Bounding the Weisfeiler–Leman Dimension via a Depth Analysis of I/R-Trees

Sandra Kiefer
sandra.kiefer@cs.ox.ac.uk
University of Oxford
Oxford, United Kingdom

Daniel Neuen
daniel.neuen@ur.de
University of Regensburg
Regensburg, Germany

ABSTRACT

The Weisfeiler–Leman (WL) dimension is an established measure for the inherent descriptive complexity of graphs and relational structures. It corresponds to the number of variables that are needed and sufficient to define the object of interest in a counting version of first-order logic (FO). These bounded-variable counting logics were even candidates to capture graph isomorphism, until a celebrated construction due to Cai, Fürer, and Immerman [Combinatorica 1992] showed that $\Omega(n)$ variables are required to distinguish all non-isomorphic n-vertex graphs.

Still, very little is known about the precise number of variables required and sufficient to define every n-vertex graph. For the bounded-variable (non-counting) FO fragments, Pikhurko, Veith, and Verbitsky [Discret. Appl. Math. 2006] provided an upper bound of $\frac{n+3}{2}$ and showed that it is essentially tight. Our main result yields that, in the presence of counting quantifiers, $\frac{n}{4} + o(n)$ variables suffice. This shows that counting does allow us to save variables when defining graphs. As an application of our techniques, we also show new bounds in terms of the vertex cover number of the graph.

To obtain the results, we introduce a new concept called the *WL depth* of a graph. We use it to analyze branching trees within the Individualization/Refinement (I/R) paradigm from the domain of isomorphism algorithms. We extend the recursive procedure from the I/R paradigm by the possibility of splitting the graphs into independent parts. Then we bound the depth of the obtained branching trees, which translates into bounds on the WL dimension and thereby on the number of variables that suffice to define the graphs.

CCS CONCEPTS

• **Theory of computation → Finite Model Theory**; **Graph algorithms analysis**; • **Mathematics of computing → Combinatorial algorithms**.

KEYWORDS

Weisfeiler-Leman algorithm, first-order logic, counting quantifiers, individualization/refinement paradigm

LICS '24, July 8–11, 2024, Tallinn, Estonia

ACM ISBN 979-8-4007-0660-8/24/07
https://doi.org/10.1145/3661814.3662122

ACM Reference Format:
Sandra Kiefer and Daniel Neuen. 2024. Bounding the Weisfeiler–Leman Dimension via a Depth Analysis of I/R-Trees. In *39th Annual ACM/IEEE Symposium on Logic in Computer Science (LICS '24), July 8–11, 2024, Tallinn, Estonia.* ACM, New York, NY, USA, 14 pages. https://doi.org/10.1145/3661814.3662122

1 INTRODUCTION

The Weisfeiler–Leman (WL) algorithm is a combinatorial algorithm that iteratively collects and aggregates local information of structures and encodes them in colors assigned to parts of the structures. The original algorithm introduced by Weisfeiler and Leman [32] is the 2-dimensional version, which colors pairs of vertices. Its generalization to arbitrary dimension $k \geq 1$ is the k-dimensional WL algorithm (k-WL), which was independently introduced by Babai and Mathon (see [4] for a historic note) as well as by Immerman and Lander [14].

The most prominent application of the WL algorithm lies in the context of graph comparison, since the computed information can be used to discover structural differences in the graphs. Indeed, the algorithm is commonly used as a subroutine in isomorphism algorithms both in practice (see, e.g., [15, 16, 21, 22]) and theory (see, e.g., [1, 2, 5, 24, 26]), including Babai's quasipolynomial-time isomorphism test [4], which falls back on k-WL for dimension $k = O(\log n)$.

Besides that, the WL algorithm has connections to numerous other areas in (theoretical) computer science (see the survey articles [17, 23]). Among the most prominent links is the one to counting logics. It is known that k-WL distinguishes two graphs if and only if the graphs can be distinguished via a sentence in first-order logic with counting quantifiers and $k + 1$ variables, i.e., in the logic C^{k+1} [7, 14]. Via this connection, the algorithm and the study of its expressive power have become a major tool to analyze the inherent descriptive complexity of relational structures. More precisely, the *WL dimension* of a graph G is the minimum dimension of the algorithm that suffices to distinguish G from every non-isomorphic graph and it directly corresponds to the minimum number of variables that suffice to define the graph in the counting logic C.

For some time, there was hope that there would be a universal bound on the WL dimension for all graphs, which would have placed the graph isomorphism problem in the complexity class P. However, a celebrated construction due to Cai, Fürer, and Immerman [7] shows that $\Omega(n)$ variables are needed to define every graph on n vertices, i.e., the WL dimension of n-vertex graphs is in $\Omega(n)$. On the other hand, many restricted classes of graphs have finite WL dimension, for example, every graph class that excludes a fixed graph as a minor [11].

In recent years, there has been a series of results aiming to provide more precise bounds on the WL dimension of certain graph classes. For example, it was shown in [20] that the WL dimension of planar graphs is at most 3. Further examples include upper bounds on the WL dimension that are linear (with small and explicit constant factors) in the tree-width [18], rank-width [13] or genus [12] of graphs.

Surprisingly, there has only been little progress towards determining the WL dimension only with respect to the number of vertices of a graph, which is arguably the simplest and most natural graph parameter. In terms of logics, this poses the following question. *How many variables are needed and sufficient to define graphs on n vertices in* C*?* Pikhurko, Veith, and Verbitsky [28] proved that for every two non-isomorphic n-vertex graphs G and H, there is an FO-formula with at most $\frac{n+3}{2}$ variables that distinguishes G and H. For the logic FO (without counting quantifiers), in the worst case, this bound is optimal up to an additive term of one, i.e., there are non-isomorphic n-vertex graphs which can only be distinguished in FO with at least $\frac{n+1}{2}$ variables. Since every FO-formula is also a C-formula, the upper bound also holds for C, i.e., every n-vertex graph G can be defined in C with at most $\frac{n+3}{2}$ variables.[1] However, as opposed to the FO setting, it has remained open whether this bound is tight in the presence of counting quantifiers or whether they actually decrease the number of distinct variables that are needed.

Taking a closer look at the Cai-Fürer-Immerman (CFI) construction, [28] also shows that at least $0.00465n$ variables are required to define every n-vertex graph G in C. Using today's refined understanding of the CFI construction (see, e.g., [8, 25, 29]) and more recent results on expander graphs [10], we can obtain an improved lower bound of $(\frac{1}{96} - o(1))n$ on the WL dimension of all n-vertex graphs. Still, there is a considerable gap between this lower and the upper bound.

This work. Our main contribution is the following upper bound on the WL dimension of the class of all n-vertex graphs, which improves on the result obtained by Pikhurko, Veith, and Verbitsky [28].

Theorem 1.1. *The WL dimension of every n-vertex graph is at most $\frac{n}{4} + o(n)$.*

Via the characterization of the WL algorithm in terms of first-order logic with counting quantifiers, we immediately obtain the following.

Corollary 1.2. *Every n-vertex graph G can be defined in C^k, i.e., in the k-variable fragment of first-order logic enriched with counting quantifiers, where $k \in \frac{n}{4} + o(n)$.*

In particular, considering the worst-case optimality of the bound from [28] for FO without counting, our result shows that the ability to count does allow us to save variables when defining graphs.

Our techniques also allow us to obtain an improved bound on the WL dimension in terms of the vertex cover number. For a graph G, a set $S \subseteq V(G)$ is a *vertex cover* of G if $e \cap S \neq \emptyset$ for all edges $e \in E(G)$, and the *vertex cover number* of G is the minimal size of a vertex cover. It is easy to see (and also follows from [18, Theorem 6.4]) that the WL dimension of a graph is at most its vertex cover number. We obtain the following stronger bound.

Theorem 1.3. *The WL dimension of every graph with vertex cover number r is at most $\frac{2}{3}r + 3$.*

By constructing a vertex cover of small size for the CFI graphs, we also obtain a lower bound of $(\frac{1}{72} - o(1))r$ on the WL dimension of graphs with vertex cover number r.

The starting point for our analysis is the following observation. Suppose that for a graph G, there are vertices $v_1, \ldots, v_s$ such that, after individualizing these vertices (i.e., assigning a unique color to each of them) and performing 1-WL (also known as the *Color Refinement algorithm*), we obtain a discrete coloring, i.e., one where all vertices receive different colors. Then it is well known that the WL dimension of G is at most $s + 1$. This idea builds the foundation of the Individualization/Refinement (I/R) paradigm, which is most prominently used in practical graph isomorphism tools, see, e.g., [15, 16, 21, 22], but it has also been used in theoretical work, such as [2, 3, 5, 20, 31].

Unfortunately, the method does not suffice to obtain good upper bounds on the WL dimension of n-vertex graphs, since the number of vertices that need to be individualized might be high. Indeed, for the complete graph K_n on n vertices, it is easy to see that $n - 1$ vertices need to be individualized so that applying 1-WL results in a discrete coloring. To overcome this issue, we adopt a strategy inspired by practical isomorphism solvers [16], which is to allow for simple modifications to the graph without changing the problem at hand, as well as treating components of a graph independently. For example, the WL dimension of a graph G is equal to the WL dimension of G with complemented edge set. For K_n, complementing the edge set yields isolated vertices. Now, using that the WL dimension of a graph G is at most $\max\{2, k\}$, where k is the maximum dimension of its connected components, we obtain that the WL dimension of a complete graph is at most 2.

It turns out that a combination of these ideas is already very powerful and suffices for us to show Theorems 1.1 and 1.3. We concretize the approach in a new concept, which we call the *WL depth* of a graph. To obtain our results, we first show that if G has k-WL depth at most ℓ, then its WL dimension is at most $\max\{2, k\} + \ell$. We then prove that the 1-WL depth of a graph is at most $\frac{2}{3}r+1$, where r is the vertex cover number of the graph. This implies Theorem 1.3. Afterwards, we show that the 2-WL depth of any n-vertex graph is at most $\frac{n}{4} + o(n)$, resulting in Theorem 1.1. This part is our main technical contribution and may be of independent interest since it also provides bounds on the possible depth of branching trees considered by practical isomorphism tests [16].

Outline. After covering the necessary preliminaries in the next section, we introduce the WL depth of a graph in Section 3 and prove various basic properties for it. This notion is the key concept underlying our main results. After that, we prove Theorem 1.3 in Section 4 and Theorem 1.1 in Section 5. Finally, we give the lower bounds on the WL dimension in Section 6. All omitted proofs can be found in the full version [19].

[1] Note that, while we can well speak about definability of a graph in C, i.e., it being distinguished from every second graph, we need to restrict ourselves to the comparison of graphs with equal numbers of vertices in the bounded-variable fragments of FO, since we cannot determine the number n of vertices without using $n + 1$ variables or counting.

2 PRELIMINARIES

2.1 Graphs and Colorings

An (undirected) *graph* is a pair $G = (V(G), E(G))$ of a finite, nonempty *vertex set* $V(G)$ and an *edge set* $E(G) \subseteq \{\{u,v\} \mid u, v \in V(G), u \neq v\}$. For $v, w \in V(G)$, we also write vw as a shorthand for $\{v, w\}$. The *neighborhood* of v in G is $N_G(v) := \{w \mid \{v, w\} \in E(G)\}$ and the *degree* of v in G is $\deg_G(v) := |N_G(v)|$. The *closed neighborhood* of v in G is $N_G[v] := N_G(v) \cup \{v\}$. For $W \subseteq V(G)$, we also define $N_G(W) := (\bigcup_{v \in W} N(v)) \setminus W$. If the graph is clear from the context, we usually omit the subscript.

A set $S \subseteq V(G)$ is a *vertex cover* of G if $S \cap e \neq \emptyset$ for all $e \in E(G)$. The *vertex cover number* of G is the smallest integer $r \geq 0$ such that G has a vertex cover of size r.

For a graph G and $U, W \subseteq V(G)$, we define $E_G(U, W) := \{uw \in E(G) \mid u \in U, w \in W\}$. We also denote by $G[W]$ the *induced subgraph* of G on the vertex set W, and define $G - W := G[V(G) \setminus W]$. For disjoint subsets $U, W \subseteq V(G)$, we define the bipartite graph $G[U, W]$ with vertex set $U \cup W$ and edge set $E_G(U, W)$. A bipartite graph G with bipartition (V_1, V_2) is called *biregular* if $\deg(u_1) = \deg(v_1)$ for all $u_1, v_1 \in V_1$, and $\deg(u_2) = \deg(v_2)$ for all $u_2, v_2 \in V_2$.

A *(vertex-)colored graph* is a tuple (G, χ) where G is a graph and $\chi\colon V(G) \to C$ is a *(vertex) coloring*, a mapping from $V(G)$ into some set C of colors. We write $\mathrm{im}(\chi) := \{\chi(v) \mid v \in V(G)\}$ to denote the image of χ. We generally assume that all graphs are colored even if not explicitly stated. Typically, the color set C is chosen to be an initial segment $[n] := \{1, \dots, n\}$ of the natural numbers. We say a coloring χ is *discrete* if it is injective, i.e., all color classes have size 1.

Let $\chi\colon U \to C$ be a coloring of the elements of some universe U. For a tuple $\bar{u} = (u_1, \dots, u_\ell) \in U^\ell$, we define $\chi[\bar{u}]$ to be the coloring obtained from χ by individualizing all elements $u_1, \dots, u_\ell$, i.e., $(\chi[\bar{u}])(u_i) = (1, \min\{j \in [\ell] \mid u_i = u_j\})$ for all $i \in [\ell]$, and $(\chi[\bar{u}])(v) = (0, \chi(v))$ for all $v \in U \setminus \{u_1, \dots, u_\ell\}$. For $u_1, \dots, u_\ell \in U$, we also write $\chi[u_1, \dots, u_\ell]$ for $\chi[(u_1, \dots, u_\ell)]$. Moreover, slightly abusing notation, for a set $S = \{u_1, \dots, u_\ell\} \subseteq U$, we write $\chi[S]$ instead of $\chi[u_1, \dots, u_\ell]$ if the order of the elements is irrelevant to us.

