On Weisfeiler-Leman Invariance:
Subgraph Counts and Related Graph Properties

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Abstract

The $k$-dimensional Weisfeiler-Leman algorithm ($k$-WL) is a fruitful approach to the Graph Isomorphism problem. 2-WL corresponds to the original algorithm suggested by Weisfeiler and Leman over 50 years ago. 1-WL is the classical color refinement routine. Indistinguishability by $k$-WL is an equivalence relation on graphs that is of fundamental importance for isomorphism testing, descriptive complexity theory, and graph similarity testing which is also of some relevance in artificial intelligence. Focusing on dimensions $k = 1, 2$, we investigate subgraph patterns whose counts are $k$-WL invariant, and whose occurrence is $k$-WL invariant. We achieve a complete description of all such patterns for dimension $k = 1$ and considerably extend the previous results known for $k = 2$.

1 Introduction

Color refinement is a classical procedure widely used in isomorphism testing and other areas. It initially colors each vertex of an input graph by its degree and refines the vertex coloring in rounds, taking into account the colors appearing in the neighborhood of each vertex. This simple and efficient procedure successfully canonizes almost all graphs in linear time [5]. Combined with individualization, it is the basis of the most successful practical algorithms for the graph isomorphism problem; see [31] for an overview and historical comments.

The first published work on color refinement dates back at least to 1965 (Morgan [33]). In 1968 Weisfeiler and Leman [43] gave a procedure that assigns colors to pairs of vertices of the input graph. The initial colors are edge, nonedge, and loop. The procedure refines the coloring in rounds by assigning a new color to each pair $(u, v)$ depending on the color types of the 2-walks $uvw$, where $w$ ranges over the vertex set. The procedure terminates when the color partition of the set of all vertex pairs stabilizes. The output coloring is an isomorphism invariant of the input

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graph. It yields an edge-colored complete directed graph with certain highly regular properties. This object, known as a coherent configuration, has independently been discovered in other contexts in statistics (Bose [8]) and algebra (Higman [26]).

A natural extension of this idea, due to Babai (see [4, 9]), is to iteratively classify \( k \)-tuples of vertices. This is the \( k \)-dimensional Weisfeiler-Leman procedure, abbreviated as \( k \)-WL. Thus, \( 2 \)-WL is the original Weisfeiler-Leman algorithm [43], and \( 1 \)-WL is color refinement. The running time of \( k \)-WL is \( n^{O(k)} \), where \( n \) denotes the number of vertices in an input graph. Cai, Fürer, and Immerman [9] showed that there are infinitely many pairs of nonisomorphic graphs \( (G_i, H_i) \) such that \( k \)-WL fails to distinguish between them for any \( k = o(n) \). Nevertheless, the Weisfeiler-Leman procedure, as an essential component in isomorphism testing, can hardly be overestimated. A constant dimension often suffices to solve the isomorphism problem for important graph classes. A striking result here (Grohe [23]) is that for any graph class excluding a fixed minor (like bounded genus or bounded treewidth graphs) isomorphism can be tested using \( k \)-WL for a constant \( k \) that only depends on the excluded minor. Moreover, Babai’s quasipolynomial-time algorithm [4] for general graph isomorphism crucially uses \( k \)-WL for logarithmic \( k \).

We call two graphs \( G \) and \( H \) \( k \)-WL-equivalent and write \( G \equiv_{k \text{-WL}} H \) if they are indistinguishable by \( k \)-WL; formal definitions are given in Sections 2 (\( k = 1 \)) and 3 (\( k \geq 2 \)). By the Cai-Fürer-Immerman result [9], we know for any given \( k \) that the \( \equiv_{k \text{-WL}} \)-equivalence is coarser than the isomorphism relation on graphs.

**Definition 1.1.** A graph property (i.e., an isomorphism-invariant family of graphs) \( \mathcal{P} \) is \( k \)-WL-invariant if for any pair of graphs \( G \) and \( H \):

\[
G \in \mathcal{P} \text{ and } G \equiv_{k \text{-WL}} H \text{ implies } H \in \mathcal{P}.
\]

In particular, a graph parameter \( \pi \) is \( k \)-WL-invariant if \( \pi(G) = \pi(H) \) whenever \( G \equiv_{k \text{-WL}} H \).

The broad question of interest in this paper is which graph properties (and graph parameters) are \( k \)-WL-invariant for a specified \( k \). The motivation for this natural question comes from various areas. Understanding the power of \( k \)-WL, even for small values of \( k \), is important for both isomorphism testing and graph similarity testing. For example, the largest eigenvalues of \( 1 \)-WL-equivalent graphs are equal [39]. Moreover, \( 2 \)-WL-equivalent graphs are cospectral [14, 20]. Consequently, by Kirchhoff’s theorem, \( 2 \)-WL-equivalent graphs have the same number of spanning trees. Also the \( 2 \)-WL-invariance of certain metric graph parameters such as diameter is easy to show. Fürer [19] recently asked which basic combinatorial parameters are \( 2 \)-WL-invariant. While it is readily seen that \( 2 \)-WL-equivalence preserves the number of 3-cycles, Fürer pointed out, among other interesting observations, that also the number of \( s \)-cycles is \( 2 \)-WL-invariant for each \( s \leq 6 \). More recently, Dell, Grohe, and Rattan [15] characterized \( k \)-WL-equivalence in terms of homomorphism profiles. Specifically, they show that \( G \equiv_{k \text{-WL}} H \) if and only if the number of homomorphisms from \( F \) to \( G \) and to \( H \) are equal for all graphs \( F \) of treewidth at most \( k \).
As a heuristic for graph similarity testing, the Weisfeiler-Leman procedure has been applied in artificial intelligence; see [40] for an 1-WL-based application and [34] for a multidimensional version. It is noteworthy that 1-WL turns out to be exactly as powerful as graph neural networks [35]. Comparing subgraph frequencies is also widely used for testing graph similarity and detecting structure of large real-life graphs; see, e.g., [21, 22, 32, 42]. For example, just knowing the number of triangles is valuable information about a social network; see, e.g., [24]. Important structural information can also be found from the number of paths of length 2 and from the degree distribution, i.e., the statistics of star subgraphs; see [36]. This poses a natural question on how much the two approaches — one based on k-WL-equivalence and one based on subgraph statistics — are related to each other.

Finally, k-WL-equivalence is of fundamental importance for finite and algorithmic model theory. A graph property $\mathcal{P}$ is k-WL-invariant exactly when $\mathcal{P}$ is definable in the $(k+1)$-variable infinitary counting logic. Showing a graph property $\mathcal{P}$ to be not $\equiv_{k-WL}$-invariant for any $k$ will imply $\mathcal{P}$ is not definable in fixed-point logic with counting (FPC); see, e.g., the survey [13]. A systematic study of k-WL-invariant constraint satisfaction problems was undertaken by Atserias, Bulatov, and Dawar [3].

**Our results**

Let $F$ be a fixed pattern graph and $G$ be any given graph. The main focus of our paper is to investigate the $k$-WL-invariance of: (a) the property that $G$ contains $F$ as a subgraph, and (b) the number of subgraphs of $G$ isomorphic to $F$. We use $\text{sub}(F, \cdot)$ to denote the subgraph count function. Thus, $\text{sub}(F, G)$ denotes the number of subgraphs of $G$ isomorphic to $F$.

**Definition 1.2.** Let $\mathcal{C}(k)$ denote the class of all pattern graphs $F$ for which the subgraph count $\text{sub}(F, \cdot)$ is $\equiv_{k-WL}$-invariant. Furthermore, $\mathcal{R}(k)$ consists of all pattern graphs $F$ such that the property of a graph containing $F$ as a subgraph is $\equiv_{k-WL}$-invariant.

The concepts of $\mathcal{C}(k)$ and $\mathcal{R}(k)$ correspond to algorithmic counting and recognition problems respectively. Note that $\mathcal{C}(k) \subseteq \mathcal{R}(k)$. We use this notation to state some consequences of prior work. The $k$-WL-equivalence characterization [15], stated above, can be used to show that $\mathcal{C}(k)$ contains every $F$ such that all homomorphic images of $F$ have treewidth no more than $k$. We say that such an $F$ has *homomorphism-hereditary treewidth* at most $k$; see Section 3 for details. The striking result by Anderson, Dawar, and Holm [1] on the expressibility of the matching number in FPC implies that there is some $k$ such that $\mathcal{R}(k)$ contains all matching graphs $sK_2$, where $sK_2$ denotes the disjoint union of $s$ edges. On the other hand, there is no $k$ such that $\mathcal{R}(k)$ contains all cycle graphs $C_s$. This readily follows from the result by Dawar [12, 13] that the property of a graph having a Hamiltonian cycle is not $\equiv_{k-WL}$-invariant for any $k$.

Our results are as follows.
**Complete description of C(1) and R(1) (invariance under color refinement).** We prove that, up to adding isolated vertices, C(1) consists of all star graphs $K_{1,s}$ and the 2-matching graph $2K_2$. Hence, C(1) contains exactly the pattern graphs of homomorphism-hereditary treewidth equal to 1. Another noteworthy consequence is that, for every $F \in C(1)$, the subgraph count $\text{sub}(F, G)$ is determined just by the degree sequence of a graph $G$.

We obtain a complete description of $R(1)$ by proving that this class consists of the graphs in $C(1)$ and three forests $P_3 + P_2$, $P_3 + 2P_2$, and $2P_3$, where $P_s$ denotes the path graph on $s$ vertices.

**Case study for C(2) and R(2) (invariance under the original Weisfeiler-Leman algorithm).** An explicit characterization of $C(2)$ and $R(2)$ appears challenging. Indeed, it is not a priori clear whether testing membership in these graph classes is possible in polynomial time. While it is unknown whether $C(2)$ consists exactly of graphs with homomorphism-hereditary treewidth bounded by 2, we prove that this is indeed the case for some standard graph sequences. These results are related to questions that have been discussed in the literature.

- Beezer and Farrell [6] proved that the first five coefficients of the matching polynomial of a strongly regular graph are determined by its parameters. I.e., if $G$ and $H$ are strongly regular graphs with the same parameters, then $\text{sub}(sK_2, G) = \text{sub}(sK_2, H)$ for $s \leq 5$. We prove that $sK_2 \in C(2)$ if and only if $s \leq 5$. It follows that the Beezer-Farrell result extends to 2-WL-equivalent graphs. I.e., if $G$ and $H$ are any two 2-WL-equivalent graphs, then the first five coefficients of their matching polynomials coincide. Moreover, this result is tight and cannot be extended to a larger $s$. Note that strongly regular graphs with the same parameters are the simplest example of 2-WL-equivalent graphs.

- Fürer [19] proved that $C_s \in C(2)$ for $3 \leq s \leq 6$ and $C_s \notin C(2)$ for $8 \leq s \leq 16$. We close the gap and show that $C_7$ is the largest cycle graph in $C(2)$. We also prove that $C(2)$ contains $P_1, \ldots, P_7$ and no other path graphs. The result on cycles admits the following generalization. First, we observe that the girth $g(G)$ of a graph $G$ is a 2-WL-invariant parameter. Then, we prove that if $G \equiv_{2-WL} H$, then $\text{sub}(C_s, G) = \text{sub}(C_s, H)$ for each $3 \leq s \leq 2g(G) + 1$. Neither the factor of 2, nor the additive term of 1 can here be improved.

