defined as the graph $G[S]$ with vertices $V(G[S]) = S$ and edges $E(G[S]) = \{\{u, v\} \in E(G) \mid u, v \in S\}$.*

The following definition indicates whether a pair of nodes is connected by an edge or not.

Definition 15 (Atomic Type). *For a tuple of nodes (u_1, u_2), the* atomic type *$\mathrm{atp}_G((u_1, u_2))$ of G over (u_1, u_2) indicates where $\{u_1, u_2\} \in E(G)$, i.e., $\mathrm{atp}_G((u_1, u_2)) = 1$ if $\{u_1, u_2\} \in E(G)$ and zero otherwise.*

We continue by defining *tree graphs*, an important class of graphs that is closely related to the 1-WL test.

Definition 16 (Tree Graph). *A graph T is called a* tree (graph) *if it is connected and does not contain cycles. A* rooted tree *$T^s = (V(T^s), E(T^s))$ is a tree in which a node $s \in V(T^s)$ is singled out. This node is called the* root *of the tree. For each vertex $t \in V(T^s)$, we define its* depth *$\mathrm{dep}_{T^s}(t) := \mathrm{dist}_{T^s}(t, s)$, where dist denotes the shortest path distance between t and s. The* depth *of T^s is then the maximum depth among all nodes $t \in V(T)$. We define $\mathrm{Desc}_{T^s}(t)$ the set of* descendants *of t, i.e., $\mathrm{Desc}_{T^s}(t) = \{t' \in T^s \mid \mathrm{dep}_{T^s}(t') = \mathrm{dep}_{T^s}(t) + \mathrm{dist}_{T^s}(t, t')\}$. For each $t \in V(T^s) \setminus \{s\}$, we define the* parent node *$\mathrm{pa}_{T^s}(t)$ of t as the unique node $t' \in \mathcal{N}(t)$ such that $\mathrm{dep}_{T^s}(t) = \mathrm{dep}_{T^s}(t') + 1$. We define the* subtree of *T^s* rooted at *node t by $T^s[t]$, i.e., $T^s[t] := T^s[\mathrm{Desc}_{T^s}(t)]$.*

The remainder of this section is structured as follows. Appendix D.1 introduces the basics on tree decompositions. In Appendix D.2, we present the class of fan cactus graphs, encompassing all cactus graphs, and develop its canonical tree decomposition. For technical reasons, we present an alternative formulation of r-ℓWL in Appendix D.3. Subsequently, in Appendix D.4 we define the unfolding tree of r-ℓWL and illustrate its relation to the r-ℓWL colors and canonical tree decompositions of fan cactus graphs. Finally, in Appendix D.4.1, we establish the groundwork to conclude the proof of Theorem 2, a simple corollary of all the results in this section.

D.1. Tree Decomposition Preliminaries

Along with its notation, this subsection closely adheres to the conventions outlined by B. Zhang et al. (2024, Section C). In the following, we provide a formal definition of a *tree decomposition* for a graph.

Definition 17 (Tree Decomposition). *Let $G = (V(G), E(G))$. A* tree decomposition *of G is a tree $T = (V(T), E(T))$ together with a function $\beta_T : V(T) \to 2^{V(G)}$ satisfying the following conditions:*

1. *Each tree node $t \in V(T)$ is mapped to a non-empty subset of vertices $\beta_T(t) \subset V(G)$ in G, referred to as a bag. We say tree node t contains vertex u if $u \in \beta_T(t)$.*
2. *For each edge $\{u, v\} \in E(G)$, there exists at least one tree node $t \in V(T)$ such that $\{u, v\} \subset \beta_T(t)$.*
3. *For each vertex $u \in V(G)$, all tree nodes t containing u form a connected subtree, i.e., the induced subgraph $T[\{t \in V(T) : u \in \beta_T(t)\}]$ is connected.*

If (T, β_T) is a tree decomposition of G, we refer to the tuple (G, T, β_T) as a tree-decomposed graph. The width of the tree decomposition T of G is defined as

$$\max_{t \in V(T)} |\beta_T(t)| - 1.$$

If T has root s, we also denote it as (G, T^s, β_T).

Definition 18 (Treewidth)**.** *The* treewidth *of a graph G, denoted as $\mathrm{tw}(G)$, is the minimum positive integer k such that there exists a tree decomposition of width k.*

D.2. Cactus Graphs and their Canonical Tree Decomposition

Cactus graphs play a crucial role in graph theory due to their unique structural properties. Before delving into their canonical tree decomposition, we define the concept of a rooted r-cactus graph. To simplify the notation, we assume that graphs in this section are connected and that $V(G) \subseteq \mathbb{N}$ for all graphs G. Further, we assume that $r \in \mathbb{N}$ throughout this section.

Definition 19 (Rooted r-Cactus Graph)**.** *A* cactus graph *is a graph where every edge lies on at most one simple cycle. An* r-cactus graph *is a cactus graph where every simple cycle has at most r vertices. A rooted cactus (graph) G^s is a cactus graph G with a root node $s \in V(G)$.*

Now, we introduce the notion of a fan cactus, which is an essential concept for our subsequent discussions on the canonical tree decomposition of these graphs.

Definition 20 (Fan Cactus)**.** *Let G^s be a rooted r-cactus. For every simple cycle C in G let v_C be the unique vertex in C that is closest to s. We obtain a* fan r-cactus *F^s from a rooted r-cactus G^s by adding an arbitrary number of edges $\{v_C, w\}$ to any cycle C with $w \in V(C)$. Let $\mathcal{M}^{r+2}$ be the class of graphs F with $s \in V(F)$ such that F^s is a fan r-cactus.*

Remark 1. *Every r-cactus is a fan r-cactus. Every fan r-cactus is outerplanar. Every outerplanar graph has tree-width at most 2.*

Figure 7 shows an example of a fan 6-cactus. As fan cacti are outerplanar, graph isomorphism can be decided in linear time. One way to do so is to use a *canonicalization* function, that maps graphs to a unique representative of each set of isomorphic graphs. We denote the set of all such representatives as $\mathcal{M}^{r+2}/\cong \subseteq \mathcal{M}^{r+2}$.

Lemma 3 (Colbourn et al. (1981))**.** *There exists a function* $\mathrm{canon} : \mathcal{M}^{r+2} \to \mathcal{M}^{r+2}/\cong$ *such that*

1. $G \cong \mathrm{canon}(G)$
2. $G \cong H \iff V(\mathrm{canon}(G)) = V(\mathrm{canon}(H)) \wedge E(\mathrm{canon}(G)) = E(\mathrm{canon}(H))$.

Moreover, given $G \in \mathcal{M}^{r+2}$, $\mathrm{canon}(G)$ *can be computed in linear time.*

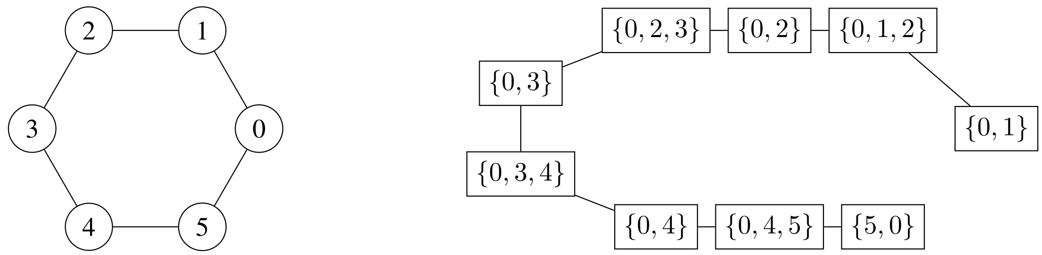
For each $G \in \mathcal{M}^{r+2}$ we denote the isomorphism between G and $\mathrm{canon}(G)$ as canon_G. Colbourn et al. (1981) describe a bottom-up algorithm to obtain $\mathrm{canon}(G)$ of a fan r-cactus G. We will implicitly use the results of this canonicalization to define a canonical *tree decomposition* of fan r-cacti. The crucial point in the algorithm is a simple way to decide which "direction" to use when dealing with a cycle in the underlying cactus graph. Each undirected, rooted cycle allows for a choice between two directions when building a tree decomposition. We will first define a tree decomposition for a rooted cycle which depends on a choice of direction and then define a canonical direction of cycles in G based on canon_G.

Definition 21 (Tree Decomposition of Rooted Cycle)**.** *Let C_n be a cycle graph on n nodes v_0 to v_{n-1}. The path T on nodes $w_1, \ldots, w_{2n-3}$ with bags $\beta(w_1) = \{v_0, v_1\}$ and for $i \geq 2$*

$$\beta(w_i) = \begin{cases} \beta(w_{i-1}) \cup \{v_i\} & \textit{if } i \textit{ is even} \\ \beta(w_{i-1}) \setminus \{v_{i-2}\} & \textit{if } i \textit{ is odd} \end{cases}$$

is a tree decomposition of C_n. We say that v_0 and v_1 correspond *to w_0 and v_i* corresponds *to w_{2i-1} for $i \geq 2$.*

A depiction of the tree decomposition T^0 (right) of C_6 (left) is shown below. Note that we have to choose one of two possible orientations of the undirected cycle to construct T^0. We address this choice in the next definition.



Definition 22 (Canonical Tree Decomposition of Undirected Rooted Cycle)**.** *Let F^s be a fan r-cactus and C be a simple cycle in the underlying cactus G. Let $v_C, v_1, \ldots, v_{n-1}$ and $v_C, v_{n-1}, \ldots, v_1$ be the two directions of C rooted at v_C. We define the canonical tree decomposition of C in G as the tree decomposition of the smaller of the two orientations* $\mathrm{canon}_F(v_C), \mathrm{canon}_F(v_1), \ldots, \mathrm{canon}_F(v_{n-1})$ *and* $\mathrm{canon}_F(v_C), \mathrm{canon}_F(v_{n-1}), \ldots, \mathrm{canon}_F(v_1)$.

The choice of "smaller" does not matter as long as it defines a total order. One can, for example, use a lexicographical order. Based on Definition 22, we now define a canonical tree decomposition of fan cactus graphs, in the sense that any two isomorphic fan cactus graphs will have isomorphic tree decompositions.

Definition 23 (Canonical Tree Decomposition of Fan r-Cactus Graphs)**.** *Let F^s be a fan r-cactus and G^s its underlying r-cactus. We define the canonical tree decomposition $T^{\tilde{s}}$ of F rooted at $\tilde{s}$ as follows*

1. ***Node Gadget:*** *For all $v \in V(F)$ add a node t to $V(T)$ and set $\beta(t) = \{v\}$. We choose $\tilde{s}$ such that $\beta(\tilde{s}) = \{s\}$.*
2. ***Tree Edge Gadget:*** *For all $\{v, w\} \in E(G)$ that are not on a simple cycle in F add a node $x_{\{v,w\}}$ to $V(T)$ with $\beta(x_{\{v,w\}}) = \{v, w\}$ and edges $\{v, x_{\{v,w\}}\}$ and $\{w, x_{\{v,w\}}\}$ to $E(T)$*
3. ***Cycle Gadget:*** *For each (undirected) cycle C in the underlying cactus G, add a copy of its canonical tree decomposition $T_C^{v_C}$ of C rooted at v_C to T and connect nodes in it to the corresponding node gadgets.*

For the discussions in subsequent sections, we introduce the following definition.