An *isomorphism* from G to a graph H is a bijection $\varphi\colon V(G) \to V(H)$ such that for all $v, w \in V(G)$, it holds that $\{v, w\} \in E(G)$ if and only if $\{\varphi(v), \varphi(w)\} \in E(H)$. The graphs G and H are *isomorphic* ($G \cong H$) if there is an isomorphism from G to H. We write $\varphi\colon G \cong H$ to denote that φ is an isomorphism from G to H. Isomorphisms between colored graphs have to respect the colors of the vertices.

2.2 Logics

We give a brief introduction to the logics and notation we use here. For more background, we refer the reader to [11, 27]. We write FO to denote standard *first-order logic*. For a formula φ, we write $\varphi(x_1, \dots, x_k)$ to indicate that the free variables of φ are among the variables $\{x_1, \dots, x_k\}$. A *sentence* is a formula without free variables.

We define *first-order logic with counting quantifiers* C to be the extension of FO by counting quantifiers of the form $\exists^{\geq j} x\varphi$. The formula $\exists^{\geq j} x\varphi$ is satisfied over a graph G if there are at least j distinct elements $v \in V(G)$ that satisfy φ. For $k \geq 1$, we define C^k to be the restriction of C to formulas with at most k variables, i.e., we restrict ourselves to a set of variables of size k.

Let G and H be two graphs and let L be a logic. We say that a sentence $\varphi \in \mathsf{L}$ *distinguishes* G and H if exactly one of G and H is a model of φ.

2.3 The Weisfeiler–Leman Algorithm

Let $\chi_1, \chi_2\colon (V(G))^k \to C$ be colorings of the k-tuples of vertices of a graph G. We say χ_1 *refines* χ_2, denoted $\chi_1 \preceq \chi_2$, if $\chi_1(\bar{v}) = \chi_1(\bar{w})$ implies $\chi_2(\bar{v}) = \chi_2(\bar{w})$ for all $\bar{v}, \bar{w} \in (V(G))^k$. The colorings χ_1 and χ_2 are *equivalent*, denoted $\chi_1 \equiv \chi_2$, if $\chi_1 \preceq \chi_2$ and $\chi_2 \preceq \chi_1$. The coloring χ_1 *strictly refines* χ_2, denoted $\chi_1 \prec \chi_2$, if $\chi_1 \preceq \chi_2$ and $\chi_1 \not\equiv \chi_2$.

We describe the *k-dimensional Weisfeiler–Leman algorithm* (k-WL) for $k \geq 1$. Let (G, χ) be a colored graph. We define the initial coloring $\mathsf{WL}^k_0[G, \chi]\colon (V(G))^k \to C$ as the coloring where each tuple is colored with the isomorphism type of its underlying ordered subgraph. More precisely, for two colored graphs (G, χ) and (G, χ'), and vertices $v_1, \dots, v_k \in V(G)$ and $v'_1, \dots, v'_k \in V(G')$ we have $\mathsf{WL}^k_0[G, \chi](v_1, \dots, v_k) = \mathsf{WL}^k_0[G', \chi'](v'_1, \dots, v'_k)$ if and only if there is an isomorphism between the induced colored graphs $G[\{v_1, \dots, v_k\}]$ and $G'[\{v'_1, \dots, v'_k\}]$ mapping v_i to v'_i for all $i \in [k]$.

We then recursively define the coloring $\mathsf{WL}^k_i[G, \chi]$ obtained after i rounds of the algorithm. Suppose $k \geq 2$. For $\bar{v} = (v_1, \dots, v_k) \in (V(G))^k$, set $\mathsf{WL}^k_{i+1}[G, \chi](\bar{v}) := \big(\mathsf{WL}^k_i[G, \chi](\bar{v}), \mathcal{M}_i(\bar{v})\big)$, where

$$\mathcal{M}_i(\bar{v}) := \left\{\!\!\left\{ \big(\mathsf{WL}^k_i[G,\chi](\bar{v}[w/1]), \dots, \mathsf{WL}^k_i[G,\chi](\bar{v}[w/k])\big) \;\middle|\; w \in V(G) \right\}\!\!\right\}$$

and $\bar{v}[w/i] := (v_1, \dots, v_{i-1}, w, v_{i+1}, \dots, v_k)$ is the tuple obtained from substituting the i-th entry of $\bar{v}$ with w.

For $k = 1$, the definition is analogous, but we set

$$\mathcal{M}_i(\bar{v}) := \left\{\!\!\left\{ \mathsf{WL}^1_i[G, \chi](w) \;\middle|\; w \in N_G(v) \right\}\!\!\right\}.$$

By definition, $\mathsf{WL}^k_{i+1}[G, \chi] \preceq \mathsf{WL}^k_i[G, \chi]$ holds for all $i \geq 0$. So there is a minimal $i_\infty \geq 0$ such that $\mathsf{WL}^k_{i_\infty}[G, \chi] \equiv \mathsf{WL}^k_{i_\infty+1}[G, \chi]$, and we set $\mathsf{WL}^k[G, \chi] := \mathsf{WL}^k_{i_\infty+1}[G, \chi]$.

To simplify notation, for $\ell < k$ and vertices $v_1, \dots, v_\ell \in V(G)$, we write $\mathsf{WL}^k[G, \chi](v_1, \dots, v_\ell)$ for $\mathsf{WL}^k[G, \chi](v_1, \dots, v_\ell, v_\ell, \dots, v_\ell)$, where the latter tuple has k entries.

Also, we say a vertex coloring $\lambda\colon V(G) \to C$ is *stable with respect to k-WL* if it is not refined by k-WL. Formally, this means that $\lambda \equiv \lambda'$ where $\lambda'\colon V(G) \to C$ is defined via $\lambda'(v) := \mathsf{WL}^k[G, \lambda](v)$ for all $v \in V(G)$.

The algorithm k-WL takes a vertex-colored graph (G, χ) as input and returns $\mathsf{WL}^k[G, \chi]$. Given vertex-colored graphs (G, χ) and (H, λ), the algorithm *distinguishes* (G, χ) and (H, λ) if

$$\left\{\!\!\left\{ \mathsf{WL}^k[G, \chi](\bar{v}) \;\middle|\; \bar{v} \in (V(G))^k \right\}\!\!\right\} \neq \left\{\!\!\left\{ \mathsf{WL}^k[H, \lambda](\bar{w}) \;\middle|\; \bar{w} \in (V(H))^k \right\}\!\!\right\}.$$

We write $(G, \chi) \simeq_k (H, \lambda)$ if k-WL does not distinguish (G, χ) and (H, λ). Also, k-WL *identifies* (G, χ) if it distinguishes (G, χ) from every other non-isomorphic vertex-colored graph. From the definition, it follows that all graphs that are distinguished (and identified, respectively) by k-WL are also distinguished (and identified, respectively) by $(k + 1)$-WL. The *WL dimension* of a graph (G, χ) is the minimal integer $k \geq 1$ such that k-WL identifies (G, χ).

The following theorem connects the WL algorithm to first-order logic with counting quantifiers.

Theorem 2.1 ([7, 14]). *Let $k \geq 1$ and let G, H be two graphs. Then $G \simeq_k H$ if and only if there is no sentence in C^k that distinguishes G and H.*

We also require the following lemma.

Lemma 2.2. *Let $k \in \mathbb{N}$, let (G, χ) be a vertex-colored graph, and let $u \in V(G)$. Suppose k-WL identifies the graph $(G, \chi[u])$. Then $(k+1)$-WL identifies (G, χ).*

Proof. Suppose there is a vertex-colored graph (G', χ') with a vertex $u' \in V(G')$ such that $\mathsf{WL}^{k+1}[G', \chi'](u') = \mathsf{WL}^{k+1}[G, \chi](u)$. Hence, we have that

$$\{\!\{\mathsf{WL}^{k+1}[G, \chi](u, w_1, \dots, w_k) \mid (w_1, \dots, w_k) \in V^k(G)\}\!\}$$
$$= \{\!\{\mathsf{WL}^{k+1}[G', \chi'](u', w_1', \dots, w_k') \mid (w_1', \dots, w_k') \in V^k(G')\}\!\}.$$

Thus, the graphs $(G, \chi[u])$ and $(G', \chi'[u'])$ obtain equal colorings under k-WL. By assumption, this implies that $(G, \chi[u])$ and $(G', \chi'[u'])$ are isomorphic, which is equivalent to the existence of an isomorphism from (G, χ) to (G', χ') mapping u to u'. □

3 THE WEISFEILER–LEMAN DEPTH

In this section, we introduce the k-WL depth of a colored graph (G, χ), which is the key notion underlying our analysis. Let $k \geq 1$. Intuitively speaking, the k-WL depth is the minimum number of vertices that need to be individualized in order to obtain a discrete coloring after performing k-WL, except that we allow for some simple additional operations that do not affect the WL dimension. The first such operation is the possibility to split a graph into connected components. Indeed, it is known that if $k \geq 2$ and k-WL identifies every connected component of a graph, then k-WL also identifies G. So we may always restrict ourselves to the analysis of connected graphs when we are interested in bounding the WL dimension. In itself, this operation is of limited use, since it can only be applied at most once. For this reason, we also consider operations that allow us to decrease the number of edges (hoping to make the graph disconnected again).

The most basic operation is to complement the entire edge set of G, which is already sufficient to handle complete graphs. However, in a vertex-colored graph, we can also complement edges between two color classes without changing the WL dimension. More generally, we can choose any number of pairs of vertex colors and complement edges exactly between the chosen pairs. To formalize this idea, we introduce the notion of a flip function.

Let (G, χ) be a vertex-colored graph and let $C \coloneqq \mathrm{im}(\chi)$. A *flip function for* (G, χ) is a function $f\colon C \times C \to \{0, 1\}$ such that $f(c_1, c_2) = f(c_2, c_1)$ for all $c_1, c_2 \in C$.

Let f be a flip function for (G, χ). We define the *f-flip of* (G, χ) to be the graph $\mathrm{flip}_f(G, \chi) \coloneqq (G', \chi)$ where $V(G') = V(G)$ and

$$E(G') \coloneqq \{vw \in E(G) \mid f(\chi(v), \chi(w)) = 0\} \cup \{vw \notin E(G) \mid v \neq w, f(\chi(v), \chi(w)) = 1\}.$$

Intuitively speaking, the f-flip of (G, χ) is obtained from (G, χ) by complementing the edges between all color classes associated with $c_1, c_2 \in C$ for which $f(c_1, c_2) = 1$.

We will mostly use one particular flip function f, which aims at minimizing the number of edges in the f-flip. We define $f^*_{G,\chi}\colon C \times C \to \{0, 1\}$ via $f^*_{G,\chi}(c_1, c_2) = 1$ if and only if

$$\left|E_G(\chi^{-1}(c_1), \chi^{-1}(c_2))\right| > \frac{1}{2}\left|\left\{vw \in \binom{V(G)}{2} \;\middle|\; \chi(v) = c_1, \chi(w) = c_2\right\}\right|.$$

We define the *flip* of (G, χ) as $\mathrm{flip}^*(G, \chi) \coloneqq \mathrm{flip}_{f^*_{G,\chi}}(G, \chi)$. We say that (G, χ) *is flipped* if $(G, \chi) = \mathrm{flip}^*(G, \chi)$. Observe that flipping is idempotent, i.e., the flip of (G, χ) is flipped.

With these definitions at hand, we are now ready to formally define the k-WL depth. As already indicated above, the concept aims at describing the minimum number of vertices that need to be individualized in order to obtain a discrete coloring after performing k-WL, but we additionally allow splitting the graph into its connected components (which are then treated independently) and transitioning to the f-flip for any flip function f. More precisely, we wish to arrive at a graph with a discrete coloring by applying the operations (A) refine the coloring using k-WL, (B) move to the f-flip for any flip function f, (C) split the graph into connected components and treat them independently, and (D) individualize some vertex. In doing so, we aim to minimize the number of vertex individualizations. This is formalized in the next definition.

Definition 3.1. Let $k \geq 1$. A *k-IRC tree* of (G, χ) is a triple (T, r, γ) where T is a tree with root $r \in V(T)$, and γ maps each $t \in V(T)$ to a vertex-colored graph $\gamma(t) = (G_t, \chi_t)$ such that $\gamma(r) = (G, \chi)$, and for each leaf t of T, it holds that $|V(G_t)| = 1$, and additionally, each internal node t of T satisfies (at least) one of the following:

(A) t has exactly one child s and $G_s = G_t$ (uncolored) and $\chi_s(v) = \mathsf{WL}^k[G, \chi_t](v)$ for all $v \in V(G_t)$,
(B) t has exactly one child s and $(G_s, \chi_s) = \mathrm{flip}_f(G_t, \chi_t)$ for some flip function f of (G_t, χ_t),
(C) G_t has exactly ℓ connected components with vertex sets $A_1, \dots, A_\ell$, and t has exactly ℓ children $s_1, \dots, s_\ell$ and it holds that $(G_{s_i}, \chi_{s_i}) = (G_t[A_i], \chi_t|_{A_i})$ for all $i \in [\ell]$, or
(D) t has exactly one child s and $G_s = G_t$ and $\chi_s = \chi_t[u]$ for some $u \in V(G_t)$.

There may be situations where an internal node t satisfies more than one of the above conditions. We say the node t is an *individualization node* if it satisfies Condition (D) and none of the other conditions. We define the *individualization depth* of (T, r, γ) to be the maximum number of individualization nodes on any root-to-leaf path in (T, r). The *k-WL depth of* (G, χ) is the minimum individualization depth of a k-IRC tree of (G, χ) and we denote it by $\mathrm{depth}^k_{\mathsf{WL}}(G, \chi)$.

We start by determining the WL depth of some simple examples.

Example 3.2. A 1-IRC tree of the 6-cycle C_6 (where every vertex receives the same color) is shown in Figure 1. The 1-IRC tree has individualization depth 1, and hence $\mathrm{depth}^1_{\mathsf{WL}}(C_6) \leq 1$. Actually, it is not difficult to see that $\mathrm{depth}^1_{\mathsf{WL}}(C_6) = 1$.