Characterization of $R(2)$ appears to be still harder. Fürer [19] has shown that $R(2)$ does not contain the complete graph with 4 vertices. Building on that, we show that $R(2)$ also does not contain any graph $F$ with a unique 4-clique. In view of this

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1The result of [6] is actually stronger and applies even to distance-regular graphs: The first five coefficients of the matching polynomial of such a graph are determined by the intersection array of the graph.

2Two distance-regular graphs with the same intersection array are also 2-WL-equivalent.
result, it is natural to conjecture that $R(2)$ does not contain any graph of clique number more than 3. We also show that $R(2)$ contains only finitely many cycle graphs $C_s$. Moreover, following Dawar’s approach \cite{12}, for each $k$ we show that $R(k)$ contains only finitely many $C_s$.

**Notation.** The *girth* $g(G)$ is the minimum length of a cycle in $G$. If $G$ is acyclic, then $g(G) = \infty$. We denote the vertex set of $G$ by $V(G)$ and the edge set by $E(G)$. Furthermore, $v(G) = |V(G)|$ and $e(G) = |E(G)|$. The set of vertices adjacent to a vertex $u \in V(G)$ forms its neighborhood $N(u)$. The subgraph of $G$ induced by a subset of vertices $X \subseteq V(G)$ is denoted by $G[X]$. For two disjoint vertex subsets $X$ and $Y$, we denote by $G[X,Y]$ the bipartite graph with vertex classes $X$ and $Y$ and all edges of $G$ with one vertex in $X$ and the other in $Y$. The vertex-disjoint union of graphs $G$ and $H$ is denoted by $G + H$. Furthermore, we write $mG$ for the disjoint union of $m$ copies of $G$. We use the standard notation $K_n$ for complete graphs, $P_n$ for paths, and $C_n$ for cycles on $n$ vertices. Furthermore, $K_{s,t}$ denotes the complete bipartite graph whose vertex classes have $s$ and $t$ vertices. Likewise, $K_{1,1} = K_2$, $K_{1,2} = P_3$, $C_3 = K_3$ etc.

## 2 Color refinement invariance

Given a graph $G$, the *color-refinement* algorithm (abbreviated as 1-WL) iteratively computes a sequence of colorings $C^i$ of $V(G)$. The initial coloring $C^0$ is monochromatic, that is $C^0(u)$ is the same for all vertices $u$. Then,

$$C^{i+1}(u) = \left( C^i(u), \{ C^i(a) : a \in N(u) \} \right),$$

where $\{ \ldots \}$ denotes a multiset (i.e., the multiplicity of each element counts).

If $\phi$ is an isomorphism from $G$ to $H$, then a straightforward inductive argument shows that $C^i(u) = C^i(\phi(u))$ for each vertex $u$ of $G$. This readily implies that, if graphs $G$ and $H$ are isomorphic, then

$$\{ C^i(u) : u \in V(G) \} = \{ C^i(v) : v \in V(H) \}$$

for all $i \geq 0$. We write $G \equiv_{\text{1-WL}} H$ exactly when this condition is met.

The following fact is a direct consequence of the definition.

**Lemma 2.1.** If $A \equiv_{\text{1-WL}} B$ and $A' \equiv_{\text{1-WL}} B'$, then $A + A' \equiv_{\text{1-WL}} B + B'$.

1-WL *distinguishes* graphs $G$ and $H$ if $G \not\equiv_{\text{1-WL}} H$. In fact, the algorithm does not need to check (2) for infinitely many $i$: If Equality (2) is false for some $i$ then it is false for $i = n$, where $n$ denotes the number of vertices in each of the graphs. By this reason, we call the coloring $C^n$ *stabilized*.

The partition $P_G$ of $V(G)$ into color classes of $C^n$ is called the *stable partition* of $G$. We call the elements of $P_G$ *cells.*
The stable partition \( P_G \) is equitable. I.e., for any two (possibly equal) cells \( X \) and \( Y \), all vertices in \( X \) have equally many neighbors in \( Y \) and vice versa. The number of neighbors that a vertex of \( X \) has in \( Y \) will be denoted by \( d(X,Y) \). Thus, for each cell \( X \) the graph \( G[X] \) induced by \( X \) is regular, that is, all vertices in \( G[X] \) have the same degree, namely \( d(X,X) \). Moreover, for all pairs of cells \( X, Y \) the bipartite graph \( G[X,Y] \) induced by \( X \) and \( Y \) is biregular, that is, all vertices in \( X \) have equally many neighbors in \( Y \) and vice versa.

The degree matrix of \( P_G \) is defined as

\[
D_G = (d(X,Y))_{X,Y \in P_G}
\]

and indexed by the stabilized colors of the cells; that is, the index \( X \) of \( D_G \) is the color \( C^n(x) \) of any vertex \( x \in X \).

**Lemma 2.2.** \( G \equiv_{1-WL} H \) if and only if \( D_G = D_H \).

Indeed, the equality \( D_G = D_H \) readily implies the equality (2) for \( i = n \). On the other hand, the inequality \( D_G \neq D_H \) implies that the multisets of colors in (2) for \( i = n \) are different. If they were the same, then they would become distinct in the next refinement round, i.e., for \( i = n + 1 \) (whereas we know that if 1-WL can detect such a distinction, it is detected by the \( n \)-th round).

Let \( F \) be a graph and \( s \) be a positive integer. Note that \( F \) belongs to \( \mathcal{C}(k) \) or \( \mathcal{R}(k) \) if and only if the graph \( F + s K_1 \) belongs to this class. Therefore, we will ignore isolated vertices.

**Theorem 2.3.** Up to adding isolated vertices, the classes \( \mathcal{C}(1) \) and \( \mathcal{R}(1) \) are formed by the following graphs.

1. \( \mathcal{C}(1) \) consists of the star graphs \( K_{1,s} \) for all \( s \geq 1 \) and the 2-matching graph \( 2K_2 \).
2. \( \mathcal{R}(1) \) consists of the graphs in \( \mathcal{C}(1) \) and the following three forests:

\[
P_3 + P_2, P_3 + 2P_2, \text{ and } 2P_3. \tag{3}
\]

The proof is spread over the next four subsections.

### 2.1 Membership in \( \mathcal{C}(1) \)

If two graphs are indistinguishable by color refinement, they have the same degree sequence. Notice that

\[
\text{sub}(K_{1,s}, G) = \sum_{v \in V(G)} \binom{\text{deg} \; v}{s},
\]

where \( \text{deg} \; v \) denotes the degree of a vertex \( v \). This equality shows that \( K_{1,s} \in \mathcal{C}(1) \). Since any two edges constitute either \( 2K_2 \) or \( K_{1,2} \), we have

\[
\text{sub}(2K_2, G) = \frac{e(G)}{2} - \text{sub}(K_{1,2}, G). \tag{4}
\]
Taking into account that $e(G) = \frac{1}{2} \sum_{v \in V(G)} \deg v$, this implies that $2K_2 \in \mathcal{C}(1)$.

Note that the equality (4) has been reported in several sources; see, e.g., [17, Lemma 1] and the comments therein.

2.2 Non-membership in $\mathcal{C}(1)$

To prove that a graph $F$ is not in $\mathcal{C}(1)$, one needs to exhibit 1-WL-equivalent graphs $G$ and $H$ such that $\text{sub}(F, G) \neq \text{sub}(F, H)$. Table 1 provides a list of such witnesses for each of the three forests in (3). The non-membership of all other graphs in $\mathcal{C}(1)$ follows from their non-membership in $\mathcal{R}(1)$, which will be proved in the corresponding subsection below.

| $F$               | $P_3 + P_2$ | $2P_3$ | $P_3 + 2P_2$ |
|------------------|-------------|--------|--------------|
| $G$              | $C_6$       | $C_6$  | $C_7$        |
| $\text{sub}(F, G)$ | 12          | 3      | 7            |
| $H$              | $2C_3$      | $2C_3$ | $C_4 + C_3$  |
| $\text{sub}(F, H)$ | 18          | 9      | 6            |

Table 1: Witnesses to non-membership in $\mathcal{C}(1)$: Each pair $G$ and $H$ consists of regular graphs with the same number of vertices and of the same degree.

2.3 Membership in $\mathcal{R}(1)$

We call a graph $H$ amenable if color refinement distinguishes $H$ from any other nonisomorphic graph $G$. For each of the three forests $F$ in (3), we are able to explicitly describe the class $\text{Forb}(F)$ of $F$-free graphs. Based on this description, we can show that, with just a few exceptions, every $F$-free graph is amenable.

Lemma 2.4.

1. Every $(P_3 + P_2)$- or $2P_3$-free graph $H$ is amenable.

2. Every $(P_3 + 2P_2)$-free graph $H$ is amenable unless $H = 2C_3$ or $H = C_6$.

Proving that $F \in \mathcal{R}(1)$ means proving the following implication:

$$G \equiv_{1-WL} H \ \& \ H \in \text{Forb}(F) \implies G \in \text{Forb}(F).$$

(5)

This implication is trivial whenever $H$ is an amenable graph because then $G \cong H$. By Part 1 of Lemma 2.4, we immediately conclude that the graphs $P_3 + P_2$ and $2P_3$ are in $\mathcal{R}(1)$. Part 2 ensures (5) for all $(P_3 + 2P_2)$-free graphs except $2C_3$ and $C_6$. However, the implication (5) holds true also for each exceptional graph $H \in \{2C_3, C_6\}$ by the following trivial reason. Since $H$ has 6 vertices, any 1-WL-indistinguishable graph $G$ must have also 6 vertices and hence cannot contain a $P_3 + 2P_2$ subgraph.
The proof of Lemma 2.4 is lengthy and relies on an explicit description of the class of \( F \)-free graphs for each \( F \in \{ P_3 + P_2, 2P_3, P_3 + 2P_2 \} \). Obtaining such a description requires a scrupulous combinatorial analysis, and we postpone the proof to Appendix A.

### 2.4 Non-membership in \( \mathcal{R}(1) \)

We begin with proving that \( \mathcal{R}(1) \) can contain only forests of stars.

**Lemma 2.5** (see Bollobás [7, Corollary 2.19] or Wormald [44, Theorem 2.5]). Let \( d, g \geq 3 \) be fixed, and \( dn \) be even. Let \( G_{n,d} \) denote a random \( d \)-regular graph on \( n \) vertices. Then the probability that \( G_{n,d} \) has girth \( g \) converges to a non-zero limit as \( n \) grows large.

**Lemma 2.6.** \( \mathcal{R}(1) \) can contain only acyclic graphs.

**Proof.** Assume that a graph \( F \) has a cycle of length \( m \). We show that it cannot belong to \( \mathcal{R}(1) \). Let \( d = v(F) - 1 \). Lemma 2.5 ensures that there exists a \( d \)-regular graph \( X \) of girth strictly more than \( m \). Then \( F \) does not appear as a subgraph in \( H = (d + 1)X \) but clearly does in \( G = v(X) K_{d+1} \). It remains to notice that \( G \) and \( H \) are both \( d \)-regular and have the same number of vertices. \( \square \)

**Lemma 2.7.** \( \mathcal{R}(1) \) can contain only forests of stars.

**Proof.** Suppose that \( F \in \mathcal{R}(1) \). By Lemma 2.6, \( F \) is a forest. In order to prove that every connected component of \( F \) is a star, it is sufficient and necessary to prove that \( F \) does not contain \( P_4 \) as a subgraph. Assume, to the contrary, that \( F \) has \( P_4 \)-subgraphs.