Definition 24 (Depth in the Canonical Tree Decomposition of Fan r-Cactus Graphs)**.** *Let (F, T^s) be a canonical tree decomposition of a fan r-cactus. We define the* depth $\mathrm{dep}(t)$ *of $t \in V(T)$ recursively as follows:*

1. $\mathrm{dep}(s) = 0$
2. *For $v \in V(T)$ with parent node p:* $\mathrm{dep}(v) = \begin{cases} \mathrm{dep}(p) + 1 & \text{if } |\beta(v)| = 1 \text{ or } |\beta(p)| = 1 \\ \mathrm{dep}(p) & \text{otherwise} \end{cases}$

The depth of (F, T^s) is then the maximum depth of any node $t \in V(T^s)$.

Intuitively, for a given fan r-cactus graph F with its canonical tree decomposition T^s, Definition 24 captures the depth (see Definition 17) of the tree T^s, if cycles in F and the corresponding bags in T^s were replaced single edges.

Lemma 4. *Let F^s be a fan r-cactus. The canonical tree decomposition $(F, T^{\tilde{s}})$ is a tree decomposition of F^s.*

Proof. We need to show that (1) T is a tree, (2) for every edge $e \in E(F)$ there exists some bag $\beta(v)$ with $e \subseteq \beta(v)$, and (3) $T[\{t \in V(T) : u \in \beta(t)\}]$ is connected.

To see that T does not contain cycles, note that we replace each cycle with its cycle gadget, which is a path. It is easy to see that T is connected as G is connected.

For (2), note that tree edges $e \in V(F)$ have their own gadget node in x_e with $\beta(x_e) = e$. Similarly, each edge e on a simple cycle C of the underlying cactus F of G is contained in some bag within the cycle gadget of C. Finally, for diagonal edges $\{v_C, w\} \in E(F) \setminus E(G)$, v_C is contained in any bag of the cycle gadget of C. As a result $\{v_C, v\}$ is contained in the bag of the corresponding node of v.

For (3), note that in the tree edge gadget nodes t with $v \in \beta(t)$ are connected to the node gadget of v. In the cycle gadget, any node t with $w \in \beta(t)$ is either directly or via its neighbor connected to the node gadget of w if $w \neq v_C$. As the cycle gadget is connected and v_C is in any bag of the gadget, there also exists a path to the node gadget of v_C where every bag contains v_C. □

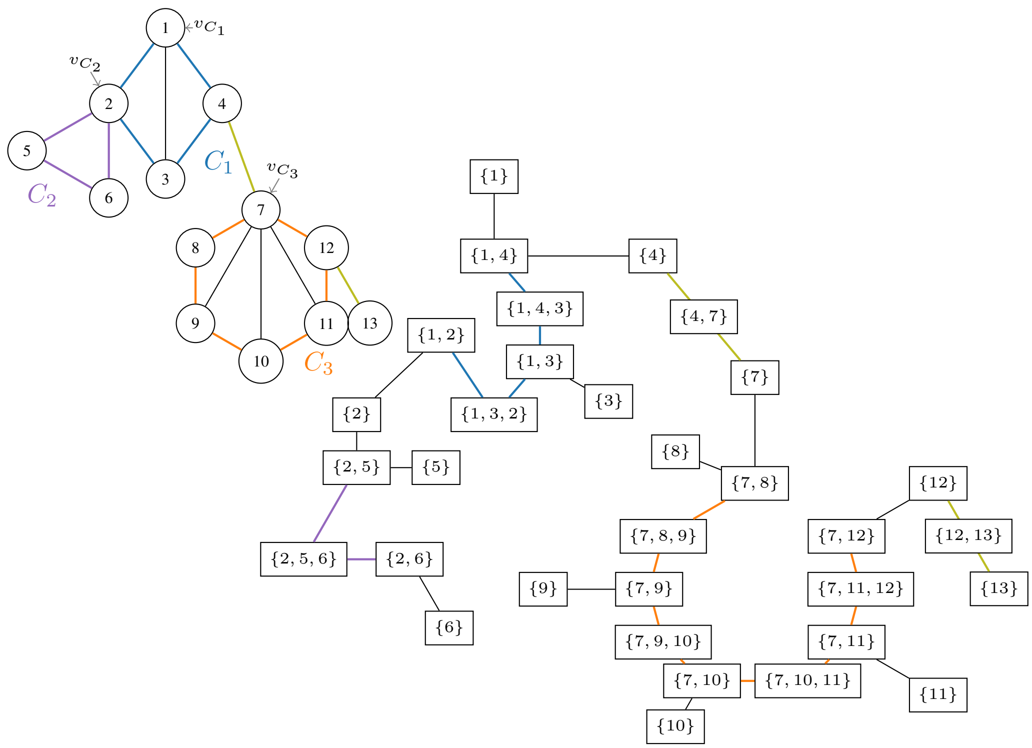


Figure 7: Example of a fan 6-cactus F^1 (left) and its canonical tree decomposition $(T, 1)$. The underlying rooted 6-cactus G^1 (on colored, thick edges) of F^1 contains three simple cycles C_1, C_2, C_3. Additional diagonal edges must have v_{C_i} as one endpoint.

We conclude this subsection with a formal definition of when two canonical tree decompositions are isomorphic and prove the main result of this section, i.e. that canonical tree decompositions of fan r-cacti G^s, H^t are isomorphic whenever G^s, H^t are isomorphic.

Definition 25 (Isomorphism between canonical tree-decomposed graphs)**.** *Given two canonical tree-decomposed graphs* (G, T^s) *and* $(\tilde{G}, \tilde{T}^{\tilde{s}})$*, a pair of mappings* (ρ, τ) *is called an* isomorphism between (G, T^s) and $(\tilde{G}, \tilde{T}^{\tilde{s}})$*, denoted by* $(G, T^s) \cong (\tilde{G}, \tilde{T}^{\tilde{s}})$*, if the following holds:*

- *ρ is an isomorphism between G and $\tilde{G}$,*
- *τ is an isomorphism between T^s and $\tilde{T}^{\tilde{s}}$,*
- *For any $t \in T^s$, we have $\rho(\beta_T(t)) = \beta_{\tilde{T}}(\tau(t))$.*

Lemma 5. *Let $G^s \cong H^t$ be rooted r-fan cacti. Then $(G^s, T[G^s]) \cong (H^t, T[H^t])$.*

Proof. Let ρ be a root preserving isomorphism between G^s and H^t. According to Lemma 3 then there exist isomorphisms canon_G and canon_H with $\rho = \mathrm{canon}_G \circ \mathrm{canon}_H^{-1}$. We construct $\tau : V(T[G^s]) \to V(T[H^t])$ from ρ as follows: It is easy to see that ρ induces a bijective mapping τ between the nodes of $T[G^s]$ and $T[H^t]$ that assigns each gadget node $v \in V(T[G^s])$ to the unique gadget node $\tau(v) \in V(T[H^t])$ with $\beta(\tau(v)) = \rho(\beta(v))$. By the same argument, τ maps the root of $T[G^s]$ to the root of $T[H^t]$.

Now assume by contradiction that τ is not an isomorphism between $T[G^s]$ and $T[H^t]$. That means that w.l.o.g. there exists $\{v, w\} \in E(T[G^s])$ with $\{\tau(v), \tau(w)\} \notin E(T[H^t])$. However, for the bags of v, w it holds $\mathrm{canon}_G(\beta(v)) = \mathrm{canon}_H(\beta(\tau(v)))$ and $\mathrm{canon}_G(\beta(w)) = \mathrm{canon}_H(\beta(\tau(w)))$. This cannot happen, as the addition of edges in Definition 23 depends only on the images of the bags under canon. $\square$

D.3. Alternative r-ℓWL

In this subsection, we define slightly modified versions of 1-WL and r-ℓWL that we consider in the subsequent sections.

Definition 26 (Alternative 1-WL and r-ℓWL)**.** *The* alternative 1-WL test *refines vertices' colors as*

$$c^{(t+1)}(v) \leftarrow \mathrm{HASH}\left(c^{(t)}(v), \left\{\!\!\left\{\left(\mathrm{atp}(v,u), c^{(t)}(u)\right) \mid u \in V(G)\right\}\!\!\right\}\right).$$

Equivalently, we define the alternative r-ℓWL *via*

$$\begin{aligned} c_r^{(t+1)}(v) \leftarrow \mathrm{HASH}_r \Bigg(& c_r^{(t)}(v), \left\{\!\!\left\{\left(\mathrm{atp}(v,u), c^{(t)}(u)\right) \mid u \in V(G)\right\}\!\!\right\}, \\ & \left\{\!\!\left\{ c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_1(v)\right\}\!\!\right\}, \\ & \vdots \\ & \left\{\!\!\left\{ c_r^{(t)}(\mathbf{p}) \mid \mathbf{p} \in \mathcal{N}_r(v)\right\}\!\!\right\} \Bigg), \end{aligned}$$

It is well-known that both the alternative 1-WL test and the standard 1-WL test are equally powerful (in terms of their expressive power). Similarly, the alternative r-WL test and the standard r-WL test are equally powerful. For the sake of simplicity in the subsequent discussion, we will refer to both the alternative 1-WL and r-WL tests simply as the 1-WL and r-WL tests, respectively. Although this practice may seem like a slight abuse of notation, it is justified because the expressive power of these tests remains unaffected.

Finally, as noted in Section 6, we alter the r-ℓWL algorithm slightly by incorporating atomic types into the path representation.

Hence, we update node features according to

$$
\begin{aligned}
c_r^{(t+1)}(v) \leftarrow \mathrm{HASH}_r \Bigg(c_r^{(t)}(v), & \left\{\!\!\left\{ \left(\mathrm{atp}(v,u), c^{(t)}(u)\right) \mid u \in V(G) \right\}\!\!\right\}, \\
& \left\{\!\!\left\{ \left(\mathrm{atp}(v,\mathbf{p}), c_r^{(t)}(\mathbf{p})\right) \mid \mathbf{p} \in \mathcal{N}_1(v) \right\}\!\!\right\}, \\
& \vdots \\
& \left\{\!\!\left\{ \left(\mathrm{atp}(v,\mathbf{p}), c_r^{(t)}(\mathbf{p})\right) \mid \mathbf{p} \in \mathcal{N}_r(v) \right\}\!\!\right\} \Bigg),
\end{aligned} \tag{8}
$$

where $\left(\mathrm{atp}(v,\mathbf{p}), c_r^{(t)}(\mathbf{p})\right) := \left(\left(\mathrm{atp}(v,p_1), c_r^{(t)}(p_1)\right), \ldots, \left(\mathrm{atp}(v,p_{q+1}), c_r^{(t)}(p_{q+1})\right)\right)$ for $\mathbf{p} = \{p_i\}_{i=1}^{q+1} \in \mathcal{N}_q(v)$. The definition of atomic types $\mathrm{atp}(\cdot,\cdot)$ is given in Definition 15. Clearly this version of r-ℓWL is more powerful than the standard version, according to Definition 6. However, it is unclear whether r-ℓWL with atomic types is strictly more powerful than standard r-ℓWL.

