The Power of the Weisfeiler-Leman Algorithm to Decompose Graphs

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Abstract

The Weisfeiler-Leman procedure is a widely-used approach for graph isomorphism testing that works by iteratively computing an isomorphism-invariant coloring of vertex tuples. Meanwhile, a fundamental tool in structural graph theory, which is often exploited in approaches to tackle the graph isomorphism problem, is the decomposition into 2- and 3-connected components.

We prove that the 2-dimensional Weisfeiler-Leman algorithm implicitly computes the decomposition of a graph into its 3-connected components. Thus, the dimension of the algorithm needed to distinguish two given graphs is at most the dimension required to distinguish the corresponding decompositions into 3-connected components (assuming dimension at least 2).

This result implies that for $k \ge 2$, the k-dimensional algorithm distinguishes k-separators, i.e., k-tuples of vertices that separate the graph, from other vertex k-tuples. As a byproduct, we also obtain insights about the connectivity of constituent graphs of association schemes.

In an application of the results, we show the new upper bound of k on the Weisfeiler-Leman dimension of graphs of treewidth at most k. Using a construction by Cai, Fürer, and Immerman, we also provide a new lower bound that is asymptotically tight up to a factor of 2.

${f 1}$ Introduction

Originally introduced in [36], the Weisfeiler-Leman (WL) algorithm has become a – if not the – fundamental subroutine in the context of isomorphism testing for graphs. It is used in theoretical as well as in practical approaches to tackle the graph isomorphism problem (see e.g. [5, 18, 30, 31, 34]), among them also Babai's recent quasipolynomial-time isomorphism test [4]. For every $k \geq 1$, there is a k-dimensional version of the algorithm which colors the vertex k-tuples of the input graph and iteratively refines the coloring in an isomorphism-invariant manner.

There are various characterizations of the algorithm, which link it to other areas in theoretical computer science (see also Further Related Work). For example, very recent results in the context of machine learning show that the 1-dimensional version of the algorithm is as expressive as graph neural networks with respect to distinguishing graphs [33]. Following Grohe [15], an indicator to investigate the expressive power of the algorithm is the so-called WL dimension of a graph, defined as the minimal dimension of the WL algorithm required in order to distinguish the graph from every other non-isomorphic graph.

There is no fixed dimension of the algorithm that decides graph isomorphism in general, as was proved by Cai, Fürer, and Immerman [9]. Still, when focusing on particular graph classes, often a bounded dimension of the algorithm suffices to identify every graph in the class. This proves that for the considered class, graph isomorphism is solvable in polynomial time, since the k-dimensional WL algorithm can be implemented in time $\mathcal{O}(n^{k+1} \log n)$ [26]. For example, it suffices to apply the 3-dimensional WL algorithm to identify every planar graph [27]. Also, the WL dimension of graphs of treewidth at most k is bounded by k + 2 [17]. More generally, by a celebrated result by Grohe, for all graph classes with an excluded minor, the WL dimension is bounded [14]. Very recent work provides explicit upper bounds on the WL dimension, which are linear in the rank width [18] and in the Euler genus [16], respectively, of the graph.

Regarding combinatorial techniques, to handle graphs with complex structures, the decomposition into connected, biconnected, and triconnected components provides a fundamental tool from structural graph theory. The decomposition can be computed in linear time (see e.g. [23, 35]). Hopcroft and Tarjan used the decomposition of a graph into its triconnected components to obtain an algorithm that decides isomorphism for planar graphs in quasi-linear time [21, 22, 24], which was improved to linear time by Hopcroft and Wong [25].

Also, in [27], to prove the bound on the WL dimension for the class of planar graphs, the challenge of distinguishing two arbitrary planar graphs is reduced to the case of two arc-colored triconnected planar graphs, by exploiting the fact that the 3-dimensional WL algorithm is able to implicitly compute the decomposition of a graph into its triconnected components. Similarly, the bound on the WL dimension for graphs parameterized by their Euler genus from [16] relies on an isomorphism-invariant decomposition of the graphs into their triconnected components.