Let \( T \) be a connected component of \( F \) containing \( P_4 \). Consider a diametral path \( v_1v_2v_3 \ldots v_d \) in \( T \), where \( d \geq 4 \). Note that \( v_1 \) is a leaf. Let \( T' \) be obtained from \( T \) by identifying the vertices \( v_1 \) and \( v_4 \). Thus, \( T' \) is a unicyclic graph, where the vertices \( v_2, v_3 \), and \( v_4 = v_1 \) form a cycle \( C_3 \). Obviously, \( v(T') < v(T) \).

Consider now the graph \( H_T = 2T' \). Identify one component of \( H_T \) with \( T' \) and fix an isomorphism \( \alpha \) from this to the other component of \( H_T \). Let \( G_T \) be obtained from \( H_T \) by removing the edges \( v_2v_4 \) and \( \alpha(v_2)\alpha(v_4) \) and adding instead the new edges \( v_2\alpha(v_4) \) and \( v_4\alpha(v_2) \). Note that, by construction, \( V(T') \subseteq V(H_T) = V(G_T) \). Note that \( G_T \) contains a subgraph isomorphic to \( T \). We now prove that

\[
G_T \equiv_{1-WL} H_T. \tag{6}
\]

Indeed, define a map \( \phi : V(G_T) \rightarrow V(T') \) by \( \phi(u) = \phi(\alpha(u)) = x \) for each \( u \in V(T') \subseteq V(G_T) \). Note that \( \phi \) is a covering map from \( G_T \) to \( T' \), that is, a surjective homomorphism whose restriction to the neighborhood of each vertex of \( G_T \) is surjective. A straightforward inductive argument shows that \( \phi \) preserves the coloring produced by 1-WL, that is, \( C^i(\phi(u)) = C^i(u) \) for all \( i \), where \( C^i \) is defined by (1). Thus, the multiset \( \{ C^i(u) : u \in V(G_T) \} \) is obtained from the multiset...
\[ \{ C^i(u) : u \in V(T') \} \] by doubling the multiplicity of each color. Since \( H_T \) consists of two disjoint copies of \( T' \), this readily implies that \( G_T \) and \( H_T \) are indistinguishable by 1-WL, and (6) follows.

If a connected component \( T \) of \( F \) does not contain \( P_4 \), we set \( G_T = H_T = 2T' \). The equivalence (6) is true also in this case. Define \( G = \sum_T G_T \) and \( H = \sum_T H_T \) where the disjoint union is taken over all connected components \( T \) of \( F \). We have \( G \equiv_{1-WL} H \) by Lemma 2.1. Since each \( G_T \) contains a subgraph isomorphic to \( T' \), the graph \( G \) contains a subgraph isomorphic to \( F \). On the other hand, \( H \) does not contain any subgraph isomorphic to \( F \). To see this, let \( F_0 \) be a non-star component of \( F \) with maximum number of vertices. Then \( H \) cannot contain even \( F_0 \) because every non-star component of \( H \) has fewer vertices than \( F_0 \). Thus, we get a contradiction to the assumption that \( F \in \mathcal{R}(1) \).

Lemma 2.7 reduces our task to proving that every star forest that is not listed in Theorem 2.3, that is, different from any of

\[ K_{1,s} \ (s \geq 1), \ 2K_{1,1}, \ K_{1,2} + K_{1,1}, \ 2K_{1,2}, \ K_{1,2} + 2K_{1,1} \quad (7) \]

does not belong to \( \mathcal{R}(1) \). Our proof of this fact sticks to the following scheme. First, we will give a direct proof of non-membership for a small amount of basic star forests. Then we will establish two derivation rules based on some closure properties of \( \mathcal{R}(1) \). Finally, we will show that these derivation rules can be used, for each star forest \( F \) under consideration, to refute the hypothesis \( F \in \mathcal{R}(1) \) by deriving from it the membership in \( \mathcal{R}(1) \) of one of the basic star forests.

**Lemma 2.8** (Basic star forests). None of the star forests \( K_{1,s} + K_{1,1} \) for any \( s \geq 3 \), \( K_{1,3} + K_{1,2} \), \( 2K_{1,3} \), and \( 2K_{1,s} + K_{1,1} \) for any \( s \geq 1 \) belongs to \( \mathcal{R}(1) \).

**Proof.** In order to prove that a graph \( F \) is not in \( \mathcal{R}(1) \), one needs to exhibit 1-WL-indistinguishable graphs \( G \) and \( H \) such that \( G \) contains \( F \) as a subgraph while \( H \) does not. Below we provide such witnesses \( G \) and \( H \) for each basic star forest \( F \) listed in the lemma; see also Fig. 1.

- \( K_{1,s} + K_{1,1}, \ s \geq 3; \ H = K_{s,s} \) and \( G \) is obtained from \( 2K_s \) by adding a perfect matching between the two \( K_s \) parts.
- \( 2K_{1,3}; \ G = 2K_4 \) and \( H \) is the Wagner graph (or 4-Möbius ladder).
- \( K_{1,3} + K_{1,2}; \ G \) is obtained from \( 2C_4 \) by adding an edge between the two \( C_4 \) parts, and \( H \) is obtained from \( C_8 \) by adding an edge between two antipodal vertices of the 8-cycle in \( H \).
- \( 2K_{1,s} + K_{1,1}, \ s \geq 1; \) Both graphs \( G \) and \( H \) are obtained from \( 2K_{1,s+1} \) by adding two edges \( e \). Let \( a \) and \( b \) be two leaves of the first copy of \( K_{1,s+1} \), and let \( a' \) and \( b' \) be two leaves of the other copy of \( K_{1,s+1} \). Then \( G \) additionally contains two edges \( aa' \) and \( bb' \), whereas \( H \) additionally contains two edges \( ab \) and \( a'b' \).
\[
F = K_{1,s} + K_{1,1}, \ s = 3
\]

\[
F = 2K_{1,3}
\]

\[
F = K_{1,3} + K_{1,2}
\]

\[
F = 2K_{1,s} + K_{1,1}, \ s = 3
\]

Figure 1: \(G/H\)-certificates for each basic star forest \(F\).

In the first two cases, the graphs \(G\) and \(H\) in each witness pair are indistinguishable by color refinement as they are regular graphs of the same degree with the same number of vertices. In the last two cases, the 1-WL-indistinguishability of \(G\) and \(H\) is easily seen directly or by computing their stable partitions and applying Lemma 2.2.

Lemma 2.9 (Derivation rules).

1. If \(K_{1,i_1} + \ldots + K_{1,i_s} + K_{1,i_{s+1}} \in \mathcal{R}(1)\), then \(K_{1,i_1} + \ldots + K_{1,i_s} \in \mathcal{R}(1)\).

2. If \(K_{1,i_1+1} + \ldots + K_{1,i_{s+1}} \in \mathcal{R}(1)\), then \(K_{1,i_1} + \ldots + K_{1,i_s} \in \mathcal{R}(1)\).

Proof. 1. Suppose that \(K_{1,i_1} + \ldots + K_{1,i_s} \notin \mathcal{R}(1)\). Let \(G\) and \(H\) be two graphs witnessing this, that is, \(G \equiv_{1-WL} H\) and \(G\) contains this star forest while \(H\) does not. Then the graphs \(G + K_{1,i_{s+1}}\) and \(H + K_{1,i_{s+1}}\), which are 1-WL-indistinguishable by Lemma 2.7, witness that \(K_{1,i_1} + \ldots + K_{1,i_s} + K_{1,i_{s+1}} \notin \mathcal{R}(1)\).

2. Suppose that \(K_{1,i_1} + \ldots + K_{1,i_s} \notin \mathcal{R}(1)\) and this is witnessed by \(G\) and \(H\). Given a graph \(X\), let \(X'\) denote the result of attaching a new degree-1 vertex \(x'\) to each vertex \(x\) of \(X\) (thus, \(v(X') = 2v(X)\)). Then the graphs \(G'\) and \(H'\) witness that \(K_{1,i_1+1} + \ldots + K_{1,i_{s+1}} \notin \mathcal{R}(1)\). Indeed, it is easy to see that \(X\) contains \(K_{1,i_1} + \ldots + K_{1,i_s}\) if and only if \(X'\) contains \(K_{1,i_1+1} + \ldots + K_{1,i_{s+1}}\) as a subgraph. The equivalence \(G' \equiv_{1-WL} H'\) follows from the equivalence \(G \equiv_{1-WL} H\).

Now, let \(F\) be a star forest not listed in (7). Assume that \(F \in \mathcal{R}(1)\). Lemma 2.9 provides us with two derivations rules:

- if a star forest \(X\) is in \(\mathcal{R}(1)\), then the result of removing one connected component from \(X\) is also in \(\mathcal{R}(1)\);
• if a star forest $X$ is in $\mathcal{R}(1)$, then the result of cutting off one leaf in each connected component of $X$ is also in $\mathcal{R}(1)$.

Note that, applying these derivation rules, $F$ can be reduced to one of the basic star forests. By Lemma 2.8 we get a contradiction, which completes the proof of Theorem 2.3.

3 Weisfeiler-Leman invariance

The original algorithm described by Weisfeiler and Leman in [43], which is nowadays more often referred to as the 2-dimensional Weisfeiler-Leman algorithm, operates on the Cartesian square $V^2$ of the vertex set of an input graph $G$. Initially it assigns each pair $(u, v) \in V^2$ one of three colors, namely $\text{edge}$ if $u$ and $v$ are adjacent, $\text{nonedge}$ if $u \neq v$ and $u$ and $v$ are non-adjacent, and $\text{loop}$ if $u = v$. Denote this coloring by $C^0$. The coloring of $V^2$ is then refined step by step. The coloring after the $i$-th refinement step is denoted by $C^i$ and is computed as

$$C^i(u, v) = C^{i-1}(u, v) \mid \{\{C^{i-1}(u, w) \mid C^{i-1}(w, v)\\}_{w \in V},$$

where $\{\}$ denotes the multiset and $\mid$ denotes the string concatenation (an appropriate encoding is assumed).

The $k$-dimensional version of the algorithm, $k$-WL, operates on $V^k$. The initial coloring of a tuple $(u_1, \ldots, u_k)$ encodes its equality type and the isomorphism type of the subgraph of $G$ induced by the vertices $u_1, \ldots, u_k$. The color refinement is performed similarly to (8). For example, if $k = 3$, then

$$C^i(u_1, u_2, u_3) = C^{i-1}(u_1, u_2, u_3) \mid \{\{C^{i-1}(w, u_2, u_3) \mid C^{i-1}(u_1, w, u_3) \mid C^{i-1}(u_1, u_2, w)\\}_{w \in V},$$

Generally, we write $WL^r_k(G, u_1, \ldots, u_k)$ to denote the color of the tuple $(u_1, \ldots, u_k)$ produced by the $k$-dimensional Weisfeiler-Leman algorithm after performing $r$ refinement steps. The length of $WL^r_k(G, u_1, \ldots, u_k)$ grows exponentially as $r$ increases, which is remedied by renaming the tuple colors after each step and retaining the corresponding color substitution tables. However, in our analysis of the algorithm we will use $WL^r_k(G, u_1, \ldots, u_k)$ in its literal, iteratively defined meaning.

