Local WL Invariance and Hidden Shades of Regularity

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Abstract

The \( k \)-dimensional Weisfeiler-Leman algorithm (\( k \)-WL) is a powerful tool for testing isomorphism of two given graphs. We aim at investigating the ability of \( k \)-WL to capture properties of vertices (or small sets of vertices) in a single input graph \( G \). In general, \( k \)-WL computes a canonical coloring of \( k \)-tuples of vertices of \( G \), which determines a canonical coloring of \( s \)-tuples for each \( s \) between 1 and \( k \). We say that a property (or a numerical parameter) of \( s \)-tuples is \( k \)-invariant if it is determined by the tuple color. Our main result establishes \( k \)-invariance of the parameters counting the number of extensions of an \( s \)-tuple of vertices to a given subgraph pattern \( F \). We state a sufficient condition for \( k \)-invariance in terms of the treewidth of \( F \) and its homomorphic images, using suitable variants of these concepts for graphs with \( s \) designated roots. As an application, we observe some non-obvious regularity properties of strongly regular graphs: For example, if \( G \) is strongly regular, then the number of paths of length 6 between vertices \( x \) and \( y \) in \( G \) depends only on whether or not \( x \) and \( y \) are adjacent (and the length 6 is here optimal). Despite the fact that \( k \)-WL indistinguishability of vertex tuples implies high degree of regularity, we prove, on the negative side, that no fixed dimension \( k \) suffices for \( k \)-WL to recognize global symmetry of a graph. Specifically, for every \( k \), there is a graph \( G \) whose vertex set is colored by \( k \)-WL uniformly while \( G \) is not vertex-transitive.

1 Introduction

The \( k \)-dimensional Weisfeiler-Leman algorithm (\( k \)-WL) was designed as a powerful tool for establishing non-isomorphism of two given graphs and plays since then a constantly significant role in isomorphism testing. Most prominently, it is used in Babai’s quasipolynomial-time algorithm for the graph isomorphism problem [3]. Since recently, various modifications of this method are also used in AI for detecting (non-)similarities in graph databases [28, 31].

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Figure 1: The Shrikhande graph $S$; vertices/edges with the same background color constitute 4-cycles (i.e., some of these edges are not depicted). Both $(a, a')$ and $(b, b')$ are non-adjacent, but the common neighbors of $a$ and $a'$ are non-adjacent, while the common neighbors of $b$ and $b'$ are adjacent. The automorphism group of $S$ acts transitively on the ordered pairs of non-adjacent vertices of each type [36].

For each $k$-tuple $\bar{x} = (x_1, \ldots, x_k)$ of vertices in an input graph $G$, the $k$-WL algorithm computes a canonical color $WL_k(G, \bar{x})$; see the details in Section 2. If the multisets of colors $\{WL_k(G, \bar{x}) : \bar{x} \in V(G)^k\}$ and $\{WL_k(H, \bar{y}) : \bar{y} \in V(H)^k\}$ are different for two graphs $G$ and $H$, then these graphs are clearly non-isomorphic, and we say that $k$-WL distinguishes them. If $k$-WL does not distinguish $G$ and $H$, we say that these graphs are $k$-WL-equivalent and write $G \equiv_{k-WL} H$. As proved by Cai, Fürer, and Immerman [9], the $k$-WL-equivalence for any fixed dimension $k$ is strictly coarser than the isomorphism relation on graphs. For $k = 2$, an example of two non-isomorphic 2-WL-equivalent graphs is provided by any pair of non-isomorphic strongly regular graphs with the same parameters. The smallest such pair consists of the Shrikhande and the $4 \times 4$ rook’s graphs. The Shrikhande graph, which will occur several times in the sequel, is the Cayley graph of the abelian group $\mathbb{Z}_4 \times \mathbb{Z}_4$ with the generating set $\{(1, 0), (0, 1), (1, 1)\}$ and can naturally be drawn on the torus; see Figure 1.

Let $\text{hom}(F, G)$ denote the number of homomorphisms from a graph $F$ to a graph $G$. A characterization of the $k$-WL-equivalence in terms of homomorphism numbers by Dell, Grohe, and Rattan [17] implies that the homomorphism count $\text{hom}(F, \cdot)$ is $k$-WL-invariant for each pattern graph $F$ of treewidth at most $k$, that is, $\text{hom}(F, G) = \text{hom}(F, H)$ whenever $G \equiv_{k-WL} H$.

Let $\text{sub}(F, G)$ denote the number of subgraphs of $G$ isomorphic to $F$. Lovász [30, Section 5.2.3] showed a close connection between the homomorphism and the subgraph counts, which found many applications in various contexts. Curticapean, Dell, and Marx [16] used this connection to design efficient algorithms for counting the number of $F$-subgraphs in an input graph $G$. In [1], we addressed WL invariance of the subgraph counts. Define the homomorphism-hereditary treewidth $htw(F)$ of a graph $F$ as the maximum treewidth of a homomorphic image of $F$. Then the invariance result for the homomorphism counts [17], combined with the Lovász relationship, implies that $\text{sub}(F, G) = \text{sub}(F, H)$ whenever $G \equiv_{k-WL} H$ for $k = htw(F)$.

In the present paper we explore a local version of this invariance result, where
by locality we mean that, under certain conditions, not only the $k$-WL-equivalence type of $G$ determines the total number of $F$-subgraphs in $G$, but even the color $\text{WL}_k(G, x_1, \ldots, x_s)$ of each $s$-tuple of vertices determines the number of extensions of this particular tuple to an $F$-subgraph. More precisely, the $k$-WL-coloring of $k$-tuples of vertices determines a canonical coloring of $s$-tuples for each $s$ between 1 and $k$. Specifically, if $s < k$, we define $\text{WL}_k(G, x_1, \ldots, x_s) = \text{WL}_k(G, x_1, \ldots, x_{s-1}, x_{s+1}, \ldots, x_k)$ just by cloning the last vertex in the $s$-tuple $k - s$ times. Let $x_1, \ldots, x_s$ be a sequence of designated vertices in a host graph $G$ and $z_1, \ldots, z_s$ be a sequence of designated vertices in a pattern graph $F$. We write $\text{sub}(F, z_1, \ldots, z_s; G, x_1, \ldots, x_s)$ to denote the number of subgraphs of $F$ with designated vertices, which we introduce in Section 3. The crucial point is that the above example illustrates actually a more general fact that the count $\text{sub}(F, z_1, \ldots, z_s; G, x_1, \ldots, x_s)$ does not enjoy anymore the above invariance property. For example, for the two vertex pairs $a, a'$ and $b, b'$ in Figure 1 we have $\text{sub}(P_6, z_2, z_3; S, a, a') = 244$ while $\text{sub}(P_6, z_2, z_3; S, b, b') = 246$ though both pairs are non-adjacent. To explain the difference between the patterns $(P_6, z_1, z_6)$ and $(P_6, z_2, z_5)$, we need an appropriate extension of the notion of treewidth and homomorphism-hereditary treewidth to graphs with designated vertices, which we introduce in Section 3. The crucial point is that $\text{htw}(P_6, z_1, z_6) = 2$ while $\text{htw}(P_6, z_2, z_5) = 3$; see Example 3.3.

Our main local-invariance result is Theorem 3.4 saying that the parameter $\text{sub}(F, z_1, \ldots, z_s; \cdot)$ is $k$-WL-invariant whenever $\text{htw}(F, z_1, \ldots, z_s) \leq k$. We now mention some applications of this fact.
**An algorithmic interpretation.** Suppose that \(\text{htw}(F, z_1, \ldots, z_s) = k + 1\) and \(\text{sub}(F, z_1, \ldots, z_s, \cdot)\) is not \(k\)-WL-invariant. In this situation, it is natural to enhance \(k\)-WL by endowing the initial coloring of a \(k\)-tuple of vertices \((x_1, \ldots, x_k)\) in an input graph \(G\) with the counts \(\text{sub}(F, z_1, \ldots, z_s; G, x_{i_1}, \ldots, x_{i_s})\) for all its \(s\)-subtuples. This would result in an isomorphism algorithm of intermediate strength between \(k\)-WL and \((k + 1)\)-WL. For example, let \(k = 2\). If we enrich the initial color of a vertex pair \((x, x')\) with the number of 6-paths \(x_1x_3x_4x_6x_6\), then the example above shows that in this way we can distinguish between the Shrikhande and the \(4 \times 4\) rook’s graphs, which was impossible for 2-WL (in the \(4 \times 4\) rook’s graph, the count \(\text{sub}(P_6, z_2, z_6; R, x, x')\) is the same for all non-adjacent \(x\) and \(x'\)).

**Combinatorial consequences (disclosing hidden regularity).** Applying our local-invariance theorem to the pattern \((P_6, z_1, z_6)\) discussed above and using the fact that 2-WL does not refine the initial coloring of \(V(G)^2\) if \(G\) is a strongly regular graph, we see that the number of 6-paths between vertices \(x\) and \(y\) in a strongly regular graph depends only on whether or not \(x\) and \(y\) are adjacent (and on the parameters of the graph). We collect such non-obvious regularity properties of strongly regular graphs in Corollaries 3.5 and 3.7.

**A logical interpretation.** Cai, Fürer, and Immerman [9] established a close connection between \(k\)-WL-equivalence and the first-order \((k + 1)\)-variable logic with counting quantifiers \(C^{k+1}\). Specifically, they show that \(\text{WL}_k(G, x_1, \ldots, x_s) = \text{WL}_k(H, y_1, \ldots, y_s)\) if and only if every formula in \(C^{k+1}\) with \(s\) free variables has the same truth value on the \(s\)-tuple \(x_1, \ldots, x_s\) in \(G\) and on the \(s\)-tuple \(y_1, \ldots, y_s\) in \(H\). A standard question in descriptive complexity and finite model theory is which decision problems are expressible in a given logical formalism. Our local WL-invariance result sheds light on the following question: Which counting problems are expressible in a counting logic?

**Further applications (related work).** In a recent paper [2] we used a special case of our locality result for a single designated vertex as a technical tool to investigate WL invariance of fractional graph packing parameters. Moreover, we showed the relevance of this topic to estimating the integrality gap between these parameters and their standard integral variants.

