The Weisfeiler-Leman Algorithm and Recognition of Graph Properties

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Abstract

The $k$-dimensional Weisfeiler-Leman algorithm ($k$-WL) is a very useful combinatorial tool in graph isomorphism testing. We address the applicability of $k$-WL to recognition of graph properties. Let $G$ be an input graph with $n$ vertices. We show that, if $n$ is prime, then vertex-transitivity of $G$ can be seen in a straightforward way from the output of $2$-WL on $G$ and on the vertex-individualized copies of $G$. However, if $n$ is divisible by $16$, then $k$-WL is unable to distinguish between vertex-transitive and non-vertex-transitive graphs with $n$ vertices as long as $k = o(\sqrt{n})$. Similar results are obtained for recognition of arc-transitivity.

1 Introduction

The $k$-dimension Weisfeiler-Leman algorithm ($k$-WL), whose original, 2-dimensional version [40] appeared in 1968, has played a prominent role in isomorphism testing already for a half century. Given a graph $G$ with vertex set $V$, $k$-WL computes a canonical coloring $\text{WL}_k(G)$ of the Cartesian power $V^k$. Let $\{\text{WL}_k(G)\}$ denote the multiset of colors appearing in $\text{WL}_k(G)$. The algorithm decides that two graphs $G$ and $H$ are isomorphic if $\{\text{WL}_k(G)\} = \{\text{WL}_k(H)\}$, and that they are non-isomorphic otherwise. While a negative decision is always correct, Cai, Fürrer, and Immerman [11] constructed examples of non-isomorphic graphs $G$ and $H$ with $n$ vertices such that $\{\text{WL}_k(G)\} = \{\text{WL}_k(H)\}$ as long as $k = o(n)$. Nevertheless, a constant dimension $k$ suffices to correctly decide isomorphism for many special classes of graphs (when $G$ is in the class under consideration and $H$ is arbitrary). For example, dimension $k = 2$ is enough if $G$ is an interval graph [19], $k = 3$ is enough for planar graphs [31], and there is a constant $k = k(M)$ sufficient for all graphs not containing a given graph $M$ as a minor [25]. Last but not least, $k$-WL is an important component in Babai’s quasipolynomial-time algorithm [6] for general graph isomorphism.

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In the present paper, we initiate discussion of the applicability of \(k\)-WL to recognition of graph properties rather than to testing isomorphism. That is, given a single graph \(G\) as input, we are interested in knowing which properties of \(G\) can be detected by looking at \(WL_k(G)\). Some regularity properties are recognized in a trivial way. For example, \(G\) is strongly regular if and only if 2-WL splits \(V^2\) just in the diagonal \(\{(u,u) : u \in V\}\), the adjacency relation of \(G\), and the complement. It is worth of mentioning that isomorphism of strongly regular graphs is considered to be a hard problem for \(k\)-WL. It is only known \cite{3} that \(k\)-WL correctly decides isomorphism of strongly regular graphs with \(n\) vertices if \(k \geq 2\sqrt{n} \log n\) (see also \cite{7}).

For a property \(P\), we use the same character \(P\) to denote also the class of all graphs possessing this property. Suppose that the isomorphism problem for graphs in \(P\) is known to be solvable by \(k\)-WL. This means that, for every \(G \in P\), \(\{WL_k(G)\}\) is a complete isomorphism invariant of \(G\) and hence, at least implicitly, \(WL_k(G)\) contains the information about all properties of \(G\). It is, however, a subtle question whether any certificate of the membership of \(G\) in \(P\) can be extracted from \(WL_k(G)\) efficiently. We can only be sure that \(k\)-WL distinguishes \(P\) from its complement, in the following sense: If \(G \in P\) and \(H \notin P\), then \(\{WL_k(G)\} \neq \{WL_k(H)\}\). However, given the last inequality, we will never know whether \(G \in P\) and \(H \notin P\) or whether \(H \in P\) and \(G \notin P\). As a particular example, the knowledge that 2-WL decides isomorphism of interval graphs or that 3-WL decides isomorphism of planar graphs does not seem to imply, on its own, any recognition algorithm for these classes.

We address the applicability of \(k\)-WL to recognition of properties saying that a graph is highly symmetric.

**Vertex-transitivity.** A graph \(G\) is **vertex-transitive** if every vertex can be taken to any other vertex by an automorphism of \(G\). It is unknown whether the class of vertex-transitive graphs is recognizable in polynomial time. The case of graphs with a prime number \(p\) of vertices is easier due to the known characterization \cite{39} of vertex-transitive graphs with \(p\) vertices as **circulant graphs**, i.e., Cayley graphs of the cyclic group of order \(p\). In this case, a polynomial-time recognition algorithm is known due to Muzychuk and Tinhofer \cite{33}. Their algorithm uses 2-WL as preprocessing and then involves a series of algebraic-combinatorial operations to find a Cayley presentation of the input graph. Our first result, Theorem \ref{thm:vertex-transitivity}, shows a very simple, purely combinatorial way to recognize vertex-transitivity of a graph \(G\) with \(p\) vertices. Indeed, vertex-transitivity can immediately be detected by looking at the outdegrees of the monochromatic digraphs in \(WL_2(G)\) and \(WL_2(G_u)\) for all copies of \(G\) with an individualized vertex \(u\). Our algorithm takes time \(O(p^4 \log p)\), which is somewhat better than the running time \(O(p^5 \log^2 p)\) of the algorithm presented in \cite{33}.

Our approach is based on the theory of coherent configurations (see a digest of main concepts in Section \ref{sec:coherent-configurations}). In fact, our exposition, apart from the well-known facts on circulants of prime order, uses only several results about the **schurity property** of certain coherent configurations.

Furthermore, we explore the limitations of the \(k\)-WL-based combinatorial ap-
approach to vertex-transitivity by proving that, if \( n \) is divisible by 16, then \( k \)-WL is unable to distinguish between vertex-transitive and non-vertex-transitive graphs with \( n \) vertices as long as \( k = o(\sqrt{n}) \) (see Theorem 4.1). This excludes extension of our positive result to the general case. Indeed, such an extension would readily imply that 3-WL distinguishes any vertex-transitive graph from any non-vertex-transitive graph, contradicting our lower bound \( k = \Omega(\sqrt{n}) \). This bound as well excludes any other combinatorial approach to recognizing vertex-transitivity as long as it is based solely on \( k \)-WL.

Our lower bound is based on the Cai-Fürer-Immerman construction [11]. We need graphs \( G \) and \( H \) such that \( G \) is vertex-transitive, \( H \) is not, and distinguishing \( G \) and \( H \) is hard for \( k \)-WL. The CFI construction uses a special gadget to convert an expander graph \( F \) into a pair of non-isomorphic graphs \( A \) and \( B \) hard for \( k \)-WL, where \( k \) depends on the expansion quality of \( F \). Assuming that both \( A \) and \( B \) are vertex-transitive, the desired pair of \( G \) and \( H \) can be obtained by taking the vertex-disjoint union of two copies of \( A \) as \( G \) and the vertex-disjoint union of \( A \) and \( B \) as \( H \). Attempting to make \( A \) and \( B \) vertex-transitive, one faces with two subtle points. First, the original CFI gadget [11, Fig. 3] (or [29, Fig. 13.24]) destroys vertex-transitivity even when the template graph \( F \) is vertex-transitive. This technical complication can be overcome by using a simplified version of the CFI gadget (see Figure 2), which apparently first appeared in [18]; see also [23, 34, 22]. In the context of vertex-transitive coherent configurations this idea was suggested by Evdokimov in his thesis [17]. The simplified gadget can be used only if \( F \) is a regular graph of degree 3. The second subtle point is that vertex-transitive expanders of degree 3 are rather rare. We use the fact shown by Babai [4] that every vertex-transitive graph of sufficiently small diameter has at least some non-trivial expansion property. Thus, our technical contribution is a careful adaptation of the CFI construction in the vertex-transitive setting, resulting in explicit bounds. Moreover, we show that this approach, with some additional subtleties, works also for arc-transitivity (see below).