Our Contribution We show that for $k \geq 2$, the k-dimensional WL algorithm implicitly computes the decomposition into the triconnected components of a given graph. More specifically, we prove that already the 2-dimensional WL algorithm distinguishes separating pairs, i.e., pairs of vertices that separate the given graph, from other vertex pairs. This improves on a result from [27], where an analogous statement was proved for the 3-dimensional WL algorithm. Using the decomposition techniques discussed there, we conclude that for the k-dimensional WL algorithm with $k \geq 2$, to identify a graph, it suffices to determine vertex orbits on all arc-colored 3-connected components of it. Since it is easy to see that k = 1 does not suffice to distinguish vertices contained in 2-separators from others, our upper bound of 2 is tight.

The expressive power of the k-dimensional algorithm corresponds to definability in the logic C^{k+1} , the extension of the (k+1)-variable fragment of first-order logic by counting quantifiers [9, 26]. Exploiting this correspondence, our results imply that for every $n \in \mathbb{N}$, there is a formula $\varphi_n(x_1, x_2) \in \mathbb{C}^3$ (first-order logic with counting quantifiers over three variables) such that for every n-vertex graph G, it holds that $G \models \varphi_n(v, w)$ if and only if $\{v, w\}$ is a 2-separator in G. With only three variables at our disposal, it is not possible to take the route of [27] by comparing certain numbers of walks between different pairs of vertices. Instead, the formulas obtained from our proof are essentially a disjunction over all n-vertex graphs and subformulas for two distinct graphs may look completely different, exploiting specific structural properties of the graphs. While this makes the proof rather involved, it also stresses the power of the 2-dimensional WL algorithm and equivalently, the expressive power of the logic \mathbb{C}^3 . We actually show that for all $n, s \in \mathbb{N}$, there is a formula $\varphi_{n,s}(x_1, x_2, x_3) \in \mathbb{C}^3$ such that for every n-vertex graph G, it holds that $G \models \varphi_{n,s}(u, v, w)$ if and only if s = |C|, where C is the vertex set of the connected component containing u after removing v and w from the graph G.

Our result can also be viewed in a combinatorial setting. In 1985, Brouwer and Mesner [8] proved that the vertex connectivity of a strongly regular graph equals its valency and that in fact, the only minimal disconnecting vertex sets are neighborhoods. Later, Brouwer conjectured

this to be true for any constituent graph of an association scheme (i.e., any graph consisting in a single color class of the association scheme) [6]. While some progress has been made on certain special cases [12], most prominently distance-regular graphs [7], the general question is still open. Our results imply that any connected constituent graph of an association scheme is either a cycle or 3-connected. Such a statement was previously only known for symmetric association schemes [29], which are far more restricted than the general ones.

A natural use case of these results is to determine or to improve upper bounds on the WL dimension of certain graph classes. As a first application in this direction, we obtain a new upper bound of k on the WL dimension for graphs of treewidth at most k. Based on [10], we also provide a new lower bound for this graph class, thus delimiting the value of the WL dimension of graphs of treewidth bounded by k to the interval $\left\lceil \left\lceil \frac{k}{2} \right\rceil - 3, k \right\rceil$.

Further Related Work Apart from its correspondence to counting logics, the Weisfeiler-Leman algorithm has further surprising links to other areas. For example, the algorithm has a close connection to Sherali-Adams relaxations of particular linear programs [3, 19] and captures the same information as certain homomorphism counts [11]. It can also be characterized via winning strategies in so-called pebble games [20], which are a particular family of Ehrenfeucht-Fraissë games.

As mentioned above, the 1-dimensional WL algorithm essentially corresponds to graph neural networks. In order to make them more powerful, the authors of [33] propose an extension of graph neural networks based on the k-dimensional WL algorithm (see also [32]).

Towards understanding the expressive power of the algorithm, in a related direction of research, it has been studied which graph properties the WL algorithm can detect, which may become particularly relevant in the graph-learning framework. In this context, Fürer [13] as well as Arvind et al. [2] obtained results concerning the ability of the algorithm to detect and count certain subgraphs.