Another theme, which we discuss in Section 5, is the ability of \(k\)-WL to recognize global symmetry of an input graph \(G\). Specifically, a graph is vertex-transitive if its automorphisms act transitively on the vertices. It is open whether this class of graphs is recognizable in polynomial time. Note that, \(\text{WL}_k(G, \alpha(x)) = \text{WL}_k(G, x)\) for any automorphism \(\alpha\) of \(G\). Thus, if \(G\) is vertex-transitive, then \(\text{WL}_k(G, x) = \text{WL}_k(G, x')\) for every two vertices \(x\) and \(x'\) of \(G\), whatever the dimension \(k\); that is, the \(k\)-WL colors of all vertices of \(G\) are the same. A natural question is whether the converse is true for some dimension \(K\). If so, then we could recognize vertex-transitivity just by running \(K\)-WL on \(G\) and checking whether the coloring of \(V(G)\) is uniform. Using the seminal Cai-Fürer-Immerman construction of \(k\)-WL-equivalent non-isomorphic graphs [9], we prove that this approach fails. This strengthens the
fact, following from [9], that no dimension $K$ is enough for $K$-WL to split the vertex set of every input graph into the orbits of its automorphism group.

A similar negative result is obtained in Section 5 also for the recognition problem of arc-transitivity. Recall that a graph is arc-transitive if its automorphisms act transitively on the ordered pairs of adjacent vertices. $G$ is called a rank 3 graph if both $G$ and its complement are arc-transitive. We also briefly discuss whether the multidimensional Weisfeiler-Leman algorithm is powerful enough to recognize rank 3 graphs, noting the relevance of this question to the long-standing Klin’s conjecture [10].

2 Formal definitions

Graph-theoretic preliminaries. The vertex set and the edge set of a graph $G$ are denoted by $V(G)$ and $E(G)$ respectively. The neighborhood of a vertex $x$ consists of all vertices adjacent to $x$ and is denoted by $N(x)$. A graph $G$ is $s$-regular if every vertex of $G$ has exactly $s$ neighbors. An $n$-vertex $s$-regular graph $G$ is strongly regular with parameters $(n, s, \lambda, \mu)$ if every two adjacent vertices of $G$ have $\lambda$ common neighbors and every two non-adjacent vertices have $\mu$ common neighbors. The Shrikhande and the $4 \times 4$ rook’s graphs, which were mentioned in Section 1, have parameters $(16, 6, 2, 2)$.

A tree decomposition of a graph $G$ is a tree $T$ and a family $\mathcal{B} = \{B_i\}_{i \in V(T)}$ of sets $B_i \subseteq V(G)$, called bags, such that the union of all bags covers all $V(G)$, every edge of $G$ is contained in at least one bag, and we have $B_i \cap B_j \subseteq B_l$ whenever $l$ lies on the path from $i$ to $j$ in $T$. The width of the decomposition is equal to $\max |B_i| - 1$. The treewidth of $G$, denoted by $tw(G)$, is the minimum width of a tree decomposition of $G$.

For $S \subseteq V(G)$, the subgraph of $G$ induced by $S$ is denoted by $G[S]$. We write $G - x = G[V(G) \setminus \{x\}]$ to denote the graph obtained from $G$ by removal of its vertex $x$.

The Weisfeiler-Leman algorithm. We use the notation $\{\}$ for multisets and write $(f(i))_{i \leq k}$ to denote a $k$-tuple $(f(1), \ldots, f(k))$.

For a $k$-tuple of vertices $\bar{x} = (x_1, \ldots, x_k)$ in $V(G)^k$, we define $WL_k^0(G, \bar{x})$ to be the $k \times k$ matrix $(m_{i,j})$ with $m_{i,j} = 1$ if $x_i x_j \in E(G)$, $m_{i,j} = 2$ if $x_i = x_j$, and $m_{i,j} = 0$ otherwise. $WL_k^0(G, \bar{x})$ encodes the isomorphism and equality type of $\bar{x}$ in $G$ and serves as an initial coloring of $V(G)^k$ for $k$-WL.

The one-dimensional algorithm $1$-WL, known as the classical color refinement procedure, refines the initial coloring step by step, computing

$$WL_{1}^{r+1}(G, x) = \{WL_1^r(G, y) : y \in N(x)\}$$

for each $r \geq 0$. If $k \geq 2$, then $k$-WL successively computes a coloring of $V(G)^k$ by

$$WL_{k}^{r+1}(G, \bar{x}) = \{(WL_k^r(G, \bar{x}_i^u))_{i \leq k} : u \in V(G)\},$$
where
\[ \bar{x}_i^u = (x_1, \ldots, x_{i-1}, u, x_{i+1}, \ldots, x_k). \]

It can easily be noticed that each coloring refines the preceding one. If \( G \) has \( n \) vertices, the color partition of \( V(G)^k \) stabilizes in at most \( n^k \) rounds. The algorithm terminates and outputs the coloring \( \text{WL}_k(G, \bar{x}) = \text{WL}_k^n(G, \bar{x}). \)

It is useful to define \( k \)-WL colorings of \( s \)-tuples \( \bar{x} = (x_1, \ldots, x_s) \) for \( s < k \) and \( s = k + 1 \). If \( s < k \), we set \( \text{WL}_k^s(G, \bar{x}) = \text{WL}_k^s(G, x_1, \ldots, x_s, \ldots, x_s) \) and, similarly, \( \text{WL}_k(G, \bar{x}) = \text{WL}_k(G, x_1, \ldots, x_s, \ldots, x_s) \), i.e., extend \( \bar{x} \) to a \( k \)-tuple by cloning the last entry. For \( k \geq 2 \) and \( \bar{x} = (x_1, \ldots, x_k, x_{k+1}) \), we define
\[ \text{WL}_k(G, \bar{x}) = (\text{WL}_k(G, \bar{x}_{-i}))_{i \leq k+1}, \]

where
\[ \bar{x}_{-i} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_{k+1}). \]

Thus, the color \( \text{WL}_k(G, \bar{x}) \) provides the information on the colors of all \( k \)-subtuples of \( \bar{x} \).

### 3 Local WL invariance and its consequences

An \( s \)-rooted graph \( G_\bar{x} \) is a graph \( G \) with a sequence of \( s \) (not necessarily distinct) designated vertices \( \bar{x} = (x_1, \ldots, x_s) \), which are referred to as roots. Sometimes we will also use more extensive notation \( G_{\bar{x}} = (G, x_1, \ldots, x_s) \). A homomorphism from an \( s \)-rooted graph \( F_\bar{y} \) to an \( s \)-rooted graph \( G_{\bar{x}} \) is a homomorphism from \( F \) to \( G \) taking \( y_i \) to \( x_i \) for every \( i \leq s \).

**Definition 3.1.** A tree decomposition of an \( s \)-rooted graph \( G_\bar{x} \) is a tree decomposition of \( G \) with a bag containing all of the roots \( x_1, \ldots, x_s \). The tree width of \( G_\bar{x} \), which we denote by \( tw(G_{\bar{x}}) \), is the minimum width of any tree decomposition of \( G_\bar{x} \). The homomorphism-hereditary treewidth of \( G_\bar{x} \), which we denote by \( htw(G_{\bar{x}}) \), is the maximum \( tw(H_\bar{y}) \) over all \( H_\bar{y} \) such that there is an edge-surjective homomorphism from \( G_{\bar{x}} \) to \( H_\bar{y} \).

**Remark 3.2.** Definition 3.1 has some easily observable consequences: If \( \bar{x} = (x_1) \) is a single vertex or \( \bar{x} = (x_1, x_2) \) is a vertex pair corresponding to an edge, then \( tw(G_{\bar{x}}) = tw(G) \) and \( htw(G_{\bar{x}}) = htw(G) \).

**Example 3.3.** Let \( P_6 \) be the path graph on the six consecutively adjacent vertices \( x_1, \ldots, x_6 \). We have \( htw(P_6, x_1, x_6) = 2 \) (see Figure 2a), while \( htw(P_6, x_2, x_5) = 3 \) (see Figure 2b).

Note that, if \( G_{\bar{x}} \) is a graph with \( s \) pairwise distinct roots and \( htw(G_{\bar{x}}) = k \), then \( s \leq k + 1 \).

Given a pattern graph \( F_\bar{y} \) with \( s \) pairwise distinct roots \( \bar{y} = (y_1, \ldots, y_s) \) and a host graph \( G_{\bar{x}} \) with \( s \) pairwise distinct roots \( \bar{x} = (x_1, \ldots, x_s) \), let \( \text{sub}(F_\bar{y}, G_{\bar{x}}) \)
Figure 2: (a) Homomorphic images of \((P_6, x_1, x_6)\) up to isomorphism and root swapping. (b) \((P_6, x_2, x_5)\) and its image under \(h\) which maps \(x_1\) to \(x_4\), \(x_6\) to \(x_3\), and fixes all other vertices. Since \(h(x_2)\) and \(h(x_5)\) must be in one bag, the treewidth increases to 3.

denote the number of subgraphs \(S\) of \(G\) with \(x_1, \ldots, x_s \in V(S)\) such that there is an isomorphism from \(F\) to \(S\) mapping \(y_i\) to \(x_i\) for all \(i \leq s\). For each pattern graph \(F_y\), the count \(\text{sub}(F_y, G_x)\) is an invariant of a host graph \(G_x\). In general, a function \(f\) of a rooted graph is an invariant if \(f(G_x) = f(H_{x'})\) whenever \(G_x\) and \(H_{x'}\) are isomorphic (note that an isomorphism, like any homomorphism, must respect the roots). We say that an invariant \(f_1\) is determined by an invariant \(f_2\) if \(f_2(G_x) = f_2(H_{x'})\) implies \(f_1(G_x) = f_1(H_{x'})\).

Theorem 3.4. For each \(s\)-rooted pattern graph \(F_y\) with \(\text{htw}(F_y) = k \geq 2\), the subgraph count \(\text{sub}(F_y, G_x)\) is determined by \(\text{WL}_k(G, \bar{x})\).

The proof of the theorem is postponed to Section 4 where it will be restated in a more general form as Theorem 4.3.

Continuing Example 3.3, note that Theorem 3.4 implies that the subgraph count \(\text{sub}(P_6, x_1, x_6; \cdot)\) is 2-WL-invariant.

In what follows, by \(s\)-path (resp. \(s\)-cycle) we mean a path graph \(P_s\) (resp. a cycle graph \(C_s\)) on \(s\) vertices.

Corollary 3.5.

1. For each \(s \leq 7\), the number of \(s\)-paths between distinct vertices \(x\) and \(y\) in a strongly regular graph \(G\) depends only on the adjacency of \(x\) and \(y\) (and on the parameters of \(G\)).