In Section 6 we discuss a hierarchy of natural regularity properties of graphs and show, as a consequence of failure of \( k \)-WL to recognize vertex-transitivity, that this hierarchy does not collapse at any level.

**Arc-transitivity.** A graph \( G \) is *arc-transitive* if every ordered pair of adjacent vertices can be taken to any other pair of adjacent vertices by an automorphism of \( G \). With just a little additional effort, our analysis of vertex-transitivity implies that arc-transitivity of a given graph \( G \) with a prime number of vertices can be immediately seen from WL\(_2\)(\( G \)) and from WL\(_2\)(\( G_u \)) for all vertex-individualized copies of \( G \) (Theorem 5.1). On the negative side, there is no fixed dimension \( k \) such that \( k \)-WL can in general distinguish between arc-transitive and non-arc-transitive graphs (Theorem 5.2). Though we are able to implement the CFI construction in the arc-transitive setting, in contrast to the vertex-transitive case this does not give us any explicit lower bound on the dimension. The reason is that, for a template graph \( F \), we need arc-transitive 3-regular graphs with non-trivial expansion. Requiring both arc-transitivity and 3-regularity is alone a rather strong condition. Such graphs
are extremely rare; the complete list of those with at most 512 vertices is known as Foster census [8]. We employ the construction of such graphs by Cheng and Oxley [15] and estimate their diameter using Tóth’s theorem [38] on the distribution of roots of quadratic equations in finite prime fields, which yields only an inherently existential result.

2 Notation and definitions

We denote the vertex set of a graph $G$ by $V(G)$ and the edge set by $E(G)$. The number of vertices in $G$ will sometimes be denoted by $v(G)$.

Cayley graphs. Let $Γ$ be a group and $Z$ be a set of non-identity elements of $Γ$ such that $Z^{-1} = Z$, that is, any element belongs to $Z$ only together with its inverse. The Cayley graph $\text{Cay}(Γ, Z)$ has the elements of $Γ$ as vertices, where $x$ and $y$ are adjacent if $x^{-1}y ∈ Z$. This graph is connected if and only if the connection set $Z$ is a generating set of $Γ$. Every Cayley graph is obviously vertex-transitive.

The Weisfeiler-Leman algorithm. The original version of the Weisfeiler-Leman algorithm, 2-WL, operates on the Cartesian square $V^2$ of the vertex set of an input graph $G$. Below it is supposed that $G$ is undirected. We also suppose that $G$ is endowed with a vertex coloring $c$, that is, each vertex $u ∈ V$ is assigned a color denoted by $c(u)$. The case of uncolored graphs is covered by assuming that $c(u)$ is the same for all $u$. 2-WL starts by assigning each pair $(u, v) ∈ V^2$ the initial color

$$\text{WL}_2^0(u, v) = (\text{type}, c(u), c(v)),$$

where type takes on one of three values, namely edge if $u$ and $v$ are adjacent, nonedge if distinct $u$ and $v$ are non-adjacent, and loop if $u = v$. The coloring of $V^2$ is then modified step by step. The $(r + 1)$-th coloring is computed as

$$\text{WL}_2^{r+1}(u, v) = \left\{ (\text{WL}_2^r(u, w), \text{WL}_2^r(w, v)) \right\}_{w ∈ V},$$

where $\{\}$ denotes the multiset. Let $S^r$ denote the partition of $V^2$ determined by the coloring $\text{WL}_2^r(·)$. It is easy to notice that $\text{WL}_2^{r+1}(u, v) = \text{WL}_2^{r+1}(u', v')$ implies $\text{WL}_2^r(u, v) = \text{WL}_2^r(u', v')$, which means that $S^{r+1}$ is finer than or equal to $S^r$. It follows that the partition stabilizes starting from some step $t ≤ n^2$, where $n = |V|$, that is, $S^{t+1} = S^t$, which implies that $S^r = S^t$ for all $r ≥ t$. As the stabilization is reached, 2-WL terminates and outputs the coloring $\text{WL}_2^t(·)$, which will be denoted by $\text{WL}_2(·)$.

Note that the length of $\text{WL}_2^r(u, v)$ grows exponentially as $r$ increases. The exponential blow-up is remedied by renaming the colors after each step.

Let $ϕ$ be an automorphism of $G$. A simple induction on $r$ shows that

$$\text{WL}_2^r(ϕ(u), ϕ(v)) = \text{WL}_2^r(u, v)$$

for all $r$ and, hence

$$\text{WL}_2(ϕ(u), ϕ(v)) = \text{WL}_2(u, v).$$

(2)
In particular, if $G$ is vertex-transitive, then the color $\text{WL}_2(u, u)$ is the same for all $u \in V$. If the last condition is fulfilled, we say that $2$-WL does not split the diagonal on $G$, where by the diagonal we mean the set of all pairs $(u, u)$.

In general, the automorphism group $\text{Aut}(G)$ of the graph $G$ acts on the Cartesian square $V(G)^2$, and the orbits of this action are called 2-orbits of $\text{Aut}(G)$. By Equality \[2\text{], the partition of } V(G)^2 \text{ into 2-orbits is finer than or equal to the stable partition } S = S^2 \text{ produced by 2-WL.}

3 Vertex-transitivity on a prime number of vertices

We begin with a few simple observations about the output produced by 2-WL on an input graph $G$. Recall that in this paper we restrict our attention to undirected graphs. Even though $G$ is undirected, the equality $\text{WL}_2(u, v) = \text{WL}_2(v, u)$ need not be true in general. Thus, the output of 2-WL on $G$ can naturally be seen as a complete colored directed graph on the vertex set $V(G)$, which we denote by $\text{WL}_2(G)$. Thus, $\text{WL}_2(G)$ contains every pair $(u, v) \in V(G)^2$ as an arc, i.e., a directed edge, and this arc has color $\text{WL}_2(u, v)$. We will see $\text{WL}_2(G)$ as containing no loops, but instead we assign each vertex $u$ the color $\text{WL}_2(u, u)$. Any directed subgraph of $\text{WL}_2(G)$ formed by all arcs of the same color is called a constituent digraph.

Let $(u, v)$ and $(u', v')$ be arcs of a constituent digraph $C$ of $\text{WL}_2(G)$. Note that the vertices $u$ and $u'$ must be equally colored in $\text{WL}_2(G)$. Indeed, since the color partition of $\text{WL}_2(G)$ is stable, there must exist $w$ such that $(\text{WL}_2(u', w), \text{WL}_2(w, v')) = (\text{WL}_2(u, w), \text{WL}_2(u, v))$. The equality $\text{WL}_2(u', w) = \text{WL}_2(u, w)$ can be fulfilled only by $w = u'$ because any non-loop $(u', w)$ is initially colored differently from the loop $(u, u)$ and, hence, they are colored differently after all refinements.

Note also that, if $u$ and $v$ are equally colored in $\text{WL}_2(G)$, then they have the same outdegree in every constituent digraph $C$; in particular, they simultaneously belong or do not belong to $V(C)$. Otherwise, contrary to the assumption that the color partition of $\text{WL}_2(G)$ is stable, the loops $(u, u)$ and $(v, v)$ would receive different colors in another refinement round of 2-WL. It follows that for each constituent digraph $C$ there is a number $d \geq 1$ such that all vertices in $C$ either have outdegree $d$ or 0. We call $d$ the outdegree of $C$.

Let $u \in V(G)$. A vertex-individualized graph $G_u$ is obtained from $G$ by assigning the vertex $u$ a special color, which does not occur in $G$. If $G$ is vertex-transitive, then all vertex-individualized copies of $G$ are obviously isomorphic.