Example 3.3. Every vertex-colored complete graph (K_n, χ) has k-WL depth 0 for all $k \geq 1$. Indeed, the graph $\mathrm{flip}^*(K_n, \chi)$ has no edges. So after splitting $\mathrm{flip}^*(K_n, \chi)$ into its connected components, we obtain that each one of them has only one vertex and thus satisfies the condition to be a leaf.

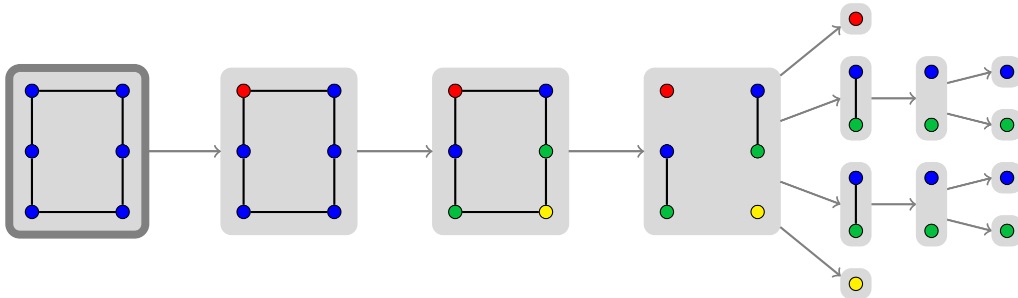

Figure 1: The figure shows a 1-IRC tree of C_6. Every gray region corresponds to one node t of the tree with the colored graph $\gamma(t)$ drawn inside. The root node is the only individualization node. Hence, the individualization depth of the 1-IRC tree is equal to 1.

Example 3.4. Let (G, χ) be a graph such that χ is a discrete coloring. Then $\text{flip}^*(G, \chi)$ has no edges, so the graph can be split into connected components of size 1. This implies that $\text{depth}^k_{\text{WL}}(G, \chi) = 0$ for all $k \geq 1$.

More generally, if applying 1-WL to a colored graph (G, χ) results in a discrete coloring, then $\text{depth}^k_{\text{WL}}(G, \chi) = 0$ for all $k \geq 1$. In particular, $\text{depth}^1_{\text{WL}}(G, \chi) = 0$ for almost all graphs (G, χ), see [6].

The following lemma will turn out to be helpful when proving upper bounds on the WL depth.

Lemma 3.5. *Let (G, χ) be a colored graph and let $k \in \mathbb{N}$. Then*

(1) $\text{depth}^k_{\text{WL}}(G, \chi) \leq \text{depth}^k_{\text{WL}}(G, \chi')$ *for the coloring χ' with $\chi'(v) = \text{WL}^k[G, \chi](v)$ for all $v \in V(G)$;*
(2) $\text{depth}^k_{\text{WL}}(G, \chi) \leq \text{depth}^k_{\text{WL}}(\text{flip}_f(G, \chi))$ *for every flip function f of (G, χ);*
(3) $\text{depth}^k_{\text{WL}}(G, \chi) \leq \max_{i \in [\ell]} \text{depth}^k_{\text{WL}}(G[A_i], \chi|_{A_i})$*, where we denote $A_1, \ldots, A_\ell$ the vertex sets of the connected components of G; and*
(4) $\text{depth}^k_{\text{WL}}(G, \chi) \leq 1 + \text{depth}^k_{\text{WL}}(G, \chi[u])$ *for every $u \in V(G)$.*

To show the inequalities, one can build a k-IRC tree for (G, χ) by using k-IRC trees for the graphs on the right-hand side as building blocks.

To demonstrate the potential of the concept of the WL depth, we show that forests have k-WL depth 0 for every $k \in \mathbb{N}$.

Lemma 3.6. *Let F be a forest and χ be a vertex coloring of F. Then $\text{depth}^k_{\text{WL}}(F, \chi) = 0$ for all $k \geq 1$.*

Proof. We show the statement by induction on the number of vertices of F. If $|V(F)| = 1$, then $\text{depth}^k_{\text{WL}}(F, \chi) = 0$ immediately follows.

So suppose $|V(F)| > 1$. If F is not connected, we split F into its connected components $F_1, \ldots, F_\ell$. By the induction hypothesis, $\text{depth}^k_{\text{WL}}(F_i, \chi|_{V(F_i)}) = 0$, so for every $i \in [\ell]$ there is a k-IRC tree (T_i, r_i, γ_i) of the graph $(F_i, \chi|_{V(F_i)})$ of individualization depth 0. Without loss of generality, assume that $V(T_i) \cap V(T_j) = \emptyset$ and $r \notin V(T_i)$ for all distinct $i, j \in [\ell]$. We build a 1-IRC tree (T, r, γ) of (F, χ) with

$$V(T) := \{r\} \cup \bigcup_{i \in [\ell]} V(T_i)$$

and

$$E(T) := \{(r, r_i) \mid i \in [\ell]\} \cup \bigcup_{i \in [\ell]} E(T_i)$$

Also, we set $\gamma(r) := (F, \chi)$ and $\gamma(t) := \gamma_i(t)$ for all $i \in [\ell]$ and $t \in V(T_i)$. Then it is easy to see that (T, r, γ) contains no individualization nodes and hence, it has individualization depth 0.

So suppose F is connected. Let $\chi^*(v) := \text{WL}^k[F, \chi](v)$ for all $v \in V(F)$. We now claim that $\text{flip}^*(F, \chi^*)$ is a disconnected forest. First note that this allows us to build a k-IRC tree (T, r, γ) as follows. The root node r has exactly one child t_1 and we set $\gamma(t_1) := (F, \chi^*)$. Then, t_1 has exactly one child t_2 and we set $\gamma(t_2) := \text{flip}^*(F, \chi^*)$. After that, since $\text{flip}^*(F, \chi^*)$ is a disconnected forest, we can proceed as before to obtain a k-IRC tree of individualization depth 0.

The following proves that $\text{flip}^*(F, \chi)$ is a disconnected forest.

Claim 3.7. *$\text{flip}^*(F, \chi)$ is a disconnected forest.*

Proof. Note that it suffices to show that $E(\text{flip}^*(F, \chi^*)) \subsetneq E(F)$.

Consider two colors $c_1, c_2 \in \text{im}(\chi^*)$. First suppose that $c_1 \neq c_2$. Since χ^* is stable with respect to 1-WL, we conclude that the set $F[(\chi^*)^{-1}(c_1), (\chi^*)^{-1}(c_2)]$ is a disjoint union of k stars $K_{1,h}$ for some $k \geq 1$ and $h \geq 0$ (for $h = 0$ the graph $K_{1,h}$ is an isolated vertex). If $k = 1$, then flipping removes all edges in $E_F(\chi^{-1}(c_1), \chi^{-1}(c_2))$. Otherwise, it has no effect on the edges in $E_F(\chi^{-1}(c_1), \chi^{-1}(c_2))$.

So consider the case $c_1 = c_2$. Then, by regularity, $F[(\chi^*)^{-1}(c_1)]$ either has no edges or is a matching. If $F[(\chi^*)^{-1}(c_1)]$ is isomorphic to K_2, flipping removes the corresponding edge. Otherwise, flipping has no effect on the edges contained in $F[(\chi^*)^{-1}(c_1)]$.

Hence, $E(\text{flip}^*(F, \chi^*)) \subseteq E(F)$. We now show that at least one edge of F is not present in $\text{flip}^*(F, \chi^*)$.

Consider the graph repeatedly obtained by removing all leaves from F until at most two vertices remain. These two vertices form a union of color classes under χ^* since χ^* is stable with respect to 1-WL. If only one vertex remains, it forms a singleton color class and all incident edges are removed by flipping the graph. Otherwise, the two vertices are connected by an edge (since F is connected), which is removed by flipping the graph. ⌟

□

Next we prove that we can always refine colorings without increasing the WL depth.

Lemma 3.8. *Let (G, χ) be a vertex-colored graph and $k \geq 1$. Also let $\chi' \colon V(G) \to C$ be a vertex coloring such that $\chi' \preceq \chi$. Then* $\mathrm{depth}^k_{\mathsf{WL}}(G, \chi') \leq \mathrm{depth}^k_{\mathsf{WL}}(G, \chi)$.

Additionally, for every k-IRC tree (T, r, γ) of (G, χ) of individualization depth d, there is a k-IRC tree (T', r', γ') of (G, χ') of individualization depth at most d such that $(T', r') = (T, r)$.

Proof. We prove the second part of the lemma; this clearly implies the first statement.

Let (T, r, γ) be a k-IRC tree of (G, χ) of individualization depth d. Also, for every $t \in V(T)$ let $(G_t, \chi_t) \coloneqq \gamma(t)$.

For every $t \in V(T)$, we construct $\gamma'(t) = (G_t, \chi'_t)$ so that (T, r, γ') is a k-IRC tree of (G, χ') of individualization depth at most d. Additionally, we ensure that $\chi'_t \preceq \chi_t$ for every $t \in V(T)$.

We describe the mapping γ' in a top-down manner starting at the root. We set $\gamma'(r) \coloneqq (G, \chi')$.

Now let $v \in V(T)$ be an internal node such that $\gamma'(t) = (G_t, \chi'_t)$ has already been defined.

First suppose t satisfies Option (A) in the k-IRC tree (T, r, γ). Let s be the unique child of t. Then $\chi_s(v) = \mathsf{WL}^k[G, \chi_t](v)$ for all $v \in V(G_t) = V(G_s)$. We set $\gamma'(s) \coloneqq (G_s, \chi'_s)$ where $\chi'_s(v) = \mathsf{WL}^k[G, \chi'_t](v)$ for all $v \in V(G_t)$. Then t also satisfies Option (A) in the k-IRC tree (T, r, γ'). Also, since $\chi'_t \preceq \chi_t$, we conclude that $\chi'_s \preceq \chi_s$ by the properties of k-WL.

Next suppose t satisfies Option (B) in the k-IRC tree (T, r, γ). Let s be the unique child of t. Then $(G_s, \chi_s) = \mathrm{flip}_f(G_t, \chi_t)$ for some flip function f of (G_t, χ_t). Let $C' \coloneqq \mathrm{im}(\chi'_t)$. We define a flip function f' of (G_t, χ'_t) as follows. Let $c'_1, c'_2 \in C'$ be two colors. Since $\chi'_t \preceq \chi_t$, there are unique colors $c_1, c_2 \in \mathrm{im}(\chi_t)$ such that $(\chi'_t)^{-1}(c'_1) \subseteq \chi_t^{-1}(c_1)$ and $(\chi'_t)^{-1}(c'_2) \subseteq \chi_t^{-1}(c_2)$. We set $f'(c'_1, c'_2) \coloneqq f(c_1, c_2)$. Let $(G'_s, \chi'_s) \coloneqq \mathrm{flip}_{f'}(G_t, \chi'_t)$. Then $G'_s = G_s$. We set $\gamma'(s) \coloneqq (G_s, \chi'_s)$. Then t satisfies Option (B) in the k-IRC tree (T, r, γ') using the flip function f'. Also, $\chi'_s = \chi'_t \preceq \chi_t = \chi_s$.

So suppose t satisfies Option (C) in the k-IRC tree (T, r, γ). Let $s_1, \dots, s_\ell$ denote the children of t. We set $\gamma'(s_i) \coloneqq (G_{s_i}, \chi'_t|_{V(G_{s_i})})$ for every $i \in [\ell]$. Then t satisfies Option (C) in the k-IRC tree (T, r, γ'). Also, $\chi'_{s_i} = \chi'_t|_{V(G_{s_i})} \preceq \chi_t|_{V(G_{s_i})} = \chi_{s_i}$ for every $i \in [\ell]$.

Finally, suppose t satisfies Option (D) in the k-IRC tree (T, r, γ). Let s be the unique child of t. Then $(G_s, \chi_s) = (G_t, \chi_t[u])$ for some $u \in V(G)$. We set $\chi'_s \coloneqq \chi'_t[u]$ and $\gamma'(s) \coloneqq (G_s, \chi'_s)$. Then t satisfies Option (D) in the k-IRC tree (T, r, γ'). Also, $\chi'_s = \chi'_t[u] \preceq \chi_t[u] = \chi_s$ since $\chi'_t \preceq \chi_t$.

Since every internal node of (T, r, γ) satisfies one of the Options (A)-(D), this completes the construction of (T, r, γ'). We get that (T, r, γ') is a k-IRC tree of (G, χ'). Also, every individualization node in (T, r, γ') is also an individualization node in (T, r, γ). So (T, r, γ') has individualization depth at most d. □

Next, we argue that we can eliminate vertices with identical neighborhoods in the graph without increasing the k-WL depth. This will become an important tool to prove the bounds on the WL dimension that we want to obtain.

Let (G, χ) be a colored graph. We say two vertices $v, w \in V(G)$ are *strong twins* if $N_G[v] = N_G[w]$ (in particular, if $v \neq w$, then $vw \in E(G)$). Also, we say that $v, w \in V(G)$ are *weak twins* if $N_G(v) = N_G(w)$ (in particular, if $v \neq w$, then $vw \notin E(G)$). Clearly, both relations are equivalence relations in G. A partition π of $V(G)$ is a *twin partition of* G if π is the partition into equivalence classes of either the strong-twin relation or the weak-twin relation in G. Let π be a twin partition of G. We define the colored graph $(G/\pi, \chi/\pi)$ where $V(G/\pi) = \pi$,

$$E(G/\pi) = \{PP' \mid P, P' \in \pi, E_G(P, P') \neq \emptyset\}$$

and $(\chi/\pi)(P) = \{\{\chi(v) \mid v \in P\}\}$. Finally, we say that G is *twin-free* if there is no non-trivial twin partition of G, i.e., there are no distinct vertices $v, w \in V(G)$ that are strong or weak twins.