Let $WL^r_k(G) = \{\{WL^r_k(G, \bar{u} : \bar{u} \in V^k)\}$ denote the color palette observed on the input graph $G$ after $r$ refinement rounds. We say that the $k$-dimensional Weisfeiler-Leman algorithm distinguishes graphs $G$ and $H$ if $WL^r_k(G) \neq WL^r_k(H)$ after some number of rounds $r$. The standard color stabilization argument shows that if $n$-vertex graphs $G$ and $H$ are distinguishable by $k$-WL, then they are distinguished after $n^k$ refinement rounds at latest. If this does not happen, we say that $G$ and $H$ are $k$-WL-equivalent and write $G \equiv_{k, \text{WL}} H$.

Obviously, isomorphic graphs are $k$-WL-equivalent for every $k$. Recall also that any two strongly regular graphs with the same parameters are 2-WL-equivalent. The smallest pair of non-isomorphic strongly regular graphs with the same parameters consists of the $4 \times 4$-rook’s graph and the Shrikhande graph (these graphs are
depicted in Fig. [2]. The 2-WL-equivalence of these graphs will be used several times below.

Note that the above description of the $k$-dimensional Weisfeiler-Leman algorithm and the $k$-WL-equivalence relation for $k \geq 2$ are meaningful as well for vertex-colored graphs (the initial coloring $C^0$ includes now also vertex colors). We will need this more general framework only once, namely in the proof of Theorem 3.9 below.

Theorem 3.1 (Dell, Grohe, and Rattan [15]). Let $\text{hom}(F,G)$ denote the number of homomorphisms from a graph $F$ to a graph $G$. For each $F$ of treewidth $k$, the homomorphism count $\text{hom}(F, \cdot)$ is $\equiv_k$-WL-invariant.

Definition 3.2. We define the homomorphism-hereditary treewidth of a graph $F$, denoted by $htw(F)$, to be the maximum treewidth $tw(F')$ over all homomorphic images $F'$ of $F$.

The following result follows directly from Theorem 3.1 and the fact established by Lovász [30, Section 5.2.3] that the subgraph count $\text{sub}(F,G)$ is expressible as a function of the homomorphism counts $\text{hom}(F',G)$ where $F'$ ranges over homomorphic images of $F$ (see also [10], where algorithmic consequences of this relationship are explored).

Corollary 3.3. $C(k)$ contains all $F$ with $htw(F) \leq k$.

It is easy to see that $htw(F) = 1$ if and only if $F$ is a star graph or the matching graph $2K_2$ (up to adding isolated vertices). Thus, Theorem 2.3 implies that $C(1)$ consists exactly of the pattern graphs $F$ with $htw(F) = 1$. We now characterize the class of graphs $F$ with $htw(F) \leq 2$.

Given a graph $G$ and a partition $P$ of the vertex set $V(G)$, we define the quotient graph $G/P$ as follows. The vertices of $G/P$ are the elements of $P$, and $X \in P$ and $Y \in P$ are adjacent in $G/P$ if and only if $X \neq Y$ and there are vertices $x \in X$ and $y \in Y$ adjacent in $G$.

Lemma 3.4. $htw(F) > 2$ if and only if there is a partition $P$ of $V(F)$ such that $F/P \cong K_4$.

Proof. Let us make two basic observations. First, $H$ is a homomorphic image of $G$ if and only if there is a partition $P$ of $V(G)$ into independent sets such that $H \cong G/P$. Second, $H$ is a minor of $G$ if and only if there is a partition $P$ of $V(G)$ such that the graph $G[X]$ is connected for every $X \in P$ and $H$ is isomorphic to a subgraph of $G/P$.

These observations imply the following fact, which is more general than stated in the lemma. Let $S_k$ be the set of the minimal forbidden minors for the class of graphs with treewidth at most $k$. Note that, since the last class of graphs is minor-closed, $S_k$ exists and is finite by the Robertson–Seymour theorem. Then $htw(F) > k$ if and only if $V(F)$ admits a partition $P$ such that $G/P$ contains a subgraph isomorphic to a graph in $S_k$. 


The lemma now follows from the well-known fact [16, Chapter 12] that $S_2 = \{K_4\}$. Note that, if $F/P$ contains $K_4$ as a subgraph, then $V(F)$ admits a partition $P'$ such that $F/P'$ is itself isomorphic to $K_4$ as the superfluous nodes of $F/P$ can be merged.

Whether or not $htw(F) \leq 2$ is a necessary condition for the membership of $F$ in $C(2)$, is open. We now show the equivalence of $F \in C(2)$ and $htw(F) \leq 2$ for several standard graph sequences.

**Theorem 3.5.** $C(2)$ contains

1. $K_2, 2K_2, 3K_2, 4K_2, 5K_2$ and no other matching graphs;
2. $C_3, \ldots, C_7$ and no other cycle graphs;
3. $P_1, \ldots, P_7$ and no other path graphs.

Theorem 3.5 is related to some questions that have earlier been discussed in the literature. Beezer and Farrell [6] proved that the first five coefficients of the matching polynomial of a strongly regular graph are determined by its parameters. In other terms, if $G$ and $H$ are strongly regular graphs with the same parameters (in fact, even distance-regular graphs with the same intersection array), then $\text{sub}(sK_2, G) = \text{sub}(sK_2, H)$ for $s \leq 5$. Part 1 of Theorem 3.5 implies that this is true in a much more general situation, namely when $G$ and $H$ are arbitrary 2-WL-equivalent graphs. Moreover, this cannot be extended to larger $s$.

Fürer [19] classified all $C_s$ for $s \leq 16$, except the $C_7$, with respect to membership in $C(2)$. Part 2 of Theorem 3.5 fills this gap and also shows that the positive result for $C_7$ is optimal.

**Proof.** 1. Lemma 3.4 makes it obvious that $htw(sK_2) \leq 2$ exactly for $s \leq 5$. This gives the positive part by Corollary 3.3. It remains to prove that $sK_2 \notin C(2)$ for all $s \geq 6$. For $6K_2$, let $G$ be the $4 \times 4$-rook’s graph and $H$ be the Shrikhande graph; see Fig. 2. Being strongly regular graphs with the same parameters $(16, 6, 2, 2)$, $G$ and $H$ are 2-WL-equivalent. As calculated in [6], $\text{sub}(6K_2, G) = 96000$ while $\text{sub}(6K_2, H) = 95872$, which certifies the non-membership of $6K_2$ in $C(2)$. In order to extend this to $sK_2$ for $s > 6$, note that

$$\text{sub}((s + 1)K_2, G + K_2) = \text{sub}((s + 1)K_2, G) + \text{sub}(sK_2, G).$$

This equality implies that if $\text{sub}(sK_2, G) \neq \text{sub}(sK_2, H)$, then it holds also one of the inequalities $\text{sub}((s + 1)K_2, G) \neq \text{sub}((s + 1)K_2, H)$ or $\text{sub}((s + 1)K_2, G + K_2) \neq \text{sub}((s + 1)K_2, H + K_2)$. Thus, if a pair $G, H$ is a certificate for $sK_2 \notin C(2)$, then $(s + 1)K_2 \notin C(2)$ is certified by the same pair $G, H$ or by the pair $G + K_2, H + K_2$. In the latter case we need to remark that $G + K_2 \equiv_{2\text{-WL}} H + K_2$ whenever $G \equiv_{2\text{-WL}} H$.

2 and 3. We have $htw(C_s) \leq 2$ if $s \leq 7$. We can use Lemma 3.4 to show this. For $s \leq 5$ this is obvious because $K_4$ has 6 edges. This is easy to see also for $s = 6$: we cannot get $K_4$ by merging just two vertices, while merging more than two vertices
results in loss of one edge. Let \( s = 7 \). The argument for \( s = 6 \) shows that \( K_4 \) cannot be obtained from \( C_7 \) if at least one edge is contracted. The assumption \( C_7/P \cong K_4 \) would, therefore, mean that \( K_4 \) has a closed walk that uses one edge twice and every other edge once. Such a walk contains an Eulerian trial in \( K_4 \), which is impossible because \( K_4 \) has all four vertices of degree 3.

Corollary 3.3 therefore implies that \( C(2) \) contains all cycle graphs \( C_s \) up to \( s = 7 \). It contains also all paths \( P_s \) up to \( s = 7 \), as the class of graphs \( \{ F : \text{htw}(F) \leq 2 \} \) is closed under taking subgraphs, which is easily seen from Lemma 3.4.

In order to obtain the negative part, we again use the Shrikhande graph \( G \) and the 4 \( \times \) 4 rook’s graph \( H \). For \( s \leq 16 \) see the table in Fig. 2 for \( P_s \) and [19] for \( C_s \). For \( s > 16 \) construct the graphs \( G_s \) and \( H_s \) by adding a vertex-disjoint path \( P_{s-16} \) to \( G \) and \( H \) respectively and by connecting both end vertices of this path to all original vertices of \( G \) and \( H \). Then

\[
\text{sub}(C_s, G_s) = \text{sub}(P_{16}, G) \neq \text{sub}(P_{16}, H) = \text{sub}(C_s, H_s),
\]

while still \( G_s \equiv_{2-\text{WL}} H_s \).

For paths, we use almost the same construction of \( G_s \) and \( H_s \), where we connect only one end vertex of \( P_{s-16} \) to the original graph. Then

\[
\text{sub}(P_s, G_s) = 2 \text{sub}(P_{16}, G) \neq 2 \text{sub}(P_{16}, H) = \text{sub}(P_s, H_s),
\]

and the pair \( G_s, H_s \) certifies that \( P_s \notin C(2) \). This works for all \( s > 17 \). If \( s = 17 \), we construct graphs \( H_{17} \) and \( G_{17} \) by adding a new neighbor of degree one to each vertex in \( G \) and \( H \). Then

\[
\text{sub}(P_{17}, G_{17}) = 2 \text{sub}(P_{16}, G) + \text{sub}(P_{15}, G)
\]
and analogously for $H$ and $H_{17}$. It remains to use the table in Fig. 2 to see that this sum is different for $G$ and $H$. 

Part 2 of Theorem 3.5 can be generalized as follows. Recall that $g(G)$ denotes the girth of a graph $G$.

**Theorem 3.6.** Suppose that $G \equiv_{2\text{-WL}} H$. Then

1. $g(G) = g(H)$.
2. $\text{sub}(C_s, G) = \text{sub}(C_s, H)$ for each $3 \leq s \leq 2g(G) + 1$.

**Proof.**

1. The proof uses the logical characterization of the $\equiv_{k\text{-WL}}$-equivalence in [9]. According to this characterization, $G \equiv_{k\text{-WL}} H$ if and only if $G$ and $H$ satisfy the same sentences in the first-order $(k + 1)$-variable logic with counting quantifiers $\exists^{\geq t}$, where an expression $\exists^{\geq t}x \Phi(x)$ for any integer $t$ means that there are at least $t$ vertices $x$ with property $\Phi(x)$.

Assume that $g(G) < g(H)$ and show that then $G \not\equiv_{2\text{-WL}} H$. It is enough to show that $G$ and $H$ are distinguishable in $3$-variable logic with counting quantifiers.

**Case 1:** $g(G)$ is odd. In this case, $G$ and $H$ are distinguishable even in the standard $3$-variable logic (with quantifiers $\exists$ and $\forall$ only). As it is well known [27], two graphs $G$ and $H$ are distinguishable in first-order $k$-variable logic if and only if Spoiler has a winning strategy in the $k$-pebble Ehrenfeucht-Fraïssé game on $G$ and $H$. In the $3$-pebble game, the players Spoiler and Duplicator have equal sets of $3$ pebbles $\{a, b, c\}$. In each round, Spoiler takes a pebble and puts it on a vertex in $G$ or in $H$; then Duplicator has to put her copy of this pebble on a vertex of the other graph. Duplicator's objective is to ensure that the pebbling determines a partial isomorphism between $G$ and $H$ after each round; when she fails, she immediately loses.