D.4. The Unfolding Tree of r-ℓWL

Given Definition 22, we assume, for the remainder of this appendix, that every fan cactus graph has a unique labeling function, allowing us to select a unique orientation for every cycle in the graph. We call this orientation the *canonical orientation*. If not otherwise mentioned, we consider the canonical orientation of cycle graphs.

We begin this section by introducing a critical concept known as *bag isomorphism* (Dell et al., 2018; B. Zhang et al., 2024).

Definition 27 (Bag Isomorphism)**.** *Let (F, T^s) be a tree-decomposed graph, and G be a graph. A homomorphism f from F to G is called a* bag isomorphism *from (F, T^s) to G if, for all $t \in V(T^s)$, the mapping f is an isomorphism from $F[\beta_{T^s}(t)]$ to $G[f(\beta_{T^s}(t))]$. We denote by $\mathrm{BIso}((F,T^s), G)$ the set of all bag isomorphisms from (F, T^s) to G, and set $\mathrm{bIso}((F,T^s),G) = |\mathrm{BIso}((F,T^s),G)|$.*

Moving forward, we proceed to define r-ℓWL unfolding trees, which intuitively construct, for a given graph and a node in the graph, the computational graph of the r-ℓWL algorithm and its canonical tree decomposition.

Definition 28 (Unfolding tree of r-ℓWL)**.** *Given a graph G, vertex $v \in V(G)$ and a non-negative $D \in \mathbb{Z}$, the* depth-$2D$ r-ℓWL unfolding tree *of a graph $G \in \mathcal{M}^{r+2}$ at node v, denoted as $\left(F^{(D)}(v), T^{(D)}(v)\right)$, is a tree-decomposition (F, T^s) constructed in the following way:*

1. ***Initialization**: $V(F) = \{v\}$ without edges, and T^s only has a root node s with $\beta_{T^s}(s) = \{v\}$. Define a mapping $V(F) \to V(G)$ as $\pi(v) = v$.*
2. ***Introduce nodes**: For each leaf node t with $|\beta_{T^s}(t)| = 1$ in T^s, do the following procedure:*

   Let $\beta_T(t) = \{g\}$. For each $w \in V(G)$ do the following:
   a) *Add a fresh child t_w to t in T^s.*
   b) *Add a fresh vertex f to F and extend π with $[f \mapsto w]$.*
   c) *Define the bag of t_w by $\beta_{T^s}(t_w) = \beta_{T^s}(t) \cup \{f\}$.*
   d) *Add an edge between f and g if $\{\pi(f), \pi(g)\}\ E(G)$.*
3. ***Introduce paths**: For each $q = 1, \ldots, r$, do:*
   For each length q path with canonical orientation $\mathbf{p} = \{p_i\}_{i=1}^{q+1} \in \mathcal{N}_q(g)$, do the following:
   a) *Add a fresh path $\mathbf{t_p} = \left\{t_{\{p_1\}}, t_{\{p_1,p_2\}}, t_{\{p_2\}}, \ldots, t_{\{p_q\}}, t_{\{p_q,p_{q+1}\}}, t_{\{p_{q+1}\}}\right\}$ to t in T^s.*
   b) *Add $q+1$ fresh vertices $f_1, \ldots, f_{q+1}$ to F and extend π with $[f_i \mapsto p_i]$ for every $i = 1, \ldots, q+1$.*
   c) *For $i = 1, \ldots, q$, let the bag of $t_{\{p_i,p_{i+1}\}}$ be defined via $\beta_{T^s}(t_{\{p_i,p_{i+1}\}}) = \beta_{T^s}(t) \cup \{f_i, f_{i+1}\}$.*
   d) *For $i = 1, \ldots, q+1$, let the bag of $t_{\{p_i\}}$ be defined via $\beta_{T^s}(t_{\{p_i\}}) = \beta_{T^s}(t) \cup \{f_i\}$.*
   e) *For $i = 1, \ldots, q+1$, add edges between f_i and f_{i+1}.*

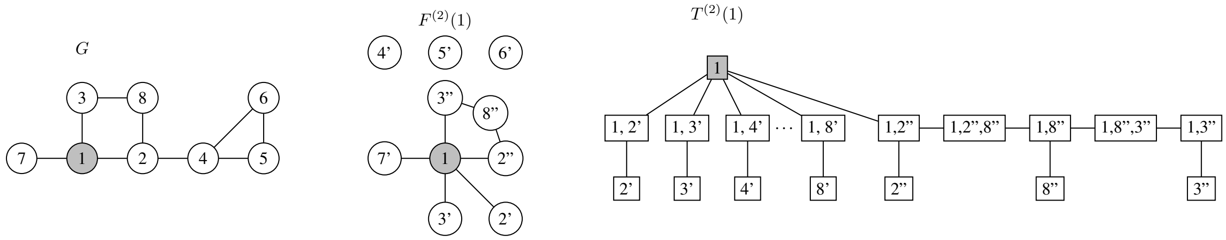


Figure 8: The depth-2 unfolding tree of graph G at vertex 1 for 2-ℓWL.

   f) *Add edges between g and $f_1, \ldots, f_{q+1}$ such that for every $i = 1, \ldots, q$, we have $F[\beta_{T^s}(t_{\{p_i,p_{i+1}\}})] = F[\{f_i, f_{i+1}, g\}] \cong G[\pi(\beta_{T^s}(t_{\{p_i,p_{i+1}\}}))]$, i.e., add edges between g and f_i if and only if there is an edge between $\{\pi(g), \pi(f_i)\} \in E(G)$.*

4. ***Forget nodes**: If t is a leaf node of T^s with $|\beta_{T^s}(t)| = 2$ and parent t' with $|\beta_{T^s}(t)| = 1$, do the following:*
   a) *Add a fresh child t_1 of t to T^s.*
   b) *Let f be that vertex introduced at t, that is, we have $\beta_{T^s}(t) \setminus \beta_{T^s}(t') = \{f\}$.*
   c) *We set $\beta_{T^s}(t_1) = \{f\}$.*

5. ***Forget paths**: If $\mathbf{t_p} = \{t_{\{p_1\}}, t_{\{p_1,p_2\}}, t_{\{p_2\}}, \ldots, t_{\{p_q\}}, t_{\{p_q,p_{q+1}\}}, t_{\{p_{q+1}\}}\}$ is a leaf path of T^s with parent t' of $t_{\{p_1\}}$, do the following:*
   a) *For $i = 2, \ldots, q+1$, add a fresh child $\tilde{t}_{\{p_i\}}$ to $t_{\{p_i\}}$.*
   b) *Let $f_2, \ldots, f_{q+1}$ be the vertices introduced at $\mathbf{t_p}$, that is, we have $\beta_{T^s}(t_{\{p_i\}}) \setminus \beta_{T^s}(t') = \{f_i\}$.*
   c) *For $i = 2, \ldots, q+1$, we set $\beta_{T^s}(\tilde{t}_{\{p_i\}}) = \{f_i\}$.*

We refer to Figure 8 for the depth-2 2-ℓWL unfolding tree of an example graph.

Theorem 5. *Let $r \geq 1$. For any graph G, any vertex $v \in V(G)$, and any non-negative integer D, let $\left(F^{(D)}(v), T^{(D)}(v)\right)$ be its depth-$2D$ r-ℓWL unfolding tree at node v. Then, $F^{(D)}(v)$ is a fan r-cactus graph, and $T^{(D)}(v)$ is an r-canonical tree decomposition of $F^{(D)}(v)$. Moreover, the constructed mapping π in Definition 28 is a bag isomorphism from $\left(F^{(D)}(v), T^{(D)}(v)\right)$ to the graph G.*

Proof. Clear by the definition of the depth-$2D$ unfolding tree of r-ℓWL. $\square$

We present the following results that fully characterize when two graphs and their respective nodes have the same r-ℓWL colors in terms of their r-ℓWL unfolding trees.

Theorem 6. *Let $r \in \mathbb{N}$. For any two connected graphs G, H, any vertices $v \in V(G)$ and $x \in V(H)$ and any $D \in \mathbb{N}$, it holds: $c_r^{(D)}(v) = c_r^{(D)}(x)$ if and only if there exists a root preserving isomorphism between $\left(F^{(D)}(v), T^{(D)}(v)\right)$ and $\left(F^{(D)}(x), T^{(D)}(x)\right)$.*

Proof of "$\Longrightarrow$". The proof is based on induction over D. When $D = 0$, the theorem obviously holds. Assume that the theorem holds for $D \leq d$, and consider $D = d+1$. We show that if $c_r^{(d+1)}(v) = c_r^{(d+1)}(x)$, then there exists an isomorphism (ρ, τ) from $\left(F^{(d+1)}(v), T^{(d+1)}(v)\right)$ to $\left(F^{(d+1)}(x), T^{(d+1)}(x)\right)$ such that $\rho(v) = x$.

If $c_r^{(d+1)}(v) = c_r^{(d+1)}(x)$, then

$$\left\{\left\{\left(\operatorname{atp}(v,u), c_r^{(d)}(u)\right) \mid u \in V(G)\right\}\right\} = \left\{\left\{\left(\operatorname{atp}(x,y), c_r^{(d)}(y)\right) \mid y \in V(H)\right\}\right\},$$

i.e., $|V(G)| = |V(H)|$, and we set $n = |V(G)|$. We enumerate $V(G) = \{w_1, \ldots, w_n\}$ and $V(H) = \{z_1, \ldots, z_n\}$ such that

$$c_r^{(d)}(w_i) = c_r^{(d)}(z_i) \tag{9}$$

for all $i = 1, \dots, n$. Also, again since $c_r^{(d+1)}(v) = c_r^{(d+1)}(x)$, we have for every $q = 1, \dots, r$,

$$\begin{aligned}&\left\{\left\{\left(\left(\operatorname{atp}(v,u_1), c_r^{(d)}(u_1)\right), \dots, \left(\operatorname{atp}(v,u_{q+1}), c_r^{(d)}(u_{q+1})\right)\right) \mid \{u_1,\dots,u_{q+1}\} = \mathbf{u} \in \mathcal{N}_q(v)\right\}\right\}\\ =&\left\{\left\{\left(\left(\operatorname{atp}(x,y_1), c_r^{(d)}(y_1)\right), \dots, \left(\operatorname{atp}(x,y_{q+1}), c_r^{(d)}(y_{q+1})\right)\right) \mid \{y_1,\dots,y_{q+1}\} = \mathbf{y} \in \mathcal{N}_q(x)\right\}\right\}.\end{aligned}$$

In particular, $|\mathcal{N}_q(v)| = |\mathcal{N}_q(x)|$ and we can enumerate the paths in $\mathcal{N}_q(v)$ and $\mathcal{N}_q(x)$ such that

$$c_r^{(d)}(\mathbf{u}_l^q) = c_r^{(d)}(\mathbf{y}_l^q) \text{ and } \operatorname{atp}(v, \mathbf{u}_l^q) = \operatorname{atp}(v, \mathbf{y}_l^q) \tag{10}$$

for every $l = 1, \dots, |\mathcal{N}_q(v)|$.