2 Preliminaries

2.1 Graphs

A graph is a pair G = (V(G), E(G)) of a vertex set V(G) and an edge set $E(G) \subseteq \{\{u, v\} \mid u, v \in V(G)\}$. All graphs considered in this paper are finite, simple (i.e., they contain no loops or multiple edges), and undirected. For $v, w \in V$, we also write vw as a shorthand for $\{v, w\}$. The neighborhood of v is denoted by N(v), and the closed neighborhood of v is $N[v] := N(v) \cup \{v\}$. The degree of v, denoted by V(v), is the number of edges incident with v. For $V(v) \cap V(v)$ we define $V(v) := \{v\}$ and $V(v) \cap V(v) \cap V(v)$.

define $N(X) \coloneqq \left(\bigcup_{v \in X} N(v)\right) \setminus X$. A walk of length k from v to w is a sequence of vertices $v = u_0, u_1, \ldots, u_k = w$ such that $u_{i-1}u_i \in E$ for all $i \in \{1, \ldots, k\}$. A path of length k from v to w is a walk of length k from v to w for which all occurring vertices are pairwise distinct. We refer to the distance between two vertices $v, w \in V(G)$ by $\operatorname{dist}(v, w)$. For a set $A \subseteq V(G)$, we denote by G[A] the induced subgraph of G on vertex set A. Also, we denote by G[A] the subgraph induced by the complement of A, that is, the graph $G - A \coloneqq G[V(G) \setminus A]$. A set $S \subseteq V(G)$ is a separator of G if G - S has more connected components than G. A k-separator of G is a separator of G of size k. A vertex $v \in V(G)$ is a cut vertex if $\{v\}$ is a separator of G. The graph G is k-connected if it is connected and has no (k-1)-separator.

An isomorphism from G to another graph H is a bijection $\varphi \colon V(G) \to V(H)$ that respects the edge relation, that is, for all $v, w \in V(G)$, it holds that $vw \in E(G)$ if and only if $\varphi(v)\varphi(w) \in V(G)$

E(H). Two 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.

A vertex-colored graph is a tuple (G, χ) , where G is a graph and $\chi \colon V(G) \to \mathcal{C}$ is a mapping into some set \mathcal{C} of colors. Similarly, an arc-colored graph is a tuple (G, χ) , where G is a graph and $\chi \colon \{(v, v) \mid v \in V(G)\} \cup \{(u, v) \mid \{u, v\} \in E(G)\} \to \mathcal{C}$ is a mapping into some color set \mathcal{C} . Typically, \mathcal{C} is chosen to be an initial segment $[n] \coloneqq \{1, \ldots, n\}$ of the natural numbers. Isomorphisms between vertex- and arc-colored graphs have to respect the colors of the vertices and arcs.

We recall the definition of the treewidth of a graph. For more background on tree decompositions and treewidth, we refer the reader to [28]. Let G be a graph. A tree decomposition of G is a pair (T,β) where T is a tree and $\beta \colon V(T) \to 2^{V(G)}$ is a function (where $2^{V(G)}$ denotes the power set of V(G)) such that

- 1. for every $v \in V(G)$, the set $\{t \in V(T) \mid v \in \beta(t)\}$ is non-empty and induces a connected subgraph in T, and
- 2. for every $e \in E(G)$, there is a $t \in V(T)$ such that $e \subseteq \beta(t)$.

The sets $\beta(t)$ for $t \in V(T)$ are the bags of the tree decomposition. The width of a tree decomposition (T, β) is

$$\operatorname{width}(T,\beta) \coloneqq \max_{t \in V(T)} |\beta(t)| - 1.$$

The treewidth of G, denoted by tw(G), is the minimum width of a tree decomposition of G.

2.2 The Weisfeiler-Leman Algorithm

Let $\chi_1, \chi_2 \colon V^k \to \mathcal{C}$ be colorings of the k-tuples of vertices of G, where \mathcal{C} is some finite set of colors. We say χ_2 refines χ_1 if for all $\bar{v}, \bar{w} \in V^k$ we have $(\chi_2(\bar{v}) = \chi_2(\bar{w}) \Rightarrow \chi_1(\bar{v}) = \chi_1(\bar{w}))$. The k-dimensional WL algorithm is a procedure that, given a graph G and a coloring χ of its k-tuples of vertices, computes an isomorphism-invariant coloring that refines χ .