Spoiler wins the game as follows. Let $C$ be a cycle of length $g(G)$ in $G$. In the first three rounds, Spoiler pebbles a $3$-path along $C$ by his pebbles $a$, $b$, and $c$ in this order. Then, keeping the pebble $a$ fixed, Spoiler moves the pebbles $b$ and $c$, in turns, around $C$ so that the two pebbled vertices are always adjacent. In the end, there arises a pebbled $acb$-path, which is impossible in $H$.

**Case 2:** $g(G)$ is even. Let $g(G) = 2m$. Consider the following statement in the $3$-variable logic with counting quantifiers:

$$\exists x \exists y \left( \text{dist}(x, y) = m \land \exists^{\geq 2} z (z \sim y \land \text{dist}(z, x) = m - 1) \right),$$

where $\text{dist}(x, y) = m$ is a $3$-variable formula expressing the fact that the distance between vertices $x$ and $y$ is equal to $m$. This statement is true on $G$ and false on $H$.

2. The proof of this part is based on the result by Dell, Grohe, and Rattan stated above as Theorem 3.1 and Lovász’ result [30, Section 5.2.3] on the expressibility of $\text{sub}(F, G)$ through the homomorphism counts $\text{hom}(F', G)$ for homomorphic images $F'$ of $F$. By these results, it suffices to prove that, if $s \leq 2g(G) + 1$ and $h$ is a
homomorphism from \( C_s \) to \( G \), then the subgraph \( h(C_s) \) of \( G \) has treewidth at most 2. Assume, to the contrary, that \( h(C_s) \) has treewidth more than 2 or, equivalently, \( h(C_s) \) contains \( K_4 \) as a minor. Since \( K_4 \) has maximum degree 3, \( h(C_s) \) contains \( K_4 \) even as a topological minor [16 Section 1.7]. Let \( M \) be a subgraph of \( h(C_s) \) that is a subdivision of \( K_4 \). Obviously, \( s \geq e(h(C_s)) \geq e(M) \). Moreover, \( s \geq e(M) + 2 \).

Indeed, the homomorphism \( h \) determines a walk of length \( s \) via all edges of the graph \( h(C_s) \). By cloning the edges traversed more than once, \( h(C_s) \) can be seen as an Eulerian multigraph with \( s \) edges. Since \( M \) has four vertices of degree 3, any extension of \( M \) to such a multigraph requires adding at least 2 edges. Thus, \( s \geq e(M) + 2 \). Note that \( M \) is formed by six paths corresponding to the edges of \( K_4 \). Moreover, \( M \) has four cycles, each cycle consists of three paths, and each of the six paths appears in two of the cycles. It follows that \( 2e(M) \geq 4g(G) \). Therefore, \( s \geq 2g(G) + 2 \), yielding a contradiction.

Moreover, Part 2 of Theorem 3.5 admits a qualitative strengthening: It turns out that even \( R(2) \) contains only finitely many cycle graphs \( C_s \). In fact, a much stronger fact is true.

**Theorem 3.7.** For each \( k \), the class \( R(k) \) contains only finitely many cycle graphs \( C_s \).

The proof of Theorem 3.7 follows a powerful approach suggested by Dawar in [12] to prove that the graph property of containing a Hamiltonian cycle is not \( \equiv_k \)-invariant for any \( k \). This fact alone immediately implies that, whatever \( k \) is, \( R(k) \) cannot contain all cycle graphs \( C_s \). An additional effort is needed to show that no \( R(k) \) can contain infinitely many \( C_s \). Specifically, Theorem 3.7 is a direct consequence of the following two facts.

**Lemma 3.8.**

1. No class \( R(k) \) contains all path graphs, that is, for very \( k \) there is \( t \) such that \( P_t \notin R(k) \).

2. If \( P_t \notin R(k) \), then \( C_s \notin R(k) \) for all \( s > t \).

**Proof.** 1. We begin with description of the main idea of Dawar’s method. The Graph Isomorphism problem (GI) is the recognition problem for the set of all pairs of isomorphic graphs. We can encode GI as a class of relational structures over vocabulary \( \langle V_1, V_2, E \rangle \), where \( V_1 \) and \( V_2 \) are unary relations describing two vertex sets and \( E \) is a binary adjacency relation (over \( V_1 \cup V_2 \)). Then GI consists of those structures where \( V_1 \) and \( V_2 \) are disjoint and the graphs \( (V_1, E) \) and \( (V_2, E) \) are isomorphic.

The starting point of the method is observing that GI is not \( \equiv_k \)-invariant for any \( k \). This follows from the seminal work by Cai, Fürer, and Immerman [9], who constructed, for each \( k \), a pair of non-isomorphic graphs \( G \) and \( H \) such that \( G \equiv_k H \). Indeed, \( G + G \in GI \) and \( G + H \notin GI \), and \( G + G \equiv_k G + H \).

Suppose now that we have two classes of relational structures \( C_1 \) and \( C_2 \) and know that \( C_1 \) is not \( \equiv_k \)-invariant for any \( k \). We can derive the same fact for \( C_2 \).
by showing a first-order reduction from $C_1$ to $C_2$, that is, a function $f$ such that $f(A) \in C_2$ iff $A \in C_1$ for any structure $A$ in the vocabulary of $C_1$, where $f(A)$ is a structure in the vocabulary of $C_2$ whose relations are relations in the universe of $A$ and are definable by first-order formulas over the vocabulary of $C_1$; see [27] for details.

There is a first-order reduction from GI to the Satisfiability problem (where for CNFs we assume a standard encoding as relational structures); see, e.g., [41]. A first-order reduction from Satisfiability to Hamiltonian Cycle is described by Dahlhaus [11]. We now describe a first-order reduction from Hamiltonian Cycle to the problem Long Path, which we define as the problem of recognizing whether a given $N$-vertex graph contains a path of length at least $\frac{3}{4}N + 2$.

To this end, we modify a standard reduction from Hamiltonian Cycle to Hamiltonian Path (which itself is not first-order as it requires selection of a single vertex from the vertex set of a given graph). Specifically, suppose we are given a graph $G$ with $n$ vertices. We expand $G$ to a graph $G'$ with $8n$ vertices as follows. For each vertex $v$ of $G$, we create its clone $v'$ with the same adjacency to the other vertices of $G$ (and their clones). Next, we connect $v$ and $v'$ by a path $v_1, v_2, v_3, v_4, v'$ via four new vertices $v_1, v_2, v_3, v_4$. Finally, for each $v \in V(G)$, we add a new neighbor $u$ to $v_2$ and a new neighbor $u'$ to $v_3$. In the resulting graph $G'$, $u$ and $u'$ have degree 1. It remains to notice that $G$ has a Hamiltonian cycle if and only if $G'$ has a path of length $6n + 2$. The vertex set and the adjacency relation of $G'$ can easily be defined by first order formulas in terms of the vertex set and the adjacency relation of $G$.

Composing the aforementioned reductions, we obtain a first-order reduction from GI to Long Path and conclude that the last problem is not $\equiv_k$-invariant for any $k$. It remains to note that the existence of a fixed $k$ for which $R(k)$ contains all path graphs, would imply the $\equiv_k$-invariance of Long Path for this $k$.

2. Consider a pair of graphs $G, H$ certifying that $P_t \notin R(k)$, that is, $G \equiv_k H$ and $G$ contains $P_t$ while $H$ does not. Without loss of generality, we can suppose that $G$ and $H$ have no isolated vertices. Like in the proof of Part 2 of Theorem 3.5, we construct the graph $G_s$ by adding a vertex-disjoint path $P_{s-1}$ to $G$ connecting both end vertices of this path to all vertices of $G$. The graph $H_s$ is obtained similarly from $H$. Note that $G_s \equiv_k H_s$ and that $G_s$ contains $C_s$ while $H_s$ does not.

It is easy to see that $K_3 \in R(2)$ (this is also a formal consequence of Part 2 of Theorem 3.5). Using the pair $G, H$ consisting of the $4 \times 4$ rook’s graph and the Shrikhande graph, Füurer [19] proved that the complete graph $K_4$ is not in $R(2)$. By padding $G$ and $H$ with new $s - 4$ universal vertices, we see that $R(2)$ contains $K_s$ if and only if $s \leq 3$. Füurer’s result on the non-membership of $K_4$ in $R(2)$ admits the following generalization.

**Theorem 3.9.** No graph containing a unique 4-clique can be in $R(2)$.

Given a graph $R$, we define a corresponding vertex-colored graph $R^*$, whose vertices are colored using four colors 1, 2, 3, 4, as follows:

- Each vertex $v$ of $R$ is replaced by four clones $v_1, v_2, v_3, v_4$, where $v_i$ has color $i$;
For vertices $v$ and $u$ of $R$, their clones $v_i$ and $u_j$ are adjacent in $R^*$ if and only if $u$ and $v$ are adjacent in $R$ and $i \neq j$.

This transformation, which we require for the proof of Theorem 3.9, is based on a reduction from the parametrized $k$-CLIQUE problem to its “colorful version” by Fellows et al. [18, Lemma 1].

Lemma 3.10.

1. $R$ contains a 4-clique if and only if $R^*$ contains a 4-clique. Moreover, the vertices of any 4-clique in $R^*$ have pairwise different colors.

2. If $R \equiv_{2-WL} S$, then $R^* \equiv_{2-WL} S^*$.

Proof. Part 1 is easy. To prove Part 2, we use the fact [25] that $G \equiv_{2-WL} H$ if and only if Duplicator has a winning strategy in the 3-pebble Hella’s bijection game on $G$ and $H$.

Like the Ehrenfeucht-Fraïssé game that we used in the proof of Theorem 3.6, the bijection game is played by two players, Spoiler and Duplicator, to whom we will refer as he and she respectively. Let $p_1, p_2, p_3$ be the three 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, $x_i$ denotes the vertex pebbled by $p_i$ in $G$, and $y_i$ 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 $x_i$ and $y_i$ can be different in different rounds. More specifically, a round is played as follows:

- Spoiler chooses $i \in \{1, 2, 3\}$;
- Duplicator responds with a bijection $f : V(G) \rightarrow V(H)$ having the property that $f(x_j) = y_j$ for all $j \neq i$ such that $p_j$ is on the board;
- Spoiler chooses a vertex $x$ in $G$ and puts $p_i$ on $x$ and its copy on $f(x)$ (this move reassigns $x_i$ to vertex $x$ and $y_i$ to vertex $f(x)$).

Duplicator’s objective is to keep the map $x_i \mapsto y_i$ a partial isomorphism during the play. Spoiler wins if the Duplicator fails. If $G$ and $H$ are vertex-colored graphs, then the Duplicator has to keep the map $x_i \mapsto y_i$ a color-preserving partial isomorphism. The description of the bijection game is complete.

The assumption $R \equiv_{2-WL} S$ implies that Duplicator has a winning strategy in the 3-pebble bijection game on $R$ and $S$. She can transform this strategy to the game on graphs $R^*$ and $S^*$. Define a projection map $\lambda : V(R^*) \cup V(S^*) \rightarrow V(R) \cup V(S)$ as follows: If a vertex $u \in V(R^*) \cup V(S^*)$ is a clone of a vertex $u \in V(R) \cup V(S)$, then $\lambda(u) = u$. Duplicator simulates a round of the game on $R$ and $S$ by assuming that

- Spoiler chooses the pebble with index $i \in \{1, 2, 3\}$ in the simulated game on $R$ and $S$ whenever he does it in the real game on $R^*$ and $S^*$;
• Spoiler chooses the vertex $\lambda(w)$ in $R$ whenever he chooses a vertex $w$ in $R^*$.