Now, by definition of the r-ℓWL tree unfolding, the graph $F^{(d+1)}(v)$ is isomorphic to the union of: a) all graphs $F^{(d)}(w_i)$ for $i = 1, \dots, n$, plus additional edges between w_i to v if $\{w_i, v\} \in E(G)$, and b) all graphs $F^{(d)}(p_{l,k}^q)$ for $q = 1, \dots, r$, $l = 1, \dots, |\mathcal{N}_q(v)|$ for any path $\mathbf{p}_l^q = \left\{p_{l,1}^q, \dots, p_{l,q+1}^q\right\} \in \mathcal{N}_q(v)$. And adding, for $k = 1, \dots q$, edges between $p_{l,k}^q$ and $p_{l,k+1}^q$. And adding, for $k = 1, \dots q+1$, edges $p_{l,k}^q$ and v if there is one in G, i.e., if $\left\{p_{l,k}^q, v\right\} \in E(G)$.

Similarly, the tree $T^{(d+1)}(v)$ is isomorphic to the disjoint union of all trees $T^{(d)}(w_i)$ (for $i = 1, \dots, n$) and $T^{(d)}(p_{l,k}^q)$ (for $q = 1, \dots, r$, $k = 1, \dots, q+1$ and $l = 1, \dots, |\mathcal{N}(v)|$). Plus adding the following fresh tree nodes and edges: a root node s, nodes t_{w_i} (for $i = 1, \dots, n$) that connects to s and the root of $T^{(d)}(w_i)$. And for $q = 1, \dots, r$, $l = 1, \dots, |\mathcal{N}_q(v)|$ for any path $\mathbf{p}_l^q \in \mathcal{N}_q(v)$ a path of length $2q$, given by $\mathbf{t}_{\mathbf{p}_l^q} = \left\{t_{\{p_{l,1}^q\}}, t_{\{p_{l,1}^q, p_{l,2}^q\}}, \dots, t_{\{p_{l,q}^q, p_{l,q+1}^q\}}, t_{\{p_{l,q+1}^q\}}\right\}$, where s is attached to $t_{\{p_{l,1}^q\}}$. And finally, connecting the trees $T^{(d)}(p_{l,k}^q)$ at root node $p_{l,k}^q$ to $t_{\{p_{l,k}^q\}}$.

By (9) and induction, there exist isomorphisms (ρ_i, τ_i) from $(F^{(d)}(w_i), T^{(d)}(w_i))$ to $(F^{(d)}(z_i), T^{(d)}(z_i))$ such that $\rho_i(w_i) = z_i$ for $i = 1, \dots, n$. By (10) and induction, there exist isomorphisms $(\rho_{l,k}^q, \tau_{l,k}^q)$ from $(F^{(d)}(u_{l,k}^q), T^{(d)}(u_{l,k}^q))$ to $(F^{(d)}(y_{l,k}^q), T^{(d)}(y_{l,k}^q))$ such $\rho_i(u_{l,k}^q) = y_{l,k}^q$ for $q = 1, \dots, r$, $k = 1, \dots, q+1$ and $l = 1, \dots, |\mathcal{N}_q(v)|$.

We now construct ρ by merging all ρ_i and $\rho_{l,k}^q$, and construct τ by merging all τ_i and $\tau_{l,k}^q$. We finally specify an appropriate mapping for the tree root, its direct children and the paths attached to the tree root. Then, it is easy to see that (ρ, τ) is well-defined and an isomorphism between $\left(F^{(d+1)}(v), T^{(d+1)}(v)\right)$ and $\left(F^{(d+1)}(x), T^{(d+1)}(x)\right)$ such that $\rho(v) = x$.

□

Proof of "$\Longleftarrow$". We now prove the other direction, again via induction over D. When $D = 0$ the assertion obviously holds. Assume that the assertion holds for $D \leq d$. Now, assume that there exists an isomorphism (ρ, τ) between $\left(F^{(d+1)}(v), T^{(d+1)}(v)\right)$ and $\left(F^{(d+1)}(x), T^{(d+1)}(x)\right)$ such that $\rho(v) = x$. We show that $c_r^{(d+1)}(v) = c_r^{(d+1)}(x)$.

We begin our proof by establishing the equality of two multisets: $\left\{\left\{(c_r^{(d)}(w), \operatorname{atp}(v, w)) | w \in V(G)\right\}\right\}$ and $\left\{\left\{(c_r^{(d)}(z), \operatorname{atp}(v, z)) | z \in V(H)\right\}\right\}$. The proof of this equivalence closely mirrors the argument presented in the proof of B. Zhang et al. (2024, Lemma C.14). Since τ is an isomorphism it maps all tree nodes $T^{(d+1)}(v)$ of depth 2 with 1 element in their bag to the corresponding tree nodes in $T^{(d+1)}(x)$. Let $s_1, \dots, s_n$ and $t_1, \dots, t_n$ be the nodes in $T^{(d+1)}(v)$ and $T^{(d+1)}(x)$ of depth 2 with 1 element in their bag, respectively. For $i = 1, \dots, n$, let s_i' and t_i' the parents of s_i and t_i, respectively. We then choose the order such that the following holds for all $i = 1, \dots, n$

1. Let $\beta_{T^{(d+1)}(v)}(s_i') = \{v, \tilde{w}_i\}$ and $\beta_{T^{(d+1)}(x)}(t_i') = \{x, \tilde{z}_i\}$. Then, $\rho(v) = x$ and $\rho(\tilde{w}_i) = \tilde{z}_i$ and thus, per assumption, $\{v, \tilde{w}_i\} \in E(F^{(d+1)}(v))$ if and only if $\{x, \tilde{z}_i\} \in E(F^{(d+1)}(x))$.
2. τ is an isomorphism from the subtree rooted at s_i in $T^{(d+1)}(v)$, i.e., $T^{(d+1)}(v)[s_i]$, the subtree rooted at t_i in $T^{(d+1)}(x)$, i.e., $T^{(d+1)}(v)[t_i]$.
3. For all $s \in \operatorname{Desc}_{T^{(d+1)}(v)}(s_i)$, it holds $\rho(\beta_{T^{(d+1)}(v)}(s)) = \beta_{T^{(d+1)}(x)}(\tau(s))$.
4. By the definition of the unfolding tree, ρ is an isomorphism from the induced subgraph $F^{(d+1)}(v)\left[T^{(d+1)}(v)[s_i]\right]$ and the induced subgraph $F^{(d+1)}(x)\left[T^{(d+1)}(x)[t_i]\right]$.

By the last three items, we get that $\left(F^{(d+1)}(v)\left[T^{(d+1)}(v)[s_i]\right], T^{(d+1)}(v)[s_i]\right)$ and $\left(F^{(d+1)}(x)\left[T^{(d+1)}(x)[t_i]\right], T^{(d+1)}(x)[t_i]\right)$ are isomorphic. By definition of the r-ℓWL unfolding tree, $\left(F^{(d+1)}(v)\left[T^{(d+1)}(v)[s_i]\right], T^{(d+1)}(v)[s_i]\right)$ is isomorphic to $(F^{(d)}(w_i), T^{(d)}(w_i))$ for some $w_i \in V(G)$ that satisfies $\{\tilde{w}_i, v\} \in E_{F^{(d+1)}(v)}$ if and only if $\{w_i, v\} \in E(G)$. And $\left(F^{(d+1)}(x)\left[T^{(d+1)}(x)[t_i]\right], T^{(d+1)}(x)[t_i]\right)$ is isomorphic to $(F^{(d)}(z_i), F^{(d)}(z_i))$ for some $z_i \in V(H)$ that satisfies $\{\tilde{z}_i, x\} \in E(F^{(d+1)}(x))$ if and only if $\{z_i, x\} \in E(G)$. Hence, by induction, we have $\operatorname{atp}(v, w_i) = \operatorname{atp}(x, z_i)$ and $c_r^{(d)}(w_i) = c_r^{(d)}(z_i)$ for all $i = 1, \ldots, n$.

It remains to show that, for every $q = 1, \ldots, r$,

$$\begin{aligned}&\left\{\!\!\left\{\left(\left(\operatorname{atp}(v, u_1), c_r^{(d)}(u_1)\right), \ldots, \left(\operatorname{atp}(v, u_{q+1}), c_r^{(d)}(u_{q+1})\right)\right) \mid \{u_1, \ldots, u_{q+1}\} = \mathbf{u} \in \mathcal{N}_q(v)\right\}\!\!\right\} \\ =&\left\{\!\!\left\{\left(\left(\operatorname{atp}(x, y_1), c_r^{(d)}(y_1)\right), \ldots, \left(\operatorname{atp}(x, y_{q+1}), c_r^{(d)}(y_{q+1})\right)\right) \mid \{y_1, \ldots, y_{q+1}\} = \mathbf{y} \in \mathcal{N}_q(x)\right\}\!\!\right\}.\end{aligned}$$

Fix $q = 1, \ldots, r$. Since τ is an isomorphism it maps all paths of length q in $T^{(d+1)}(v)$ connected to v to paths of length q in $T^{(d+1)}(x)$ connected to x.