2. For each \(3 \leq s \leq 7\), the number of \(s\)-cycles containing an edge \(xy\) of a strongly regular graph \(G\) is the same for each edge \(xy\) (depending solely on the parameters of \(G\)).

3. For each \(3 \leq s \leq 5\), the number of \(s\)-cycles containing two distinct vertices \(x\) and \(y\) of a strongly regular graph \(G\) depends only on the adjacency of \(x\) and \(y\) (and on the parameters of \(G\)).

Proof. Suppose that the path \(P_s\) goes through vertices \(x_1, \ldots, x_s\) in this order and, similarly, the cycle \(C_s\) is formed by vertices \(x_1, \ldots, x_s\) in this cyclic order. For cycles, we have \(\text{htw}(C_s, x_1, x_2) = \text{htw}(C_s) = 2\), where the first equality is due to...
| $F_{\bar{y}}$ | $G_{\bar{x}}$ | $\text{sub}(F_{\bar{y}}; G_{\bar{x}})$ |
|--------------|--------------|-----------------|
| $(P_8, x_1, x_8)$ | $(S, a, a')$  | 2500 |
| $(P_8, x_1, x_8)$ | $(S, b, b')$  | 2522 |
| $(C_8, x_1, x_2)$ | $(S, a, a')$  | 48832 |
| $(C_8, x_1, x_2)$ | $(S, b, b')$  | 48788 |
| $(C_6, x_1, x_3)$ | $(S, a, a')$  | 72 |
| $(C_6, x_1, x_3)$ | $(S, b, b')$  | 74 |
| $(C_6, x_1, x_4)$ | $(S, a, a')$  | 92 |
| $(C_6, x_1, x_4)$ | $(S, b, b')$  | 94 |

Table 1: $S$ and $\overline{S}$ denote the Shrikhande graph and its complement, respectively; $a$, $a'$, $b$, and $b'$ are the four vertices in $S$ shown in Figure 1.

Remark 3.2 and the second equality is shown in [1] for $s \leq 7$. For paths, note that $htw(P_s, x_1, x_s) \leq \max(htw(C_s, x_1, x_s), htw(C_{s-1}, x_1))$, which implies $htw(P_s, x_1, x_s) \leq 2$ again by Remark 3.2 and the estimates in [1]. A straightforward inspection shows also that $htw(C_s, x_1, x_i) = 2$ for all $i \leq s$ if $s \leq 5$. Hence, Theorem 3.4 is applicable.

The optimality of Corollary 3.5 is certified by Table 1.

Corollary 3.7 below applies to a larger class of graphs. Recall that $k$-WL, which computes a coloring of the Cartesian power $V(G)^k$, also determines a coloring of $V(G)^s$ for each $s < k$, as defined in Section 2.

**Definition 3.6.** Let $s \leq k$. A graph $G$ is called $WL_{s,k}$-homogeneous if $k$-WL does not make any non-trivial splitting of $V(G)^s$, that is, $WL_k(G, \bar{x}) \neq WL_k(G, \bar{y})$ exactly when $WL_k(G, \bar{x}) \neq WL_k(G, \bar{y})$ for every pair of $s$-tuples $\bar{x}, \bar{y} \in V(G)^s$.

Note that a graph is $WL_{1,1}$-homogeneous if and only if it is regular, and it is $WL_{2,2}$-homogeneous if and only if it is strongly regular. The class of $WL_{1,2}$-homogeneous graphs does not seem to have that clear characterization. This class obviously contains all vertex-transitive graphs. Moreover, it contains all strongly regular and all distance-regular graphs [8] (in fact, every strongly regular graph with $\lambda > 0$ is distance-regular). If $G_1$ and $G_2$ are two $WL_{1,2}$-homogeneous 2-WL-equivalent graphs, then the disjoint union of $G_1$ and $G_2$ is also $WL_{1,2}$-homogeneous. Furthermore, the class is closed under graph complementation. Note also that a graph $G$ is $WL_{1,2}$-homogeneous if and only if the coherent closure of $G$ is an association scheme; for the last concepts see [13].

**Corollary 3.7.**

1. For each $s \leq 7$, the number of $s$-paths emanating from a vertex $x$ in a $WL_{1,2}$-homogeneous graph is the same for every $x$.

2. For each $3 \leq s \leq 7$, the number of $s$-cycles containing a vertex $x$ in a $WL_{1,2}$-homogeneous graph is the same for every $x$. 
Proof. Using Remark 3.2 and the estimates of $htw(P_s)$ and $htw(C_s)$ for $s \leq 7$ in [1], we obtain $htw(P_s, x_1) = htw(P_s) \leq 2$ and $htw(C_s, x_1) = htw(C_s) = 2$. Theorem 3.4 applies.

Corollary 3.7 is optimal regarding the restriction $s \leq 7$. Indeed, consider the strongly regular graphs with parameters $(25, 12, 5, 6)$ without nontrivial automorphisms. These are two complementary graphs. Specifically, we pick $H = P_{25,02}$ (with graph6 code X)r\adeSetTjKWNJEYNRjPBgUGVTkK^YKbipMcxbk'{DlXF in the graph database [7]; this source is based on [33]. Regarding the pair $(sub(P_8, x_1, H, x), sub(C_8, x_1, H, x))$, the graph $H$ has 17 vertices $x$ with counts $(11115444, 5201448)$, 7 vertices with counts $(11115510, 5201580)$, and a single vertex with counts $(11115378, 5201316)$.

4 Proof of the local-invariance result

4.1 Logic with counting quantifiers, pebble games, and $k$-WL

Cai, Fürer, and Immerman [9] established a close connection between the Weisfeiler-Leman algorithm, first-order logic with counting quantifiers, and a variant of the Ehrenfeucht-Fraïssé game corresponding to this logic. A counting quantifier $\exists^m$ opens a logical formula saying that a graph contains at least $m$ vertices with some property. Let $C^k$ denote the set of formulas with counting quantifiers and occurrences of at most $k$ first-order variables. Furthermore, $C^{k,r}$ consists of the formulas in $C^k$ with quantifier depth at most $r$, where the quantifier depth is the maximum length of a sequence of nested quantifiers in the formula.

Let $G$ be a graph with $s \leq k$ designated vertices $(x_1, \ldots, x_s)$. The $C^{k,r}$-type of $(G, x_1, \ldots, x_s)$, which we denote by $[G, x_1, \ldots, x_s]^{k,r}$, is the set of all formulas with $s$ free variables in $C^{k,r}$ that are true on $(G, x_1, \ldots, x_s)$. The $C^k$-type of $(G, x_1, \ldots, x_s)$ is defined similarly and denoted by $[G, x_1, \ldots, x_s]^k$. Despite a rather abstract definition, we will see that the $C^{k,r}$- and $C^k$-types admit an efficient encoding by the colors produced by the Weisfeiler-Leman algorithm with appropriate parameters.

The $C^{k,r}$-types can be characterized in game-theoretic terms. For this purpose, we use the Hella’s bijection game [26]. The $k$-pebble version of the game is played on graphs $G$ and $H$ by two players,Spoiler and Duplicator. Let $p_1, \ldots, p_k$ be $k$ distinct pebbles. There are two copies of each pebble $p_i$. In one round of the game, Spoiler puts one of the pebbles $p_i$ on a vertex in $G$ and its copy on a vertex in $H$. When $p_i$ is on the board, $\alpha_i$ denotes the vertex pebbled by $p_i$ in $G$, and $\beta_i$ denotes the vertex pebbled by the copy of $p_i$ in $H$. The pebbles can change their positions during the game and, thus, the values of $\alpha_i$ and $\beta_i$ can be different in different rounds. More specifically, a round is played as follows:

- Spoiler chooses $i \in \{1, \ldots, k\}$;
- Duplicator responds with a bijection $f : V(G) \to V(H)$ having the property that $f(\alpha_j) = \beta_j$ for all $j \neq i$ such that $p_j$ is on the board;
• Spoiler chooses a vertex $\alpha$ in $G$ and puts $p_i$ on $\alpha$ and its copy $f(\alpha)$. This move reassigns $\alpha_i$ to $\alpha$ and $\beta_i$ to $f(\alpha)$.

Duplicator’s objective is to keep the map $\alpha_i \mapsto \beta_i$ a partial isomorphism between $G$ and $H$ all the time during the play. Let $\varnothing_{k,r}(G, x_1, \ldots, x_s, H, y_1, \ldots, y_s)$ denote the $r$-tound $k$-pebble game starting from the position where $\alpha_i = x_i$ and $\beta_i = y_i$ for $i \leq s$ and the other pebbles $p_i, i > s$, are off the board.

**Proposition 4.1** (Hella [26]). $[G, x_1, \ldots, x_s]^{1,r} = [H, y_1, \ldots, y_s]^{1,r}$ if and only if Duplicator has a winning strategy in the game $\varnothing_{k,r}(G, x_1, \ldots, x_s, H, y_1, \ldots, y_s)$.

We write $f_1(G, x_1, \ldots, x_s) \equiv f_2(G, x_1, \ldots, x_s)$ to say that two invariants of rooted graphs determine each other. Proposition 4.1 readily implies the following properties of $C_{k,r}$-types. Below we use the notation introduced in Section 2. In addition, if $\bar{x} = (x_1, \ldots, x_k)$, then $\bar{x}|u = (x_1, \ldots, x_k, u)$.

**Corollary 4.2.** Let $k \geq 1$ and $r \geq 0$.

1. If $s \leq k$, then

$$[G, x_1, \ldots, x_s]^{k+1,r} \equiv [G, x_1, \ldots, x_s, \ldots, x_s]^{k+1,r},$$

where the $s$-tuple $(x_1, \ldots, x_s)$ is prolonged in the right hand side by appending at most $k+1 - s$ copies of the last entry $x_s$.