Consider now a simple and still instructive example. Let $G = \overline{C}_7$ be the complement of the cycle graph on seven vertices 0, 1, \ldots, 6 passed in this order. It is not hard to see that 2-WL splits $V(G)^2$ into the four 2-orbits of $\text{Aut}(G)$; the diagonal is one of them. Note that the three constituent digraphs of $\text{WL}_2(G)$ are of the same degree 2; see Figure 1. Applying 2-WL to the vertex-individualized graph $G_0$, it can easily be seen that 2-WL again splits $V(G)^2$ into the 2-orbits of $\text{Aut}(G_0)$. Note that $\text{WL}_2(G_0)$ also has exactly three constituent digraphs of outdegree 2, while all other constituent digraphs of $\text{WL}_2(G_0)$ have outdegree 1. We see that the outdegrees of
Figure 1: The output of 2-WL on input $\overline{C_7}$ and on its vertex-individualized copy.

the constituent digraphs for $G$ and its vertex-individualized copies are distributed similarly. This similarity proves to be a characterizing property of vertex-transitive graphs on a prime number of vertices.

**Theorem 3.1.** Let $p$ be a prime, and $G$ be a graph with $p$ vertices. Suppose that $G$ is neither complete nor empty. Then $G$ is vertex-transitive if and only if the following conditions are true:

1. If run on $G$, 2-WL does not split the diagonal, that is, all vertices in $WL_2(G)$ are equally colored.
2. All constituent digraphs of $WL_2(G)$ have the same outdegree $d$ and, hence, there are $\frac{p^2-1}{d}$ constituent digraphs.
3. For every $u \in V(G)$, exactly $\frac{p^2-1}{d}$ constituent digraphs in $WL_2(G_u)$ have outdegree $d$, and all other have outdegree 1.

Since the color partition of $WL_2(G)$ for a $p$-vertex graph $G$ can be computed in time $O(p^3 \log p)$ [30], Conditions [1][3] can be verified in time $O(p^4 \log p)$, which yields an algorithm of this time complexity for recognition of vertex-transitivity of graphs with a prime number of vertices.

As it will be discussed in Remark 3.6 below, there are graphs $G$ and $H$ with a prime number of vertices such that $G$ is vertex-transitive, $H$ is not, and still they are indistinguishable by 2-WL. This implies that Theorem 3.1 is optimal in that it uses as small WL dimension as possible and, also, that the condition involving the vertex individualization cannot be dropped. Note that 1-WL, which stands for the classical degree refinement, does not suffice even when run on $G$ and all $G_u$ because the output of 1-WL on these inputs is subsumed by the output of 2-WL on $G$ alone.

### 3.1 Coherent configurations

A detailed treatment of the material presented below can be found in [14]. The stable partition $S = S^t$ of $V(G)^2$ produced by 2-WL on an input graph $G$ has certain regularity properties, which are equivalent to saying that the pair $(V, S)$
forms a coherent configuration, the concept introduced by Higman [27], which we define now.

A coherent configuration \( \mathcal{X} = (V, \mathcal{S}) \) is formed by a set \( V \), whose elements are called points, and a partition \( \mathcal{S} = \{ S_1, \ldots, S_m \} \) of the Cartesian square \( V^2 \), that is, \( \bigcup_{i=1}^{m} S_i = V^2 \) and any two \( S_i \) and \( S_j \) are disjoint. An element \( S_i \) of \( \mathcal{S} \) is referred to as a basis relation of \( \mathcal{X} \). The partition \( \mathcal{S} \) has to satisfy the following three conditions:

(A) If a basis relation \( S_i \in \mathcal{S} \) contains a loop \((u, u)\), then all pairs in \( S_i \) are loops.

(B) For every \( S_i \in \mathcal{S} \), the transpose relation \( S_i^* = \{(v, u) : (u, v) \in S_i\} \) is also in \( \mathcal{S} \).

(C) For each triple \( R, S, T \in \mathcal{S} \), the number \( p(u, v) = |\{w : (u, w) \in R, (w, v) \in S\}| \) for a pair \((u, v) \in T\) does not depend on the choice of this pair in \( T \).

In other words, if \( \mathcal{S} \) is seen as a color partition of \( V^2 \), then such a coloring is stable under 2-WL refinement.

We describe two important sources of coherent configurations. Let \( \mathcal{T} \) be an arbitrary family of subsets of the Cartesian square \( V^2 \). There exists a unique coarsest partition \( S \) of \( V^2 \) such that every \( T \in \mathcal{T} \) is a union of elements of \( S \) and \( \mathcal{X} = (V, S) \) is a coherent configuration; see [14, Section 2.6.1]. We call \( \mathcal{X} = (V, S) \) the coherent closure of \( \mathcal{T} \) and denote it by \( Cl(\mathcal{T}) \).

Given a vertex-colored undirected graph \( G \) on the vertex set \( V \), let \( \mathcal{T} \) consist of the set of the pairs \((u, v) \in V^2 \) such that \( \{u, v\} \) is an edge of \( G \) and the sets of loops \((u, u)\) for all vertices \( u \) of the same color in \( G \). Then \( Cl(\mathcal{T}) \) is exactly the stable partition produced by 2-WL on input \( G \). We denote this coherent configuration by \( Cl(G) \).

Given a coherent configuration \( \mathcal{X} = (V, S) \) and a point \( u \in V \), the coherent configuration \( \mathcal{X}_u = Cl(S \cup \{(u, u)\}) \) is called a one-point extension of \( \mathcal{X} \). This concept is naturally related to the notion of a vertex-individualized graph, in that

\[
Cl(G_u) = Cl(G)_u. \tag{3}
\]

Another source of coherent configurations is as follows. Let \( K \) be a permutation group on a set \( V \). Denote the set of 2-orbits of \( K \) by \( S \). Then \( \mathcal{X} = (V, S) \) is a coherent configuration, which we denote by \( \text{Inv}(K) \). Coherent configurations obtained in this way are said to be schurian.

We define an automorphism of a coherent configuration \( \mathcal{X} = (V, S) \) as a bijection \( \alpha \) from \( V \) onto itself such that, for every \( S \in \mathcal{S} \) and every \((u, v) \in S \), the pair \((\alpha(u), \alpha(v))\) also belongs to \( S \). The group of all automorphisms of \( \mathcal{X} \) is denoted by \( \text{Aut}(\mathcal{X}) \). A coherent configuration \( \mathcal{X} \) is schurian if and only if

\[
\mathcal{X} = \text{Inv}(\text{Aut}(\mathcal{X})). \tag{4}
\]

Note also that the connection between the coherent closure of a graph and 2-WL implies that

\[
\text{Aut}(Cl(G)) = \text{Aut}(G). \tag{5}
\]
A set of points \(X \subseteq V\) is called a fiber of \(\mathcal{X}\) if the set of loops \(\{(x, x) : x \in X\}\) is a basis relation of \(\mathcal{X}\). Denote the set of all fibers of \(\mathcal{X}\) by \(F(\mathcal{X})\). By Property A, \(F(\mathcal{X})\) is a partition of \(V\). Property C implies that for every basis relation \(S\) of \(\mathcal{X}\) there are, not necessarily distinct, fibers \(X\) and \(Y\) such that \(S \subseteq X \times Y\). We use the notation \(N_S(x) = \{y : (x, y) \in S\}\) for the set of all points in \(Y\) that are in relation \(S\) with \(x\). Note that \(|N_S(x)| = |N_S(x')|\) for any \(x, x' \in X\). We call this number the valency of \(S\). If every basis relation \(S\) of \(\mathcal{X}\) has valency 1, then \(\mathcal{X}\) is called semiregular.

**Proposition 3.2** (see [13 Exercise 2.7.35]). A semiregular coherent configuration is schurian.

Given a set of points \(U \subseteq V\) that is a union of fibers, let \(\mathcal{S}_U\) denote the set of all basis relations \(S \in \mathcal{S}\) such that \(S \subseteq X \times Y\) for some, not necessarily distinct, fibers \(X \subseteq U\) and \(Y \subseteq U\). As easily seen, \(\mathcal{X}_U = (U, \mathcal{S}_U)\) is a coherent configuration.