By construction of the r-ℓWL unfolding tree and since (ρ, τ) is an isomorphism, it holds $|\mathcal{N}_q(v)| = |\mathcal{N}_q(x)|$. Denote the relevant bags at depth 2 by $s'^q_{l,k}$ for $l = 1, \ldots, |\mathcal{N}_q(v)|$ and $k = 1, \ldots, q+1$. Denote by $s^q_{l,k}$ and $t^q_{l,k}$ the parents of $s'^q_{l,k}$ and $t'^q_{l,k}$, respectively. We then choose the order $l = 1, \ldots, |\mathcal{N}_q(v)|$ and $k = 1, \ldots, q+1$ such that it holds

1. Let $\beta_{T^{(d+1)}}(s'^q_{l,k}) = \left\{v, \tilde{w}^q_{l,k}\right\}$ and $\beta_{T^{(d+1)}}(t'^q_{l,k}) = \left\{x, \tilde{z}^q_{l,k}\right\}$. Then, $\rho(\tilde{w}^q_{l,k}) = \tilde{z}^q_{l,k}$ and thus, per assumption, $\left\{v, \tilde{w}^q_{l,k}\right\} \in E(F^{(d+1)}(v))$ if and only if $\left\{x, \tilde{z}^q_{l,k}\right\} \in E(F^{(d+1)}(x))$
2. τ is an isomorphism from the subtree rooted at $s^q_{l,k}$ in $T^{(d+1)}(v)$, i.e., $T^{(d+1)}(v)[s^q_{l,k}]$, to the subtree rooted at $t^q_{l,k}$ in $T^{(d+1)}(x)$, i.e., $T^{(d+1)}(x)[t^q_{l,k}]$.
3. For all $s \in \operatorname{Desc}_{T^{(d+1)}(v)}(s^q_{l,k})$, it holds $\rho(\beta_{T^{(d+1)}(v)}(s)) = \beta_{T^{(d+1)}(x)}(\tau(s))$.
4. By the definition of the unfolding tree, ρ is an isomorphism from the induced subgraph $F^{(d+1)}(v)\left[T^{(d+1)}(v)[s^q_{l,k}]\right]$ and the induced subgraph $F^{(d+1)}(x)\left[T^{(d+1)}(x)[t^q_{l,k}]\right]$.

By the last three items, we get that $\left(F^{(d+1)}(v)\left[T^{(d+1)}(v)[s^q_{l,k}]\right], T^{(d+1)}(v)[s^q_{l,k}]\right)$ and $\left(F^{(d+1)}(x)\left[T^{(d+1)}(x)[t^q_{l,k}]\right], T^{(d+1)}(x)[t^q_{l,k}]\right)$ are isomorphic. By definition of the r-ℓWL unfolding tree, $\left(F^{(d+1)}(v)\left[T^{(d+1)}(v)[s^q_{l,k}]\right], T^{(d+1)}(v)[s^q_{l,k}]\right)$ is isomorphic to $(F^{(d)}(w^q_{l,k}), T^{(d)}(w^q_{l,k}))$ for $w^q_{l,k} \in V(G)$ that satisfies $\left\{\tilde{w}^q_{l,k}, v\right\} \in E_{F^{(d+1)}(v)}$ if and only if $\left\{w^q_{l,k}, v\right\} \in E(G)$.

And $\left(F^{(d+1)}(x)\left[T^{(d+1)}(x)[t^q_{l,k}]\right], T^{(d+1)}(x)[t^q_{l,k}]\right)$ is isomorphic to $(F^{(d)}(z^q_{l,k}), T^{(d)}(z^q_{l,k}))$ for $z^q_{l,k} \in V(G)$ that satisfies $\left\{\tilde{z}^q_{l,k}, v\right\} \in E(F^{(d+1)}(v))$ if and only if $\left\{z^q_{l,k}, v\right\} \in E(G)$. Hence, by induction, we have $c_r^{(d)}(w^q_{l,k}) = c_r^{(d)}(z^q_{l,k})$ for all indices. By Item 1, we then have $c_r^{(d)}(\mathbf{w^q_l}) = c_r^{(d)}(\mathbf{z^q_l})$ and $\operatorname{atp}(v, \mathbf{w}^q_l) = \operatorname{atp}(v, \mathbf{z}^q_l)$ for every $q = 1, \ldots, r$ and $l = 1, \ldots, |\mathcal{N}_q(v)|$. $\square$

We introduce the following definition that provides a similarity measure between a graph and a tree-decomposed graph.

Definition 29. *Given a graph G and a tree-decomposed graph (F, T^s), define*

$$\operatorname{cnt}((F, T^s), G) = \left|\left\{v \in V \mid \exists D \in \mathbb{N} \text{ s.t. } (F^{(D)}(v), T^{(D)}(v)) \cong (F, T^s)\right\}\right|,$$

where $(F^{(D)}(v), T^{(D)}(v))$ is the depth-$2D$ r-ℓWL unfolding tree of G at v.

The counting function $\operatorname{cnt}((F, T^s), G)$ serves as a key metric, allowing us to draw connections between r-ℓWL colorings of two different graphs.

Corollary 2. *Let $r \in \mathbb{N}$. Let G and H be two graphs. Then, $c_r(G) = c_r(H)$ if and only if* $\operatorname{cnt}((F,T^s),G) = \operatorname{cnt}((F,T^s),H)$ *holds for all graphs* $(F,T^s) \in \mathcal{M}^{r+2}$.

Proof of "$\Longrightarrow$". Let $c_r(G) = c_r(H)$, i.e.,

$$\{\{c_r(v) \,|\, v \in V(G)\}\} = \{\{c_r(x) \,|\, x \in V(H)\}\}\,.$$

Assume, by contradiction, that there exists a tuple $(F,T^s) \in \mathcal{M}^{r+2}$ such that $\operatorname{cnt}((F,T^s),G) \neq \operatorname{cnt}((F,T^s),H)$. Let $c_1,\ldots,c_k$ be the final colors. Then, define for $i = 1,\ldots,k$

$$\operatorname{cnt}((F,T^s),G[c_i]) := \left|\left\{v \in V(G) \,|\, c_r(v) = c_i \text{ and } \exists D \in \mathbb{N} \text{ s.t. } (F^{(D)}(v),T^{(D)}(v)) \cong (F,T^s)\right\}\right|.$$

We have

$$\operatorname{cnt}((F,T^s),G) = \sum_{i=1}^{k} \operatorname{cnt}((F,T^s),G[c_i])\,,$$

and

$$\operatorname{cnt}((F,T^s),H) = \sum_{i=1}^{k} \operatorname{cnt}((F,T^s),H[c_i])\,.$$

Since $\operatorname{cnt}((F,T^s),G) \neq \operatorname{cnt}((F,T^s),H)$, there exist an index $i = 1,\ldots,k$ such that

$$\operatorname{cnt}((F,T^s),G[c_i]) \neq \operatorname{cnt}((F,T^s),H[c_i])\,. \tag{11}$$

Furthermore, there exists $i_n \in \mathbb{N}$ such that there are exactly n nodes $v_1,\ldots,v_n$ and $x_1,\ldots,x_n$ such that

$$c_r(v_1) = \ldots = c_r(v_{i_n}) = c_i \text{ and } c_r(x_1) = \ldots = c_r(x_{i_n}) = c_i.$$

Hence, as c_r refines $c_r^{(D)}$, we have

$$c_r^{(D)}(v_1) = \ldots = c_r^{(D)}(v_{i_n}) = c_r^{(D)}(x_1) = \ldots = c_r^{(D)}(x_{i_n}).$$

By (11), there exists some $D \in \mathbb{N}$ such that (without loss of generality) $(F^{(D)}(v_1),T^{(D)}(v_1)) \cong (F,T^s)$. Then, by Theorem 6, we have

$$\begin{aligned}(F^{(D)}(v_1),T^{(D)}(v_1)) \cong \ldots \cong (F^{(D)}(v_{i_n}),T^{(D)}(v_{i_n})) &\cong (F^{(D)}(x_{i_n}),T^{(D)}(x_{i_n}))\\ &\cong \ldots \cong (F^{(D)}(x_1),T^{(D)}(x_1)).\end{aligned}$$

There does not exist any other node w with $c_r(w) = c_1$ such that the corresponding unfolding tree is isomorphic to $(F^{(D)}(v_1),T^{(D)}(v_1))$. Hence, $\operatorname{cnt}((F,T^s),G[c_i]) = \operatorname{cnt}((F,T^s),H[c_i])$, which is a contradiction.

Proof of "$\Longleftarrow$". Suppose that $\operatorname{cnt}((F,T^s),G) = \operatorname{cnt}((F,T^s),H)$ for all $(F,T^s) \in \mathcal{M}^{r+2}$. Let $c_1,\ldots,c_{k_G}$ with multiplicities $m_1,\ldots,m_{k_G}$ and $\tilde{c}_1,\ldots,\tilde{c}_{k_H}$ with multiplicities $\tilde{m}_1,\ldots,\tilde{m}_{k_G}$ be the final colors of r-ℓWL applied to G and H, respectively. Consider some $v \in V(G)$ such that $c_r(v) = c_1$. Let D be sufficiently large (any D after convergence of r-ℓWL), then $\operatorname{cnt}((F^{(D)}(v),T^{(D)}(v)),G) = \operatorname{cnt}((F^{(D)}(v),T^{(D)}(v)),H)$ since $(F^{(D)}(v),T^{(D)}(v)) \in \mathcal{M}^{r+2}$. Hence, without loss of generality, $c_1 = \tilde{c}_1$ and $m_1 = \tilde{m}_1$. Repeating this argument for all colors finishes the proof. □

D.4.1. Proof of Theorem 2

In this section, we employ techniques adapted from the works of Dell et al. (2018) and B. Zhang et al. (2024) to derive a proof for Theorem 2 from the established result in Corollary 2.

Definition 30 (Definition 20 in (Dell et al., 2018))**.** *Let (F,T^t) and $(\tilde{F},\tilde{T}^s)$ be two tree-decomposed graphs. A pair of mappings (ρ,τ) is said to be a* bag isomorphism homomorphism *from (F,T^t) to $(\tilde{F},\tilde{T}^s)$ if it satisfies the following conditions*

1. *ρ is a homomorphism from F to $\tilde{F}$.*
2. *τ is a homomorphism from T^t to $\tilde{T}^s$.*
3. *τ is depth-surjective, i.e., the image of T^t under τ contains vertices at every depth present in $\tilde{T}^s$.*
4. *For all $t' \in T^t$, we have $\operatorname{dep}_{T^t}(t') = \operatorname{dep}_{\tilde{T}^s}(\tau(t'))$ and $F[\beta_{T^t}(t')] \cong \tilde{F}[\beta_{\tilde{T}^s}(\tau(t'))]$.*
5. *For all $t' \in T^t$, the set equality $\rho(\beta_{T^t}(t')) = \beta_{\tilde{T}^s}(\tau(t'))$ holds.*
6. *The depth of T^t and $\tilde{T}^s$ is equal.*

We denote the set of bag isomorphism homomorphisms from (F, T^t) to $(\tilde{F}, \tilde{T}^s)$ by $\operatorname{BIsoHom}\left((F, T^t), (\tilde{F}, \tilde{T}^s)\right)$ and set $\operatorname{bIsoHom}\left((F, T^t), (\tilde{F}, \tilde{T}^s)\right) = |\operatorname{BIsoHom}\left((F, T^t), (\tilde{F}, \tilde{T}^s)\right)|$.

We continue with the following lemma that shows a linear relation between the number of bag isomorphisms and the output of the counting function in Definition 29.