2. If $\bar{x} = (x_1, \ldots, x_{k+1})$, then

$$[G, \bar{x}]^{k+1,r} \equiv \left\langle [G, \bar{x}]^{k+1,0}, ([G, \bar{x}_{i-1}]^{k+1,r})_{i \leq k+1} \right\rangle.$$

3. If $\bar{x} = (x_1, \ldots, x_k)$, then

$$[G, \bar{x}]^{k+1,r+1} \equiv \left\{ ([G, \bar{x}]^{k+1,r})_{u \in V(G)} \right\}.$$

4. If $\bar{x} = (x_1, \ldots, x_{k+1})$, then

$$[G, \bar{x}]^{k+1,r+1} \equiv \left\langle [G, \bar{x}]^{k+1,0}, \left\{ ([G, \bar{x}_{i-1}]^{k+1,r})_{u \in V(G)} \right\}_{i \leq k+1} \right\rangle.$$

5. If $k \geq 2$ and $\bar{x} = (x_1, \ldots, x_k)$, then

$$[G, \bar{x}]^{k+1,r+1} \equiv \left\{ ([G, \bar{x}_i]^{k+1,r})_{i \leq k} \right\}_{u \in V(G)}.$$

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Let $k \geq 2$. Part 5 of Corollary 4.2 reveals that $[G, x_1, \ldots, x_k]^{k+1} \equiv WL_k(G, x_1, \ldots, x_k)$. Parts 1 and 2 show that

$$[G, x_1, \ldots, x_s]^{k+1} \equiv WL_k(G, x_1, \ldots, x_s)$$

also for $s < k$ and $s = k + 1$ (cf. the definitions in Section 2). This equivalence is true also for $k = 1$ and $s = 2$ if we define $WL_1(G, x_1, x_2)$ as the quadruple consisting of $WL_1(G, x_1)$, $WL_1(G, x_2)$, $WL_0(G, x_1, x_2)$, and $\{WL_1(G, x)\}_{x \in V(G)}$.

We also remark that the $C^k$-type $[G, x_1, \ldots, x_k]^k$ for every $k \geq 2$ admits an alternative encoding in terms of a dual version of the Weisfeiler-Leman algorithm; see [24, Section 3.5 in the preliminary online version]. Specifically, given $\bar{x} = (x_1, \ldots, x_k)$, let $dWL_k(G, \bar{x}) = WL_0(G, \bar{x})$ and

$$dWL_k^{r+1}(G, \bar{x}) = \left\langle dWL_k^0(G, \bar{x}), \left(\{dWL_k^r(G, \bar{x}^u) : u \in V(G)\}\right)_{1 \leq k}\right\rangle$$

for $r \geq 0$. Color refinement is terminated after stabilization, and the final coloring is denoted by $dWL_k(G, \bar{x})$. Part 4 of Corollary 4.2 implies that $[G, x_1, \ldots, x_k]^k \equiv dWL_k(G, x_1, \ldots, x_k)$.

Taking into account the above discussion, Theorem 3.4 can be restated as follows (recall that, if $htw(F_y) = k$ for an $s$-rooted graph $F_y$, then $s \leq k + 1$).

**Theorem 4.3.** For each $s$-rooted pattern graph $F_y$, the subgraph count $\text{sub}(F_y, G_{\bar{x}})$ is determined by the $C^{k+1}$-type of $(G, \bar{x})$, where $k = htw(F_y)$.

The proof of Theorem 4.3 takes the next two subsections.

In fact, Theorem 4.3 is more general than Theorem 3.4, as it applies also for the WL dimension $k = 1$. In this case, Theorem 4.3 yields the following fact.

**Corollary 4.4.** Let $F_y$ be an $s$-rooted graph with $htw(F_y) = 1$. If $s = 1$, then the subgraph count $\text{sub}(F_y, G_{\bar{x}})$ is determined by the pair $WL_1(G, x_1)$ and $\{WL_1(G, x)\}_{x \in V(G)}$. If $s = 2$, then $\text{sub}(F_y, G_{\bar{x}})$ is determined by the triple $WL_1(G, x_1)$, $WL_1(G, x_2)$, and $\{WL_1(G, x)\}_{x \in V(G)}$, along with (non)adjacency of $x_1$ and $x_2$.

As easily seen, $htw(F_y) = 1$ if and only if $F_y$ is a star graph $K_{1,n}$ or the 4-vertex graph with 2 non-adjacent edges, in each case either with one root or with two adjacent roots. Corollary 4.4 has applications in the context of [2]. It implies, in particular, that the optimum value of a fractional packing of $F$-subgraphs in a host graph is 1-WL-invariant for each star pattern $F = K_{1,n}$.

### 4.2 Local invariance of the homomorphism counts

Given two $s$-rooted graphs $F_y$ and $G_{\bar{x}}$ (with not necessarily distinct roots), let $\text{hom}(F_y, G_{\bar{x}})$ denote the number of homomorphisms from $F_y$ and $G_{\bar{x}}$ (recall that a homomorphism must map the root $y_i$ to the root $x_i$ for every $i \leq s$). The following theorem is a local version of the result by Dell, Grohe, and Rattan [17].
Theorem 4.5. For each s-rooted graph $F_y$, the homomorphism count $\text{hom}(F_y, G_{\bar{x}})$ is determined by the $C^{k+1}$-type of $(G, \bar{x})$, where $k = \text{tw}(F_y)$.

Our treatment is different from [17]. While the elegant approach of [17] exploits algebraic properties of the matrices $(\text{hom}(F, G))_{F,G}$ and $(\text{sub}(F, G))_{F,G}$, indexed by the pattern and the host graphs (cf. [30, Theorem 5.43]), we use a more direct inductive argument.

A width-$k$ tree decomposition $(\mathcal{B}, T)$ is called normalized if $|B_i| = k + 1$ for all bags and $|B_i \cap B_j| = k$ whenever $i$ and $j$ are adjacent in $T$. It is known [25, Lemma 2] that every graph $F$ of treewidth $k$ admits a normalized width-$k$ tree decomposition. Moreover, every tree decomposition $(\mathcal{A}, S)$ of $F$ can be converted to a normalized tree decomposition $(\mathcal{B}, T)$ of the same width such that every bag $A \in \mathcal{A}$ is contained in some bag $B \in \mathcal{B}$. When speaking of a width-$k$ tree decomposition $(\mathcal{B}, T)$ of a rooted graph $F_y$, this allows us to suppose that $(\mathcal{B}, T)$ is normalized. Let $B_p$ be a bag containing all roots $y_1, \ldots, y_s$. If $s \leq k$, for technical reasons it will also be convenient to put the new bag $B_q = \{y_1, \ldots, y_s\} \in \mathcal{B}$ and add the new vertex $q$ to $T$ connecting it by an edge to $p$. If $s = k + 1$, then $(\mathcal{B}, T)$ does not need to be modified, and we just set $q = p$. We consider $T$ an ordered tree rooted at $q$ and refer to $(\mathcal{B}, T, q)$ as a rooted normalized tree decomposition of $F_y$. The depth of $(\mathcal{B}, T, q)$ is the longest distance from $q$ to any other node in $T$.

Lemma 4.6. Let $F_y$ be an s-rooted graph with pairwise distinct roots and $(\mathcal{B}, T, q)$ be a rooted normalized tree decomposition of $F_y$ of width $k$ and depth $r$. Suppose that $s = k$ or $s = k + 1$. Then the homomorphism count $\text{hom}(F_y, G_{\bar{x}})$ is determined by the $C^{k+1,r}$-type of $(G, \bar{x})$.

Proof. We use induction on $r$. If $r = 0$, then $B_q = V(F) = \{y_1, \ldots, y_s\}$ is the only bag, and $\text{hom}(F_y, G_{\bar{x}})$ is clearly determined by the $C^{k+1,0}$-type of $(G, \bar{x})$ (which is the isomorphism and equality type of $\bar{x}$ in $G$). Suppose that $r \geq 1$. Each child $c$ of $q$ in $T$ corresponds to a subtree $T_c$ of $T$, which we define as the connected component of $T - q$ containing $c$. Furthermore, $T_c$ determines the subgraph $F^c = F[\bigcup_{j \in V(T_c)} B_j]$ of $F$. We endow $F^c$ with the sequence of roots $\bar{y}^c$ which is obtained from $\bar{y}$ by deleting the entry in $B_q \setminus B_c$ (if any) and appending the vertex in $B_c \setminus B_q$ as the last entry. Note that $(\{B_j\}_{j \in V(T_c)}, T_c, c)$ is a rooted normalized tree decomposition of $F^c_{\bar{y}^c}$ of width $k$ and depth $r - 1$.

Assume first that $s = k$. In this case, $B_q \subset B_c$ for any child $c$ of $q$. Clearly, every homomorphism from $F^c$ to $G$ that extends the map $\bar{y}^c \mapsto \bar{x}|u$ for some vertex $u \in V(G)$ is compatible with the map $\bar{y} \mapsto \bar{x}$. It follows that

$$\text{hom}(F_y, G_{\bar{x}}) = \prod_{c \in N(q)} \sum_{u \in V(G)} \text{hom}(F^c_{\bar{y}^c}, G_{\bar{x}|u}).$$

By the induction assumption, each homomorphism count $\text{hom}(F^c_{\bar{y}^c}, G_{\bar{x}|u})$ is determined by the type $[G, \bar{x}|u]^{k+1,r-1}$. By Part 3 of Corollary 4.2, this implies that $\text{hom}(F_y, G_{\bar{x}})$ is determined by $[G, \bar{x}|u]^{k+1,r}$. 

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In the case case of \( s = k + 1 \), we split the set \( N(q) \) of all children of \( q \) into \( k + 1 \) parts \( N_i(q) \), \( i \leq k + 1 \), by putting \( c \) in \( N_i(q) \) if \( B_c \setminus B_q = \{ y_i \} \). For each \( i \leq k + 1 \), let \( T_i \) be the tree formed by the branches \( T_c \) for all \( c \in N_i(q) \) and the new vertex \( i \) adjacent to each \( c \in N_i(q) \). Accordingly, \( F^i = F^i \cup \{ V(F^c) \} \), where \( F^c \) is as defined above. We root \( F^i \) at the sequence of vertices \( \bar{y}_{-1-i} \). Furthermore, \( B_i \) is obtained by taking the union of \( \{ B_j \}_{j \in \mathcal{V}(T_i)} \) over all \( c \in N_i(q) \) and adding the new bag \( B_i \) consisting of all roots of \( F^i \) except \( y_i \). Note that \( (B_i, T_i, i) \) is a rooted normalized tree decomposition of \( F^i \) of width \( k \). The tree \( T_i \) still has depth \( r \) but, since \( |B_i| = k \), we can proceed by induction as in the first case. Doing so, for each \( i \leq k + 1 \) we conclude that the homomorphism count \( \text{hom}(F^i_{\bar{y}_{-1-i}}, G_{\bar{x}_{-i}}) \) is determined by the type \([G, \bar{x}_{-i}]^{k+1,r} \). Now, note that the type \([G, \bar{x}]^{k+1,0} \) determines whether or not the map \( \bar{y} \mapsto \bar{x} \) is a partial homomorphism from \( F \) to \( G \). If not, then \( \text{hom}(F_{\bar{y}}, G_x) = 0 \). If so, then

\[
\text{hom}(F_{\bar{y}}, G_x) = \prod_{1 \leq i \leq k+1} \text{hom}(F^i_{\bar{y}_{-1-i}}, G_{\bar{x}_{-i}}).
\]

Taking into account Part 2 of Corollary 4.2 we see that the count \( \text{hom}(F_{\bar{y}}, G_x) \) is determined by \([G, \bar{x}]^{k+1,r} \).