We describe the mechanisms of the algorithm in the following. For an integer k > 1 and a vertex-colored graph (G, χ) , we let $\chi^0_{G,k} \colon V^k \to \mathcal{C}$ be the coloring where each k-tuple is colored with the isomorphism type of its underlying ordered colored subgraph. More formally, $\chi^0_{G,k}(v_1,\ldots,v_k) = \chi^0_{G,k}(w_1,\ldots,w_k)$ if and only if for all $i \in [k]$ it holds that $\chi(v_i) = \chi(w_i)$, and for all $i,j \in [k]$, it holds that $v_i = v_j \Leftrightarrow w_i = w_j$ and $v_iv_j \in E(G) \Leftrightarrow w_iw_j \in E(G)$. If G is arc-colored, the arc colors must be respected accordingly.

We then recursively define the coloring $\chi_{G,k}^i$ obtained after i rounds of the algorithm. Let $\chi_{G,k}^{i+1}(v_1,\ldots,v_k) := (\chi_{G,k}^i(v_1,\ldots,v_k);\mathcal{M})$, where \mathcal{M} is a multiset defined as

$$\left\{\!\!\left\{ \left(\chi_{G,k}^{i}(\bar{v}[w/1]),\chi_{G,k}^{i}(\bar{v}[w/2]),\ldots,\chi_{G,k}^{i}(\bar{v}[w/k])\right) \,\middle|\, w \in V \right\}\!\!\right\}$$

where $\bar{v}[w/i] := (v_1, \dots, v_{i-1}, w, v_{i+1}, \dots, v_k).$

For the 1-dimensional algorithm (i.e. k=1), the definition is similar, but we iterate only over the neighbors of v_1 , that is, the multiset \mathcal{M} equals $\{\!\!\{\chi^i_{G,1}(w)\mid w\in N(v_1)\}\!\!\}$.

By definition, every coloring $\chi_{G,k}^{i+1}$ induces a refinement of the partition of the k-tuples of vertices of the graph G with coloring $\chi_{G,k}^i$. Thus, there is a minimal i such that the partition of the vertex k-tuples induced by $\chi_{G,k}^{i+1}$ is not strictly finer than the one induced by $\chi_{G,k}^i$. For this value of i, we call the coloring $\chi_{G,k}^i$ the *stable* coloring of G and denote it by $\chi_{G,k}$.

The original WL algorithm is its 2-dimensional variant [36]. Since that version is the central algorithm of this paper, we omit the index 2 and write χ_G instead of $\chi_{G,2}$.

For $k \in \mathbb{N}$, the k-dimensional WL algorithm takes as input a (vertex- or arc-)colored graph (G,χ) and returns the coloring $\chi_{G,k}$. The procedure can be implemented in time $O(n^{k+1}\log n)$ [26]. For two graphs G and H, we say that the k-dimensional WL algorithm distinguishes G and H if there is a color c such that the sets $\{\bar{v} \mid \bar{v} \in (V(G))^k, \chi_{G,k}(\bar{v}) = c\}$ and $\{\bar{w} \mid \bar{w} \in (V(H))^k, \chi_{H,k}(\bar{w}) = c\}$ have different cardinalities. We write $G \simeq_k H$ if the k-dimensional WL algorithm does not distinguish G and H. The algorithm identifies G if it distinguishes G from every non-isomorphic graph H.

Pebble Games For further analysis, it is often cumbersome to work with the WL algorithm directly and more convenient to use the following characterization via pebble games, which is known to capture the same information. Let $k \in \mathbb{N}$. For graphs G and H on the same number of vertices and with vertex colorings χ and χ' , respectively, we define the *bijective k-pebble game* $BP_k(G, H)$ as follows:

- The game has two players called Spoiler and Duplicator.
- The game proceeds in rounds, each of which is associated with a pair of positions (\bar{v}, \bar{w}) with $\bar{v} \in (V(G))^{\ell}$ and $\bar{w} \in (V(H))^{\ell}$, where $0 \le \ell \le k$.
- The initial position of the game is a pair of vertex tuples of equal length ℓ with $0 \le \ell \le k$. If not specified otherwise, the initial position is the pair ((),()) of empty tuples.
- Each round consists of the following steps. Suppose the current position of the game is $(\bar{v}, \bar{w}) = ((v_1, \dots, v_\ell), (w_1, \dots, w_\ell))$. First, Spoiler chooses whether to remove a pair of pebbles or to play a new pair of pebbles. The first option is only possible if $\ell > 0$, and the latter option is only possible if $\ell < k$.