Lemma 6. *Let $r \in \mathbb{N}$. For any tree-decomposed graph $(F, T^s) \in \mathcal{M}^{r+2}$ and any graph G, it holds*

$$\operatorname{bIso}((F, T^s), G) = \sum_{(\tilde{F}, \tilde{T}^t) \in \mathcal{M}^{r+2}} \operatorname{bIsoHom}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right) \cdot \operatorname{cnt}\left(\left(\tilde{F}, \tilde{T}^t\right), G\right). \tag{12}$$

Proof. Let (F, T^s) be a tree-decomposed graph such that T^s has depth $2D$. The sum is over all isomorphism types $(\tilde{F}, \tilde{T}^t)$ of tree-decomposed graphs. Since $\operatorname{bIsoHom}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right) = 0$ holds if $\tilde{T}^t$ has depth larger than $2D$ or nodes with $\geq (r+1) \cdot (|V(G)| - 1)$ children the sum is finite and thus well-defined.

Assume that for the root bag of (F, T^s) it holds $\beta_{T^s}(s) = \{v\}$ and the depth of (F, T^s) is $2D$. Let $x \in V(G)$ be any vertex in G, and denote by $(F^{(D)}(x), T^{(D)}(x))$ the depth-$2D$ r-ℓWL-unfolding tree at node x. Define the following two sets,

$$\begin{aligned} S_1(x) &= \{h \in \operatorname{BIso}((F, T^s), G) \mid h(v) = x\}, \\ S_2(x) &= \left\{(\rho, \tau) \in \operatorname{BIsoHom}\left((F, T^s), \left(F^{(D)}(x), T^{(D)}(x)\right)\right) \mid \rho(v) = x\right\}. \end{aligned}$$

We prove that $|S_1(x)| = |S_2(x)|$ for every $x \in V(G)$, which is equivalent to (12). For this, we show for any bag isomorphism h from (F, T^s) to G with $h(v) = x$, there exists a *unique* bag isomorphism homomorphism σ from (F, T^s) to $(F^{(D)}(x), T^{(D)}(x))$ with $\sigma(v) = x$ such that $h = \pi \circ \sigma$, where π is the bag isomorphism from $(F^{(D)}(x), T^{(D)}(x))$ to G, defined in Definition 28 and Theorem 5, respectively. To visualize this proof idea, see Figure 9.

First, define $\rho(v) := x$. Let $v_1, \ldots, v_n \in V(F)$ be nodes that correspond to bags in T^s of depth 2 with one element inside the bag and their parents having two elements in their bag, i.e., $\{v_i\}$ are the corresponding bags. Similarly, set $x_1, \ldots, x_m \in V(F^{(D)}(x))$ nodes that correspond to bags of depth 2 in $T^{(D)}(x)$, with one element inside the bag and their parents having two elements in their bag. Since h is a bag isomorphism and π as well, for every $i = 1, \ldots, n$ there exists a j_i such that $h(v_i) = \tilde{x}_{j_i} = \pi(x_{j_i})$, where $\tilde{x}_{j_i} \in V(G)$ and $x_{j_i} \in V\left(F^{(D)}(x)\right)$. Since π and h are bag isomorphisms, we have

$$F[\{\{v, v_i\}\}] \cong G[\{\{x, \tilde{x}_{j_i}\}\}] \cong F^{(D)}(x)[\{\{x, x_{j_i}\}\}]. \tag{13}$$

Now, set $\rho(v_i) = x_{j_i}$ for every $i = 1, \ldots, n$. Based on (13), we can easily define τ such that τ satisfies Definition 30 with respect to bags that are of depth 1 and 2.

For $q = 1, \ldots, r$ and $l = 1, \ldots, |\mathcal{N}_q(v)|$, let $\mathbf{p}_l^q$ be a path of length $2q$ starting from the root node s in T^s. Every such path $\mathbf{p}_l^q$ in T^s corresponds to unique path $\mathbf{v}_l^q$, that is in $\mathcal{N}_q(x)$, of length q in F. We represent the path by $\left\{v_{l,1}^q, v_{l,2}^q, \ldots, v_{l,q+1}^q\right\}$, where every consecutive node is connected to each other and for $k = 1, \ldots q+1$, we have $\left\{v, v_{l,k}^q\right\} \in E(F)$ iff $\left\{h(v), h(v_{l,k}^q)\right\} \in E(G)$ as h is a bag isomorphism. Further for every node $k = 1, \ldots, q+1$ there exists a $j_{l,k}^q$ such that

$h(v^q_{l,k}) = \tilde{x}_{j^q_{l,k}} = \pi(x_{j^q_{l,k}})$, where $\tilde{x}_{j^q_{l,k}} \in V(G)$, $\left\{\tilde{x}_{j^q_{l,1}}, \ldots, \tilde{x}_{j^q_{l,q+1}}\right\} \in \mathcal{N}_q(x)$ and $\left\{x_{j^q_{l,1}}, \ldots, x_{j^q_{l,q+1}}\right\} \in \mathcal{N}_q(x)$. We set $\sigma(v^q_{l,k}) = x_{j^q_{l,k}}$ for every $k = 1, \ldots, q+1$. Clearly, we have

$$F\left[\{\{v, v_i, v_{i+1}\}\}\right] \cong G\left[\left\{\left\{x, \tilde{x}_{j_i}, \tilde{x}_{j_{i+1}}\right\}\right\}\right] \cong F^{(D)}(x)\left[\left\{\left\{x, x_{j_i}, x_{j_{i+1}}\right\}\right\}\right]. \tag{14}$$

Now, based on (14), we can easily define τ such that τ satisfies Definition 30 with respect to bags that correspond to paths in $\mathcal{N}_q(v)$ for $q = 1, \ldots, r$. Now, following this construction recursively leads to a bag isomorphism ρ such that $h = \pi \circ \rho$.

It remains to show that (ρ, τ) is unique (up to isomorphism). For this, let (ρ_1, τ_1) be another bag isomorphism homomorphism between (F, T^s) and $(F^{(D)}(x), T^{(D)}(x))$ such that $\rho_1(v) = x$ and $h = \pi \circ \rho_1$. We show that $\rho = \rho_1$.

We begin by showing that $\rho(v) = \rho_1(v)$ for every v that is not in a cycle. Adopting the previous notations, consider $v_1, \ldots, v_n \in V(F)$ and $x_1, \ldots, x_m \in V(F^{(D)}(x))$. For each $i = 1, \ldots, n$, let k_i and l_i be the indices such that $\rho(v_i) = x_{k_i}$ and $\rho_1(v_i) = x_{l_i}$. Consequently, $\pi(x_{k_i}) = \pi(x_{l_i})$. We note that the image of $h(v_i)$ is not contained in a cycle in G, as otherwise, h would not be a bag isomorphism. Similarly, x_{k_i} and x_{l_i} are not contained in a cycle; otherwise, ρ and ρ_1 would not be bag isomorphisms. Now, π is an injective mapping if the domain is restricted to nodes that are of depth 1 and 2, and not contained in a cycle. Hence, $x_{k_i} = x_{l_i}$.

We continue by showing that for every $w \in V(F)$, that is contained in a cycle, we have $\rho(w) = \rho_1(w)$. This follows a similar argument as the nodes that are not included in any cycle. We summarize the argument shortly: It must hold that $\rho(w)$ and $\rho_1(w)$ are contained in a cycle, and $\pi(\rho(w))$ and $\pi(\rho_1(w))$ as well. Now, π is injective if the domain is restricted to nodes that are only contained in cycles. Hence, $\rho_1 = \rho$.

$\square$

We continue this subsection by introducing the concept of a *bag extension* in the context of tree-decomposed graphs. This definition formalizes the notion of one tree-decomposed graph being an extension of another.

Definition 31 (Definition 20 in (Dell et al., 2018)). *Let (F, T^t) be a tree-decomposed graph. A* bag extension *of (F, T^t) is a graph (H, T^t) with $V(H) = V(F)$ such that for every $t \in V(T^t)$ the induced subgraph $H[\beta_{T^t}(t)]$ is an extension of $F[\beta_{T^t}(T)]$, i.e., if $e \in E(F[\beta_{T^t}(T)])$, then $e \in E(H[\beta_{T^t}(T)])$. We define* $\mathrm{bExt}\left((F, T^t), (\tilde{F}, \tilde{T}^s)\right)$ *as the number of bag extensions of (F, T^t) that are isomorphic to $(\tilde{F}, \tilde{T}^s)$.*

Intuitively, a bag extension of a tree-decomposed graph (F, T^s) can be achieved by adding an arbitrary number of edges to F. Each added edge must be contained within a bag that corresponds to a node in the tree T^s.

Definition 32 (Definition C.28 in (B. Zhang et al., 2024)). *Given a tree-decomposed graph (F, T^r) and a graph G, a* bag-strong homomorphism *from (F, T^s) to G is a homomorphism f from F to G such that, for all $t \in V(T^r)$, f is a strong homomorphism from $F[\beta_{T^s}(t)]$ to $G[f(\beta_{T^s}(t))]$, i.e., $\{u, v\} \in E(F[\beta_{T^s}(t)])$ iff $\{f(u), f(v)\} \in E(G[f(\beta_{T^s}(t))])$. Denote $\mathrm{BStrHom}((F, T^s), G)$ to be the set of all bag-strong homomorphisms from (F, T^s) to G, and denote $\mathrm{bStrHom}((F, T^s), G) = |\mathrm{BStrHom}((F, T^s), G)|$.*

We continue with decomposing the number of homomorphism from a fan cactus graph to any graph.

Lemma 7. *Let $r \in \mathbb{N}$. For any tree-decomposed graph $(F, T^s) \in \mathcal{M}^{r+2}$ and any graph G, it holds*

$$\hom(F, G) = \sum_{(\tilde{F}, \tilde{T}^t) \in \mathcal{M}^{r+2}} \mathrm{bExt}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right) \cdot \mathrm{bStrHom}\left(\left(\tilde{F}, \tilde{T}^t\right), G\right). \tag{15}$$

Proof. The proof follows the lines of Lemma C.29. in (B. Zhang et al., 2024). First, (15) is well-defined as T^s is finite, hence, there can only be finitely many bag extensions of (F, T^s).

Further, consider the set

$$S = \left\{\left(\left(\tilde{F}, \tilde{T}^t\right), (\rho, \tau), g\right) \mid \left(\tilde{F}, \tilde{T}^t\right) \in \mathcal{M}^{r+2}, (\rho, \tau) \in \mathrm{BExt}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right), g \in \mathrm{BstrHom}\left(\left(\tilde{F}, \tilde{T}^t\right), G\right)\right\}.$$

We consider the mapping σ from S to $\hom(F, G)$ via $((\rho, \tau), g) \mapsto g \circ \rho$. We show that for every homomorphism h there exists a unique, up to automorphisms, $\left(\tilde{F}, \tilde{T}^t\right) \in \mathcal{M}^{r+2}$, (ρ, τ) and g such that $h = g \circ \rho$.