Proof of Theorem 4.3 If \( s = k \) or \( s = k + 1 \), then we are done by Lemma 4.6 Suppose that \( s < k \). Let \((B, T)\) be a normalized width-\( k \) tree decomposition of \( F \) which contains all roots \( y_1, \ldots, y_s \) in one bag \( B_s \). We choose \((B, T)\) and \( B_i \) lexicographically first according to a natural encoding. Set \( y'_i = y_i \) for all \( i \leq s \) and let \( y'_{s+1}, \ldots, y'_{k+1} \) be the remaining vertices in \( B_i \setminus \{ y_1, \ldots, y_s \} \). Evidently,

\[
\text{hom}(F_{\bar{y}}, G_x) = \sum_{x' \in V(G)^{k+1} : (x'_1, \ldots, x'_s) = \bar{x}} \text{hom}(F_{y'}, G_{x'}).
\]

By Lemma 4.6 each summand is determined by the pair \((F_{y'}, [G, \bar{x}]^{k+1})\). Note that \( F_{y'} \) depends only on \( F_{\bar{y}} \) due to our choice of \( B_i \). Applying Part 3 of Corollary 4.2 iteratively, we see that the multiset \([ [G, \bar{x}]^{k+1} : x' \in V(G)^{k+1}, (x'_1, \ldots, x'_s) = \bar{x} ] \) and, hence, the count \( \text{hom}(F_{\bar{y}}, G_x) \) are determined by the type \([G, \bar{x}]^{k+1} \).

We have tacitly assumed so far that the roots \( \bar{y} \) are pairwise distinct. The general case follows from this one if \( y_i = y_j \) implies \( x_i = x_j \) for all pairs of indices \( 1 \leq i < j \leq s \). Whether or not the last condition is true is determined by the type \([G, \bar{x}]^{k+1,0} \). If it is violated, then \( \text{hom}(F_{\bar{y}}, G_x) = 0 \).

**4.3 From the homomorphism to the subgraph counts**

Let \( \text{hom}^*(F_{\bar{y}}, G_x) \) denote the number of injective homomorphisms from \( F_{\bar{y}} \) to \( G_x \). Counting injective homomorphisms and subgraphs is essentially equivalent, since

\[
\text{sub}(F_{\bar{y}}, G_x) = \frac{\text{hom}^*(F_{\bar{y}}, G_x)}{|\text{Aut}(F_{\bar{y}})|}.
\]
where \( \text{Aut}(F) \) is the automorphism group of \( F \) (as any homomorphism, automorphisms have to respect the roots). This allows us to directly obtain Theorem 4.3 from the following lemma, which we prove using the inductive approach due to Lovász [29].

**Lemma 4.7.** For each pattern graph \( F \) with \( s \) pairwise distinct roots, the injective homomorphism count \( \text{hom}^*(F, G) \) is determined by the \( C^{k+1} \)-type of \((G, \bar{x})\), where \( k = htw(F) \).

**Proof.** We use induction on the number of vertices in \( F \). The base case, namely \( V(F) = \{ y_1 \} \), is obvious. Suppose that \( F \) has at least two vertices.

Call a partition \( \alpha \) of \( V(F) \) proper if every element of \( \alpha \) is an independent set of vertices in \( F \). The partition of \( V(F) \) into singletons is called discrete. A proper partition \( \alpha \) determines the homomorphic image \( F/\alpha \) of \( F \) where \( V(F/\alpha) = \alpha \) and two elements \( A \) and \( B \) of \( \alpha \) are adjacent if between the vertex sets \( A \) and \( B \) there is at least one edge in \( F \). Let \( \bar{y}/\alpha = (A_1, \ldots, A_s) \) where \( A_i \) is the element of the partition \( \alpha \) contains \( y_i \). The \( s \)-rooted graph \( F_{\bar{y}}/\alpha \) is defined by \( F_{\bar{y}}/\alpha = (F/\alpha)_{\bar{y}/\alpha} \).

Note that

\[
\text{hom}(F_{\bar{y}}, G) = \text{hom}^*(F_{\bar{y}}, G) + \sum_{\alpha} \text{hom}^*(F_{\bar{y}}/\alpha, G)
\]

where the sum goes over the non-discrete proper partitions of \( V(F) \). Note that the number of roots in each \( F_{\bar{y}}/\alpha \) stays \( s \), but some of the roots may become equal to each other. In this case, we have \( \text{hom}^*(F_{\bar{y}}/\alpha, G) = 0 \), and all such \( \alpha \) can be excluded from consideration.

Now, \( \text{hom}(F_{\bar{y}}, G) \) is determined by the \( C^{k+1} \)-type of \((G, \bar{x})\) by Theorem 4.5 because \( ttw(F) \leq htw(F) \). Each \( \text{hom}^*(F_{\bar{y}}/\alpha, G) \) is determined by the \( C^{k+1} \)-type of \((G, \bar{x})\) by the inductive assumption. It follows that \( \text{hom}^*(F_{\bar{y}}, G) \) is also determined.

The proof of Theorem 4.3 is complete.

**Remark 4.8.** The result by Dell, Grohe, and Rattan [17] about the global WL invariance of homomorphism counts admits a generalization to vertex-colored graphs. The same holds true for the relationship between the homomorphism and the subgraph counts shown by Lovász [29, 30]. Using these generalizations, we can obtain a weaker version of the local-invariance result by using special vertex colors to designate roots. Specifically, if \( F' \) is an \( s \)-rooted version of \( F \), then \( \text{sub}(F', \cdot) \) is \( k'-\text{WL-invariant} \) for \( k' = htw(F') + s \). The result of Theorem 3.4 is finer due to the strict inequality \( htw(F') < htw(F) + s \).

### 4.4 Extensions

**Vertex-colored graphs.** Theorems 3.4 and 4.3 hold true for vertex-colored graphs, which is important for the applications of the local-invariance results in [2]. The \( k \)-WL algorithm on a vertex-colored input graph begins with an initial coloring of
V(G)k including the colors of all vertices in each k-tuple (x1, . . . , xk). The refinement step remains the same if k ≥ 2. If k = 1, then the (r + 1)-th color must explicitly include the preceding r-th color of a vertex. Speaking about the Ck+1-type of (G, ¯x) for a vertex-colored graph G, we suppose that our first-order language contains a unary relation symbol for each vertex color. The homomorphism-hereditary treewidth is defined as in Definition 3.1, with keeping in mind that homomorphisms of rooted vertex-colored graphs have to respect also vertex colors.

With these clarifications, Theorem 4.3 makes perfect sense for vertex-colored graphs, and its proof goes virtually without changes. Only the proof of Lemma 4.7 needs a little care. Specifically, any proper partition α of V(F) consists of independent set of equally colored vertices in F, and the graph F/α inherits the vertex coloring of F.

Pattern graphs with many roots. According to Definition 3.1 of the (homomorphism-hereditary) treewidth of a rooted graph, if F ¯y has s roots and tw(F ¯y) = k, then s ≤ k + 1. This relationship can be relaxed by modifying the definition as follows. As before, we define a tree decomposition (B, T) of F ¯y to be a tree decomposition of F with a designated bag B∗ containing all roots y1, . . . , ys. We say that the width of (B, T) is equal to max |B|−1 over all bags B ∈ B except B = B∗. This change affects the parameters tw(F ¯y) and htw(F ¯y), which we now denote by tw*(F ¯y) and htw*(F ¯y), respectively. Now, the last parameter can be arbitrarily smaller than the number of roots. Suppose that s > k. We can define the Ck-type of an arbitrarily long s-tuple of vertices ¯x in a graph G as the sequence of the Ck-types of all k-subtuples of ¯x. Theorem 4.3 is true for k = htw*(F ¯y) with virtually the same proof.

5 Failure of symmetry detection

Looking back at the WL-homogeneity concept introduced in Definition 3.6, denote the class of all WLs,k-homogeneous graphs by WL(s, k). We first note that the WL(s, k) hierarchy collapses as the parameter s increases. To show this, we relate it to two known graph-theoretic symmetry and regularity concepts.

A graph G is s-ultrahomogeneous if every isomorphism between two induced subgraphs of G with at most s vertices extends to an automorphism of the whole graph G. Denote the class of all s-ultrahomogeneous graphs by U(s). Note that 1-ultrahomogeneous graphs are exactly vertex-transitive graphs, and 2-ultrahomogeneous graphs are rank 3 graphs. Cameron [11] proved that every 5-ultrahomogeneous graph is s-ultrahomogeneous for all s ≥ 5, i.e., U(s) = U(5) for s ≥ 5. All graphs in U(5) were identified by Gardiner [23]. Those are mKn (the vertex-disjoint union of m copies of the complete graph Kn), their complements mKn (i.e., the regular multipartite graphs), the 5-cycle graph C5, and the 3 × 3-rook’s graph (or, the same, the line graph L(K3,3) of the complete bipartite graph K3,3).

A graph G is called s-tuple regular (or, sometimes, s-isoregular) if the number of common neighbors of any set S of at most s vertices in G depends only on the
isomorphism type of the induced subgraph $G[S]$. Let us denote the class of all $s$-tuple regular graphs by $R(s)$. Note that 1-tuple regular graphs are exactly regular graphs, and 2-tuple regular graphs are exactly strongly regular graphs. Cameron [11] (see also [10, Theorem 8.21]) and, independently, Gol’fand (see the historical comments in [4, 9]) proved that $R(5) = U(5)$. As a consequence, $R(s) = R(5)$ for all $s \geq 5$.