If Spoiler wishes to remove a pair of pebbles, he picks some $i \in [\ell]$ and the game moves to position $(\bar{v} \setminus i, \bar{w} \setminus i)$ where $\bar{v} \setminus i := (v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_{\ell})$, and the tuple $(\bar{w} \setminus i)$ is defined in the analogous way. Otherwise, the following steps are performed.

- (D) Duplicator picks a bijection $f: V(G) \to V(H)$.
- (S) Spoiler chooses $v \in V(G)$ and sets w := f(v). Then the game moves to position $((v_1, \ldots, v_\ell, v), (w_1, \ldots, w_\ell, w))$.

If for the current position $((v_1, \ldots, v_\ell), (w_1, \ldots, w_\ell))$, the induced ordered subgraphs of G and H are not isomorphic, Spoiler wins the play. More precisely, Spoiler wins if there is an $i \in [\ell]$ such that $\chi(v_i) \neq \chi'(w_i)$, or there are $i, j \in [\ell]$ such that $v_i = v_j \Leftrightarrow w_i = w_j$ or $v_i v_j \in E(G) \Leftrightarrow w_i w_j \in E(H)$. If there is no position of the play such that Spoiler wins, then Duplicator wins.

We say that Spoiler (and Duplicator, respectively) wins the bijective k-pebble game $BP_k(G, H)$ if Spoiler (and Duplicator, respectively) has a winning strategy for the game.

The following theorem describes the correspondence between the Weisfeiler-Leman algorithm and the introduced pebble games.¹

Theorem 2.1 (see e.g. [9]). Let G and H be two graphs. Then $G \simeq_k H$ if and only if Duplicator wins the game $BP_{k+1}(G, H)$.

¹The pebble games in [9] are defined slightly differently. Still, a player has a winning strategy in the game described there if and only if they have one in our game and thus, Theorem 2.1 holds for both versions of the game.

Association Schemes Let V be a set. An association scheme on V is an ordered partition (R_0, \ldots, R_d) of V^2 such that

- 1. $R_0 = \{(v, v) \mid v \in V\}$, and
- 2. for every $i \in [d]$, there is a $j \in [d]$ such that the set $R_i^{\mathsf{T}} := \{(w, v) \mid (v, w) \in R_i\}$ equals R_j , and
- 3. for all $i, j, k \in [d]$, there are numbers $p_{i,j}^k$ such that for all $(v, w) \in R_k$,

$$p_{i,j}^k = |\{x \in V \mid (v,x) \in R_i \text{ and } (w,x) \in R_j\}|.$$

An association scheme is symmetric if $R_i^{\mathsf{T}} = R_i$ for all $i \in [d]$. With each R_i , we associate a directed constituent graph $G(R_i)$ of the association scheme, defined as $G(R_i) := (V, R_i \cup R_i^{\mathsf{T}})$.

Every association scheme induces a coloring on V^2 , in which every (v, w) is colored with the relation it is contained in. This coloring is stable in the sense that it is not refined by the 2-dimensional WL algorithm (when V is interpreted as the vertex set of a complete directed graph). That is, for all $j \in [d]$ and all $(v_1, v_2), (w_1, w_2) \in R_j$, it holds that $\chi_{G(R_i)}(v_1, v_2) = \chi_{G(R_i)}(w_1, w_2)$. Conversely, every colored graph G with $\chi_{G}(v, v) = \chi_{G}(w, w)$ for all $v, w \in V(G)$ induces an association scheme in which the relations R_i are the color classes of the coloring $\chi_{G} = \chi_{G,2}$.

3 One Color

Our first goal is to prove that the 2-dimensional WL algorithm distinguishes vertex pairs that are separators in a graph from other pairs of vertices. We start with an analysis of the graphs in which all vertices are assigned the same color by the algorithm. In particular, this includes all constituent graphs of association schemes.