Note that, by the definition of twins, every edge PP' in G/π corresponds to a complete bipartite graph between the elements of P and the elements of P' in G. Also note that for all $P, P' \in V(G/\pi)$ with $(\chi/\pi)(P) \neq (\chi/\pi)(P')$ and every $v \in P, v' \in P'$, it holds that $\mathsf{WL}^k[G, \chi](v) \neq \mathsf{WL}^k[G, \chi](v')$, since for $k \geq 2$, the algorithm k-WL distinguishes vertices for which the multisets of colors of siblings in the twin relation are not equal.

Lemma 3.9. *Let $k \geq 2$. Let (G, χ) be a colored graph and let π be a twin partition of G. Then*

$$\mathrm{depth}^k_{\mathsf{WL}}(G, \chi) \leq \mathrm{depth}^k_{\mathsf{WL}}(G/\pi, \chi/\pi).$$

Proof sketch. Let $k \geq 2$ be fixed. We show that for every colored graph (G, χ), every twin partition π of G, and every k-IRC tree (T', r', γ') of $(G', \chi') \coloneqq (G/\pi, \chi/\pi)$ of individualization depth d, it holds that $\mathrm{depth}^k_{\mathsf{WL}}(G, \chi) \leq d$. We prove this statement by induction on the height h of the tree (T', r').

In the base case, $h = 0$. Then $|V(G')| = 1$, which means that all vertices in (G, χ) are twins. Then G is a complete graph or has no edges and in both cases, $\mathrm{depth}^k_{\mathsf{WL}}(G, \chi) = 0 \leq d$ (see Example 3.3).

So as the inductive hypothesis, assume the statement holds for all graphs (H, λ) and twin partitions σ of H for which $(H/\sigma, \lambda/\sigma)$ has a k-IRC tree of height less than h. Let (G, χ) be a colored graph for which $(G', \chi') \coloneqq (G/\pi, \chi/\pi)$ has a k-IRC tree (T', r', γ') of height h. Let d be the individualization depth of (T', r', γ').

Let $t'_1, \dots, t'_\ell$ denote the children of r'. For $i \in [\ell]$, let $(G'_i, \chi'_i) \coloneqq \gamma'(t'_i)$ and let T'_i denote the subtree of T' rooted at t'_i. Observe that $(T'_i, t'_i, \gamma'|_{V(T'_i)})$ is a k-IRC tree of (G'_i, χ'_i) and has height less than h. Let d_i denote the individualization depth of $(T'_i, t'_i, \gamma'|_{V(T'_i)})$. Observe that $d_i \leq d$, and if r' is an individualization node, then it even holds that $d_i \leq d - 1$.

First suppose that $\ell = 1$, $G'_1 = G'$, and $\chi'_1(v) = \mathsf{WL}^k[G', \chi'](v)$ for all $v \in V(G')$. Let $\chi_1(v) \coloneqq \mathsf{WL}^k[G, \chi](v)$ for all $v \in V(G)$. Note that $\chi_1/\pi \equiv \chi'_1$ since $k \geq 2$. Furthermore, we know that (G'_1, χ'_1) has a k-IRC tree of height less than h and individualization depth at most d (for instance $(T'_1, t'_1, \gamma'|_{V(T'_1)})$). Thus, by Lemma 3.8, the same holds for $(G', \chi_1/\pi)$. Hence, we can apply the induction hypothesis to (G, χ_1) and π and obtain that

$$\begin{aligned}\mathrm{depth}^k_{\mathsf{WL}}(G, \chi) \overset{\text{L. 3.5(1)}}{\leq} \mathrm{depth}^k_{\mathsf{WL}}(G, \chi_1) &\overset{\text{IH}}{\leq} \mathrm{depth}^k_{\mathsf{WL}}(G', \chi_1/\pi) \\ \overset{\text{L. 3.8}}{=} \mathrm{depth}^k_{\mathsf{WL}}(G', \chi'_1) &\leq d.\end{aligned}$$

The other cases can be dealt with similarly, using Lemma 3.5 to "descend towards children of (G, χ)", the induction hypothesis to factor out twins, and Lemma 3.8 to transition to (G', χ'). We refer to the full version [19] for the details. □

Our main motivation to study the k-WL depth of graphs is to obtain improved bounds on the k-WL dimension of graphs. Towards this end, the following lemma relates the k-WL depth of a graph to its k-WL dimension.

LEMMA 3.10. *Let $k, d \in \mathbb{N}$ and let (G, χ) be a colored graph with $\text{depth}^k_{\text{WL}}(G, \chi) \leq d$. Then the $(\max\{2, k\} + d)$-dimensional Weisfeiler–Leman algorithm identifies (G, χ).*

PROOF. Let (T, r, γ) be a k-IRC tree of (G, χ) of individualization depth d. Let h be the height of (T, r). We prove the statement by induction on h.

In the base case, $h = 0$. Then $|V(G)| = 1$ and (G, χ) is identified by k-WL for every $k \in \mathbb{N}$.

So as the inductive hypothesis, assume the statement holds for all graphs (H, λ) that have a k-IRC tree of height smaller than h and of individualization depth at most d.

Let $t_1, \ldots, t_\ell$ denote the children of r. For $i \in [\ell]$, let $(G_i, \chi_i) :=$ $\gamma(t_i)$ and let T_i denote the subtree of T rooted at t_i. Observe that $(T_i, t_i, \gamma|_{V(T_i)})$ is a k-IRC tree of (G_i, χ_i) of height smaller than h. Let d_i denote the individualization depth of $(T_i, t_i, \gamma|_{V(T_i)})$. Observe that $d_i \leq d$, and if r is an individualization node, then it even holds that $d_i \leq d - 1$.

First suppose that $\ell = 1$, $G_1 = G$, and $\chi_1(v) = \text{WL}^k[G, \chi](v)$ for all $v \in V(G)$. By the induction hypothesis, (G_1, χ_1) is identified by $(\max\{2, k\} + d)$-WL. Hence, (G, χ) is identified by $(\max\{2, k\} + d)$-WL.

Next, suppose that $\ell = 1$ and $(G_1, \chi_1) = \text{flip}_f(G, \chi)$ for some flip function f of (G, χ). By the induction hypothesis, (G_1, χ_1) is identified by $(\max\{2, k\} + d)$-WL. Consider a colored graph (G', χ') with $(G', \chi') \simeq_{\max\{2,k\}+d} (G, \chi)$. Then it has to have the same vertex color classes and sizes as (G, χ). We conclude that $\text{flip}_f(G'\chi') \simeq_{\max\{2,k\}+d} (G_1, \chi_1)$, which implies that there is an isomorphism $\varphi\colon \text{flip}_f(G'\chi') \cong (G_1, \chi_1)$ (since (G_1, χ_1) is identified by $(\max\{2, k\} + d)$-WL). But then φ is also an isomorphism from (G', χ') to (G, χ). Hence, (G, χ) is identified by $(\max\{2, k\}+d)$-WL.

Now, suppose that G is disconnected and consists of connected components with vertex sets $A_1, \ldots, A_\ell$. So we have $(G_i, \chi_i) =$ $(G[A_i], \chi|_{A_i})$ for all $i \in [\ell]$. By the induction hypothesis, each $(G[A_i], \chi|_{A_i})$ is identified by $(\max\{2, k\} + d)$-WL. Since 2-WL distinguishes pairs of vertices in the same connected component from pairs of vertices in different connected components, the algorithm $(\max\{2, k\}+d)$-WL distinguishes (G, χ) from any graph whose multiset of isomorphism types of connected components is different. Hence, (G, χ) is identified by $(\max\{2, k\} + d)$-WL.

Finally, suppose that $\ell = 1$ and there is some $u \in V(G)$ such that $(G_1, \chi_1) = (G, \chi[u])$. By the induction hypothesis, $(G, \chi[u])$ is identified by $(\max\{2, k\} + d - 1)$-WL. Hence, by Lemma 2.2, (G, χ) is identified by $(\max\{2, k\} + d)$-WL. □

In analyzing the k-WL depth of (vertex-colored) graphs (G, χ), the challenge is when only the last option is applicable, i.e., (G, χ) is connected and flipped, and χ is stable with respect to k-WL, that is, it is not refined by it. In such a case, we say that (G, χ) is *k-robust*.

LEMMA 3.11. *Let $k \geq 1$ and suppose that (G, χ) is k-robust and $|V(G)| \geq 2$. Then $|\chi^{-1}(c)| \geq 2$ for every color $c \in \text{im}(\chi)$.*

PROOF. Suppose $|\chi^{-1}(c)| = 1$ for some color c, and let $v \in V(G)$ denote the unique vertex of color c. Since G is connected and $|V(G)| \geq 2$, there is some $w \in N(v)$. Let $D := \{w' \in V(G) \mid \chi(w') = \chi(w)\}$. Since χ is stable with respect to k-WL, we conclude that $D \subseteq N(v)$. But this contradicts (G, χ) being flipped since all edges are present between the color classes $\{v\}$ and D. □

For a graph G, a vertex coloring χ and a set $U \subseteq V(G)$, we define the coloring $\chi_{k,U}$ via $\chi_{k,U}(v) := \text{WL}^k[G, \chi[U]](v)$ for all $v \in V(G)$. For a single vertex $u \in V(G)$, we also set $\chi_{k,u} := \chi_{k,\{u\}}$.

Now, a simple strategy to bound the k-WL depth of a graph is, given a k-robust graph, to individualize a small set of vertices U so that the number of colors in $\chi_{k,U}$ increases as much as possible.

LEMMA 3.12. *Let $\xi, k \geq 1$ be integers. Suppose that, for every k-robust graph (G, χ) with $n > 1$ vertices, there is a set $U \subseteq V(G)$ such that $|\text{im}(\chi_{k,U})| \geq |\text{im}(\chi)| + \xi|U|$. Then*

$$\text{depth}^k_{\text{WL}}(G, \chi) \leq \frac{n-1}{\xi}$$

for every colored graph (G, χ).

PROOF. We prove that

$$\text{depth}^k_{\text{WL}}(G, \chi) \leq \frac{|V(G)| - |\text{im}(\chi)|}{\xi}. \tag{1}$$

for every colored graph (G, χ).

We prove (1) by induction on the tuple $(|V(G)|, |\text{im}(\chi)|, |E(G)|)$. Consider the set $M := \{(n, \ell, m) \in \mathbb{Z}^3_{\geq 0} \mid \ell \leq n\}$ and observe that $(|V(G)|, |\text{im}(\chi)|, |E(G)|) \in M$. For the induction, we define a linear order $\prec$ on M via $(n, \ell, m) \prec (n', \ell', m')$ if $n < n'$, or $n = n'$ and $\ell > \ell'$, or $n = n'$ and $\ell = \ell'$ and $m < m'$. Note that we use the inverse order on the second component, i.e., $(n, \ell, m) \prec (n, \ell', m')$ if $\ell > \ell'$. Still, since $\ell \leq n$ for every $(n, \ell, m) \in M$, there are no infinite decreasing chains in M.

For the base case, suppose $|V(G)| = 1$. Then $\text{depth}^1_{\text{WL}}(G, \chi) =$ $0 = \frac{|V(G)|-|\text{im}(\chi)|}{\xi}$ and the statement holds.

For the inductive step, suppose that (G, χ) is a colored graph with $|V(G)| > 1$. We distinguish several cases.

- First suppose that χ is not stable with respect to k-WL, i.e., $\chi^* \prec \chi$ where $\chi^*(v) := \text{WL}^k[G, \chi](v)$ for all $v \in V(G)$. Observe that $|\text{im}(\chi^*)| > |\text{im}(\chi)|$, so $(|V(G)|, |\text{im}(\chi^*)|, |E(G)|) \prec$ $(|V(G)|, |\text{im}(\chi)|, |E(G)|)$. Hence, by the induction hypothesis, we get

$$\text{depth}^k_{\text{WL}}(G, \chi^*) \leq \frac{|V(G)| - |\text{im}(\chi^*)|}{\xi}.$$

  Also, $\text{depth}^k_{\text{WL}}(G, \chi) \leq \text{depth}^k_{\text{WL}}(G, \chi^*)$ by Lemma 3.5(1). Together, we obtain that

$$\text{depth}^k_{\text{WL}}(G, \chi) \leq \text{depth}^k_{\text{WL}}(G, \chi^*) \leq \frac{|V(G)| - |\text{im}(\chi^*)|}{\xi} \leq \frac{|V(G)| - |\text{im}(\chi)|}{\xi}.$$

- Next, assume that (G, χ) is not flipped. Let $(G', \chi') := \text{flip}^*(G, \chi)$. Observe that $V(G') = V(G)$, $\chi' = \chi$ and $|E(G')| < |E(G)|$ hold.

Thus, $(|V(G')|, |\operatorname{im}(\chi')|, |E(G')|) \prec (|V(G)|, |\operatorname{im}(\chi)|, |E(G)|)$. Hence, by the induction hypothesis, we get

$$\operatorname{depth}^k_{\mathrm{WL}}(G', \chi') \leq \frac{|V(G')| - |\operatorname{im}(\chi')|}{\xi}.$$

Also, $\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^k_{\mathrm{WL}}(G', \chi')$ by Lemma 3.5(2). Together, we obtain that

$$\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^k_{\mathrm{WL}}(G', \chi') \leq \frac{|V(G')| - |\operatorname{im}(\chi')|}{\xi} = \frac{|V(G)| - |\operatorname{im}(\chi)|}{\xi}.$$

- Suppose G is not connected and let $A_1, \dots, A_\ell$ be the vertex sets of the connected components of G. Observe that $|A_i| < |V(G)|$ for all $i \in [\ell]$. By the induction hypothesis, we get

$$\operatorname{depth}^k_{\mathrm{WL}}(G[A_i], \chi|_{A_i}) \leq \frac{|A_i| - |\operatorname{im}(\chi|_{A_i})|}{\xi}$$

for all $i \in [\ell]$. Together with Lemma 3.5(3) we obtain

$$\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \max_{i \in [\ell]} \operatorname{depth}^k_{\mathrm{WL}}(G[A_i], \chi|_{A_i}) \leq \max_{i \in [\ell]} \frac{|A_i| - |\operatorname{im}(\chi|_{A_i})|}{\xi}.$$

Also, since $|A_i| - |\operatorname{im}(\chi|_{A_i})| \geq 0$, we get that

$$\max_{i \in [\ell]}(|A_i| - |\operatorname{im}(\chi|_{A_i})|) \leq \sum_{i \in [\ell]} (|A_i| - |\operatorname{im}(\chi|_{A_i})|) = |V(G)| - \sum_{i \in [\ell]} |\operatorname{im}(\chi|_{A_i})| \leq |V(G)| - |\operatorname{im}(\chi)|.$$

So $\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{\xi}$.