Let $s \leq k$. It is clear that

$$U(s) \subseteq WL(s,k) \subseteq R(s).$$

It follows that

$$WL(s,k) = \{mK_n, \overline{mK_n}\}_{m,n} \cup \{C_5, L(K_{3,3})\} \text{ if } k \geq s \geq 5.$$

### 5.1 Vertex-transitivity

Let us fix the first parameter to $s = 1$. Since the $WL(s,k)$ hierarchy collapses with respect to the parameter $k$ for each $s \geq 5$, it is natural to ask whether the hierarchy of the classes $WL(1,k)$ collapses with respect to $k$. This question has a clear algorithmic meaning. Let $VT = U(1)$ denote the class of all vertex-transitive graphs.

**Lemma 5.1.** $WL(1,l) = WL(1,k)$ for all $l \geq k$ if and only if $VT = WL(1,k)$.

**Proof.** If $VT = WL(1,k)$, then $WL(1,l) = WL(1,k)$ for each $l \geq k$ because $VT \subseteq WL(1,l) \subseteq WL(1,k)$. For the other direction, assume that $WL(1,k)$ contains a graph $G$ which is not vertex-transitive. Let $n$ denote the number of vertices in $G$ and note that $G$ does not belong to $WL(1,l)$ for any $l \geq n$. \hfill $\square$

Assume now that $VT = WL(1,K)$ for some dimension $K$. We could then recognize whether a given graph $G$ is vertex-transitive just by running $K$-WL on $G$ and looking whether the obtained partition of $V(G)$ is non-trivial. However, this approach does not work: There is no dimension $K$ such that $K$-WL is strong enough to recognize vertex-transitivity and, equivalently, the $WL(1,k)$ hierarchy does not collapse. This fact strengthens the result by Cai, Fürer, and Immerman [9] that no dimension $K$ is enough for $K$-WL to split the vertex set of every graph into the orbits of its automorphism group. In what follows, $v(G)$ denotes the number of vertices in a graph $G$.

**Theorem 5.2.** There is an infinite family of graphs such that every graph $G$ in the family is $WL_{1,k}$-homogeneous for all $k \leq 0.001 v(G)$ but not vertex-transitive.

The proof, which takes the rest of this section, is based on the Cai-Fürer-Immerman construction [9]. More specifically, in place of the standard CFI gadget [9, Fig. 3], we use its simplified version shown in Figure 3, which appears in various contexts in [18, 21, 22, 32].
Given a connected 3-regular graph $H$ on $n$ vertices, we construct a 6-regular graph $A$ with $4n$ vertices as follows. For two disjoint sets of vertices $X$ and $Y$ in a graph $G$, we write $G[X, Y]$ to denote the bipartite graph with vertex classes $X$ and $Y$ and all edges from $E(G)$ between $X$ and $Y$.

(i) Each vertex $v$ of $H$ is replaced with a set $Q(v) = \{v_1, v_2, v_3, v_4\}$ of four new vertices, which are put in $V(A)$.

(ii) For each edge $vu$ of $H$, the bipartite graph $A[Q(v), Q(u)]$ is isomorphic to the disjoint union of two 4-cycles. Note that each of these 4-cycles contains exactly 2 vertices of $Q(v)$. We say that such two vertices are matched and, thus, the subgraph $A[Q(v), Q(u)]$ determines a matching on $Q(v)$ (i.e., a splitting of $Q(v)$ into two pairs), which we denote by $M_{v,u}$.

(iii) For each vertex $v$ of $H$, it is required that the matchings $M_{v,a}$, $M_{v,b}$, and $M_{v,c}$ for the three neighbors $a$, $b$, and $c$ of $v$ are pairwise distinct.

To fulfill Condition (iii), for each vertex $v \in V(H)$ with $N(v) = \{a, b, c\}$ we fix an assignment of matchings $M_{v,a}$, $M_{v,b}$, and $M_{v,c}$ and then, for each edge $vu \in E(H)$, connect each pair in $M_{v,u}$ with a pair in $M_{u,v}$ by a 4-cycle (or, equivalently, by a complete bipartite graph $K_{2,2}$) so that the resulted subgraph $A[Q(v), Q(u)]$ of $A$ is as described by Condition (ii). Note that, for each $vu \in E(H)$, this step can be done in two different ways. The operation of changing $A[Q(v), Q(u)]$ for its bipartite complement will be called a twist.

Fix a graph $A$ chosen as described above. For a set $S \subseteq E(H)$, let $A^S$ denote the graph obtained from $A$ by twisting the subgraph $A[Q(v), Q(u)]$ for all edges $vu \in S$. The following fact is a version of [9, Lemma 6.2].

**Lemma 5.3.** $A \cong A^S$ if and only if $|S|$ is even. Moreover, if $|S|$ is even, then there exists an isomorphism from $A$ to $A^S$ mapping every set $Q(x)$ onto itself.

**Proof-sketch.** The lemma can be proved similarly to [9, Lemma 6.2], and we only outline the argument for one direction, as a similar argument will be used several times below. Specifically, if $|S|$ is even, we will describe how to find an isomorphism from $A$ to $A^S$ taking each $Q(x)$ onto itself.
We need some preliminaries on the local structure of $A$. Given a 4-element set $X = \{x_1, x_2, x_3, x_4\}$, let $K(X)$ denote the group of permutations of $X$ preserving each of the three matchings on $X$, that is, a permutation $\phi : X \to X$ is in $K(X)$ if and only if, for every two elements $x_i, x_j \in X$, either $\phi(\{x_i, x_j\}) = \{x_i, x_j\}$ or $\phi(\{x_i, x_j\}) = X \setminus \{x_i, x_j\}$. Specifically,

$$K(X) = \{\text{id}_X, (x_1x_2)(x_3x_4), (x_1x_3)(x_2x_4), (x_1x_4)(x_2x_3)\}.$$

Note that $K(X)$ is isomorphic to the Klein four-group.

Let $\phi \in K(X)$ and $M$ be a matching on $X$. Note that two cases are possible: the matched pairs in $M$ are either preserved or swapped by $\phi$. We say that $\phi$ fixes the matching in the former case and that $\phi$ flips the matching in the latter case. For example, $\phi = (x_1x_2)(x_3x_4)$ fixes $M = \{\{x_1, x_2\}, \{x_3, x_4\}\}$ and flips the other two matchings on $X$. In fact, every non-identity $\phi \in K(X)$ fixes one of the matchings and flips the other two.

Suppose that $|S| = 2n$ and use induction on $n$. Consider the base case $n = 1$. Assume first that the two edges in $S$ are adjacent, say, those are $vu$ and $uw$. Let $\phi_{vuw}$ be the permutation in $K(Q(u))$ which flips each of the matchings $M_{u,v}$ and $M_{u,w}$. Clearly, $\phi_{vuw}$ twists each of the subgraphs $A[Q(u), Q(v)]$ and $A[Q(u), Q(w)]$ and does not change anything else in the graph. Therefore, $\phi_{vuw}$ is an isomorphism from $A$ to $A^S$.

If $S$ consists of two non-adjacent edges $vu'$ and $ww'$, consider a shortest path connecting these edges, say, $vu_1 \ldots u_k w$. The permutation

$$\phi_{vu'v} \phi_{vu_1u_2} \phi_{u_1u_2u_3} \cdots \phi_{u_{k-1}u_kw} \phi_{ukw}$$

is an isomorphism from $A$ to $A^S$ because it twists both subgraphs $A[Q(v'), Q(v)]$ and $A[Q(w), Q(w')]$ and changes nothing else (each of the intermediate subgraphs $A[Q(u_1), Q(u_2)]$ etc. is twisted twice).

Suppose now that $n \geq 2$. Choose two edges $e_1$ and $e_2$ in $S$ and denote $S' = S \setminus \{e_1, e_2\}$. Note that $A^S = (A^{S'})^{e_1e_2}$. We have $A^S \cong A^{S'}$ as in the base case and $A^S \cong A$ by the induction assumption. \hfill \square

Let $B = A^{(e)}$ for an edge $e$ of $H$. It follows from Lemma 5.3 that the isomorphism type of $B$ does not depend on the choice of $e$. Lemma 5.3 also implies that $A$ and $B$ are not isomorphic.

Given $X \subset V(H)$, let $H \setminus X$ denote the graph obtained from $H$ by removal of all vertices in $X$. We call a set $X$ a separator of $H$ if every connected component of the graph $H \setminus X$ has at most $n/2$ vertices. The number of vertices in a separator is called its size. We denote the minimum size of a separator of $H$ by $s(H)$. The following fact is a version of [9] Theorem 6.4, with virtually the same proof.

**Lemma 5.4.** $A \cong k$-WL $B$ for all $k < s(H)$.

We will need also the following property of the construction.

**Lemma 5.5.** If $H$ is vertex-transitive, then both $A$ and $B$ are vertex-transitive.
Proof. Since the outcome of our construction is determined only up to twists and $A$ is an arbitrarily chosen outcome graph, it is enough to prove the lemma for $A$.

Claim A. For every two vertices $v$ and $u$ of $H$, there is an automorphism of $A$ taking the set $Q(v)$ onto the set $Q(u)$.

Proof of Claim A. Let $f$ be an automorphism of $H$ such that $f(v) = u$. Fix a permutation $\psi$ of $V(A)$ with the following two properties:

- $\psi(Q(x)) = Q(f(x))$ for every $x \in V(H)$.
- $\psi$ transform the matching $M_{x,y}$ into the matching $M_{f(x),f(y)}$ for every $xy \in E(H)$.

Denote the image of $A$ under $\psi$ by $A^\psi$. Note that, for every $xy \in E(H)$, either $A^\psi[Q(x), Q(y)] = A[Q(x), Q(y)]$ or $A^\psi[Q(x), Q(y)]$ is the twisted version of $A[Q(x), Q(y)]$. Since $A^f \cong A$, the number of subgraphs $A[Q(x), Q(y)]$ twisted by $\psi$ is even by Lemma 5.3. By the same lemma, there is an isomorphism $\phi$ from $A^f$ to $A$ mapping each $Q(x)$ onto itself. The composition $\phi \psi$ is an automorphism of $H$ mapping each $Q(x)$ onto $Q(f(x))$, in particular, $Q(v)$ onto $Q(u)$.  

Claim B. For every $u \in V(H)$ and every two vertices $u_i, u_j \in Q(u)$, there is an automorphism of $A$ transposing $u_i$ and $u_j$.