A main tool for the analysis are distance patterns of vertices. For a graph G and a vertex $v \in V(G)$, let $D(v) := \{\{\operatorname{dist}(v,w) \mid w \in V(G)\}\}$. Note that for vertices $u,v \in V(G)$, it holds that $\chi_G(u,u) \neq \chi_G(v,v)$ whenever $D(u) \neq D(v)$, since the 2-dimensional WL algorithm detects distances between vertex pairs.

Lemma 3.1. Let G be a graph and $uv \in E(G)$. Suppose that D(u) = D(v). Then

$$\{ \{ \operatorname{dist}(u, w) \mid w \in V(G) \colon \operatorname{dist}(u, w) < \operatorname{dist}(v, w) \} \}$$

$$= \{ \{ \operatorname{dist}(v, w) \mid w \in V(G) \colon \operatorname{dist}(v, w) < \operatorname{dist}(u, w) \} \}.$$

Proof. We have $|\operatorname{dist}(v,w) - \operatorname{dist}(u,w)| \leq 1$ for all $w \in V(G)$ since $uv \in E(G)$. Suppose the statement is false and let $d \in \mathbb{N}$ be the maximal number such that d has distinct multiplicities in the two multisets. Let m_1 be the multiplicity of d in the first multiset and m_2 be the multiplicity of d in the second. Without loss of generality, assume that $m_1 > m_2$. Then

$$m_1 = |\{w \in V(G) \mid \text{dist}(u, w) = d \land \text{dist}(v, w) = d + 1\}|$$

and

$$m_2 = |\{w \in V(G) \mid \text{dist}(v, w) = d \land \text{dist}(u, w) = d + 1\}|.$$

But

$$\begin{aligned} &|\{w \in V(G) \mid \mathrm{dist}(u,w) = d+1 \wedge \mathrm{dist}(v,w) = d+1\}| \\ &= |\{w \in V(G) \mid \mathrm{dist}(v,w) = d+1 \wedge \mathrm{dist}(u,w) = d+1\}| \end{aligned}$$

and

$$|\{w \in V(G) \mid \operatorname{dist}(u, w) = d + 2 \wedge \operatorname{dist}(v, w) = d + 1\}|$$

= $|\{w \in V(G) \mid \operatorname{dist}(v, w) = d + 2 \wedge \operatorname{dist}(u, w) = d + 1\}|$,

where the first equality is trivial and the second equality follows from the maximality of d. However, then D(u) and D(v) contain the number d+1 in distinct multiplicities, a contradiction.

Throughout the remainder of this section, if not explicitly stated otherwise, we make the following assumption.

Assumption 3.2. G is a connected graph on n vertices with the following properties:

- 1. $\chi_G(u,u) = \chi_G(v,v)$ for all $u,v \in V(G)$, and
- 2. G has a 2-separator $\{w_1, w_2\}$.

In the rest of this section, we analyze the structure of G and ultimately prove that G must be a cycle. In particular, this completely characterizes constituent graphs of association schemes that are connected, but not 3-connected.

Note that Assumption 3.2 implies that G is regular, i.e., deg(u) = deg(v) for all $u, v \in V(G)$.

Lemma 3.3. G is 2-connected, i.e., G does not contain any cut vertex.

This is a consequence of Condition 1 in Assumption 3.2, since the 2-dimensional WL algorithm distinguishes cut vertices from other vertices (see [27, Corollary 7]) and it is easy to see that it is not possible that every vertex in G is a cut vertex. Note that the lemma implies that each of w_1 and w_2 has at least one neighbor in each of the connected components of $G - w_1 w_2$.

Lemma 3.4. Let C be the vertex set of a connected component of $G - w_1w_2$ such that $|C| < \frac{n}{2}$ and let $v \in C$. Then there is no vertex $u \in N(v)$ such that $\operatorname{dist}(u, w_1) < \operatorname{dist}(v, w_1)$ and $\operatorname{dist}(u, w_2) < \operatorname{dist}(v, w_2)$.