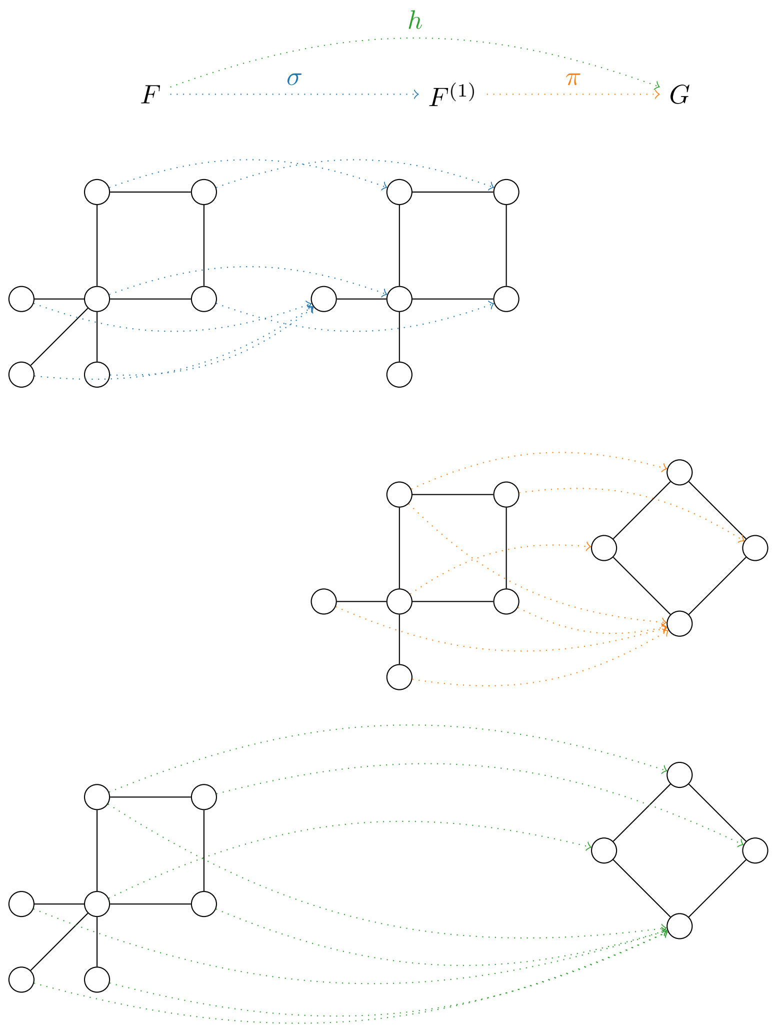


Figure 9: Visualization of proof idea of Lemma 6

We begin with the existence part. For $h \in \hom(F, G)$, we define $\left(\tilde{F}, \tilde{T}^t\right) \in \mathcal{M}^{r+2}$, (ρ, τ) and g as follows.

- We define $\tilde{F}$ by adding the edges given by
$$\{\{u, v\} \mid u, v \in V(F), \exists t \in T^s \text{ s.t. } \{u, v\} \in \beta_{T^s}(t), \{h(u), h(v)\} \in E(G)\}\,. \tag{16}$$
We define $\tilde{T}^t := T^s$. Clearly, $\left(\tilde{F}, \tilde{T}^t\right) \in \mathcal{M}^{r+2}$ and it is a bag extension as only edges are added that are contained within a bag that corresponds to a node in T^s.
- We define ρ and τ as the identity mappings on their respective domain, leading to $(\rho, \tau) \in \mathrm{BExt}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right)$.
- We define $g = h$. For $x \in \tilde{T}^t$, we show that g is a strong homomorphism from $\tilde{F}[\beta_{\tilde{T}^t}(x)]$ to $G[g(\beta_{\tilde{T}^t}(x))]$. Let $\{u, v\} \in E\left(\tilde{F}[\beta_{\tilde{T}^t}(x)]\right)$, then $\{g(u), g(v)\} \in E\left(G[g(\beta_{\tilde{T}^t}(x))]\right)$ as h is a homomorphism with respect to the edges $E(F)$ and in (16) only edge $\{u, v\}$ were added that satisfy $\{h(u), h(v)\} \in E(G)$. On the other hand $\{g(u), g(v)\} \in E\left(G[g(\beta_{\tilde{T}^t}(x))]\right)$, but $\{u, v\} \notin E\left(\tilde{F}[\beta_{\tilde{T}^t}(x)]\right)$ would contradict (16) as u, v are contained in the same bag $\beta_{\tilde{T}^t}(x)$. Hence, $g \in \mathrm{BstrHom}\left(\left(\tilde{F}, \tilde{T}^t\right), G\right)$.

We finally prove the uniqueness part, i.e., that $\sigma\left((\tilde{F}_1, \tilde{T}_1^{t_1}), (\rho_1, \tau_1), g_1\right) = h$ implies that there exists an isomorphism $(\tilde{\rho}, \tilde{\tau})$ from $\left(\tilde{F}_1, \tilde{T}_1^{t_1}\right)$ to $\left(\tilde{F}, \tilde{T}^t\right)$ such that $\tilde{\rho} \circ \rho_1 = \rho$, $\tilde{\tau} \circ \tau_1 = \tau$. We first prove that $\tilde{F}_1 \cong \tilde{F}$ and $\tilde{T}_1^{t_1} \cong \tilde{T}^t$.

1. For any $u, v \in V(F)$, we obviously have $\rho(u) = \rho(v)$ iff $u = v$ iff $\rho_1(u) = \rho_1(v)$ as ρ and ρ_1 are injective mappings.
2. Let $u, v \in V(F)$. Consider $\{\rho_1(u), \rho_1(v)\} \in E(\tilde{F}_1)$, we show that $\{\rho(u), \rho(v)\} \in E(\tilde{F})$. If $\{u, v\} \in E(F)$, then clearly $\{\rho(u), \rho(v)\} \in E(\tilde{F})$ as ρ is a homomorphism. Hence, assume that $\{u, v\} \notin E(F)$. Then, u, v must be contained in the same bag of T^s as ρ_1 is a bag extension and only node pairs are added if they are in the same bag. Hence, $\rho(u)$ and $\rho(v)$ are contained in the same bag. As g_1 is a homomorphism, we have $\{g_1(\rho_1(u)), g_1(\rho_1(v))\} \in E(G)$. But, then also $\{g(\rho(u)), g(\rho(v))\} \in E(G)$, and as g is a strong homomorphism (with respect to the bag in which $\rho(u)$ and $\rho(v)$ are contained), we have $\{\rho(u), \rho(v)\} \in E(\tilde{F})$. By symmetry of the argument, we have $\{\rho_1(u), \rho_1(v)\} \in E(\tilde{F}_1)$ iff $\{\rho(u), \rho(v)\} \in E(\tilde{F})$.
3. Since ρ_1 and ρ are bag extension, they are bijective on their respective domain. Hence, $\tilde{\rho} = \rho \circ \rho_1^{-1}$ defines an isomorphism from $\tilde{F}_1$ to $\tilde{F}$. On the other hand, $\tilde{T}_1^{t_1} \cong \tilde{T}^t$ trivially holds, again with $\tilde{\tau} = \tau \circ \tau_1^{-1}$.

We have $\tilde{\rho} \circ \rho_1 = \rho$, $\tilde{\tau} \circ \tau_1 = \tau$. We show that the tuple $(\tilde{\rho}, \tilde{\tau})$ is an isomorphism, i.e., it remains to show that for any $b \in \tilde{T}_1^{t_1}$, we have $\tilde{\rho}(\beta_{\tilde{T}_1^{t_1}}(b)) = \beta_{\tilde{T}^t}(\tilde{\tau}(b))$. Since τ_1 is surjective, we can choose a such that $\tau_1(a) = b$. Then,

$$\tilde{\rho}(\beta_{\tilde{T}_1^{t_1}}(\tau_1(a))) = \tilde{\rho}(\rho_1(\beta_{T^s}(a))) = \rho(\beta_{T^s}(a)) = \beta_{\tilde{T}^t}(\tau(a)) = \beta_{\tilde{T}^t}(\tilde{\tau} \circ \tau_1(a)) = \beta_{\tilde{T}^t}(\tilde{\tau}(b)).$$

The first and third equalities hold since (ρ_1, τ_1) and (ρ, τ) are bag extensions. $\square$

Definition 33 (Definition 30 in (B. Zhang et al., 2024))**.** *Given two tree-decomposed graphs (F, T^s) and $(\tilde{F}, \tilde{T}^t)$, a homomorphism (ρ, τ) from (F, T^s) to $(\tilde{F}, \tilde{T}^t)$ is called* bag-strong surjective *if ρ is a bag-strong homomorphism from (F, T^s) to $\tilde{F}$ and is surjective on both vertices and edges, and τ is an isomorphism from T^s to $\tilde{T}^t$ such that for all $x \in V(T^s)$, we have $\rho(\beta_{T^s}(x)) = \beta_{\tilde{T}^t}(\tau(x))$. Denote* $\mathrm{BStrSurj}((F, T^s), (\tilde{F}, \tilde{T}^t))$ *to be the set of all bag-strong subjective homomorphisms from (F, T^s) to $(\tilde{F}, \tilde{T}^t)$, and denote* $\mathrm{bStrSurj}((F, T^s), (\tilde{F}, \tilde{T}^t)) = |\mathrm{BStrSurj}((F, T^s), (\tilde{F}, \tilde{T}^t))|$.

Lemma 8. *Let $r \in \mathbb{N}$. For any tree-decomposed graph $(F, T^s) \in \mathcal{M}^{r+2}$ and any graph G, it holds*

$$\mathrm{bStrHom}\left((F, T^s), G\right) = \sum_{(\tilde{F}, \tilde{T}^t) \in \mathcal{M}^{r+2}} \mathrm{bStrSurj}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t\right)\right) \frac{\mathrm{bIso}\left(\left(\tilde{F}, \tilde{T}^t\right), G\right)}{\mathrm{aut}\left(\tilde{F}, \tilde{T}^t\right)}, \tag{17}$$

where $\mathrm{aut}(\tilde{F}, \tilde{T}^t)$ counts the number of automorphisms of $(\tilde{F}, \tilde{T}^t)$.

Proof. The proof follows the lines of Lemma C.31. in (B. Zhang et al., 2024).

Consider the set

$$S = \left\{ \left(\left(\tilde{F}, \tilde{T}^t \right), (\rho, \tau), g \right) \mid \left(\tilde{F}, \tilde{T}^t \right) \in \mathcal{M}^{r+2}, (\rho, \tau) \in \text{BStrSurj}\left((F, T^s), \left(\tilde{F}, \tilde{T}^t \right) \right), g \in \text{BIso}\left(\left(\tilde{F}, \tilde{T}^t \right), G \right) \right\}.$$

We consider the mapping σ from S to $\text{BStrHom}\left((F, T^s), G\right)$ via $((\rho, \tau), g) \mapsto g \circ \rho$. We show that for every bag-strong homomorphism h there exists a unique, up to automorphisms, $\left(\tilde{F}, \tilde{T}^t \right) \in \mathcal{M}^{r+2}$, bag-strong surjective homomorphism (ρ, τ) and g such that $h = g \circ \rho$.