- Finally, suppose that (G, χ) is connected and flipped, $|V(G)| > 1$, and χ is stable with respect to k-WL. By assumption, there is a $U \subseteq V(G)$ such that $|\operatorname{im}(\chi_{k,U})| \geq |\operatorname{im}(\chi)| + \xi|U|$. In particular, $|\operatorname{im}(\chi_{k,U})| > |\operatorname{im}(\chi)|$, hence $(|V(G)|, |\operatorname{im}(\chi_{k,U})|, |E(G)|) \prec (|V(G)|, |\operatorname{im}(\chi)|, |E(G)|)$. Thus, by the induction hypothesis, we get

$$\operatorname{depth}^k_{\mathrm{WL}}(G, \chi_{k,U}) \leq \frac{|V(G)| - |\operatorname{im}(\chi_{k,U})|}{\xi}.$$

Also, applying Lemma 3.5(4) a total of $|U|$ many times and then Lemma 3.5(1), we obtain

$$\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^k_{\mathrm{WL}}(G, \chi[U]) + |U| \leq \operatorname{depth}^k_{\mathrm{WL}}(G, \chi_{k,U}) + |U|.$$

Together, it follows that

$$\operatorname{depth}^k_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^k_{\mathrm{WL}}(G, \chi_{k,U}) + |U| \leq \frac{n - |\operatorname{im}(\chi_{k,U})|}{\xi} + |U| \leq \frac{n - (|\operatorname{im}(\chi)| + \xi|U|) + \xi|U|}{\xi} = \frac{n - |\operatorname{im}(\chi)|}{\xi}. \quad \square$$

With this tool at hand, we can already obtain a first bound on the 1-WL depth of general graphs.

For a vertex-colored graph (G, χ), we define the graph $G[[\chi]]$ with vertex set $V(G[[\chi]]) \coloneqq \operatorname{im}(\chi)$ and edges

$$E(G[[\chi]]) \coloneqq \{(c_1, c_2) \mid E_G(\chi^{-1}(c_1), \chi^{-1}(c_2)) \neq \emptyset\}.$$

Here, we explicitly define $G[[\chi]]$ to contain self-loops, i.e., there is a loop $(c_1, c_1) \in E(G[[\chi]])$ if $E_G(\chi^{-1}(c_1), \chi^{-1}(c_1)) \neq \emptyset$. For $c_1 \in V(G[[\chi]])$, we set $\deg_{G[[\chi]]}(c_1) \coloneqq |\{c_2 \in V(G[[\chi]]) \mid (c_1, c_2) \in E(G[[\chi]])\}|$.

Lemma 3.13. *Let (G, χ) be a 1-robust graph such that $|V(G)| > 1$. Let $c \in \operatorname{im}(\chi)$ and set $\xi \coloneqq \deg_{G[[\chi]]}(c) + 1$. Then $|\operatorname{im}(\chi_{1,u})| \geq |\operatorname{im}(\chi)| + \xi$ for every $u \in \chi^{-1}(c)$.*

Proof. Let $c_1, \dots, c_d$ be the neighbors of c in the graph $G[[\chi]]$. We have that $|\operatorname{im}(\chi[u])| \geq |\operatorname{im}(\chi)| + 1$. Hence, it suffices to argue that $|\operatorname{im}(\chi_{1,u})| \geq |\operatorname{im}(\chi[u])| + d$. Let $i \in [d]$ and first suppose that $c_i \neq c$. Then the graph $G[\chi^{-1}(c), \chi^{-1}(c_i)]$ is biregular, because χ is stable with respect to 1-WL. Moreover, this graph contains at least one edge since $(c, c_i) \in E(G[[\chi]])$, and it is not a complete bipartite graph since (G, χ) is flipped. So, after individualizing u and performing 1-WL, the color class c_i is split.

For $c = c_i$, the same argument applies. The graph $G[\chi^{-1}(c)]$ contains at least one edge, since $(c, c) \in E(G[[\chi]])$, and it is not a complete graph, since (G, χ) is flipped. So, after individualizing u and performing 1-WL, the color class c is split one more time (following the split that occurs from individualizing u). □

Corollary 3.14. *Let (G, χ) be a colored graph. Then it holds that $\operatorname{depth}^1_{\mathrm{WL}}(G, \chi) \leq \frac{n-1}{2}$.*

Proof. Let (G, χ) be a 1-robust graph such that $|V(G)| > 1$. Then $\deg_{G[[\chi]]}(c) \geq 1$ for all $c \in \operatorname{im}(\chi)$. So the corollary follows from Lemmas 3.12 and 3.13 by setting $\xi = 2$. □

In combination with Lemma 3.10, we obtain that the WL dimension of every n-vertex graph is at most $\frac{n+3}{2}$ which essentially recovers the result from [28] using simpler arguments. In the following, we extend this type of argument to obtain improved bounds.

4 BOUNDING THE WL DEPTH IN THE VERTEX COVER NUMBER

In this section, we prove Theorem 1.3. On a high level, the strategy for the proof is similar to the one for Corollary 3.14, in which we have argued that for every 1-robust graph there is some vertex $u \in V(G)$ such that, after individualizing u and performing 1-WL, the number of colors in G increases by at least 2.

Let (G, χ) be a colored graph and let S be a vertex cover of G. An example is given in Figure 2. We intend to find a vertex $u \in V(G)$ such that, after individualizing u and performing 1-WL, the number of colors *in the set* S grows as much as possible. Indeed, as soon as all vertices in S have pairwise different colors, one can prove easily that the 1-WL depth is equal to 0.

To actually implement this idea, we rely on some additional instruments. First of all, note that a color appearing in the set S may also appear outside of S (i.e., there may be vertices $v \in S$ and $w \notin S$ with $\chi(v) = \chi(w)$). Here, our intuition is that it is preferable if colors only appear in the set S. This motivates us to consider a different progress measure which, instead of only

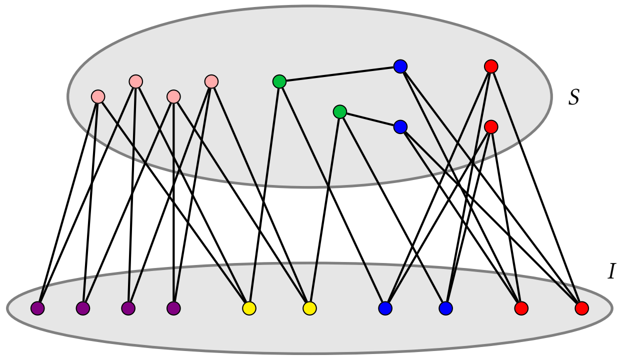

Figure 2: A colored graph (G, χ) and a vertex cover S of G. We set $I := V \setminus S$. The set $\chi(S)$ contains the colors red, blue, green and pink. The set $\chi(S) \setminus \chi(I)$ contains only green and pink. Hence, $p = 4 + 2 = 6$ in this example.

counting colors in S, also gives additional weight to colors that only appear in S. More precisely, we aim to increase the parameter $p := |\chi(S)| + |\chi(S) \setminus \chi(V \setminus S)|$ as much as possible using a single individualization followed by performing 1-WL. Since the maximum value of p is equal to $2|S|$, we need to increase p by at least 3 with a single individualization to achieve the desired bound.

To achieve this goal, we distinguish two cases. In the first case $\chi(S) \cap \chi(V \setminus S) \neq \emptyset$, and we prove that we have either reached the goal, or individualizing a single vertex and refining the coloring with 1-WL renders the two color sets disjoint. This is covered in Lemma 4.1 below. Note that, as opposed to Lemma 3.13, it is not possible to restrict our analysis to 1-robust graphs, since arbitrary flips in the edge set may change the vertex cover number. For this reason, we restrict ourselves to flips that only remove edges.

The second case $\chi(S) \cap \chi(V \setminus S) = \emptyset$ is then covered in Lemma 4.2. Here, we need to individualize up to two vertices together to ensure that the number of colors always increases by the desired amount.

Lemma 4.1. *Let (G, χ) be a colored graph such that $|V(G)| > 1$, G is connected and χ is stable with respect to 1-WL. Also let $S \subseteq V(G)$ be a vertex cover of G and define $I := V(G) \setminus S$.*

Then there are colors $c, d \in \text{im}(\chi)$ such that $|\chi^{-1}(c) \cup \chi^{-1}(d)| \geq 2$ and $vw \in E(G)$ for all distinct $v \in \chi^{-1}(c), w \in \chi^{-1}(d)$, or there is some vertex $u \in V(G)$ such that, for $\chi' := \text{WL}^1[G, \chi[u]]$, it holds that

(a) $|\chi'(S)| \geq |\chi(S)| + 2$ and $|\chi'(S) \setminus \chi'(I)| \geq |\chi(S) \setminus \chi(I)| + 1$,
(b) $|\chi'(S)| \geq |\chi(S)| + 1$ and $|\chi'(S) \setminus \chi'(I)| \geq |\chi(S) \setminus \chi(I)| + 2$, or
(c) $\chi'(S) \cap \chi'(I) = \emptyset$.

The proof of the lemma relies on a lengthy case distinction and can be found in the full version [19].

Lemma 4.2. *Let (G, χ) be a colored graph that is 1-robust and suppose $|V(G)| > 1$. Also let $S \subseteq V(G)$ be a vertex cover of G and define $I := V(G) \setminus S$. Moreover, suppose that $\chi(S) \cap \chi(I) = \emptyset$. Then*

(i) there is a vertex $u \in V(G)$ such that $|\chi_{1,u}(S)| \geq |\chi(S)| + 2$, or
(ii) there are vertices $u_1, u_2 \in V(G)$ such that $|\chi_{1,\{u_1,u_2\}}(S)| \geq |\chi(S)| + 3$.

Proof. We distinguish three cases.

- First suppose there are $u, w \in S$ such that $uw \in E(G)$. We claim that $|\chi_{1,u}(S)| \geq |\chi(S)| + 2$. Let $c := \chi(u)$, $d := \chi(w)$ and define $C := \chi^{-1}(c)$, $D := \chi^{-1}(d)$. We have that $|C|, |D| \geq 2$ since G is 1-robust (see Lemma 3.11).
  If $C \neq D$, then $D \not\subseteq N(u)$ since G is flipped. Hence, $|\chi_{1,u}(C)| \geq 2$ and $|\chi_{1,u}(D)| \geq 2$, which implies that $|\chi_{1,u}(S)| \geq |\chi(S)| + 2$.
  Otherwise, $C = D$. We have $C \cap N(u) \neq \emptyset$ and $C \setminus (N[u]) \neq \emptyset$. So $|\chi_{1,u}(C)| \geq 3$, which implies that $|\chi_{1,u}(S)| \geq |\chi(S)| + 2$.
- Next, suppose there are no $u, w \in S$ such that $uw \in E(G)$, and $|\chi(S)| \geq 2$. Then there is some $u \in I$ such that $|\chi(N(u))| \geq 2$, i.e., u is adjacent to least two color classes within S (observe that $N(u) \subseteq S$). Pick distinct $c, d \in \chi(N(u))$ and let $C := \chi^{-1}(c)$, $D := \chi^{-1}(d)$. Since G is flipped, we conclude that $C \setminus N(u) \neq \emptyset$ and $D \setminus N(u) \neq \emptyset$. So $|\chi_{1,u}(C)| \geq 2$ and $|\chi_{1,u}(D)| \geq 2$, which implies that $|\chi_{1,u}(S)| \geq |\chi(S)| + 2$.
- Finally, suppose there are no $u, w \in S$ such that $uw \in E(G)$, and $|\chi(S)| = 1$. Since G is flipped, we get that $|N(v)| \leq \frac{1}{2}|S|$ for all $v \in I$. Since G is connected, there must be vertices $u_1, u_2 \in I$ such that $N(u_1) \cap N(u_2) \neq \emptyset$ and $N(u_1) \not\subseteq N(u_2)$ and $N(u_2) \not\subseteq N(u_1)$. Then $N(u_1) \cup N(u_2) \neq S$ using that $|N(u_i)| \leq \frac{1}{2}|S|$ for both $i \in \{1, 2\}$. It follows that $|\chi_{1,\{u_1,u_2\}}(S)| \geq 4 = |\chi(S)| + 3$. □

With Lemmas 4.1 and 4.2 at our disposal, we can now bound the 1-WL depth in terms of the vertex cover number.

Theorem 4.3. *Let (G, χ) be a colored graph with vertex cover number r. Then*

$$\text{depth}^1_{\text{WL}}(G, \chi) \leq \frac{2}{3} \cdot r + 1.$$

The proof of the theorem follows the outline given above. On a technical level, it relies on an induction similar to the proof of Lemma 3.12. The details are given in the full version [19].

Corollary 4.4. *Let (G, χ) be a colored graph with vertex cover number r. Then (G, χ) has WL dimension at most $\frac{2}{3} \cdot r + 3$.*

Proof. This follows from Lemma 3.10 and Theorem 4.3. □

5 ADVANCED BOUNDS USING 2-WL

In this section, we improve on the bound on the WL depth of n-vertex graphs stated in Corollary 3.14 and prove Theorem 1.1. Towards this end, we need to rely on the 2-dimensional Weisfeiler–Leman algorithm. More precisely, we analyze the 2-WL depth of n-vertex graphs. The following theorem is the main result of this section.

Theorem 5.1. *Let (G, χ) be a colored graph. Then it holds that* $\text{depth}^2_{\text{WL}}(G, \chi) \leq \frac{n}{4} + o(n)$.

Together with Lemma 3.10, this immediately gives the following corollary.