Proof of Claim B. Without loss of generality, suppose that $i = 1$ and $j = 2$. Consider the permutation $\phi = (u_1 u_2)(u_3 u_4)$. We will use the notation introduced in the proof of Lemma 5.3. Note that $\phi$ belongs to the Klein group $K(Q(u))$. Moreover, there are neighbors $v$ and $w$ of $u$ such that $\phi = \phi_{vw}$. It easily follows from the vertex-transitivity of $H$ that the path $vwu$ extends to a cycle $vwux_1 \ldots x_kv$. The permutation

$$\phi_{vw} \phi_{wux_1} \phi_{wx_1x_2} \phi_{x_1x_2x_3} \ldots \phi_{x_kvu}$$

is an automorphism of $A$ and transposes $u_1$ and $u_2$.  

Combining Claims A and B we obtain the lemma.  

We now define a graph $G$ as the vertex-disjoint union of $A$ and $B$. Since $A$ and $B$ are connected non-isomorphic graphs, $G$ is not vertex-transitive.

Lemma 5.6. $G$ is $\mathrm{WL}_{1,k}$-homogeneous for all $k < s(H)$.

Proof. Since both $A$ and $B$ are vertex-transitive (Lemma 5.5), for every dimension $k$ we have $\mathrm{WL}_k(A,a) = \mathrm{WL}_k(A,a')$ for all vertices $a, a'$ in $A$ and $\mathrm{WL}_k(B,b) = \mathrm{WL}_k(B,b')$ for all vertices $b, b'$ in $B$. Moreover, let $k < s(H)$. Since $A \equiv_{k, \mathrm{WL}} B$ (Lemma 5.4), we have $\mathrm{WL}_k(A,a) = \mathrm{WL}_k(B,b)$ for all vertices $a \in V(A)$ and $b \in V(B)$. By Proposition 4.1 and Equivalence 11, this is equivalent to the condition that Duplicator has a winning strategy in the $(k + 1)$-pebble bijection game $\mathcal{D}_{k+1,r}(A,a,B,b)$ for every number of rounds $r$ (recall that the game starts from the position where the vertex $a$ is pebbled in $A$ and the vertex $b$ is pebbled in $B$).
We now have to show that Duplicator has a winning strategy in the game $D_{k+1,r}(G, u, G, v)$ for any $u, v \in V(G)$ and every number of rounds $r$.

If both $u$ and $v$ are in $A$ or both are in $B$, then Lemma 5.5 implies that there is an automorphism $\alpha$ of $G$ such that $\alpha(u) = v$. Duplicator wins the game by exhibiting the bijection $f = \alpha$ in each round.

It remains to consider the case that $u \in V(A)$ and $v \in V(B)$ (the case of $u \in V(B)$ and $v \in V(A)$ is similar). Duplicator wins by combining her winning strategies in the game $D_{k+1,r}(A, u, B, v)$ and in the game $D_{k+1,r}(B, A)$ starting from the empty board.

To complete the proof of Theorem 5.2, we use an infinite family of connected 3-regular graphs such that every graph $H$ in this family is vertex-transitive and has $s(H) > 0.008 v(H) = 0.001 v(G)$.

An appropriate family of connected 3-regular graphs has been found by Chiu [15]. Every graph $H$ in this family is a Cayley graph of a finite group and, hence, vertex-transitive. Moreover, every $H$ is a Ramanujan graph. In general, a $d$-regular graph $H$ is a Ramanujan graph if its second eigenvalue $\lambda_2(H)$ is smaller than or equal to $2\sqrt{d - 1}$. In our case $d = 3$ and $\lambda_2(H) \leq 2\sqrt{2}$.

The edge expansion of $H$ is defined as

$$ h(H) = \min_{0 < |S| \leq n/2} \frac{|\partial S|}{|S|}, $$

where $S \subset V(H)$ and $\partial S$ denotes the set of edges of $H$ between one vertex in $S$ and the other vertex outside. It is known [27, Theorem 2.4] that

$$ h(H) \geq (d - \lambda_2(H))/2 $$

for a $d$-regular $H$. For $H$ constructed in [15] we, therefore, have $h(H) \geq \frac{3 - 2\sqrt{2}}{2}$. The vertex expansion of $H$ is defined as

$$ h_{\text{out}}(H) = \min_{0 < |S| \leq n/2} \frac{|\partial_{\text{out}}(S)|}{|S|}, $$

where $\partial_{\text{out}}(S)$ denotes the set of vertices of $H$ outside $S$ with at least one neighbor in $S$. As easily seen, $h_{\text{out}}(H) \geq h(H)/d$ for $d$-regular graphs, which yields $h_{\text{out}}(H) \geq \frac{3 - 2\sqrt{2}}{6}$ in our case. Finally, we use the estimate

$$ s(H) \geq \frac{h_{\text{out}}(H)}{3 + h_{\text{out}}(H)} n \quad (2) $$

(see [34, Lemma 7.10 in the preliminary version]), which in our case implies $s(H) > 0.009 n$, as desired. The proof of Theorem 5.2 is complete.
5.2 Rank 3 graphs

The discussion in the beginning of the preceding subsection makes perfect sense also for the parameter \( s = 2 \). Let \( \text{R}3\text{G} = \text{U}(2) \) denote the class of all rank 3 graphs. An analog of Lemma 5.1 says that the \( \text{WL}(2, k) \) hierarchy collapses to the \( K \)-th level if and only if rank 3 graphs are recognizable by \( K \)-WL, that is, \( \text{R}3\text{G} = \text{WL}(2, K) \). The definition of a rank 3 graph is rather restrictive (see [12, Section 6]), and we conjecture that the last equality is true. In fact, it follows from a stronger conjecture that remains open since a long time.

We say that a graph \( G \) satisfies the \( t \)-vertex condition if, for every 2-rooted graph \((F, y_1, y_2)\) with at most \( t \) vertices, the subgraph \( \text{sub}(F, y_1, y_2; G, x_1, x_2) \) depends only on whether the vertices \( x_1 \) and \( x_2 \) are equal and, if not, whether they are adjacent (we here allow the possibility that \( y_1 = y_2 \) and \( x_1 = x_2 \)). Obviously, every rank 3 graph satisfies the \( t \)-vertex condition for all \( t \). Klin’s conjecture [19] (see also the references in [35]) says that there is \( T \) such that, conversely, every graph \( G \) satisfying the \( T \)-vertex condition is a rank 3 graph. Note that the subgraph count \( \text{sub}(F, y_1, y_2; G, x_1, x_2) \) for all patterns with \( k + 1 \) or fewer vertices are determined by \( \text{WL}_k(G, x_1, x_2) \). Therefore, every \( \text{WL}_{2,k} \)-homogeneous graph satisfies the \((k+1)\)-vertex condition, and Klin’s conjecture implies the existence of \( K \) such that \( \text{R}3\text{G} = \text{WL}(2, K) \).

5.3 Arc-transitivity

Arc-transitive graphs form an intermediate class between VT and R3G. If \( G \) is arc-transitive, then \( \text{WL}_k(G, u, v) = \text{WL}_k(G, u', v') \) for every two pairs \( uv \) and \( u'v' \) of adjacent vertices in \( G \), whatever \( k \). If the converse is true for some dimension \( K \), this would mean that arc-transitivity is recognizable by \( K \)-WL. Extending our argument for vertex-transitivity in Subsection 5.1, we prove that this is, unfortunately, not the case.

**Theorem 5.7.** For every \( k \) there exists a non-arc-transitive graph \( G \) such that \( \text{WL}_k(G, u, v) = \text{WL}_k(G, u', v') \) for every two pairs \( uv \) and \( u'v' \) of adjacent vertices in \( G \).

The proof takes the rest of this section. For a given a connected 3-regular graph \( H \), let \( A \) and \( B \) be the graphs constructed in Subsection 5.1.

**Lemma 5.8.** If \( H \) is arc-transitive, then both \( A \) and \( B \) are arc-transitive.

**Proof.** Since \( A \) was chosen arbitrarily up to twisting, it suffices to prove the lemma for \( A \). The proof of the following fact is similar to the proof of Claim \( A \).

**Claim C.** For every two pairs \( vu \) and \( v'u' \) of adjacent vertices of \( H \), there is an automorphism of \( A \) mapping \( Q(v) \) onto \( Q(v') \) and \( Q(u) \) onto \( Q(u') \).

1The standard definition of the \( t \)-vertex condition refers to induced subgraphs. The two variants are equivalent; cf. [30, Section 5.2.3].
Claim [C] reduces proving that $A$ is arc-transitive to proving the following fact.

**Claim D.** Let $uv \in E(H)$. For every two pairs of adjacent vertices $u_i v_j$ and $u_s v_t$ of $A$, there is an automorphism of $A$ taking $u_i$ to $u_s$ and $v_j$ to $v_t$.

**Proof of Claim D.** Without loss of generality, suppose that the subgraph $A[Q(u), Q(v)]$ consists of the 4-cycle with edges $u_1v_1, u_1v_2, u_2v_1,$ and $u_2v_2$ and the 4-cycle with edges $u_3v_3, u_3v_4, u_4v_3,$ and $u_4v_4$. Notice first that there is an automorphism $\phi$ of $A$ transposing these cycles. Indeed, let $C$ be a cycle in $H$ containing the edge $uv$ and consider the permutation $\phi$, constructed as in the proof of Claim [B], that twists the subgraph $A[Q(x), Q(y)]$ twice for each edge $xy$ along $C$.

It remains to show that $A$ has an automorphism $\phi$ transposing $u_1$ and $u_2$ and fixing each of $v_1$ and $v_2$ (the argument works as well for the other symmetric cases). Consider a shortest cycle $S$ in $H$ and let $a$ be a vertex of $S$. Let $b$ be the neighbor of $a$ different from its two neighbors on $S$. Since $S$ has the minimum possible length, $b$ does not belong to $S$. By the arc-transitivity of $H$, we conclude that for every edge $xy$ of $H$ there is a cycle containing $x$ and not containing $y$.

Now, let $C$ be a cycle containing $u$ and not containing $v$ and $\phi$ be the automorphism of $A$ twisting, like the above, all the subgraphs $A[Q(x), Q(y)]$ along $C$ twice. Recall that $\phi$ contains the factor $(u_1u_2)(u_3u_4)$ and does not touch any vertex in $Q(v)$, as desired. \(\triangleright\)

The proof of the lemma is complete. \(\square\)

Like in the proof of Theorem 5.2, let $G$ be the vertex-disjoint union of $A$ and $B$. Since these are connected non-isomorphic graphs, $G$ is not arc-transitive (in fact, even not vertex-transitive). The following fact is proved similarly to Lemma 5.6.