We begin with the existence part. For $h \in \text{BStrHom}\left((F, T^s), G\right)$, we define $\left(\tilde{F}, \tilde{T}^t \right) \in \mathcal{M}^{r+2}$, (ρ, τ) and g as follows.

We define $\tilde{F}$ by defining an equivalence relation $\sim$ on $V(F)$: $u \sim v$ if $h(u) = h(v)$ and there exists a path P in T^s with endpoints $t_1, t_2 \in V(T^s)$ such that $u \in \beta_{T^s}(t_1), v \in \beta_{T^s}(t_2)$, and all nodes t on the path P satisfies that $h(u) = h(v) \in h(\beta_{T^s}(t))$. We then define ρ as the quotient map with respect to $\sim$ and set $\tilde{F} = F/\sim$, i.e.,

$$V(\tilde{F}) = \{\rho(u) \mid u \in V(F)\}, E(\tilde{F}) = \{\{\rho(u), \rho(v)\} \mid \{u, v\} \in E(F)\},$$

which is well-defined as $\{u, v\} \in E(F)$ imples $\rho(u) \neq \rho(v)$ since h is a homomorphism. Then, ρ is surjective per construction.

We define the mapping $g : V(\tilde{F}) \to V(G)$ such that $g(\rho(u)) = h(u)$ for all $u \in V(F)$. This mapping g is well-defined since $\rho(u) = \rho(v)$ implies $h(u) = h(v)$, and $\rho : V(F) \to V(\tilde{F})$ is surjective. This leads to the equality $h = g \circ \rho$. To demonstrate that g is a homomorphism, consider any edge $(x, y) \in E(\tilde{F})$. There exists an edge $(u, v) \in E(F)$ such that $\rho(u) = x$ and $\rho(v) = y$, which implies $(h(u), h(v)) \in E(G)$, since h is a homomorphism. Consequently, this means $(g(x), g(y)) \in E(G)$.

We continue by defining the tree $\tilde{T}^t := (V(T), E(T), \beta_{\tilde{T}^t})$. We set $t = s$, and define τ to be the identity. Furthermore, we have $\beta_{\tilde{T}^t}(x) = \rho(\beta_{T^s}(x))$ for all $x \in V(T)$. It remains to prove that $(\tilde{F}, \tilde{T}^t) \in \mathcal{M}^{r+2}$ is a valid tree decomposition. For this, it suffices to prove that for any vertex $x \in V(\tilde{F})$ the subgraph $B_{\tilde{T}^t}(x)$ is connected. For this, let $x \in V(\tilde{F})$ and $t_1, t_2 \in B_{\tilde{T}^t}(x)$. Then, there exists $u \in \beta_{T^s}(t_1), v \in \beta_{T^s}(t_2)$ such that $\rho(u) = x, \rho(v) = x$. Therefore, $u \sim v$. As such, there exists a path $P \in T^s$ such that all nodes b on P satisfy $h(u) \in h(\beta_{T^s}(b))$. Hence, for every $b \in P$ there exists some $w_b \in \beta_{T^s}(b)$ such that $h(w_b) = h(u)$, and consequently $w_b \sim u$. Finally, $x = \rho(u) = \rho(w_b) \in \rho(\beta_{T^s}(b)) = \beta_{\tilde{T}^t(b)}$ for all b in the path P. Hence, $\left(\tilde{F}, \tilde{T}^t \right) \in \mathcal{M}^{r+2}$.

It remains to prove that ρ is a bag-strong surjective homomorphism and g is a bag isomorphism. We begin by showing that ρ is a bag-strong surjective homomorphism. For this, let $t \in V(T^s)$ and $u, v \in \beta_{T^s}(t)$. If $\{u, v\} \notin E(F)$, then $\{h(u), h(v)\} \notin E(G)$ (since h is a bag-strong homomorphism). Therefore, $\{\rho(u), \rho(v)\} \notin E(\tilde{F})$ since g is a homomorphism. Hence, ρ is a bag-strong surjective homomorphism.

We show that g is a bag isomorphism. Let $x \in V(\tilde{T}^t)$, and consider $\tilde{u}, \tilde{v} \in \beta_{\tilde{T}^t}(x)$. Since ρ is surjective, there exist $u, v \in \beta_{T^s}(x)$ such that $\rho(u) = \tilde{u}$ and $\rho(v) = \tilde{v}$. We have $\{\rho(u), \rho(v)\} \notin E(\tilde{F})$ iff $\{h(u), h(v)\} \notin E(G)$, since both ρ and h are bag-strong homomorphisms. Therefore, g is a bag isomorphism.

We finally prove that $\sigma\left((\tilde{F}_1, \tilde{T}^{t_1}), (\rho_1, \tau_1), g_1 \right) = \sigma\left((\tilde{F}, \tilde{T}^t), (\rho, \tau), g \right)$ implies there exists an isomorphism $(\tilde{\rho}, \tilde{\tau})$ from $(\tilde{F}_1, \tilde{T}_1^{t_1})$ to $(\tilde{F}, \tilde{T}^t)$ such that $\tilde{\rho} \circ \rho_1 = \rho, \tilde{\tau} \circ \tau_1 = \tau, g_1 = g \circ \tilde{\rho}$. Let $h = g_1 \circ \rho_1 = g \circ \rho$. We will only show that $\tilde{F}_1 \cong \tilde{F}$ since the remaining procedure is almost the same as in previous proofs. It suffices to prove that, for all $u, v \in V(F)$, $\rho_1(u) = \rho_1(v)$ iff

a) $h(u) = h(v)$, and

b) There exists a path P in T^s with endpoints $t_1, t_2 \in V(T)$ such that $u \in \beta_{T^s}(t_1), v \in \beta_{T^s}(t_2)$, and all node x on path P satisfies that $h(u) \in h(\beta_{T^s}(x))$.

We begin by showing the first direction, i.e., $\rho_1(u) = \rho_1(v)$ implies Items a) and b). If $\rho_1(u) = \rho_1(v)$, we clearly have $h(u) = h(v)$ as g_1 is well-defined. Also, there exists $x_1 \in B_{T^s}(u), x_2 \in B_{T^s}(v)$, i.e., $u \in \beta_{T^s}(x_1)$ and $v \in \beta_{T^s}(x_2)$.

Hence, $\rho(u) \in \rho(\beta_{T^s}(x_1)) \subset \beta_{\tilde{T}_1^{t_1}}(\tau_1(x_1))$ and $\rho_1(u) = \rho_1(v) \in \rho_1(\beta_{T^s}(x_2)) \subset \beta_{\tilde{T}_1^{t_1}}(\tau_1(x_2))$ since (ρ_1, τ_1) is a homomorphism. Hence, $\tau_1(x_1), \tau_1(x_2) \in B_{\tilde{T}_1^{t_1}}(\rho_1(u))$. Since $\tilde{T}_1^{t_1}[B_{\tilde{T}_1^{t_1}}(\rho_1(u))]$ is connected, there is a path P in $\tilde{T}_1^{t_1}[B_{\tilde{T}_1^{t_1}}(\rho_1(u))]$ with endpoints $\tau_1(x_1), \tau_1(x_2)$ such that all nodes x on P satisfies $\rho_1(u) \in \beta_{\tilde{T}_1^{t_1}}(x) = \beta_{\tilde{T}_1^{t_1}}(\tau \circ \tau^{-1}(x)) = \rho_1\left(\beta_{T^s}(\tau_1^{-1}(x))\right)$. We conclude $h(u) = g_1(\rho_1(u)) \in g_1(\rho_1(\beta_{T^s}(\tau_1^{-1}(x)))) = h(\beta_{T^s}(\tau_1^{-1}(x)))$.

We continue by showing the second direction, i.e., $\rho_1(u) = \rho_1(v)$ if Items a) and b). We prove this by contradiction, i.e., assume $\rho_1(u) \neq \rho_1(v)$ but the above items (a) and (b) hold. We consider two cases.First, assume that u and v are in the same bag of T^s. Then, as (ρ_1, τ_1) is a homomorphism, the nodes $\rho_1(u)$ and $\rho_1(v)$ are in the same bag of $\tilde{T}_1^{t_1}$. Since g_1 is a bag isomorphism, we have $g_1(\rho_1(u)) \neq g_1(\rho_1(v))$. This contradicts Item (a) above.

Now, consider the second case. For this, assume that u and v are not in the same bag of T^s. Then, there exist two adjacent nodes x_1, x_2 on path P such that $u \in \beta_{T^s}(x_1), u \notin \beta_{T^s}(x_2)$. We have $\beta_{T^s}(x_2) \subset \beta_{T^s}(x_1)$ as for every pair of nodes t_1, t_2 in a canonical tree decomposition with $\{t_1, t_2\} \in E(T^s)$ we have either $\beta_{T^s}(t_1) \subset \beta_{T^s}(t_2)$ or $\beta_{T^s}(t_2) \subset \beta_{T^s}(t_1)$. Now, item (b) implies that there exists $w \in \beta_{T^s}(x_2)$ such that $w \neq u$ and $h(w) = h(u)$. Then, $\rho_1(w) \in \rho_1\left(\beta_{T^s}(x_2)\right) \subset \rho_1\left(\beta_{T^s}(x_1)\right) \subset \beta_{\tilde{T}_1^{t_1}}(\tau_1(x_1))$. Therefore, $\rho_1(u)$ and $\rho_1(w)$ are two different nodes in $\beta_{\tilde{T}_1^{t_1}}\left(\tau_1(x_1)\right)$ with $g_1(\rho_1(u)) = h(u) = h(w) = g_1(\rho_1(w))$. This contradicts the condition that g_1 is a bag isomorphism. This yields the desired result that $\tilde{F} \cong \tilde{F}_1$. □

Finally, we restate Theorem 2, with its proof now being a straightforward corollary of the preceding results in this section.

Theorem 2 (Homomorphism Counting Power of r-ℓWL)**.** *Let $r \geq 0$. Then, r-ℓWL can homomorphism-count $\mathcal{M}^{r+2}$.*

Proof. According to Corollary 2, if $c_r(G) = c_r(H)$, then $\mathrm{cnt}(F, G) = \mathrm{cnt}(F, H)$ for every $F \in \mathcal{M}^{r+2}$. Utilizing Lemma 6, we extend this result to bag isomorphism counts: $\mathrm{bIso}(F, G) = \mathrm{bIso}(F, H)$ holds for every $F \in \mathcal{M}^{r+2}$. Finally, invoking Lemma 7 and Lemma 8, we conclude that $\hom(F, G) = \hom(F, H)$ for all $F \in \mathcal{M}^{r+2}$. □