Whenever Duplicator’s strategy in the simulated game on $R$ and $S$ yields a bijection $f : V(R) \rightarrow V(S)$, in the real game on $R^*$ and $S^*$ Duplicator responds with the bijection $f^* : V(R^*) \rightarrow V(S^*)$ taking each clone of a vertex $v \in V(R)$ to the clone of $f(v)$ that has the same color. This completes description of Duplicator’s strategy for the game on $R^*$ and $S^*$.

Note that, whenever $x_i \in V(R^*)$ and $y_i \in V(S^*)$ are pebbled by $p_i$, then $\lambda(x_i) \in V(R)$ and $\lambda(y_i) \in V(S)$ are pebbled by $p_i$ in the simulated game. This, along with the facts that Duplicator always succeeds in the simulated game and $f^*$ always preserves the vertex colors, readily implies that Duplicator succeeds in each round of the game on $R^*$ and $S^*$. Thus, she has a winning strategy in this game, and we conclude that $R^* \equiv_{2\text{-WL}} S^*$.

**Proof of Theorem 3.9.** Let $R$ be the $4 \times 4$-rook’s graph and $S$ be the Shrikhande graph. Recall that $R$ contains a 4-clique, while $S$ does not. Consider now $G = R^*$ and $H = S^*$. By Lemma 3.10 $G$ contains a 4-clique, $H$ does not, and $G \equiv_{2\text{-WL}} H$.

Let $c_G : V(G) \rightarrow \{1, 2, 3, 4\}$ and $c_H : V(H) \rightarrow \{1, 2, 3, 4\}$ denote the vertex colorings of $G$ and $H$ respectively.

Now, let $F$ be a graph that contains exactly one $K_4$. Suppose that $V(F) = \{1, \ldots, l\}$ and $F[\{1, 2, 3, 4\}] \cong K_4$. Denote $F' = F[\{5, \ldots, l\}]$. We define a graph $G'$ as $V(G') = V(G) \cup V(F')$ and

$$E(G') = E(G) \cup E(F') \cup \{\{u, v\} : u \in V(G), v \in V(F'), \{c_G(u), v\} \in E(F)\}.$$ 

In other words, each of the vertices 1, 2, 3, and 4 of $F$ is cloned to 16 copies with the same adjacency to the other vertices. Further, the set of the 64 clones, whose names 1, 2, 3, 4 are now regarded as colors, is endowed with edges to create a copy of $G$. The graph $H'$ is defined similarly.

Note that $H'$ does not contain $F$ or even any copy of $K_4$. Indeed, $K_4$ appears neither in $H$ nor in $F'$, and any copy $K$ of $K_4$ in $H'$ with an edge between $V(H)$ and $V(F')$ would give rise to one more copy of $K_4$ in $F$ (note that $K$ can use only differently colored vertices from $H$ because each color class of $H$ is an independent set). On the other hand, $G'$ contains $F$ as a subgraph. Indeed, $G$ contains a 4-clique with colors 1, 2, 3, 4, which completes the $F'$ fragment of $G'$ to a copy of $F'$.

It remains to prove that $G' \equiv_{2\text{-WL}} H'$. It suffices to prove that Duplicator has a winning strategy in the 3-pebble bijection game on $G'$ and $H'$. Since $G \equiv_{2\text{-WL}} H$, Duplicator has a winning strategy in the 3-pebble bijection game on $G$ and $H$. She can win the game on $G'$ and $H'$ by simulating the game on $G$ and $H$ as follows. She assumes that

• Spoiler chooses the pebble with index $i \in \{1, 2, 3\}$ in the simulated game on $G$ and $H$ whenever he does it in the real game on $G'$ and $H'$;

• Spoiler chooses a vertex $x$ in $G$ whenever he chooses this vertex in $G'$ (recall that $V(G') = V(G) \cup V(F')$).
Whenever Duplicator’s strategy in the simulated game on $G$ and $H$ yields a bijection $f : V(G) \to V(H)$, in the real game on $G'$ and $H'$ Duplicator responds with the bijection $f' : V(G') \to V(H')$ that coincides with $f$ on $V(G)$ and is the identity map on $V(H')$. The bijection $f'$ does not change if Spoiler chooses a vertex $x$ in $V(F') \subset V(G')$.

In order to check that this strategy is winning for Duplicator, consider the vertices pebbled in $G'$ and $H'$ by $p_i$ and $p_j$ for any $i, j \in \{1, 2, 3\}$. Without loss of generality, suppose that $i = 1$ and $j = 2$. According to our notation, $p_1$ occupies vertices $x_1 \in V(G')$ and $y_1 \in V(H')$, and $p_2$ occupies vertices $x_2 \in V(G')$ and $y_2 \in V(H')$. Duplicator’s strategy ensures that $x_i \in V(F')$ exactly when $y_i \in V(F')$ for each $i = 1, 2$. If both $x_1$ and $x_2$ are in $V(G)$, then both $y_1$ and $y_2$ are in $V(H)$ and are adjacent if and only if $x_1$ and $x_2$ are adjacent. The last condition is true because the vertices in $V(G) \cup V(H)$ are pebbled according to Duplicator’s winning strategy in the game on $G$ and $H$. If both $x_1$ and $x_2$ are in $V(F')$, then $y_1$ and $y_2$ is the identical vertex pair in the graph $F$, and the adjacency relation is preserved by trivial reasons. Finally, suppose that $x_1 \in V(G)$ while $x_2 \in V(F')$ and, hence, $y_1 \in V(H)$ and $y_2 \in V(F')$. Since $x_1$ and $y_1$ were pebbled according to Duplicator’s winning strategy in the game on $G$ and $H$, they have the same color. Moreover, $x_2$ and $y_2$ are identical vertices in $F$. It follows by the construction of $G'$ and $H'$ that $y_1$ and $y_2$ are adjacent in $H'$ if and only if $x_1$ and $x_2$ are adjacent in $G'$.

4 Concluding discussion

An intriguing open problem is whether Corollary 3.3 yields a complete description of the class $\mathcal{C}(k)$. Our Theorem 2.3 gives an affirmative answer in the one-dimensional case. Moreover, this theorem gives a complete description of the class $\mathcal{R}(1)$. The class $\mathcal{R}(2)$ remains a mystery. For example, it contains either finitely many matching graphs $sK_2$ or all of them, and we currently do not know which of these is true. In other words, is the matching number preserved by $\equiv_{2\text{-WL}}$-equivalence? Note that non-isomorphic strongly regular graphs with the same parameters cannot yield counterexamples to this. The Brouwer-Haemers conjecture states that every connected strongly regular graph is Hamiltonian except the Petersen graph, and Pyber 37 has shown there are at most finitely many exceptions to this conjecture. Since the Petersen graph has a perfect matching, it is therefore quite plausible that every connected strongly regular graph has an (almost) perfect matching.

By Corollary 3.3 the subgraph count $\text{sub}(F, G)$ is $k$-WL-invariant for $k = \text{htw}(F)$. Interestingly, the parameter $\text{htw}(F)$ appears in a result by Curticapean, Dell, and Marx 10 who show that $\text{sub}(F, G)$ is computable in time $e(F)^{O(e(F))} \cdot v(G)^{\text{htw}(F)+1}$. An interesting area is to explore connections between $k$-WL-invariance and algorithmics, which are hinted by this apparent coincidence.

Which induced subgraphs and their counts are $k$-WL-invariant for different $k$ deserves study. We note that the induced subgraph counts have been studied in the context of finite model theory by Kreutzer and Schweikardt 29.
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A Proof of Lemma 2.4

We prove Lemma 2.4 by splitting it into Lemmas A.5, A.9, and A.8 below. The proof is based on an explicit description of the class of $F$-free graphs for each $F \in \{P_3 + P_2, P_3 + 2P_2, 2P_3\}$.

A.1 Forbidden forests

Let $\text{Forb}(F)$ denote the class of all graphs that do not have subgraphs isomorphic to $F$. Describing $\text{Forb}(F)$ explicitly is a hard task in general, even if $F$ is a simple pattern like a matching graph $sP_2$. Nevertheless, we will need explicit characterization of $\text{Forb}(F)$ in several simple cases. As the simplest fact, note that

$$\text{Forb}(2P_2) = \{ K_{1,s} + tK_1, K_3 + tK_1 \}_{s \geq 1, t \geq 0}.$$  

For a characterization of $\text{Forb}(3P_2)$, recall some standard graph-theoretic concepts.

The join of graphs $G$ and $H$, denoted by $G \ast H$, is obtained from the disjoint union of $G$ and $H$ by adding all possible edges between a vertex of $G$ and a vertex of $H$.

The line graph $L(H)$ of a graph $G$ has $E(H)$ as the set of vertices, and $e$ and $e'$ from $E(H)$ are adjacent in $L(H)$ if and only if they share a vertex in $H$. A clique cover of size $k$ of a graph $G$ is a set of cliques $C_1, \ldots, C_k$ in $G$ such that $V(G) = \bigcup_{i=1}^{k} C_i$. Note that cliques in $L(H)$ are exactly star or triangle subgraphs of $H$. It follows that $H$ is in $\text{Forb}(2P_2)$ exactly when $L(H)$ is a complete graph or, in other words, has a clique cover of size 1. This admits an extension to the 3-matching pattern.

**Lemma A.1.** 1. Let $v(H) \geq 6$. Then $H$ is in $\text{Forb}(3P_2)$ exactly when $L(H)$ has a clique cover of size at most 2.

2. Up to adding isolated vertices, $H \in \text{Forb}(3P_2)$ exactly in these cases:

   i. $v(H) \leq 5$,
ii. $H$ is a subgraph of one of the following graphs:

- $2K_3$,
- $K_1 \ast (K_3 + sK_1)$, $s \geq 0$,
- $K_2 \ast sK_1$, $s \geq 1$.

Members of the last two families are depicted in Figure 3. Note that $K_2 \ast sK_1$ is the complete split graph with the clique part of size 2.

Note that Lemma A.1 does not hold true without the assumption $v(H) \geq 6$. As an example, consider the complement of $P_3 + 2K_1$. This graph does not contain any 3-matching, while its line graph has clique cover number 3.

Proof. 1. In one direction, suppose that $E(H) = E_1 \cup E_2$, where both $E_1$ and $E_2$ are cliques in $L(H)$. Among any three edges $e_1, e_2, e_3$ of $H$, at least two belong to one of these cliques. By this reason, $e_1, e_2, e_3$ cannot form a $3P_2$ subgraph of $H$.

For the other direction, assume that $H$ does not contain any $3P_2$ subgraph. If $H$ does not contain even any $2P_2$ subgraph, then we are done because, as it was already mentioned, $H$ has a clique cover of size 1 in this case. Assume, therefore, that $H$ contains two non-adjacent edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$. Call any vertex in $V(H) \setminus \{u_1, v_1, u_2, v_2\}$ external. Since $\{e_1, e_2\}$ cannot be extended to a 3-matching subgraph, we can state the following facts.

(A) Every two external vertices in $H$ are non-adjacent.

(B) If $u_i$ has an external neighbor $x$, then $v_i$ has no external neighbor possibly except $x$. Symmetrically, the same holds true for $u_i$ and $v_i$ swapped.