If a coherent configuration has a single fiber, it is called association scheme.

### 3.2 Proof of Theorem 3.1

**Necessity.** Given a vertex-transitive graph \(G\) with \(p\) vertices, where \(p\) is prime, we have to check Conditions 1-3. Condition 1 follows immediately from vertex-transitivity; see the discussion in the end of Section 2. For Condition 2, we use two basic results on vertex-transitive graphs with a prime number of vertices. First, every such graph is isomorphic to a circulant graph, i.e., a Cayley graph of a cyclic group, because every transitive group of permutations of a set of prime cardinality \(p\) contains a \(p\)-cycle (Turner [39]). Let \(\mathbb{F}_p\) denote the \(p\)-element field, \(\mathbb{F}_p^+\) its additive group, i.e., the cyclic group of order \(p\), and \(\mathbb{F}_p^\times\) its multiplicative group, which is isomorphic to the cyclic group of order \(p - 1\). Another useful fact (Alspach [1]) is that, if a set \(Z \subset \mathbb{F}_p\) is non-empty and \(Z \neq \mathbb{F}_p^\times\), then the automorphism group of the circulant graph \(\text{Cay}(\mathbb{F}_p^+, Z)\) consists of the maps

\[
x \mapsto ax + b, \quad x \in \mathbb{F}_p, \quad \text{for all } a \in M, \ b \in \mathbb{F}_p^+,
\]

where \(M = M(Z)\) is the largest subgroup of \(\mathbb{F}_p^\times\) of even order such that \(Z\) is a union of cosets of \(M\). This subgroup is well defined because the condition \(Z = -Z\) implies that \(Z\) is split into pairs \(\{z, -z\}\) and, hence, is a union of cosets of the multiplicative subgroup \(\{1, -1\}\). For example, \(\text{Cay}(\mathbb{F}_7^+, \{2, 3, 4, 5\})\) and \(M(\{2, 3, 4, 5\}) = \{1, -1\}\). Without loss of generality we assume that \(G = \text{Cay}(\mathbb{F}_p^+, Z)\) and denote \(K = \text{Aut}(G)\).

Let \(\mathcal{X} = (\mathbb{F}_p^+, \mathcal{S})\) be the coherent closure of \(G\). Recall that \(\mathcal{S}\) is exactly the stable partition of \(V(G)^2\) produced by 2-WL on input \(G\). The irreflexive basis relations of \(\mathcal{X}\) are exactly the constituent digraphs of \(\text{WL}_2(G)\), and we have to prove that all of them have the same valency.

Condition 1 says that \(\mathcal{X}\) is an association scheme. In general, not all association schemes with a prime number of points are schurian (see, e.g., [14, Section 4.5]). Nevertheless, the theorem by Leung and Man on the structure of Schur rings over cyclic groups implies the following fact.
Proposition 3.3 (see [14, Theorem 4.5.1]). Let $X = (V, S)$ be an association scheme with a prime number of points. If $\text{Aut}(X)$ acts transitively on $V$, then $X$ is schurian.

By Equality (5), $\text{Aut}(X) = K$. Since the group $K$ is transitive, Proposition 3.3 implies that $X$ is schurian, and we have $X = \text{Inv}(K)$ by Equality (1). This yields Condition 2 for $d = |M|$. Indeed, every irreflexive basis relation $S \in S$ has valency $|M|$. To see this, it is enough to count the number of pairs $(0, y)$ in $S$. Fix an arbitrary pair $(0, y) \in S$. A pair $(0, y')$ is in the 2-orbit containing $(0, y)$ if and only if $y' = ay$ for $a \in M$, for which we have $|M|$ possibilities.

It remains to prove Condition 3. By vertex-transitivity, all vertex-individualized copies of $G$ are isomorphic and, therefore, it is enough to consider $G_0$. We have to count the frequencies of valencies in $X_0$. Note that $X_0 = \text{Cl}(G_0)$ by Equality (3).

It is generally not true that a one-point extension of a schurian coherent configuration is schurian; see [14, Section 3.3.1]. Luckily, this is the case in our setting. The proof of the following statement is rather involved.

Proposition 3.4 (see [14, Theorem 4.4.14]). If $X = \text{Inv}(K)$, where $K$ is the group of permutations of the form (6) for a subgroup $M$ of $\mathbb{F}_p^\times$, then the one-point extension $X_0$ is schurian.

Taking into account Equality (5), we have

$$\text{Aut}(X_0) = \text{Aut}(\text{Cl}(G_0)) = \text{Aut}(G_0) = \text{Aut}(G)_0 = K_0,$$

where $K_0$ is the one-point stabilizer of 0 in $K$, that is, the subgroup of $K$ consisting of all permutations $\alpha \in K$ such that $\alpha(0) = 0$. Obviously, $K_0 = \{ x \mapsto ax, x \in \mathbb{F}_p \}_{a \in M}$.

Let $S$ be a 2-orbit of $K_0$. If $S$ contains a pair $(0, y)$, then it consists of all pairs $(0, y')$ for $y' \in My$ and, hence, has valency $|M|$. If $S$ contains a pair $(z, y)$ with $z \neq 0$ and $y \neq z$, then $(z, y)$ is the only element of $S$ with the first coordinate $z$, and $S$ has valency 1. The proof of Condition 3 is complete.

Sufficiency. Let $G$ be a graph satisfying Conditions 1–3 stated in the theorem. Let $X = \text{Cl}(G)$. Condition 1 says that $X$ is an association scheme. By Equality (5), it suffices to prove that the group $\text{Aut}(X)$ is transitive. The proof is based on the following lemma. Though a stronger fact is established in [32, Theorem 7.1], we here include a proof of the lemma for the reader’s convenience. We closely follow [32] but provide a bit more details for non-experts in algebraic graph theory.

Lemma 3.5. Let $X = (V, S)$ be an association scheme. Suppose that the following two conditions are true for every point $u \in V$:

(I) the coherent configuration $(X_u)_{V \setminus \{u\}}$ is semiregular, and

(II) $F(X_u) = \{ N_S(u) : S \in S \}$.

Then the group $\text{Aut}(X)$ acts transitively on $V$. 

Proof. Let \( u \in V \). By Condition \([1]\) and Proposition \([3.2]\), the coherent configuration \( \mathcal{X}' = (\mathcal{X}_u)_{V \setminus \{u\}} \) is schurian. We claim that the coherent configuration \( \mathcal{X}_u = (V, S_u) \) is schurian also. Let \( K' = \text{Aut}(\mathcal{X}') \) and define \( K \) to be a permutation group on \( V \) that, for each \( \alpha' \in K' \), contains the permutation \( \alpha \) which fixes \( u \) and coincides with \( \alpha' \) on \( V \setminus \{u\} \). Consider a basis relation \( S \in S_u \). If \( S \) is a basis relation of \( \mathcal{X}' \), then it is a 2-orbit of \( K' \) and, hence, of \( K \). If \( S \) is not a basis relation of \( \mathcal{X}' \), then \( S = \{u\} \times X \) for some fiber \( X \in F(\mathcal{X}') \). Since \( X \) is an orbit of \( K' \) and, hence, of \( K \), \( S \) is a 2-orbit of \( K \) also in this case. Thus, \( \mathcal{X}_u = \text{Inv}(K) \).

Let \( A = \text{Aut}(\mathcal{X}) \). Since \( \text{Aut}(\mathcal{X}_u) = \text{Aut}(\mathcal{X})_u = A_u \) (where \( A_u \) denotes the one-point stabilizer of \( u \) in \( A \)) and \( \mathcal{X}_u \) is schurian, \( \mathcal{X}_u = \text{Inv}(A_u) \). Condition \([1]\) implies that, for every \( S \in \mathcal{S} \), \( N_S(u) \) is an orbit of \( A_u \).