Corollary 5.2. *The WL dimension of every n-vertex colored graph (G, χ) is at most $\frac{n}{4} + o(n)$.*

In particular, we obtain Theorem 1.1. Also, together with Theorem 2.1, we obtain Corollary 1.2.

On a high level, the proof of Theorem 5.1, which covers the rest of this section, again follows a similar strategy as the one for

Corollary 3.14. However, to obtain the improved bound, the details become significantly more intricate and we have to distinguish several cases.

Let (G, χ) be a vertex-colored graph and suppose that χ is stable with respect to 2-WL. We define

$$\mu_{G,\chi}(c_1, c_2) := |\{\mathsf{WL}^2[G, \chi](v_1, v_2) \mid v_1 \in \chi^{-1}(c_1), v_2 \in \chi^{-1}(c_2), v_1 \neq v_2\}|$$

for all $c_1, c_2 \in \mathrm{im}(\chi)$. Also, similarly as in Lemma 3.13, as a lower bound on the progress, i.e., how many new colors we get from a 2-WL refinement of a coloring after a vertex individualization, we set

$$\xi_{G,\chi}(c_1) := \sum_{c_2 \in \mathrm{im}(\chi)} (\mu_{G,\chi}(c_1, c_2) - 1).$$

Note that $\xi_{G,\chi}(c_1) \geq \deg_{G[[\chi]]}(c_1)$ for all colors $c_1 \in \mathrm{im}(\chi)$.

As before, we can restrict our attention to 2-robust graphs (G, χ) for which $|V(G)| > 1$. Towards this end, a vertex-colored graph (G, χ) is called *nice* if it is connected, flipped, $|V(G)| > 1$, and χ is stable with respect to 2-WL.

The next lemma, which is similar in nature to Lemma 3.13, forms the starting point of our analysis.

Lemma 5.3. *Let (G, χ) be a nice graph. Let $c \in \mathrm{im}(\chi)$ and set $\xi := \xi_{G,\chi}(c)+1$. Then $|\mathrm{im}(\chi_{2,u})| \geq |\mathrm{im}(\chi)|+\xi$ for every $u \in \chi^{-1}(c)$.*

Proof. Clearly, $\chi_{2,u} \preceq \chi$. So

$$\begin{aligned} |\mathrm{im}(\chi_{2,u})| &= \sum_{c' \in \mathrm{im}(\chi)} |\chi_{2,u}(\chi^{-1}(c'))| \\ &\geq 1 + \sum_{c' \in \mathrm{im}(\chi)} \mu_{G,\chi(c,c')} = |\mathrm{im}(\chi)| + \xi \end{aligned}$$

where the inequality follows from χ being stable with respect to 2-WL. □

If $\xi_{G,\chi}(c) \geq 3$, then $\xi \geq 4$ in the statement of the lemma. Thus, individualizing any vertex u of color c yields an increase in the number of color classes by at least 4, which is sufficient to show $\mathrm{depth}^2_{\mathsf{WL}}(G, \chi) \leq \frac{n}{4} + o(n)$. In the following, we thus consider nice graphs (G, χ) such that $\xi_{G,\chi}(c) \leq 2$ for all colors $c \in \mathrm{im}(\chi)$. In particular, this means that $G[[\chi]]$ has maximum degree 2. To cover the remaining cases, we rely on several tools from [2, 3].

Let (G, χ) be a colored graph and let $\lambda := \mathsf{WL}^2[G, \chi]$. For every $c \in \mathrm{im}(\lambda)$, we define the *constituent graph of c* to be the (undirected) graph F_c with vertex set $V(F_c) := V(G)$ and edge set

$$E(F_c) := \{vw \mid \lambda(v, w) = c\}.$$

Theorem 5.4 ([3, Theorem 2.1]). *Let (G, χ) be a colored graph and suppose that $\lambda := \mathsf{WL}^2[G, \chi]$. Also assume that*

(A) $c_0 := \lambda(v, v) = \lambda(w, w)$ for all $v, w \in V(G)$,
(B) $|\mathrm{im}(\lambda)| \geq 3$, and
(C) F_c is connected for every color $c \in \mathrm{im}(\lambda) \setminus \{c_0\}$.

Then there is a set $U \subseteq V(G)$ of size

$$|U| < 4\sqrt{n} \log n$$

such that $\chi_{2,U}$ is discrete.

For two sets A and B, we let $A \triangle B := (A \setminus B) \cup (B \setminus A)$ denote the symmetric difference of A and B.

Lemma 5.5 ([2]). *Let (G, χ) be a graph and let $D \subseteq V(G)$ such that $|N(v) \triangle N(w)| \geq \ell$ for all distinct $v, w \in D$. Then there is a set $U \subseteq V(G)$ such that $|U| \leq \frac{n}{\ell}(1 + 2 \log n)$ and $\chi_U(v, v) \neq \chi_U(w, w)$ for all distinct $v, w \in D$.*

A *hypergraph* is a pair $\mathcal{H} = (V, \mathcal{E})$ where V is a non-empty finite set of vertices and $\mathcal{E} \subseteq 2^V$ is the set of *hyperedges*. A hypergraph $\mathcal{H} = (V, \mathcal{E})$ is *non-empty* if $\mathcal{E} \neq \emptyset$. Also, $\mathcal{H}$ is *r-uniform* if $|E| = r$ for all $E \in \mathcal{E}$. Moreover, $\mathcal{H}$ is *k-regular* if for every $v \in V$, it holds that $|\{E \in \mathcal{E} \mid v \in E\}| = k$. We say $\mathcal{H}$ is *regular* if $\mathcal{H}$ is k-regular for some $k \geq 0$.

Lemma 5.6 ([2, Lemma 3.4]). *Suppose that $1 \leq d < r < n$. Let $\mathcal{H} = (V, \mathcal{E})$ be a non-empty regular r-uniform hypergraph such that $|E \cap E'| \geq d$ for all $E, E' \in \mathcal{E}$. Then $r^2 > nd$.*

Also, our analysis relies on the following auxiliary lemma. For a mapping $\lambda\colon V^2 \to C$ and two sets $U, W \subseteq V$, we let $\lambda(U, W) := \{\lambda(u, w) \mid u \in U, w \in W\}$.

Lemma 5.7. *Let (G, χ) be a colored graph and suppose that $\lambda := \mathsf{WL}^2[G, \chi]$. Also assume that there is a partition (V_1, V_2) of $V(G)$ such that*

(A) $|V_1| \geq 4$ and $|V_2| \geq 4$,
(B) $2 \leq |N_G(v_1) \cap V_2| \leq |V_2| - 2$ for all $v_1 \in V_1$, and
(C) $|\lambda(V_1, V_1)| = 2$, $|\lambda(V_2, V_2)| = 2$ and $\lambda(V_1, V_1) \cap \lambda(V_2, V_2) = \emptyset$.

Then there is a set $U \subseteq V(G)$ of size

$$|U| < 6\sqrt{n} \log n$$

such that $\chi_{2,U}$ is discrete.

Proof. Combining (A) and (C), we conclude that $k_1 := \deg(v_1) = \deg(v_1')$ for all $v_1, v_1' \in V_1$. Similarly, $k_2 := \deg(v_2) = \deg(v_2')$ for all $v_2, v_2' \in V_2$. We also have $\lambda(v_1, v_1') = \lambda(v_1'', v_1''')$ for all $v_1, v_1', v_1'', v_1''' \in V_1$ such that $v_1 \neq v_1'$ and $v_1'' \neq v_1'''$. In particular, $\mu_1 := |N(v_1) \cap N(v_1')| = |N(v_1'') \cap N(v_1''')|$ for all $v_1, v_1', v_1'', v_1''' \in V_1$ such that $v_1 \neq v_1'$ and $v_1'' \neq v_1'''$. Similarly, $\lambda(v_2, v_2') = \lambda(v_2'', v_2''')$ for all $v_2, v_2' v_2'', v_2''' \in V_2$ such that $v_2 \neq v_2'$ and $v_2'' \neq v_2'''$. We get that $2 \leq k_2 \leq |V_1| - 2$ and $\mu_2 := |N(v_2) \cap N(v_2')| = |N(v_2'') \cap N(v_2''')|$ for all $v_2, v_2', v_2'', v_2''' \in V_1$ such that $v_2 \neq v_2'$ and $v_2'' \neq v_2'''$.

Without loss of generality, assume that $|V_1| \leq |V_2|$. By transitioning to the complement of G, we may also suppose that $k_2 \leq \frac{1}{2} \cdot |V_1|$. Also note that $\mu_1 \geq 1$ by Condition (B). Moreover, $k_1 \cdot k_2 \geq |V_2| - 1$ and $|V_1| \cdot k_1 = |V_2| \cdot k_2$.

Claim 5.8. *$k_1^2 > \mu_1 |V_2|$ and $k_2^2 > \mu_2 |V_1|$.*

Proof. By symmetry, it suffices to prove the first statement. We define a hypergraph $\mathcal{H} = (V_2, \mathcal{E})$ where

$$\mathcal{E} := \{N(v_1) \mid v_1 \in V_1\}.$$

Then $\mathcal{H}$ is a regular and k_1-uniform hypergraph such that $|E \cap E'| \geq \mu_1$ for all $E, E' \in \mathcal{E}$. So $k_1^2 > \mu_1 |V_2|$ by Lemma 5.6. ⌟

Since $k_2 \leq \frac{1}{2}|V_1|$, we get that $\frac{1}{2}k_2 > \mu_2$. By the same argument, $\frac{1}{2}k_1 > \mu_1$.

Let $v_1, v_1' \in V_1$. Then $|N(v_1) \triangle N(v_1')| = 2(k_1 - \mu_1) > k_1$. So, by Lemma 5.5, there is a set $U \subseteq V(G)$ such that $|U| \leq \frac{n}{k_1}(1 + 2 \log n)$ and $\chi_U(v_1, v_1) \neq \chi_U(v_1', v_1')$ for all distinct $v_1, v_1' \in V_1$. This implies that χ_U is discrete. Also, $k_1^2 \geq |V_2| - 1 \geq \frac{1}{2}(n-1) \geq \frac{1}{4}n$ which implies that

$$\frac{n}{k_1}(1 + 2\log n) \leq 2\sqrt{n}(1 + 2\log n) \leq 6\sqrt{n}\log n. \qquad \square$$

Recall that, with Lemma 5.3 at hand, we can restrict our attention to nice graphs (G, χ) such that $\xi_{G,\chi}(c) \leq 2$ for all colors $c \in \operatorname{im}(\chi)$. Also, with Lemma 3.9 in mind, we may assume that (G, χ) is twin-free. The next lemma covers the first case in which $|\operatorname{im}(\chi)| \geq 4$.

Lemma 5.9. *Let (G, χ) be a nice and twin-free graph. Also suppose $\xi_{G,\chi}(c) \leq 2$ for all colors $c \in \operatorname{im}(\chi)$, and $|\operatorname{im}(\chi)| \geq 4$.*

Then there is a set $U \subseteq V(G)$ of size

$$|U| < 6\sqrt{n}\log n$$

such that $\chi_{2,U}$ is discrete.

Proof. There are $c_1, c_2, c_3, c_4 \in \operatorname{im}(\chi)$ such that

(i) $\mu_{G,\chi}(c_1, c_2) = \mu_{G,\chi}(c_2, c_3) = \mu_{G,\chi}(c_3, c_4) = 2$.

Note that this implies $\mu_{G,\chi}(c_2, c_2) = \mu_{G,\chi}(c_3, c_3) = 1$. Let $V_2 := \chi^{-1}(c_2)$ and $V_3 := \chi^{-1}(c_3)$.

First observe that G cannot induce a matching between V_2 and V_3, since otherwise $\mu_{G,\chi}(c_2, c_4) = \mu_{G,\chi}(c_3, c_4) = 2$. But this is not possible since $\xi_{G,\chi}(c_1) \leq 2$.

So we can apply Lemma 5.7 to obtain a set $U \subseteq V(G)$ of size

$$|U| < 6\sqrt{n}\log n$$

such that $\chi_{2,U}$ is discrete on the sets V_2 and V_3. However, then $\chi_{2,U}$ is discrete (on the entire vertex set of G) since G is twin-free and $\xi_{G,\chi}(c) \leq 2$ for all colors $c \in \operatorname{im}(\chi)$. $\square$

The next lemma allows us to cover the case $|\operatorname{im}(\chi)| \in \{2, 3\}$.

Lemma 5.10. *Let (G, χ) be a nice and twin-free graph. Also suppose $\xi_{G,\chi}(c) \leq 2$ for all colors $c \in \operatorname{im}(\chi)$, and $|\operatorname{im}(\chi)| \in \{2, 3\}$.*

Then there is some $U \subseteq V(G)$ such that $1 \leq |U| \leq 2$ and $|\operatorname{im}(\chi_{2,U})| \geq |\operatorname{im}(\chi)| + 4 \cdot |U|$, or there is a set $U \subseteq V(G)$ of size

$$|U| \leq 6n^{3/4}\log n$$

such that $\chi_{2,U}$ is discrete.

The proof can be found in the full version [19].

Finally, it remains to the cover the case $|\operatorname{im}(\chi)| = 1$. For $m \geq 1$ define the graph $L_{2,m}$ with vertex set $L_{2,m} := [2] \times [m]$ and edge set

$$E(L_{2,m}) := \{(i, j)(i', j') \mid i = i' \vee j = j'\}.$$

Lemma 5.11. *Let (G, χ) be a nice and twin-free graph. Also suppose that $|\operatorname{im}(\chi)| = 1$ and $\xi_{G,\chi}(c_0) \leq 2$ for the unique color $c_0 \in \operatorname{im}(\chi)$.*

Then one of the following holds:

(i) there is a set $U \subseteq V(G)$ of size $1 \leq |U| \leq 2$ such that $|\operatorname{im}(\chi_{2,U})| \geq 1 + 4 \cdot |U|$,

(ii) there is a set $U \subseteq V(G)$ of size

$$|U| < \max(6\sqrt{n}\log n, 24\log n)$$

such that $\chi_{2,U}$ is discrete, or

(iii) G is isomorphic to $L_{2,m}$ for some $m \geq 3$.