We split our further analysis into three cases.

Case 1: There are external vertices $x_1$ and $x_2$ such that $x_1u_1v_1$ and $x_2u_2v_2$ are triangles. Claims (A) and (B) imply that $H$ has no other edge. Thus, $H = 2K_3$, and $E(H)$ is covered by two triangle cliques.

Case 2: There is a triangle $x_1u_1v_1$ and no triangle $x_2u_2v_2$. By Claim (B), none of the vertices $x_1$, $u_1$, and $v_1$ has an external neighbor. One of the vertices $u_2$ and $v_2$, say $u_2$ must have at least one external neighbor $x$. If there are also other external
vertices, all of them are adjacent to \( u_2 \) by Claim (B). The edges \( u_1v_2 \) and \( v_1v_2 \) are impossible in \( H \) because they would form a 3-matching together with \( x_1v_1 \), \( u_2x \) and \( x_1u_1, u_2x \) respectively. Thus, \( H \) can only look as shown in Figure 4(a). We see that \( E(H) \) is covered by the triangle \( x_1u_1v_1 \), and the neighborhood star of \( u_2 \).

**Case 3:** There is no external vertex \( x \) such that \( xu_1v_1 \) or \( xu_2v_2 \) is a triangle. If one of the edges \( e_1 \) and \( e_2 \) has no external neighbor, then all edges between \( e_1 \) and \( e_2 \) are possible and, by Claims (A) and (B), \( H \) looks as shown in Figure 4(b). Thus, also in this case \( E(H) \) is covered by a star and a triangle (or by a star and a small star \( K_{1,t} \) with \( t = 1, 2 \)).

If both \( e_1 \) and \( e_2 \) have external neighbors, then the assumption \( v(H) \geq 6 \) implies that there is an external neighbor \( x_1 \) for \( e_1 \) and there is an external neighbor \( x_2 \neq x_1 \) for \( e_2 \). Without loss of generality, suppose that \( x_i \) is adjacent to \( u_i \) for both \( i = 1, 2 \). Then \( v_1 \) and \( v_2 \) cannot be adjacent for else \( H \) would contain a 3\( P_2 \) formed by \( x_1u_1 \), \( x_2u_2 \), and \( v_1v_2 \). By Claim (B), any other external vertex is adjacent to \( u_1 \) or to \( u_2 \), or to both of them. Thus, \( H \) looks as in Figure 4(c), and \( E(H) \) is covered by the neighborhood stars of \( u_1 \) and \( u_2 \).

2. This part follows from Part 1. Let \( v(H) \geq 6 \). If \( E(H) \) is covered by two triangles, then \( H \) is a subgraph of \( 2K_3 \). If \( E(H) \) is covered by a triangle and a star, then \( H \) is a subgraph of \( K_1 \ast (K_3 + sK_1) \). Finally, if \( E(H) \) is covered by two stars, then \( H \) is a subgraph of \( K_2 * sK_1 \).

As usually, \( \Delta(G) \) denotes the maximum degree of a vertex in the graph \( G \).

**Lemma A.2.** Let \( F \in \{ P_3 + P_2, P_3 + 2P_2, 2P_3 \} \). Up to adding isolated vertices, the classes \( \text{Forb}(F) \) consist of the following graphs.

1. \( H \in \text{Forb}(P_3 + P_2) \) exactly in these cases:

   i. \( v(H) \leq 4 \),

   ii. \( \Delta(H) = 1 \), that is, \( H = sK_2 \),

   iii. \( H = K_{1,s} \).

2. \( H \in \text{Forb}(P_3 + 2P_2) \) exactly in these cases:

   i. \( v(H) \leq 6 \),

   ii. \( \Delta(H) = 1 \),
iii. $H$ is a subgraph of one of the following graphs:
- $K_1 \ast (K_3 + sK_1)$, $s \geq 0$,
- $K_2 \ast sK_1$, $s \geq 1$.

3. $H \in \text{Forb}(2P_3)$ exactly in these cases:
   i. $H = H_0 + sK_2$, $s \geq 0$, where $v(H_0) \leq 5$,
   ii. $H = N + sK_2$, $s \geq 0$, where $N$ is the 6-vertex net graph shown in Figure 5
   iii. $H$ is a subgraph of the graph $K_1 \ast sK_2$ for some $s \geq 1$.

Note that Part 2.iii includes all $3P_2$-free graphs with at least 7 vertices; see Figure 3.

The graphs in Part 3.ii–iii are shown in Figure 5. Note also that $K_1 \ast sK_2$ are known as friendship graphs, and they are a part of the more general class of windmill graphs.

Proof. 1. Any graph satisfying Conditions i–iii obviously does not contain $P_3 + P_2$. For the other direction, let $H$ be $(P_3 + P_2)$-free. Suppose that $\Delta(H) \geq 2$. Then $H$ must be connected (recall that we assume that $H$ has no isolated vertex). Furthermore, suppose that $H$ has at least 5 vertices. If $\Delta(H) = 2$, then $H$ is a path or a cycle with at least 5 vertices, but all of them contain $P_3 + P_2$. It follows that $\Delta(H) \geq 3$, that is, $H$ contains a 3-star $K_{1, 3}$. Call any vertex outside this star subgraph external. If an external vertex is adjacent to a leaf of the 3-star, this clearly results in a $P_3 + P_2$ subgraph. We conclude that all external vertices are adjacent to the central vertex $x$ of the 3-star. Thus, $V(H) = N(x) \cup \{x\}$. Since $v(H) \geq 5$, the vertex $x$ has at least 4 neighbors. As a consequence, no two neighbors of $x$ can be adjacent, as this would yield a $P_3 + P_2$. We conclude that $H = K_{1, s}$ for some $s \geq 4$.

2. If $H$ satisfies at least one of Conditions i–ii, it obviously does not contain any subgraph $P_3 + 2P_2$. If $H$ satisfies Condition iii, then it does not contain even $3P_2$. For the other direction, suppose that $H$ is $(P_3 + 2P_2)$-free.

If $H$ has three or more connected components, then obviously $H = sK_2$ for $s \geq 3$ (recall the assumption that $H$ has no isolated vertex).

Consider now the case that $H$ has exactly two connected components. If one of them is $P_2$, then the other must (and can) be an arbitrary connected $P_3 + P_2$-free graph. By Part 1 of the lemma, the second component has at most 4 vertices or
is a star. In the former case, \( v(H) \leq 6 \). In the latter case, \( H \) is a subgraph of \( K_1 * (K_3 + sK_1) \) for some \( s \). If none of the connected components of \( H \) is \( P_2 \), then both of them contain a \( P_3 \) and, therefore, both must be \( 2P_2 \)-free. Since every \( 2P_2 \)-free graph is a star or a triangle, this leaves three possibilities for \( H \). If \( H = 2K_3 \), then \( v(H) \leq 6 \). If \( H = K_3 + K_{1,s} \), then \( H \) is a subgraph of \( K_1 * (K_3 + sK_1) \). Finally, if \( H = K_{1,s} + K_{1,t} \), then \( H \) is a subgraph of \( K_2 * (s+t)K_1 \).

It remains to consider the case that \( H \) is connected. Suppose that \( v(H) \geq 7 \). Then the condition that \( H \) does not contain any \( P_3 + 2P_2 \) implies that \( H \) does not contain even any \( 3P_2 \) subgraph. By Lemma [A.1] \( H \) is a subgraph of \( K_1 * (K_3 + sK_1) \) or \( K_2 * sK_1 \).

3. Like in the previous cases, it suffices to prove the theorem in one direction. Let \( H \) be \( 2P_3 \)-free. If \( H \) is disconnected, all but one connected components must be \( P_2 \). As a single non-\( P_2 \) component, an arbitrary connected \( 2P_3 \)-free graph is allowed. Since the class of all graphs satisfying Conditions i–iii is closed under addition of isolated edges, it is enough to prove the claim in the case of a connected \( H \).

Note first that \( H \) contains no cycle \( C_n \) for \( n \geq 6 \) because such a cycle contains a \( 2P_3 \). Suppose that \( v(H) \geq 6 \). Then \( H \) contains also neither \( C_5 \) nor \( C_4 \). Indeed, if \( H \) contains a \( C_5 \), then \( H \) must contain also a subgraph \( \begin{array}{c} \text{D} \end{array} \), which contains a \( 2P_3 \). If \( H \) contains a \( C_4 \), then \( H \) must contain one of subgraphs

\[
\begin{array}{c}
\text{D}, \quad \text{E}, \quad \text{F}, \quad \text{G},
\end{array}
\]

and all of them contain a copy of \( 2P_3 \).

Suppose that \( H \) contains a 3-cycle \( xyz \) and call any further vertex of \( H \) external. An external vertex can be adjacent to at most one of the vertices \( x, y, \) and \( z \) for else \( H \) would contain a \( C_4 \). Assume first that two vertices of the 3-cycle, say, \( x \) and \( y \) have external neighbors \( x' \) and \( y' \) respectively, which must be distinct. Since \( v(H) \geq 6 \), there must be yet another external vertex \( z' \). The only possibility avoiding appearance of a \( 2P_3 \) is that \( z' \) is adjacent to \( z \), and no other adjacencies and further vertices are possible. Thus, in this case \( v(H) = 6 \) and \( H \) is the net graph.

Assume now that only one of the vertices of the 3-cycle, say \( x \), has external neighbors. The distance from any external vertex \( v \) to \( x \) is at most 2 for else a copy of \( 2P_3 \) appears. If this distance is equal to 2, denote the common external neighbor of \( x \) and \( v \) by \( v' \) and note that \( v' \) has degree 2 in \( H \) and \( v \) has degree 1. If an external vertex \( u \) does not appear in such 3-path \( xv'v \), then it is adjacent only to \( x \) or, possibly, also to one vertex \( u' \) of the same kind. Then \( u \) has degree 1 in \( H \) in the former case and degree 2 in the latter case. It follows that \( H \) is a subgraph of a windmill graph \( K_1 * sK_2 \).

It remains to consider the case that \( H \) is a tree. The diameter of \( H \) is at most 4 for else \( H \) would contain a \( P_6 \) and, hence, a \( 2P_3 \). If the diameter is equal to 4, then \( H \) contains a \( P_3 \) subgraph. Let \( x \) be the middle vertex along this copy of \( P_3 \). Note that none of the four other vertices cannot have any further neighbor in \( H \). Moreover, any branch of \( H \) from \( x \) can be \( P_2 \) or \( P_3 \) and nothing else. It follows that \( H \) is a subgraph of a windmill graph \( K_1 * sK_2 \).
Suppose now that the diameter of a tree \( H \) is equal to 3. Let \( x_1x_2x_3x_4 \) be a copy of \( P_4 \) in \( H \). Call any other vertex in \( H \) external. Since \( v(H) \geq 6 \), there are at least two external vertices. None of them can be adjacent to \( x_1 \) or \( x_4 \) because then the diameter would be larger. It is also impossible that one external vertex is adjacent to \( x_2 \) and another to \( x_3 \) because then \( H \) would contain a \( 2P_3 \). Without loss of generality, assume that \( x_3 \) has no external vertex. Due to the assumption on the diameter of \( H \), all the external vertices are adjacent to \( x_2 \). This simple tree is obviously a subgraph of a windmill graph.

It remains to note that the trees of diameter 2 are exactly the stars and that a single tree of diameter 1 is \( P_2 \).