**Lemma 5.9.** If $k < s(H)$, then $\text{WL}_k(G, u, v) = \text{WL}_k(G, u', v')$ for every two pairs $uv$ and $u'v'$ of adjacent vertices in $G$.

To derive Theorem 5.7 from Lemma 5.9 we need connected arc-transitive 3-regular graphs with arbitrarily large minimal separator size. Requiring both arc-transitivity and 3-regularity is alone a rather strong condition. Such graphs are rare; the complete list of those with at most 512 vertices is known as Foster census [6]. Cheng and Oxley [14] proved that, for every prime $p$ with $p \equiv 1 \pmod{3}$, up to isomorphism there exists exactly one arc-transitive 3-regular graph with $2p$ vertices. Denote this graph by $H_p$. Let $D_{2p}$ be the dihedral group with generators $a$ and $b$, where $a$ corresponds to a reflection and $b$ corresponds to a rotation in $2\pi/p$. It is known [20] that $H_p$ is isomorphic to the Cayley graph on $D_{2p}$ with the generating set \{a, ab, ab^{r+1}\} where $r \neq 1$ is a cube root of unity in the multiplicative group $\mathbb{Z}/p^*$. Babai [3] estimated the vertex expansion of a connected vertex-transitive graph $H$ from below in terms of the diameter of $H$, which we denote by $D(H)$. Specifically,

$$h_{\text{out}}(H_p) \geq \frac{1}{D(H_p)}.$$ 

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It follows by (2) that
\[ s(H_p) \geq \frac{2p}{6D(H_p) + 1}. \]
We, therefore, have to show that there is an infinite sequence of graphs \( H_p \) with \( D(H_p) = o(p) \).

As easily seen,
\[ D(H_p) \leq \frac{p}{2r} + r + 1 \] (3)
for every prime \( p \) with \( p \equiv 1 \pmod{3} \) and \( r = r(p) \) as specified above. Obviously, \( r \geq \sqrt{p} \) and, hence, \( \frac{p}{2r} \leq \frac{1}{2} p^{2/3} \). We also need smallness of the second term in (3).

To this end, we use the following result by Tóth [37]. Let \( q(x) = ax^2 + bx + c \) be a quadratic polynomial such that the discriminant \( b^2 - 4ac \) is not a square. Let \( P \) be an arithmetic progression containing infinitely many primes. Then, as \( p \) runs through the primes in \( P \), the fractions \( r/p \) for the roots \( r \) of \( q(x) \) in \( \mathbb{Z}_p \) are uniformly distributed in the interval \((0, 1)\).

Now, let \( q(x) = x^2 + x + 1 \) and \( P = \{3n+1 : n \geq 1\} \). Tóth’s theorem implies in this case that, for every \( \varepsilon > 0 \), there are infinitely many primes \( p \) with a cube root \( r \) of unity in \( \mathbb{Z}_p^* \) such that \( 1 < r < \varepsilon p \). This completes the proof of Theorem 5.7.

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References

[1] V. Arvind, F. Fuhlbrück, J. Köbler, and O. Verbitsky. On Weisfeiler-Leman invariance: Subgraph counts and related graph properties. In Fundamentals of Computation Theory. Proc. of the 22nd International Symposium, (FCT’19), volume 11651 of Lecture Notes in Computer Science, pages 111–125. Springer, 2019.

[2] V. Arvind, F. Fuhlbrück, J. Köbler, and O. Verbitsky. On the Weisfeiler-Leman dimension of Fractional Packing. In Language and Automata Theory and Applications (LATA’20), volume 12038 of Lecture Notes in Computer Science. Springer, 2020.

[3] L. Babai. Local expansion of vertex-transitive graphs and random generation in finite groups. In Proceedings of the 23rd Annual ACM Symposium on Theory of Computing (STOC’91), pages 164–174. ACM, 1991.

[4] L. Babai. Automorphism groups, isomorphism, reconstruction. In Handbook of Combinatorics, chapter 27, pages 1447–1540. Elsevier, 1995.
[5] L. Babai. Graph isomorphism in quasipolynomial time. In *Proceedings of the 48th Annual ACM Symposium on Theory of Computing (STOC’16)*, pages 684–697, 2016.

[6] I. Bouwer, W. Chernoff, B. Monson, and Z. Star, editors. *The Foster census. R. M. Foster’s census of connected symmetric trivalent graphs*. Winnipeg: Charles Babbage Research Centre, 1988.

[7] A. E. Brouwer. Paulus graphs. <https://www.win.tue.nl/~aeb/drg/graphs/paulus/p25_02>.

[8] A. E. Brouwer, A. M. Cohen, and A. Neumaier. *Distance-regular graphs*, volume 18 of *Ergebnisse der Mathematik und ihrer Grenzgebiete. 3. Folge*. Berlin etc.: Springer-Verlag, 1989.

[9] J. Cai, M. Führer, and N. Immerman. An optimal lower bound on the number of variables for graph identifications. *Combinatorica*, 12(4):389–410, 1992.

[10] P. Cameron and J. van Lint. *Designs, graphs, codes and their links*, volume 22 of *London Mathematical Society Student Texts*. Cambridge etc.: Cambridge University Press, 1991.

[11] P. J. Cameron. 6-transitive graphs. *J. Comb. Theory, Ser. B*, 28(2):168–179, 1980.

[12] P. J. Cameron. Strongly regular graphs. In *Topics in algebraic graph theory*, pages 203–221. Cambridge: Cambridge University Press, 2004.

[13] G. Chen and I. Ponomarenko. *Coherent configurations*. Central China Normal University Press, 2019.

[14] Y. Cheng and J. G. Oxley. On weakly symmetric graphs of order twice a prime. *J. Comb. Theory, Ser. B*, 42(2):196–211, 1987.

[15] P. Chiu. Cubic Ramanujan graphs. *Combinatorica*, 12(3):275–285, 1992.

[16] R. Curticapean, H. Dell, and D. Marx. Homomorphisms are a good basis for counting small subgraphs. In *Proceedings of the 49th Annual ACM SIGACT Symposium on Theory of Computing (STOC’17)*, pages 210–223. ACM, 2017.

[17] H. Dell, M. Grohe, and G. Rattan. Lovász meets Weisfeiler and Leman. In *45th International Colloquium on Automata, Languages, and Programming (ICALP’18)*, volume 107 of *LIPIcs*, pages 40:1–40:14. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2018.

[18] S. Evdokimov and I. Ponomarenko. On highly closed cellular algebras and highly closed isomorphisms. *Electr. J. Comb.*, 6, 1999.
[19] I. Faradžev, M. Klin, and M. Muzichuk. Cellular rings and groups of automorphisms of graphs. In *Investigations in algebraic theory of combinatorial objects*, pages 1–152. Dordrecht: Kluwer Academic Publishers, 1994.

[20] Y. Feng and J. H. Kwak. Constructing an infinite family of cubic 1-regular graphs. *Eur. J. Comb.*, 23(5):559–565, 2002.

[21] F. Fuhlbrück, J. Köbler, and O. Verbitsky. Identifiability of graphs with small color classes by the Weisfeiler-Leman algorithm. In *37th Symposium on Theoretical Aspects of Computer Science (STACS’20)*, volume 154 of *LIPIcs*. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2020.

[22] M. Führer. On the combinatorial power of the Weisfeiler-Lehman algorithm. In *Algorithms and Complexity — 10th International Conference (CIAC’17) Proceedings*, volume 10236 of *Lecture Notes in Computer Science*, pages 260–271, 2017.

[23] A. Gardiner. Homogeneity conditions in graphs. *J. Comb. Theory, Ser. B*, 24(3):301–310, 1978.

[24] M. Grohe. *Descriptive complexity, canonisation, and definable graph structure theory*, volume 47 of *Lecture Notes in Logic*. Cambridge University Press, 2017. A preliminary online version is available at [http://www.lics.cms.rwth-aachen.de/global/show_document.asp?id=aaaaaaaaaabbbtvh](http://www.lics.cms.rwth-aachen.de/global/show_document.asp?id=aaaaaaaaaabbbtvh).

[25] D. J. Harvey and D. R. Wood. Parameters tied to treewidth. *Journal of Graph Theory*, 84(4):364–385, 2017.

[26] L. Hella. Logical hierarchies in PTIME. *Inf. Comput.*, 129(1):1–19, 1996.

[27] S. Hoory, N. Linial, and A. Widgerson. Expander graphs and their applications. *Bulletin of the American Mathematical Society. New Series*, 43(4):439–561, 2006.

[28] N. M. Kriege, F. D. Johansson, and C. Morris. A survey on graph kernels. Technical report, [abs/1903.11835](https://arxiv.org/abs/1903.11835), 2019.

[29] L. Lovász. On the cancellation law among finite relational structures. *Periodica Mathematica Hungarica*, 1(2):145–156, 1971.

[30] L. Lovász. *Large Networks and Graph Limits*, volume 60 of *Colloquium Publications*. American Mathematical Society, 2012.

[31] C. Morris, K. Kersting, and P. Mutzel. Glocalized Weisfeiler-Lehman graph kernels: Global-local feature maps of graphs. In *2017 IEEE International Conference on Data Mining (ICDM’17)*, pages 327–336. IEEE Computer Society, 2017.
[32] D. Neuen and P. Schweitzer. Benchmark graphs for practical graph isomorphism. In 25th Annual European Symposium on Algorithms (ESA’17), volume 87 of LIPIcs, pages 60:1–60:14. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2017.

[33] A. J. L. Paulus. Conference matrices and graphs of order 26. Technical report, Eindhoven University of Technology, 1973.

[34] O. Pikhurko, H. Veith, and O. Verbitsky. The first order definability of graphs: Upper bounds for quantifier depth. Discrete Applied Mathematics, 154(17):2511–2529, 2006. A preliminary version is available at arxiv.org/abs/math/0311041.

[35] S. Reichard. A criterion for the t-vertex condition of graphs. J. Comb. Theory, Ser. A, 90(2):304–314, 2000.

[36] S. S. Sane. The Shrikhande graph. Resonance, 20:903–918, 2015.

[37] A. Tóth. Roots of quadratic congruences. IMRN. International Mathematics Research Notices, 2000(14):719–739, 2000.