Denote the orbit of \( A_u \) containing a point \( x \) by \( A_u(x) \). We claim that \( |A_u(x)| = |A_u| \) for every point \( x \neq u \). Indeed, if \( \alpha(x) = \beta(x) \) for two different permutations in \( A_u \), then the stabilizer \( (A_u)_x \) contains a non-identity permutation, namely \( \alpha^{-1} \beta \). Therefore, the 2-orbit of \( A_u \) containing a pair \((x, y)\) with \( y \notin \{u, x\} \) contains also the pair \((x, \alpha^{-1} \beta(y))\). Choosing \( y \) to be a point moved by \( \alpha^{-1} \beta \), we get a contradiction with Condition \([1]\).

We conclude that \( |N_S(u)| = |A_u| \) for every irreflexive \( S \in \mathcal{S} \). The right hand side of this equality does not depend on \( S \). The left hand side does not depend on \( u \) because \( \mathcal{X} \) is an association scheme. It follows that there exists a number \( k \) such that \( |A_u| = k \) for all \( u \in V \).

Let \( Q \) be an orbit of \( A \). Since \( A_u \) is a subgroup of \( A, Q \) is a union of orbits of \( A_u \). Choosing a point \( u \) in \( Q \), we conclude that \( |Q| \equiv 1 \pmod{k} \). If there was a point \( u' \notin Q \), the same argument would yield \( |Q| \equiv 0 \pmod{k} \). Therefore, such \( u' \) does not exist, and \( Q = V \), as desired. \( \square \)

Let \( u \) be an arbitrary vertex \( u \) of \( G \). By Equality \([3]\), \( \mathcal{X}_u = Cl(G_u) \). All what we now need is to derive Conditions \([1][3]\) in the lemma from Conditions \([1][3]\) in the theorem.

For a fiber \( X \in F(\mathcal{X}_u) \), note that \( \{u\} \times X \) must be a basis relation of \( \mathcal{X}_u \). Since this relation has valency \(|X|\), Condition \([3]\) implies that every fiber in \( F(\mathcal{X}_u) \) is either singleton or consists of \( d \geq 2 \) points. Denote the number of singletons in \( F(\mathcal{X}_u) \) by \( a \). Besides of them, \( F(\mathcal{X}_u) \) contains \((p-a)/d\) fibers of size \( d \).

For every \( X, Y \in F(\mathcal{X}_u) \) with \(|X| = 1 \text{ and } |Y| = d \), \( X \times Y \) is a basis relation of \( \mathcal{X}_u \) of valency \( d \). It follows from Condition \([3]\) that

\[
\frac{p - 1}{d} \geq \frac{a(p-a)}{d}.
\]

Therefore, \( p - 1 \geq a(p-a) \) or, equivalently, \( p(a-1) \leq (a-1)(a+1) \). Assume for a while that \( a > 1 \). It immediately follows that \( a \geq p - 1 \). Since the equality \( a = p - 1 \) is impossible, we conclude that \( a = p \). However, this implies that \( d = 1 \), a contradiction. Thus, \( a = 1 \). Consequently, every fiber of the coherent configuration \( \mathcal{X}' = (\mathcal{X}_u)_{V \setminus \{u\}} \) is of cardinality \( d \), and \(|F(\mathcal{X}')| = (p-1)/d\).

Let \( S \) be a basis relation of \( \mathcal{X} \). If \( S \) is reflexive, then \( N_S(u) = \{u\} \). If \( S \) is irreflexive, then \( N_S(u) \) must be a union of fibers in \( F(\mathcal{X}') \). By Condition \([2]\) the
number of irreflexive basis relations in $S$ is $(p-1)/d$. It follows that $N_S(u)$ actually coincides with one of the fibers of $\mathcal{X}'$. This proves Condition [11].

Since $\mathcal{X}_u$ contains $(p-1)/d$ basis relations of the kind $\{u\} \times X$ for $X \in F(\mathcal{X}')$, Condition [3] implies that every basis relation of $\mathcal{X}'$ is of valency 1, yielding Condition [11].

The proof of Theorem [3.1] is complete.

Remark 3.6. We now argue that there is a vertex transitive graph $G$ and a non-vertex-transitive graph $H$ such that $G$ and $H$ are indistinguishable by 2-WL. Recall that a strongly regular graph with parameters $(n, d, \lambda, \mu)$ is an $n$-vertex $d$-regular graph where every two adjacent vertices have $\lambda$ common neighbors, and every two non-adjacent vertices have $\mu$ common neighbors. As easily seen, two strongly regular graphs with the same parameters are indistinguishable by 2-WL, and our example will be given by $G$ and $H$ of this kind. Let $p$ be a prime (or a prime power) such that $p \equiv 1 \pmod{4}$. The Paley graph on $p$ vertices is the Cayley graph $\text{Cay}(\mathbb{F}_p^+, Y_p)$ where $Y_p$ is the subgroup of $\mathbb{F}_p^*$ formed by all quadratic residues modulo $p$. The assumption $p \equiv 1 \pmod{4}$ ensures that $-1$ is a quadratic residue modulo $p$ and, hence, $Y_p = -Y_p$. The Paley graph on $p$ vertices is strongly regular with parameters $(p, \frac{p-1}{2}, \frac{p-5}{4}, \frac{p-1}{4})$.

Let $G$ be the Paley graph on 29 vertices. It is known (Bussemaker and Spence; see, e.g., [10] Section 9.9]) that there are 40 other strongly regular graphs with parameters $(29, 14, 6, 7)$. Let $H$ be one of them. We have only to show that $H$ is not vertex-transitive. Otherwise, by [39] this would be a circulant graph, that is, we would have $H = \text{Cay}(\mathbb{F}_p^+, Z)$ for some connection set $Z$. In this case, the coherent closure $\mathcal{C}(H)$ must be schurian by Proposition [3.3]. Since $H$ is strongly regular, 2-WL colors all pairs of adjacent vertices uniformly and, therefore, they form a 2-orbit of $\text{Aut}(H)$. It follows that the stabilizer $\text{Aut}(H)_0$ acts transitively on $N(0)$, the neighborhood of 0 in $H$. The aforementioned result of Alspach, implies that $Z$ is the subgroup of $\mathbb{F}_p^*$ of order $(p-1)/2$ i.e., $M = Z$ in (6). This means that $Z = Y_p$ and $H = G$, a contradiction.

4 A lower bound for the WL dimension

We now prove a negative result on the recognizability of vertex-transitivity by $k$-WL. We begin with a formal definition of the $k$-dimensional algorithm. Let $k \geq 2$. Given a graph $G$ with vertex set $V$ as input, $k$-WL operates on $V^k$. The initial coloring of $\bar{u} = (u_1, \ldots, u_k)$ encodes the equality type of this $k$-tuple and the ordered isomorphism type of the subgraph of $G$ induced by the vertices $u_1, \ldots, u_k$. The color refinement is performed similarly to [11]. Specifically, $k$-WL iteratively colors $V^k$ by $WL_{k}^{t+1}(\bar{u}) = \{ (WL_{k}^{t}(\bar{u}_{i,w}^{w})), \ldots, WL_{k}^{t}(\bar{u}_{i,w}^{w}) ) : w \in V(G) \}$, where $\bar{u}_{i,w}^{w} = (u_1, \ldots, u_{i-1}, w, u_{i+1}, \ldots, u_k)$. If $G$ has $n$ vertices, the color partition stabilizes in $t \leq n^k$ rounds, and $k$-WL outputs the coloring $WL_{k}^{t}(\cdot) = WL_{k}^{\infty}(\cdot)$.