The proof of this lemma can also be found in the full version [19]. With this, we are finally ready to give the proof of Theorem 5.1.

Proof of Theorem 5.1. We define

$$f(n) := \max\left(6n^{3/4}\log n, 24\log n\right).$$

We prove that

$$\operatorname{depth}^2_{\mathrm{WL}}(G, \chi) \leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|). \tag{2}$$

for every vertex-colored graph (G, χ).

We prove (2) by induction on the tuple $(|V(G)|, |\operatorname{im}(\chi)|, |E(G)|)$. Consider the set $M := \{(n, \ell, m) \in \mathbb{Z}^3_{\geq 0} \mid \ell \leq n\}$ and observe that $(|V(G)|, |\operatorname{im}(\chi)|, |E(G)|) \in M$. For the induction, we define a linear order $\prec$ on M via $(n, \ell, m) \prec (n', \ell', m')$ if $n < n'$, or $n = n'$ and $\ell > \ell'$, or $n = n'$ and $\ell = \ell'$ and $m < m'$. Note that we use the inverse order on the second component, i.e., $(n, \ell, m) \prec (n, \ell', m')$ if $\ell > \ell'$. Still, since $\ell \leq n$ for every $(n, \ell, m) \in M$, there are no infinite decreasing chains in M.

For the base case, suppose $|V(G)| = 1$. Then $\operatorname{depth}^1_{\mathrm{WL}}(G, \chi) = 0 = \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|)$ and the statement holds.

For the inductive step, suppose (G, χ) is a colored graph with $|V(G)| > 1$. We distinguish several cases.

- First suppose that χ is not stable with respect to 2-WL, i.e., $\chi^* \prec \chi$ where $\chi^*(v) := \mathrm{WL}^2[G, \chi](v)$ for all $v \in V(G)$. Observe that $|\operatorname{im}(\chi^*)| > |\operatorname{im}(\chi)|$, so $(|V(G)|, |\operatorname{im}(\chi^*)|, |E(G)|) \prec (|V(G)|, |\operatorname{im}(\chi)|, |E(G)|)$. Hence, by the induction hypothesis, we get

$$\operatorname{depth}^2_{\mathrm{WL}}(G, \chi^*) \leq \frac{|V(G)| - |\operatorname{im}(\chi^*)|}{4} + f(|V(G)|).$$

  Also, $\operatorname{depth}^2_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^2_{\mathrm{WL}}(G, \chi^*)$ by Lemma 3.5(1). Together, we obtain that

$$\begin{aligned}\operatorname{depth}^2_{\mathrm{WL}}(G, \chi) &\leq \operatorname{depth}^2_{\mathrm{WL}}(G, \chi^*)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi^*)|}{4} + f(|V(G)|)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|).\end{aligned}$$

- Next, suppose that (G, χ) is not flipped. Define $(G', \chi') := \operatorname{flip}^*(G, \chi)$. Observe that $V(G') = V(G)$, $\chi' = \chi$ and $|E(G')| < |E(G)|$ hold. We conclude that $(|V(G')|, |\operatorname{im}(\chi')|, |E(G')|) \prec (|V(G)|, |\operatorname{im}(\chi)|, |E(G)|)$. Hence, by the induction hypothesis, we get

$$\operatorname{depth}^2_{\mathrm{WL}}(G', \chi') \leq \frac{|V(G')| - |\operatorname{im}(\chi')|}{4} + f(|V(G')|).$$

  Also, $\operatorname{depth}^2_{\mathrm{WL}}(G, \chi) \leq \operatorname{depth}^2_{\mathrm{WL}}(G', \chi')$ by Lemma 3.5(2). Together, we obtain that

$$\begin{aligned}\operatorname{depth}^2_{\mathrm{WL}}(G, \chi) &\leq \operatorname{depth}^2_{\mathrm{WL}}(G', \chi')\\ &\leq \frac{|V(G')| - |\operatorname{im}(\chi')|}{4} + f(|V(G')|)\\ &= \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|).\end{aligned}$$

- Suppose that G is not connected and let $A_1, \dots, A_\ell$ be the vertex sets of the connected components of G. Observe that $|A_i| < |V(G)|$ for all $i \in [\ell]$. By the induction hypothesis, we get

$$\operatorname{depth}^2_{\mathrm{WL}}(G[A_i], \chi|_{A_i}) \leq \frac{|A_i| - |\operatorname{im}(\chi|_{A_i})|}{4} + f(|A_i|)$$

for all $i \in [\ell]$. Together with Lemma 3.5(3), we obtain

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq \max_{i\in[\ell]} \text{depth}^2_{\text{WL}}(G[A_i],\chi|_{A_i})\\ &\leq \max_{i\in[\ell]} \frac{|A_i| - |\operatorname{im}(\chi|_{A_i})|}{4} + f(|A_i|).\end{aligned}$$

Also, since $|A_i| - |\operatorname{im}(\chi|_{A_i})| \geq 0$, we get that

$$\begin{aligned}\max_{i\in[\ell]}(|A_i| - |\operatorname{im}(\chi|_{A_i})|) &\leq \sum_{i\in[\ell]}(|A_i| - |\operatorname{im}(\chi|_{A_i})|)\\ &= |V(G)| - \sum_{i\in[\ell]} |\operatorname{im}(\chi|_{A_i})|\\ &\leq |V(G)| - |\operatorname{im}(\chi)|.\end{aligned}$$

Additionally, f is monotonically increasing. So $\text{depth}^2_{\text{WL}}(G,\chi) \leq \frac{|V(G)|-|\operatorname{im}(\chi)|}{4} + f(|V(G)|)$.

- So we may assume that (G,χ) is nice. Next, suppose (G,χ) is not twin-free and let π be a twin-partition of G. Observe that $|\pi| < |V(G)|$, so by the induction hypothesis we get

$$\text{depth}^2_{\text{WL}}(G/\pi,\chi/\pi) \leq \frac{|\pi| - |\operatorname{im}(\chi/\pi)|}{4} + f(|\pi|).$$

In combination with Lemma 3.9, we conclude that

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq \text{depth}^2_{\text{WL}}(G/\pi,\chi/\pi)\\ &\leq \frac{|\pi| - |\operatorname{im}(\chi/\pi)|}{4} + f(|\pi|).\end{aligned}$$

We have that $|\operatorname{im}(\chi)| \geq |\operatorname{im}(\chi/\pi)|$ using that χ is not refined by 2-WL. So

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq \frac{|\pi| - |\operatorname{im}(\chi/\pi)|}{4} + f(|\pi|)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|)\end{aligned}$$

using again that f is monotonically increasing.

- So we may suppose that (G,χ) is nice and twin-free. Next, suppose there is some $c \in \operatorname{im}(\chi)$ such that $\xi_{G,\chi}(c) \geq 3$. Let $u \in \chi^{-1}(c)$. Then $|\operatorname{im}(\chi_{2,u})| \geq |\operatorname{im}(\chi)| + 4$ by Lemma 5.3. So

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq 1 + \text{depth}^2_{\text{WL}}(G,\chi_{2,u})\\ &\leq 1 + \frac{|V(G)| - |\operatorname{im}(\chi_{2,u})|}{4} + f(|V(G)|)\\ &\leq 1 + \frac{|V(G)| - (|\operatorname{im}(\chi)| + 4)}{4} + f(|V(G)|)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|)\end{aligned}$$

where the first inequality follows from Lemma 3.5 and the second inequality holds by the induction hypothesis.

- So we may additionally assume that $\xi_{G,\chi}(c) \leq 2$ for every $c \in \operatorname{im}(\chi)$. Finally, we distinguish several cases based on $|\operatorname{im}(\chi)|$.
  - First suppose that $|\operatorname{im}(\chi)| \geq 4$. By Lemma 5.9, there is a set $U \subseteq V(G)$ of size

$$|U| < 6\sqrt{n}\log n \leq f(n)$$

such that $\chi_{2,U}$ is discrete. By Lemma 3.5 we conclude that

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq |U| + \text{depth}^2_{\text{WL}}(G,\chi_{2,U})\\ &\leq |U| + 0 \leq f(|V(G)|)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|)\end{aligned}$$

where the second inequality holds since $\chi_{2,U}$ is discrete (see also Example 3.4).

  - Next, suppose that $|\operatorname{im}(\chi)| \in \{2,3\}$. We apply Lemma 5.10 and obtain a set $U \subseteq V(G)$ such that $1 \leq |U| \leq 2$ and $|\operatorname{im}(\chi_{2,U})| \geq |\operatorname{im}(\chi)| + 4 \cdot |U|$, or a set $U \subseteq V(G)$ of size

$$|U| \leq 6n^{3/4}\log n \leq f(n)$$

such that $\chi_{2,U}$ is discrete. In the latter case, we get that $\text{depth}^2_{\text{WL}}(G,\chi) \leq f(n) \leq \frac{|V(G)|-|\operatorname{im}(\chi)|}{4} + f(|V(G)|)$ similar to the previous case. In the former case, we have

$$\begin{aligned}\text{depth}^2_{\text{WL}}(G,\chi) &\leq |U| + \text{depth}^2_{\text{WL}}(G,\chi_{2,U})\\ &\leq |U| + \frac{|V(G)| - |\operatorname{im}(\chi_{2,U})|}{4} + f(|V(G)|)\\ &\leq |U| + \frac{|V(G)| - (|\operatorname{im}(\chi)| + 4|U|)}{4} + f(|V(G)|)\\ &\leq \frac{|V(G)| - |\operatorname{im}(\chi)|}{4} + f(|V(G)|)\end{aligned}$$

where the first inequality follows from Lemma 3.5 and the second inequality holds by the induction hypothesis.

  - Finally, assume that $|\operatorname{im}(\chi)| = 1$, in which case we use Lemma 5.11. If Option (i) or (ii) is satisfied, we proceed as in the previous case. So suppose Option (iii) is satisfied, i.e., G is isomorphic to $L_{2,m}$ for some $m \geq 3$. Then it is easy to check that $\text{depth}^2_{\text{WL}}(G,\chi) = 1 \leq \frac{|V(G)|-|\operatorname{im}(\chi)|}{4} + f(|V(G)|)$ (after individualizing an arbitrary vertex and performing 2-WL, repeatedly flipping and splitting into connected components results in graphs with only a single vertex). □

6 LOWER BOUND ON THE WL DIMENSION

In this section, we provide lower bounds on the WL dimension. First, we show a lower bound in terms of the number of vertices. The proof is based on the following theorem, which can be obtained from [10, Lemma 5 and Corollary 7].

For a graph G, we use $\text{tw}(G)$ to denote the tree-width of G. Since we do not need the actual definition of the tree-width, we skip it here and refer to graph-theory textbooks for it (for example, [9]).

Theorem 6.1. *There exists an integer n_0 such that for every even $n \geq n_0$, there exists a 3-regular graph G on n vertices such that*

$$\text{tw}(G) \geq \frac{1}{24}n - 1.$$

To obtain graphs with high WL dimension from 3-regular graphs of large tree-width, we rely on the Cai-Fürer-Immerman construction [7]. In order to keep the number of vertices as small as possible, we rely on a slightly modified construction (see, e.g., [25, 29]).

Let G be a graph and let $U \subseteq V(G)$. For $v \in V(G)$, we define $\delta_{v,U} := |\{v\} \cap U|$. Also, we let $E(v) := \{e \in E(G) \mid v \in e\}$, i.e., $E(v)$ denotes the set of edges incident to v. We define the graph

$\mathrm{CFI}(G, U)$ with vertex set

$$V(\mathrm{CFI}(G,U)) \coloneqq \{(v,S) \mid v \in V(G), S \subseteq E(v), |S| \equiv \delta_{v,U} \bmod 2\}$$

and edge set

$$E(\mathrm{CFI}(G,U)) \coloneqq \{(v,S)(u,T) \mid uv \in E(G), uv \notin S \triangle T\}.$$

Note that if G is a 3-regular graph with n vertices, then we have

$$|V(\mathrm{CFI}(G,U))| = 4n.$$

The following lemma is well known (see, e.g., [7, 29]).

Lemma 6.2. *Let G be a connected graph and let $U, U' \subseteq V(G)$. Then $\mathrm{CFI}(G,U) \cong \mathrm{CFI}(G,U')$ if and only if $|U| \equiv |U'| \bmod 2$.*

We define $\mathrm{CFI}(G) \coloneqq \mathrm{CFI}(G, \emptyset)$ and $\mathrm{CFI}^{\times}(G) \coloneqq \mathrm{CFI}(G, \{u\})$ for some $u \in V(G)$.

The next lemma relates the WL dimension of $\mathrm{CFI}(G)$ to the tree-width of the base graph G. A variant of this lemma already appears for example in [8] with the underlying ideas dating back to [7]. The concrete statement given below follows for example from [25, Lemma 12] and [7, 14].

Lemma 6.3. *Let G be a connected graph. Then $\mathrm{CFI}(G) \simeq_k \mathrm{CFI}^{\times}(G)$ for every $k < \mathrm{tw}(G)$. In particular, the Weisfeiler–Leman dimension of $\mathrm{CFI}(G)$ is at least $\mathrm{tw}(G)$.*

Now, we can combine Theorem 6.1 and Lemma 6.3 to obtain a concrete lower bound on the WL dimension in terms of the number of vertices.

Theorem 6.4. *There exists an integer n_0 such that for every $n \geq n_0$ that is divisible by 8, there is an n-vertex graph G_n whose Weisfeiler–Leman dimension is at least $\frac{1}{96}n - 1$.*

Proof. Let n_0' denote the constant from Theorem 6.1 and define $n_0 \coloneqq 4n_0'$. Let $n \geq n_0$ denote an integer that is divisible by 8, and let $n' \coloneqq \frac{n}{4}$. Observe that n' is even. So by Theorem 6.1, there exists a 3-regular graph B_n on n' vertices such that

$$\mathrm{tw}(B_n) \geq \frac{1}{24}n' - 1.$$

We define $G_n \coloneqq \mathrm{CFI}(B_n)$. We have $|V(G_n)| = 4n' = n$ as desired. Thus, by Lemma 6.3, the WL dimension of G_n is at least

$$\mathrm{tw}(B_n) \geq \frac{1}{24}n' - 1 = \frac{1}{96}n - 1. \qquad \square$$

Next, we modify the argument to obtain a better lower bound on the WL dimension in terms of the vertex cover number. To this end, we construct a vertex cover for the CFI graphs.