We conclude this subsection with a straightforward characterization of a class of graphs appearing in Lemma [A.1]2.ii and Lemma [A.2]2.iii. The vertex cover number \( \tau(G) \) is equal to the minimum size of a vertex cover in a graph \( G \).

**Lemma A.3.** \( \tau(H) \leq 2 \) if and only if \( H \) is a subgraph of the complete split graph \( K_2 * sK_1 \) for some \( s \geq 1 \).

### A.2 Amenability

In [2], we defined the concept of a graph being amenable to color refinement. Specifically, we call a graph \( H \) amenable if 1-WL distinguishes \( H \) from any other graph \( G \) that is not isomorphic to \( H \). In other words, a graph is amenable if it is identifiable by 1-WL up to isomorphism. In logical terms, a graph is amenable exactly if it is definable in the two-variable first-order logic with counting quantifiers. We now show that, with just a few exceptions, every \( F \)-free graph for each \( F \) from the preceding subsection is amenable.

Efficiently verifiable amenability criteria are obtained in [2] and [28] but we do not use these powerful tools here as more simple and self-contained arguments are sufficient for our purposes. We will use the following auxiliary facts.

**Lemma A.4.** 1. Every forest is amenable.

2. Let \( K \) be a forest. Then the disjoint union \( H + K \) is amenable if and only if \( H \) is amenable.

Part 1 of Lemma [A.4] follows from [38] Theorem 2.5; see also [2] Corollary 5.1. A proof of Part 2 can be found in [2], Section 5].

A straightforward inspection shows that every graph with at most 4 vertices is amenable. The following fact is, therefore, a straightforward consequence of Lemmas [A.2]1 and [A.4]1.

**Lemma A.5.** Every \((P_3 + P_2)\)-free graph is amenable.

Below we examine amenability of \( F \)-free graphs for \( F \in \{3P_2, P_3 + 2P_2, 2P_3\} \). As the simplest application of Lemma [A.4]2, while proving the amenability, one can always assume that the graph under consideration has no isolated vertex.
Lemma A.6. If $\tau(H) \leq 2$, then $H$ is amenable.

The subgraph of a graph $G$ induced by a subset of vertices $X \subseteq V(G)$ is denoted by $G[X]$. For two disjoint vertex subsets $X$ and $Y$, we denote by $G[X,Y]$ the bipartite graph with vertex classes $X$ and $Y$ and all edges of $G$ with one vertex in $X$ and the other in $Y$.

Proof. Let $\{u, v\}$ be a vertex cover of $H$. The set $V(H) \setminus \{u, v\}$ consists of three parts: the common neighborhood of $u$ and $v$, the neighbors solely of $u$, and the neighbors solely of $v$; see Figure 6(a). Denote the first part by $C$ and the last two parts by $A$ and $B$ respectively.

If $H$ is a forest, we are done by Lemma A.4.1. Suppose, therefore, that $H$ has a cycle, that is, $|C| \geq 2$ or $|C| = 1$ and $u$ and $v$ are adjacent. Thus, both $\deg u \geq 2$ and $\deg v \geq 2$, which means that $A \cup B$ is exactly the set of all pendant vertices in $H$.

If $|A| \neq |B|$, then the stable partition $\mathcal{P}_H$ consists of the cells $A, B, C, D = \{u\}$, and $E = \{v\}$; see Figure 6(a). In degenerate cases, $A$ or $B$ can be an empty set. A key observation is that the graph $H[X]$ for every cell $X \in \mathcal{P}_H$ is empty. Moreover, for every two cells $X, Y \in \mathcal{P}_H$, the bipartite graph $H[X,Y]$ is either complete or empty. Suppose that $G \equiv_{1-WL} H$. Let $A', B', C', D', E'$ be the cells of $G$ with the same stabilized colors as $A, B, C, D, E$ respectively. We have $|X| = |X'|$ for each $X \in \mathcal{P}_H$ and its counterpart $X' \in \mathcal{P}_G$. Moreover, Lemma 2.2 implies that every $G[X]$ is empty and $G[X', Y']$ is complete or empty in full accordance with $H[X, Y]$.

It follows that any bijection $f : V(H) \to V(G)$ taking each cell $X$ to its counterpart $X'$ is an isomorphism from $H$ to $G$. A similar argument will repeatedly be used throughout this subsection.

If $|A| = |B|$, then $\mathcal{P}_H$ consists of three cells $A \cup B, C, D \cup E$, where $C$ can be empty; see Figure 6(b). Note that both $H[A \cup B]$ and $H[C]$ are empty, while $H[D \cup E]$ is either complete or empty depending on adjacency of $u$ and $v$. Moreover, $H[C, D \cup E]$ is complete, $H[C, A \cup B]$ is empty, and $H[D \cup E, A \cup B] \cong 2K_{1,|A|}$, where the two stars are centered at $u$ and $v$. Denote the corresponding cells in a 1-WL-indistinguishable graph $G$ by $(A \cup B)'$, $C'$, and $(D \cup E)'$. Lemma 2.2 implies, in particular, that $d((D \cup E)', (A \cup B)) = d(D \cup E, A \cup B) = |A|$ and $d((A \cup B)', (D \cup E)) = d(A \cup B, D \cup E) = 1$. This determines the graph $G[(D \cup E)', (A \cup B)]$ up to

\footnote{We call a vertex $v$ pendant if $\deg v = 1$.}
isomorphism, namely $G[(D \cup E)']$, $(A \cup B)' \cong H[D \cup E, A \cup B]$. Similarly to
the preceding case, consider a cell-preserving bijection $f : V(H) \to V(G)$, assuming
additionally that $f$ is an isomorphism from $H[D \cup E, A \cup B]$ to $G[(D \cup E)']$, $(A \cup B)'$.
As easily seen, $f$ is an isomorphism from the whole graph $H$ to $G$. \hfill \Box

**Lemma A.7.** Every $3P_2$-free graph $H$ is amenable unless $H = 2C_3$.

**Proof.** We use the description of the class of $3P_2$-free graph provided by Lemma [A.1]2. An easy direct inspection reveals that all graphs with at most 5 vertices are
amenable. In view of Lemmas [A.3] and [A.6], it remains to consider the case that $H$
is a subgraph of the graph $K_1 \ast (K_3 + sK_1)$ for some $s \geq 2$; see Figure 3.

Denote the set of pendant vertices of $K_1 \ast (K_3 + sK_1)$ by $A$. We suppose that
at least two vertices from $A$ are in $H$ for else $v(H) \leq 5$. Denote the non-pendant
vertices of $K_1 \ast (K_3 + sK_1)$ by $x_0, x_1, x_2, \text{ and } x_3$, where $x_0$ is the common
neighbor of all pendant vertices. By our general assumption, $H$ has no isolated vertex, which
implies that $x_0$ belongs to $H$ and all vertices in $A$ are adjacent to $x_0$ in $H$. Assume
first that none of the vertices $x_1, x_2, \text{ and } x_3$ is pendant in $H$. Then $\mathcal{P}_H$ includes the
cells $A$ and $\{x_0\}$. Note that any other cell in $\mathcal{P}_H$ contains at most 3 vertices. As
easily seen, for any $X, Y \in \mathcal{P}_H$ the graph $H[X]$ is complete or empty and $H[X, Y]$ is
a complete or empty bipartite graph. Due to this fact, any cell-respecting bijection
from $V(H)$ to the vertex set of an 1-WL-indistinguishable graph $G$ provides an
isomorphism from $H$ to $G$.

If any of $x_1, x_2, \text{ and } x_3$ is pendant in $H$, then it joins the cell $A$, and the previous
argument applies. \hfill \Box

**Lemma A.8.** Every $(P_3 + 2P_2)$-free graph $H$ is amenable unless $H = 2C_3$ or $H = C_6$.

**Proof.** We use the description of the class $\text{Forb}(P_3 + 2P_2)$ provided by Lemma [A.2]2.
A direct inspection shows that all graphs with at most 6 vertices except $2C_3$ and $C_6$
are amenable. Each graph $sK_2$, like any forest, is amenable. Every graph in Part
iii of Lemma [A.2]2 is even $3P_2$-free and, therefore, amenable by Lemma [A.7]. \hfill \Box

**Lemma A.9.** Every $2P_3$-free graph $H$ is amenable.

**Proof.** We use the description of the class $\text{Forb}(2P_3)$ provided by Lemma [A.2]3.
If $H$ is as in Part i or ii, then its amenability follows from Lemma [A.4]2 and the
aforementioned fact that all graphs with at most 6 vertices except $2C_3$ and $C_6$ are
amenable. Suppose, therefore, that $H$ is a subgraph of some windmill graph.

If $H$ contains no triangle, it is acyclic and amenable by Lemma [A.4]1. If $H$
contains $C_3$ as a connected component, then $H = C_3 + sK_2$, and this graph is
amenable by Lemma [A.4]2. In any other case, $H$ contains a triangle with one
vertex of degree at least 3. This is the only vertex of degree at least 3 in $H$; let us
denote it by $u$. The stable partition of $H$ looks as shown in Figure 7. Specifically,
$\mathcal{P}_H = \{A, B, C, D, E\}$, where $A$ consists of those neighbors of $u$ which are adjacent

\[\text{This also follows easily from the characterization of the amenability in [2].}\]
Figure 7: Proof of Lemma A.9.

to another neighbor of \( u \), \( B \) of the pendant neighbors of \( u \), \( C \) of the remaining neighbors of \( u \), \( D \) of all non-neighbors of \( u \) and, finally, \( E = \{u\} \) (\( B, C, \) and \( D \) can be empty).

Suppose that \( G \cong 1\text{-}WL \ H \), and let \( A', B', C', D', E' \) be the cells of \( G \) with the same stabilized colors as \( A, B, C, D, E \) respectively. For any cell \( X \neq A \), the graph \( H[X] \) is empty. By Lemma 2.2, \( G[X'] \) is also empty unless \( X' = A' \). Furthermore, \( H[A] \cong tK_2 \), where \( t = |A|/2 \), and hence \( d(A) = 1 \). By Lemma 2.2, \( d(A') = 1 \) as well, which implies that \( G[A'] \cong tK_2 \cong H[A] \).

For any two cells \( X, Y \in P_H \), the bipartite graph \( H[X,Y] \) is empty or complete unless \( \{X,Y\} = \{C,D\} \). By Lemma 2.2, the bipartite graph \( G[X',Y'] \) is empty or complete in the exact accordance with \( H[X,Y] \) unless \( \{X',Y'\} = \{C',D'\} \). Furthermore, \( H[C,D] \cong qK_2 \), where \( q = |C| = |D| \), is a matching between \( C \) and \( D \). Therefore, \( d(C,D) = d(D,C) = 1 \). By Lemma 2.2, \( d(C',D') = d(D',C') = 1 \), which implies that \( G[C',D'] \) is a matching between \( C' \) and \( D' \), and \( G[C',D'] \cong qK_2 \cong H[C,D] \).

We construct an isomorphism \( f \) from \( H \) to \( G \) as follows. First of all, \( f \) takes each cell \( X \in P_H \) onto the corresponding cell \( X' \in P_G \). In particular, \( f(u) = u' \), where \( E' = \{u'\} \). On the cells \( B \) and \( C \), the map \( f \) is defined arbitrarily. On the cell \( A \), the map \( f \) is fixed to be an arbitrary isomorphism from \( H[A] \) to \( G[A] \). Finally, \( f \) is defined on \( D \) so that the restriction of \( f \) to \( C \cup D \) is an isomorphism from \( H[C,D] \) to \( G[C',D'] \). \(\square\)