We say that $k$-WL distinguishes graphs $G$ and $H$ if the final color palettes are different for $G$ and $H$, that is, $\{ WL_{k}(\bar{u}) : \bar{u} \in V(G)^k \} \neq \{ WL_{k}(\bar{u}) : \bar{u} \in V(H)^k \}$ (note that color renaming in each refinement round must be the same on $G$ and $H$).
Figure 2: The simplified CFI gadget

\textbf{Theorem 4.1.}

1. For every $n$ divisible by 16 there are $n$-vertex graphs $G$ and $H$ such that $G$ is vertex-transitive, $H$ is not, and $G$ and $H$ are indistinguishable by $k$-WL as long as $k \leq 0.01 \sqrt{n}$.

2. Let $n = 8p(p - 1)(p + 1)$ where $p$ is a prime and $p - 1$ is divisible by 104. Then there are $n$-vertex graphs $G$ and $H$ such that $G$ is vertex-transitive, $H$ is not, and $G$ and $H$ are indistinguishable by $k$-WL as long as $k \leq 0.001n$.

The proof, which takes the rest of this section, is based on the Cai-Fürer-Immerman construction \cite{11}. As discussed in Section \cite{1} in place of the standard CFI gadget, we use its simplified version shown in Figure 2

Given a connected 3-regular graph $F$ on $m$ vertices, we construct a 6-regular graph $A$ with $4m$ 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 $F$ 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 $F$, 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 $F$, 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 $v \in V(F)$ with neighborhood $N(v) = \{a, b, c\}$ we fix an assignment of matchings $M_{v,a}$, $M_{v,b}$, and $M_{v,c}$ and then, for each edge $vu \in E(F)$, 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 $vu \in E(F)$, 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. Since the template graph $F$ is connected, $A$ is connected too. For a set $S \subseteq E(F)$, 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 Lemma 6.2.

**Lemma 4.2.** $A \cong A^S$ 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 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 $M = \{\{x_1x_2\}, \{x_3x_4\}\}$ 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 $ww$. Let $\phi_{vuw}$ be the permutation in $K(Q(u))$ which flips each of the matchings $M_{u,v}$ and $M_{u,w}$. We extend $\phi_{vuw}$ to the whole vertex set of $A$ by identity. 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 $vv'$ and $ww'$, consider a shortest path connecting these edges, say, $vu_1 \ldots u_kw$. The permutation

$$\phi_{vu_1 \ldots u_kw} \phi_{vu_1u_2u_3} \phi_{u_1u_2u_3} \cdots \phi_{u_{k-1}u_kw} \phi_{u_kw} \phi_{vu_1u_2u_3} \phi_{vu_1u_2u_3} \phi_{u_1u_2u_3} \cdots \phi_{u_{k-1}u_kw} \phi_{u_kw} \phi_{vu_1u_2u_3} \phi_{vu_1u_2u_3} \phi_{u_1u_2u_3} \cdots \phi_{u_{k-1}u_kw} \phi_{u_kw}$$

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 $A[Q(v), Q(u_1)], A[Q(u_1), Q(u_2)]$ 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 $A^S = (A^{S'})^{\{e_1, e_2\}}$. We have $A^S \cong A^{S'}$ as in the base case and $A^{S'} \cong A$ by the induction assumption. \qed

Let $B = A^{(e)}$ for an edge $e$ of $F$. It follows from Lemma 4.2 that the isomorphism type of $B$ does not depend on the choice of $e$. Lemma 4.2 also implies that $A$ and $B$ are not isomorphic.
Given \( X \subset V(F) \), let \( F \setminus X \) denote the graph obtained from \( F \) by removal of all vertices in \( X \). We call a set \( X \) a separator of \( F \) if every connected component of the graph \( F \setminus X \) has at most \( v(F)/2 \) vertices. The number of vertices in a separator is called its size. We denote the minimum size of a separator of \( F \) by \( s(F) \). The following fact is a version of [11, Theorem 6.4], with virtually the same proof.

**Lemma 4.3.** \( A \) and \( B \) are indistinguishable by k-WL for all \( k < s(F) \).

We will need also the following property of the construction.

**Lemma 4.4.** If \( F \) 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 \( F \), 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 \( F \) 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 \( x \in V(F) \).
- \( \psi \) transforms the matching \( M_{x,y} \) into the matching \( M_{f(x),f(y)} \) for every \( xy \in E(F) \).

Denote the image of \( A \) under \( \psi \) by \( A^\psi \). Note that, for every \( xy \in E(F) \), 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 4.2. 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 \( F \) mapping each \( Q(x) \) onto \( Q(f(x)) \), in particular, \( Q(v) \) onto \( Q(u) \). \( \Box \)

**Claim B.** For every \( u \in V(F) \) 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 4.2. 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 \( F \) that the path \( vwv \) extends to a cycle \( vwv \times 1 \ldots x_3 \).

The permutation

\[
\phi_{vwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv} \phi_{uwv}
\]

is an automorphism of \( A \) and transposes \( u_1 \) and \( u_2 \). \( \Box \)

Combining Claims A and B we obtain the lemma. \( \Box \)

We now define a graph \( G \) as the vertex-disjoint union of two copies of \( A \), and \( H \) as the vertex-disjoint union of \( A \) and \( B \). Since \( A \) is vertex-transitive, \( G \) is vertex-transitive as well. On the other hand, \( H \) is not vertex-transitive because \( A \) and \( B \) are connected and non-isomorphic.
The graphs $A$ and $B$ are indistinguishable by $k$-WL for all $k < s(F)$ by Lemma 4.3 and two copies of the graph $A$ are indistinguishable by $k$-WL for every $k$ just because they are isomorphic. It follows that $G$ and $H$ are indistinguishable by $k$-WL for all $k < s(F)$. This implication can be directly seen from the game characterization of the $k$-WL-equivalence relation in [11]. To complete the proof of Theorem 4.1, we therefore need a family of connected 3-regular vertex-transitive graphs $F$ with sufficiently large value of the parameter $s(F)$.

The vertex expansion of a graph $F$ is defined as 

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

where $S \subset V(F)$ and $\partial_{\text{out}}(S)$ denotes the set of vertices of $F$ outside $S$ with at least one neighbor in $S$. We use the estimate 

$$s(F) \geq \frac{h_{\text{out}}(F)}{3 + h_{\text{out}}(F)} v(F)$$

(see Lemma 7.10 in the preliminary version of [36]). Babai [4] estimated the vertex expansion of a connected vertex-transitive graph $F$ from below in terms of the diameter of $F$, which we denote by diam($F$). Specifically,

$$h_{\text{out}}(F) \geq \frac{1}{2 \text{diam}(F)}.$$ 

By (7), this yields

$$s(F) \geq \frac{v(F)}{6 \text{diam}(F) + 1}. \quad (8)$$

To obtain Part 1 of the theorem, consider $F = \text{Cay}(D_{2q}, \{a, ab, ab^r\})$ for positive integer parameters $q$ and $r$. Here $D_{2q}$ is the dihedral group with generators $a$ and $b$, where $a$ corresponds to a reflection and $b$ corresponds to a rotation in $2\pi/q$. Note that, like $a$, the elements $ab$ and $ab^r$ correspond to reflections and, hence, are involutory. Being a Cayley graph, $F$ is vertex-transitive. The following simple fact will be needed also in Section 5.