Theorem 6.5. *There exists an integer r_0 such that for every $r \geq r_0$ that is divisible by 6, there is a graph G_r of vertex cover number at most r whose Weisfeiler–Leman dimension is at least $\frac{1}{72}r - 1$.*

Proof. Let n_0' denote the constant from Theorem 6.1 and define $r_0 \coloneqq 3n_0'$. Let $r \geq r_0$ denote an integer that is divisible by 6, and let $n' \coloneqq \frac{r}{3}$. Just like in the proof of Theorem 6.4, there is a 3-regular graph B_r on n' vertices such that the WL dimension of $G_r \coloneqq \mathrm{CFI}(B_r)$ is at least $\frac{1}{24}n' - 1 = \frac{1}{72}r - 1$.

Since B_r is 3-regular, we can greedily construct an independent set I in B_r of size at least $\frac{n'}{4}$. Indeed, for every vertex that we include in I, at most three of the remaining vertices are disqualified, so altogether, we can include at least $\frac{n'}{4}$ vertices in I.

Define $C \coloneqq V(B_r) \setminus I$. Note that C is a vertex cover of B_r. Also, it is easy to see that the set

$$C' \coloneqq \{(v,S) \in V(G_r) \mid v \in C\}$$

is a vertex cover of G_r. We have

$$|C'| = 4 \cdot |C| \leq 4 \cdot \frac{3}{4} \cdot n' = 3n' = r,$$

i.e., the graph G_r has vertex cover number at most r. $\square$

7 CONCLUSION

We have shown that the WL dimension of every n-vertex graph is in $(\frac{1}{4} + o(1))n$. This implies that every n-vertex graph can be defined in the counting logic C with $(\frac{1}{4} + o(1))n$ many variables. Our contribution improves on the previous bound of $\frac{n+3}{2}$ on the number of variables [28]. In fact, they proved that for every two non-isomorphic n-vertex graphs G and H, there is an FO-formula with at most $\frac{n+3}{2}$ variables that distinguishes G and H. Since their bound is (essentially) tight for the logic FO, our results for C also yield that the ability to count does allow us to reduce the number of variables that are needed to define arbitrary n-vertex graphs.

To obtain the results, we have introduced the concept of the k-*WL depth* of a graph and have proved that the 2-WL depth of every n-vertex graph is at most $(\frac{1}{4} + o(1))n$. Still, there is a significant gap towards the lower bound of $(\frac{1}{96} - o(1))n$ that can be obtained via the CFI construction. By pushing the arguments developed in this paper, it seems possible to obtain further improvements of the upper bound, but the case analyses will become significantly more complex. Independently and after the submission of this work, Schneider and Schweitzer published an upper bound of $(\frac{3}{20} + o(1))n$ on the WL dimension of n-vertex graphs [30]. Future work may explore to what extent their methods can be combined with ours to make further progress.

The WL depth is a concept that might raise interest in the context of graph identification beyond the scope of this work. We have shown that the 1-WL depth of a graph with vertex cover number r is at most $\frac{2}{3}r + 1$, which implies the first non-trivial upper bound on the WL dimension in terms of r. Can similar results be obtained for other graph parameters? For example, it is not difficult to show that the k-WL depth of a graph G is at most the tree-depth of G (for every $k \geq 1$). Are there a $k \in \mathbb{N}$ and an $\varepsilon > 0$ such that

$$\mathrm{depth}^{k}_{\mathrm{WL}}(G, \chi) \leq (1 - \varepsilon + o(1)) \cdot t$$

holds for every vertex-colored graph (G, χ) of tree-depth at most t?

ACKNOWLEDGMENTS

Sandra Kiefer's research was supported by the Glasstone Benefaction, University of OxfordViolette and Samuel Glasstone Research Fellowships in Science 2022] as well as Jesus College in Oxford

Daniel Neuen was partially funded by the European Union (ERC CountHom, 101077083). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

REFERENCES

[1] Vikraman Arvind, Roman Nedela, Ilia Ponomarenko, and Peter Zeman. 2022. Testing Isomorphism of Chordal Graphs of Bounded Leafage is Fixed-Parameter Tractable (Extended Abstract). In *Graph-Theoretic Concepts in Computer Science - 48th International Workshop, WG 2022, Tübingen, Germany, June 22-24, 2022, Revised Selected Papers (Lecture Notes in Computer Science, Vol. 13453)*, Michael A. Bekos and Michael Kaufmann (Eds.). Springer, 29–42. https://doi.org/10.1007/978-3-031-15914-5_3

[2] László Babai. 1980. On the Complexity of Canonical Labeling of Strongly Regular Graphs. *SIAM J. Comput.* 9, 1 (1980), 212–216. https://doi.org/10.1137/0209018

[3] László Babai. 1981. On the order of uniprimitive permutation groups. *Ann. of Math. (2)* 113, 3 (1981), 553–568. https://doi.org/10.2307/2006997

[4] László Babai. 2016. Graph isomorphism in quasipolynomial time [extended abstract]. In *Proceedings of the 48th Annual ACM SIGACT Symposium on Theory of Computing, STOC 2016, Cambridge, MA, USA, June 18-21, 2016*, Daniel Wichs and Yishay Mansour (Eds.). ACM, 684–697. https://doi.org/10.1145/2897518.2897542

[5] László Babai, Xi Chen, Xiaorui Sun, Shang-Hua Teng, and John Wilmes. 2013. Faster Canonical Forms for Strongly Regular Graphs. In *54th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2013, 26-29 October, 2013, Berkeley, CA, USA*. IEEE Computer Society, 157–166. https://doi.org/10.1109/FOCS.2013.25

[6] László Babai, Paul Erdős, and Stanley M. Selkow. 1980. Random Graph Isomorphism. *SIAM J. Comput.* 9, 3 (1980), 628–635. https://doi.org/10.1137/0209047

[7] Jin-yi Cai, Martin Fürer, and Neil Immerman. 1992. An optimal lower bound on the number of variables for graph identification. *Comb.* 12, 4 (1992), 389–410. https://doi.org/10.1007/BF01305232

[8] Anuj Dawar and David Richerby. 2007. The Power of Counting Logics on Restricted Classes of Finite Structures. In *Computer Science Logic, 21st International Workshop, CSL 2007, 16th Annual Conference of the EACSL, Lausanne, Switzerland, September 11-15, 2007, Proceedings (Lecture Notes in Computer Science, Vol. 4646)*, Jacques Duparc and Thomas A. Henzinger (Eds.). Springer, 84–98. https://doi.org/10.1007/978-3-540-74915-8_10

[9] Reinhard Diestel. 2012. *Graph Theory, 4th Edition*. Graduate texts in mathematics, Vol. 173. Springer.

[10] Zdenek Dvorák and Sergey Norin. 2016. Strongly Sublinear Separators and Polynomial Expansion. *SIAM J. Discret. Math.* 30, 2 (2016), 1095–1101. https://doi.org/10.1137/15M1017569

[11] Martin Grohe. 2017. *Descriptive Complexity, Canonisation, and Definable Graph Structure Theory*. Lecture Notes in Logic, Vol. 47. Cambridge University Press. https://doi.org/10.1017/9781139028868

[12] Martin Grohe and Sandra Kiefer. 2019. A Linear Upper Bound on the Weisfeiler–Leman Dimension of Graphs of Bounded Genus. In *46th International Colloquium on Automata, Languages, and Programming, ICALP 2019, July 9-12, 2019, Patras, Greece (LIPIcs, Vol. 132)*, Christel Baier, Ioannis Chatzigiannakis, Paola Flocchini, and Stefano Leonardi (Eds.). Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 117:1–117:15. https://doi.org/10.4230/LIPIcs.ICALP.2019.117

[13] Martin Grohe and Daniel Neuen. 2023. Canonisation and Definability for Graphs of Bounded Rank Width. *ACM Trans. Comput. Log.* 24, 1 (2023), 6:1–6:31. https://doi.org/10.1145/3568025

[14] Neil Immerman and Eric Lander. 1990. Describing Graphs: A First-Order Approach to Graph Canonization. In *Complexity Theory Retrospective: In Honor of Juris Hartmanis on the Occasion of His Sixtieth Birthday, July 5, 1988*, Alan L. Selman (Ed.). Springer New York, New York, NY, 59–81. https://doi.org/10.1007/978-1-4612-4478-3_5

[15] Tommi A. Junttila and Petteri Kaski. 2007. Engineering an Efficient Canonical Labeling Tool for Large and Sparse Graphs. In *Proceedings of the Nine Workshop on Algorithm Engineering and Experiments, ALENEX 2007, New Orleans, Louisiana, USA, January 6, 2007*. SIAM. https://doi.org/10.1137/1.9781611972870.13

[16] Tommi A. Junttila and Petteri Kaski. 2011. Conflict Propagation and Component Recursion for Canonical Labeling. In *Theory and Practice of Algorithms in (Computer) Systems - First International ICST Conference, TAPAS 2011, Rome, Italy, April 18-20, 2011. Proceedings (Lecture Notes in Computer Science, Vol. 6595)*, Alberto Marchetti-Spaccamela and Michael Segal (Eds.). Springer, 151–162. https://doi.org/10.1007/978-3-642-19754-3_16

[17] Sandra Kiefer. 2020. The Weisfeiler–Leman algorithm: an exploration of its power. *ACM SIGLOG News* 7, 3 (2020), 5–27. https://doi.org/10.1145/3436980.3436982

[18] Sandra Kiefer and Daniel Neuen. 2022. The Power of the Weisfeiler-Leman Algorithm to Decompose Graphs. *SIAM J. Discret. Math.* 36, 1 (2022), 252–298. https://doi.org/10.1137/20m1314987

[19] Sandra Kiefer and Daniel Neuen. 2024. Bounding the Weisfeiler-Leman Dimension via a Depth Analysis of I/R-Trees. *CoRR* abs/2402.03274 (2024). https://doi.org/10.48550/arXiv.2402.03274 arXiv:2402.03274

[20] Sandra Kiefer, Ilia Ponomarenko, and Pascal Schweitzer. 2019. The Weisfeiler–Leman Dimension of Planar Graphs Is at Most 3. *J. ACM* 66, 6 (2019), 44:1–44:31. https://doi.org/10.1145/3333003

[21] Brendan D. McKay. 1981. Practical graph isomorphism. *Congr. Numer.* 30 (1981), 45–87.

[22] Brendan D. McKay and Adolfo Piperno. 2014. Practical graph isomorphism, II. *J. Symb. Comput.* 60 (2014), 94–112. https://doi.org/10.1016/j.jsc.2013.09.003

[23] Christopher Morris, Yaron Lipman, Haggai Maron, Bastian Rieck, Nils M. Kriege, Martin Grohe, Matthias Fey, and Karsten Borgwardt. 2023. Weisfeiler and Leman go machine learning: the story so far. *J. Mach. Learn. Res.* 24, 333 (2023), 1–59. http://jmlr.org/papers/v24/22-0240.html

[24] Daniel Neuen. 2022. Isomorphism Testing for Graphs Excluding Small Topological Subgraphs. In *Proceedings of the 2022 ACM-SIAM Symposium on Discrete Algorithms, SODA 2022, Virtual Conference / Alexandria, VA, USA, January 9 - 12, 2022*, Joseph (Seffi) Naor and Niv Buchbinder (Eds.). SIAM, 1411–1434. https://doi.org/10.1137/1.9781611977073.59

[25] Daniel Neuen. 2024. Homomorphism-Distinguishing Closedness for Graphs of Bounded Tree-Width. In *41st International Symposium on Theoretical Aspects of Computer Science, STACS 2024, March 12-14, 2024, Clermont-Ferrand, France (LIPIcs, Vol. 289)*, Olaf Beyersdorff, Mamadou Moustapha Kanté, Orna Kupferman, and Daniel Lokshtanov (Eds.). Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 53:1–53:12. https://doi.org/10.4230/LIPICS.STACS.2024.53

[26] Daniel Neuen. 2024. Isomorphism Testing Parameterized by Genus and Beyond. *SIAM J. Discret. Math.* 38, 1 (2024), 453–484. https://doi.org/10.1137/22m1514076

[27] Martin Otto. 2017. *Bounded Variable Logics and Counting: A Study in Finite Models*. Lecture Notes in Logic, Vol. 9. Cambridge University Press. https://doi.org/10.1017/9781316716878

[28] Oleg Pikhurko, Helmut Veith, and Oleg Verbitsky. 2006. The first order definability of graphs: Upper bounds for quantifier depth. *Discret. Appl. Math.* 154, 17 (2006), 2511–2529. https://doi.org/10.1016/J.DAM.2006.03.002

[29] David E. Roberson. 2022. Oddomorphisms and homomorphism indistinguishability over graphs of bounded degree. *CoRR* abs/2206.10321 (2022). arXiv:2206.10321

[30] Thomas Schneider and Pascal Schweitzer. 2024. An Upper Bound on the Weisfeiler-Leman Dimension. *CoRR* abs/2403.12581 (2024). https://doi.org/10.48550/arXiv.2403.12581 arXiv:2403.12581

[31] Daniel A. Spielman. 1996. Faster Isomorphism Testing of Strongly Regular Graphs. In *Proceedings of the Twenty-Eighth Annual ACM Symposium on the Theory of Computing, Philadelphia, Pennsylvania, USA, May 22-24, 1996*, Gary L. Miller (Ed.). ACM, 576–584. https://doi.org/10.1145/237814.238006

[32] Boris Weisfeiler and Andrei Leman. 1968. The reduction of a graph to canonical form and the algebra which appears therein. *NTI, Series 2* (1968). English translation by Grigory Ryabov available at https://www.iti.zcu.cz/wl2018/pdf/wl_paper_translation.pdf.