**Lemma 4.5.** The diameter of $\text{Cay}(D_{2q}, \{a, ab, ab^r\})$ does not exceed $\frac{2q}{r} + r + 1$.

**Proof.** The diameter of a Cayley graph $\text{Cay}(\Gamma, Z)$ is equal to the minimum $d$ such that every element of $\Gamma$ is representable as a product of at most $d$ elements in $Z$. Every element $b^s r$ of $D_{2q}$, where $-\lfloor q/r \rfloor \leq s \leq \lfloor q/r \rfloor$ can be represented as a product of at most $2\lfloor q/r \rfloor$ elements $a$ and $ab^r$, just because $b^s r = (aab^r)^s$. To obtain an arbitrary element $b^i$ from the nearest $b^s r$, it is enough to make at most $2\lceil (r-1)/2 \rceil$ extra multiplications by $a$ and $ab$. An element $ab^i$ is obtainable similarly to $b^{-i}$, with one multiplication by $a$ omitted. \qed

Setting $r = \lfloor \sqrt{2q} \rfloor$, we obtain a 3-regular vertex-transitive graph $F$ on $2q$ vertices of diameter less than $2\sqrt{2q} + 2$. The graph $F$ results in $G$ and $H$ with $n = 16q$ vertices. By (8), $s(F) > q/(6\sqrt{2q} + 7) > 0.01\sqrt{n}$, implying Part 1.
For Part 2 we need 3-regular vertex-transitive graphs with \( s(F) = \Omega(v(F)) \). A family of such graphs has been found by Chiu [16]. Every graph \( F \) in this family is a Cayley graph of the projective general linear group \( \text{PGL}(2, \mathbb{F}_p) \) for a prime \( p \) such that such that \( -2 \) and \( 13 \) are quadratic residues modulo \( p \); any prime \( p \) such that \( p \equiv 1 \pmod{104} \) is suitable. Moreover, every \( F \) is a Ramanujan graph. In general, a \( d \)-regular graph \( F \) is a Ramanujan graph if its second eigenvalue \( \lambda_2(F) \) is smaller than or equal to \( 2\sqrt{d-1} \). In our case \( d = 3 \) and \( \lambda_2(F) \leq 2\sqrt{2} \).

The edge expansion of \( F \) is defined as
\[
h(F) = \min_{0 < |S| \leq v(F)/2} \frac{|\partial S|}{|S|},
\]
where \( S \subset V(F) \) and \( \partial S \) denotes the set of edges of \( F \) between one vertex in \( S \) and another vertex outside. It is known [28, Theorem 2.4] that
\[
h(F) \geq \frac{d - \lambda_2(F)}{2}
\]
for a \( d \)-regular \( F \). For \( F \) constructed in [16] we, therefore, have \( h(F) \geq \frac{3 - 2\sqrt{2}}{2} \).

As easily seen, \( h_{\text{out}}(F) \geq h(F)/d \) for \( d \)-regular graphs, which yields \( h_{\text{out}}(F) \geq \frac{3 - 2\sqrt{2}}{6} \). Bound (7) implies in this case that \( s(F) > 0.008v(F) = 0.001n \), as desired. The proof of Theorem 4.1 is complete.

5 Arc-transitivity

We begin with a positive result. Equality (2) implies that, if \( G \) is arc-transitive, then the color \( \text{WL}_2(u, v) \) is the same whenever \( u \) and \( v \) are adjacent. If this condition is fulfilled, we say that 2-WL does not split the adjacency relation. The following result reduces recognition of arc-transitivity of graphs with a prime number of vertices to verification that Conditions 1–3 listed in Theorem 3.1 are met and the adjacency relation is not split.

**Theorem 5.1.** A vertex-transitive graph \( G \) with a prime number of vertices is arc-transitive if and only if 2-WL does not split the adjacency relation of \( G \).

**Proof.** The necessity part is clear. To prove the sufficiency, assume that a vertex-transitive graph \( G \) with prime number of vertices is not arc-transitive. This means that the adjacency relation of \( G \) consists of two or more 2-orbits of the automorphism group \( \text{Aut}(G) \). By Proposition 3.3 the coherent closure \( \text{Cl}(G) \) is schurian. In other words, 2-WL splits the Cartesian square \( V(G)^2 \) into 2-orbits of \( \text{Aut}(\text{Cl}(G)) = \text{Aut}(G) \) and, therefore, it splits the adjacency relation of \( G \). \( \square \)

The method following from Theorem 5.1, like any other method based on \( k \)-WL with a fixed dimension \( k \), cannot be extended to detecting arc-transitivity on all input graphs. We show this by elaborating on the approach presented in Section 4.

**Theorem 5.2.** For every \( k \) there exists a pair of graphs \( G \) and \( H \) indistinguishable by \( k \)-WL such that \( G \) is arc-transitive and \( H \) is not.
Lemma 5.3. If $F$ 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 $F$, there is an automorphism of $A$ mapping $Q(v)$ onto $Q(v')$ and $Q(u)$ onto $Q(u')$.

Claim $C$ reduces proving that $A$ is arc-transitive to proving the following fact.

Claim D. Let $uv \in E(F)$. For every two pairs of adjacent vertices $u_iv_j$ and $u_sv_t$ 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 $F$ 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 $F$ 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 $F$, we conclude that for every edge $xy$ of $F$ 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. $\Box$

The proof of the lemma is complete. $\square$

Like in the proof of Theorem 4.1, let $G$ be the vertex-disjoint union of two copies of $A$, and $H$ be the vertex-disjoint union of $A$ and $B$. Since these are connected non-isomorphic graphs, $H$ is not arc-transitive (in fact, even not vertex-transitive). The graph $G$ is obviously arc-transitive. Recall that $G$ and $H$ are indistinguishable by $k$-WL for all $k < s(F)$. To obtain Theorem 5.2, we therefore need connected arc-transitive 3-regular graphs with arbitrarily large minimum separator size.

Cheng and Oxley [15] 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 $F_p$. It is known (e.g., [21]) that $F_p$ is isomorphic to a Cayley graph of the dihedral group $D_{2p}$. In fact, we can set $F_p = Cay(D_{2p}, \{ab, ab^r, ab^{r^2}\})$, where $r \neq 1$ is a cube root of unity in the multiplicative group $\mathbb{F}_p^\times$. In order to show that this graph is arc-transitive, it suffices to check that $\text{Aut}(F_p)$ acts transitively on the neighborhood of the identity element $e$ of $D_{2p}$ in $F_p$, that is, on the set $N(e) = \{ab, ab^r, ab^{r^2}\}$. Define a map $\alpha_s : D_{2p} \to D_{2p}$ by $\alpha_s(b^r) = b^{sr}$.
and \( \alpha_s(ab^i) = ab^{si} \). If \( s \) is coprime to \( p \), then \( \alpha_s \) is an automorphism of \( D_{2p} \) and, therefore, it is an automorphism of \( F_p \). It remains to note that \( \{\alpha_1, \alpha_r, \alpha_{r^2}\} \) is a subgroup of \( \text{Aut}(F_p) \) acting transitively on \( N(e) \).

We now estimate the diameter of \( F_p \).

**Lemma 5.4.** Let \( p \equiv 1 \pmod{3} \) be a prime and \( r \) be an integer such that \( 1 < r < p \) and \( r^3 \equiv 1 \pmod{p} \). Then

\[
\text{diam}(F_p) \leq \frac{2p}{r+1} + r + 2.
\]  

**Proof.** Define a map \( \beta_t : D_{2p} \to D_{2p} \) by \( \beta_t(b^i) = b^i \) and \( \alpha_s(ab^i) = ab^{i+t} \). This is an automorphism of \( D_{2p} \) for every \( t \). The composition \( \gamma = \beta_1 \circ \alpha_{r-1} \), where \( \alpha_s \) is as defined above, is an automorphism of \( D_{2p} \). Note that \( \gamma(a) = ab, \gamma(ab) = a^{br}, \) and \( \gamma(ab^{r+1}) = ab^{r^2} \). It follows that \( F_p \) is isomorphic to \( \text{Cay}(D_{2p}, \{a, ab, ab^{r+1}\}) \), and the desired bound follows from Lemma 4.5. \(
\)

According to Bound (8),

\[
\text{diam}(F_p) \leq \frac{2p}{r+1} + r + 2.
\]

We, therefore, have to show that there is an infinite sequence of primes \( p \) with \( p \equiv 1 \pmod{3} \) for which \( \text{diam}(F_p) = o(p) \). Let \( r = r(p) \) be as specified in Lemma 5.4. Obviously, \( r \geq \sqrt[3]{p} \) and, hence, \( \frac{2p}{r+1} \leq 2p^{2/3} \). We also need smallness of the second term in (9).

To this end, we use the following result by Tóth [38]. 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 \( \mathbb{F}_p \) 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 \( \epsilon > 0 \), there are infinitely many primes \( p \) with a cube root \( r \) of unity in \( \mathbb{F}_p \) such that \( 1 < r < \epsilon p \). This completes the proof of Theorem 5.2.

### 6 The Weisfeiler-Leman regularity hierarchy

The stabilized \( k \)-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 \( \text{WL}_k(x_1, \ldots, x_s) = \text{WL}_k(x_1, \ldots, x_s, \ldots, x_s) \) just by cloning the last vertex in the \( s \)-tuple \( k-s \) times.

**Definition 6.1.** Let \( s \leq k \). A graph \( G \) is called \( \text{WL}_{s,k} \)-regular if \( k \)-WL does not make any non-trivial splitting of \( V(G)^s \), that is, \( \text{WL}_k(\bar{x}) \neq \text{WL}_k(\bar{y}) \) exactly when \( \text{WL}_k(\bar{x}) \neq \text{WL}_k^0(\bar{y}) \) for every pair of \( s \)-tuples \( \bar{x}, \bar{y} \in V(G)^s \).
Note that a graph is $WL_{1,1}$-regular if and only if it is regular, and it is $WL_{2,2}$-regular if and only if it is strongly regular. The class of $WL_{1,2}$-regular graphs does not seem to have that clear characterization. This class obviously contains all vertex-transitive graphs. Moreover, it contains all constituent graphs of association schemes (i.e., symmetric closures of basis relations in association schemes). The last class, in turn, contains strongly regular and distance-regular graphs (in fact, every strongly regular graph with $\mu > 0$ is distance-regular). If two $WL_{1,2}$-regular graphs $G_1$ and $G_2$ are indistinguishable by 2-WL, then the disjoint union of $G_1$ and $G_2$ is also $WL_{1,2}$-regular. Furthermore, the class is closed under graph complementation. Note also that a graph $G$ is $WL_{1,2}$-regular if and only if the coherent closure of $G$ is an association scheme.

Denote the class of all $WL_{s,k}$-regular 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 [13] proved that every 5-ultrahomogeneous graph is $s$-ultrahomogeneous for all $s \geq 5$, i.e., $U(s) = U(5)$ for $s \geq 5$. All graphs in $U(5)$ were identified by Gardiner [24]. Those are $mK_n$ (the vertex-disjoint union of $m$ copies of the complete graph $K_n$), their complements $\overline{mK_n}$ (i.e., the regular multipartite graphs), the 5-cycle graph $C_5$, and the $3 \times 3$-rook’s graph (or, the same, the line graph $L(K_{3,3})$ of the complete bipartite graph $K_{3,3}$).

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 [13] (see also [12, Theorem 8.21]) and, independently, Gol’fand (see the historical comments in [3, 11]) 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

$$WL(s,k) = \{mK_n, \overline{mK_n}\}_{m,n} \cup \{C_5, L(K_{3,3})\} \text{ if } k \geq s \geq 5.$$
where \( VT = U(1) \) denotes the class of all vertex-transitive graphs. We say that the hierarchy (10) \textit{collapses at level} \( K \) if \( WL(1, k) = WL(1, K) \) for all \( k \geq K \). Theorem 4.1 has the following consequence.

\textbf{Corollary 6.2.} \textit{The hierarchy (10) does not collapse at any level.}

\textit{Proof.} Note that the equality \( VT = WL(1, K) \) would mean that vertex-transitivity were recognizable just by running \( K \)-WL on \( G \) and looking whether the resulting partition of \( V(G) \) is non-trivial. Theorem 4.1, therefore, implies that \( VT \neq WL(1, K) \) for any \( K \). Let \( G \) be a non-vertex-transitive graph in \( WL(1, K) \). Let \( k \) denote the number of vertices in \( G \). Since \( G \) obviously does not belong to \( WL(1, k) \), we conclude that \( WL(1, k) \) is a proper subclass of \( WL(1, K) \). \( \square \)

\section{Concluding discussion}

We have suggested a new, very simple combinatorial algorithm recognizing, in polynomial time, vertex-transitivity of graphs with a prime number of vertices. The algorithm consists, in substance, in running \( 2 \)-WL on an input graph and all its vertex-individualized copies.

One can consider another, conceptually even simpler approach. If an input graph \( G \) is vertex-transitive, then \( k \)-WL colors all diagonal \( k \)-tuples \((u, \ldots, u), u \in V(G)\), in the same color. Is this condition for a possibly large, but fixed \( k \) sufficient to claim vertex-transitivity? In general, a negative answer immediately follows from Theorem 4.1. Does there exist a fixed dimension \( k \) such that the answer is affirmative for graphs with a prime number of vertices? This is apparently a hard question; it seems that we cannot even exclude that \( k = 3 \) suffices.

Another interesting question is whether \( k \)-WL is able to efficiently recognize vertex-transitivity on \( n \)-vertex input graphs for \( n \) in a larger range than the set of primes. The lower bound of Theorem 4.1 excludes this only for \( n \) divisible by 16. It is known [2], for example, that all vertex-transitive graphs with \( 2p \) vertices for a prime \( p \equiv 3 \pmod{4} \) are Cayley graphs. Does this or any other available structural information help to design a \( k \)-WL-based recognition algorithm? Conversely, can the negative result of Theorem 4.1 be extended to a larger range of \( n \)?

The above questions make a perfect sense also for arc-transitivity. In contrast to Theorem 4.1 which gives an explicit lower bound on the WL dimension for an explicit range of \( n \), our negative result for arc-transitivity in Theorem 5.2 is implicit in both of these respects. Obtaining a constructive version of Theorem 5.2 is a well-motivated problem as it is otherwise not excluded that arc-transitivity of input graphs on any number \( n \) of vertices is recognizable by \( k \)-WL with dimension \( k = k(n) \) being a slowly increasing function of \( n \).

We conclude with a brief discussion of the concept of a \textit{rank 3 graph}, which is a "2-dimensional" analog of vertex-transitivity. While the automorphism group of a vertex-transitive graph acts transitively on its vertex set, the automorphism group of a rank 3 graph acts transitively not only on the vertices, but also on the ordered pairs of adjacent vertices and on the ordered pairs of non-adjacent vertices. Thus, \( G \)
is a rank 3 graph if and only if both $G$ and its complement are arc-transitive. Since this concept is more stringent than vertex- and arc-transitivity, the corresponding recognition problem has a priori better chances to be solvable by $k$-WL, though its complexity status is wide open.

Let $P$ be a pattern graph with designated vertices $u_1$ and $u_2$. For vertices $x_1$ and $x_2$ of a graph $G$, let $s_P(x_1, x_2)$ denote the number of copies of $P$ in $G$ such that $u_1$ is placed at $x_1$ and $u_2$ is placed at $x_2$. A graph $G$ satisfies the $t$-vertex condition if, for every $P$ with at most $t$ vertices, the count $s_P(x_1, x_2)$ depends only on (non)equality and (non)adjacency of $x_1$ and $x_2$ (Higman [26]). If $G$ is a rank 3 graph, then the $t$-vertex condition is obviously satisfied for every $t$. The long-standing Klin’s conjecture [20] (see also the references in [37, 35]) says that there is an integer $T$ such that, conversely, every graph $G$ satisfying the $T$-vertex condition is a rank 3 graph. We remark that, if this conjecture is true, then $T$-WL recognizes the class of 3 rank graphs in a straightforward way. This follows from a simple observation that, if the color of a $T$-tuple $(x_1, x_2, \ldots, x_2)$ in $WL_T(G)$ depends only on the type of the pair $(x_1, x_2)$ (like for rank 3 graphs), then $G$ satisfies the $T$-vertex condition.

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