Proof. Suppose towards a contradiction that such a vertex $u \in N(v)$ exists. For all $w \in V(G)$, we have $|\operatorname{dist}(v,w)-\operatorname{dist}(u,w)| \leq 1$, since $uv \in E(G)$. Furthermore, we have $\sum_{w \in V(G)} \left(\operatorname{dist}(v,w)-\operatorname{dist}(u,w)\right) = 0$ because D(v) = D(u) due to Condition 1 in Assumption 3.2. But $\operatorname{dist}(v,w) > \operatorname{dist}(u,w)$ for all $w \in V(G) \setminus C$, and $|V(G) \setminus C| > \frac{n}{2}$. This is a contradiction.

Lemma 3.5. Let $d := \operatorname{dist}(w_1, w_2)$ and let C be the vertex set of a connected component of $G - w_1 w_2$ such that $|C| \le \frac{n-2}{2}$. Then for all $v \in C \cup \{w_1, w_2\}$ and all $i \in \{1, 2\}$, it holds that $\operatorname{dist}(v, w_i) \le d$.

Proof. By symmetry, it suffices to prove $\operatorname{dist}(v, w_2) \leq d$. The statement is proved by induction on $\ell := \operatorname{dist}(v, w_1)$. For $\ell = 0$, it holds that $v = w_1$ and $\operatorname{dist}(w_1, w_2) = d$. So suppose the statement holds for all $u \in C \cup \{w_1, w_2\}$ with $\operatorname{dist}(u, w_1) \leq \ell$. Obviously, the statement is true if $v = w_1$ or $v = w_2$. So pick $v \in C$ with $\operatorname{dist}(v, w_1) = \ell + 1$. Let $u \in N(v)$ such that $\operatorname{dist}(u, w_1) \leq \ell$. Then $\operatorname{dist}(v, w_2) \leq \operatorname{dist}(u, w_2) \leq d$ by Lemma 3.4 and the induction hypothesis.

Lemma 3.6. $w_1w_2 \notin E(G)$.

Proof. Suppose towards a contradiction that $w_1w_2 \in E(G)$. Let C be the vertex set of a connected component of $G - w_1w_2$ such that $|C| \leq \frac{n-2}{2}$. By Lemma 3.5, we conclude that $C \subseteq N(w_1) \cap N(w_2)$. Let $v \in C$. Since G is 2-connected, the vertex w_1 must have at least one neighbor in $V(G) \setminus C$, in addition to being adjacent to C and to w_2 . Thus, $\deg(w_1) \geq |C| + 2 > |C| - 1 + |\{w_1, w_2\}| \geq \deg(v)$, which contradicts G being a regular graph. \square

Lemma 3.7. Suppose that $N(w_1) \cap N(w_2) \neq \emptyset$. Then G is a cycle.

Proof. By Lemma 3.6, it holds that $w_1w_2 \notin E(G)$. Furthermore, by the assumption of the lemma, we have $\operatorname{dist}(w_1, w_2) = 2$. Let C be the vertex set of a connected component of $G - w_1w_2$ such that $|C| \leq \frac{n-2}{2}$. Also let $C' := V(G) \setminus (C \cup \{w_1, w_2\})$. For $i, j \geq 1$ let

$$C_{i,j} := \{v \in C \mid \operatorname{dist}(v, w_1) = i \text{ and } \operatorname{dist}(v, w_2) = j\}.$$

By Lemma 3.5, we conclude that $C_{i,j} = \emptyset$ unless $(i,j) \in \{(1,1),(1,2),(2,1),(2,2)\}.$

Suppose there exists $v \in C_{1,2}$. We have $D(v) = D(w_1)$ and, by Lemma 3.3, also $N(w_1) \cap C' \neq \emptyset$. Thus, there is a vertex $u' \neq w_1$ such that $\operatorname{dist}(w_1, u') < \operatorname{dist}(v, u')$ and therefore, by Lemma 3.1, there is also a vertex $u \neq v$ such that $\operatorname{dist}(v, u) < \operatorname{dist}(w_1, u)$. For every such vertex u, it holds that $\operatorname{dist}(w_1, u) \leq 2$ and thus, $u \in N(v)$. Therefore, by Lemma 3.1, for every vertex $v' \neq w_1$ with $\operatorname{dist}(w_1, v') < \operatorname{dist}(v, v')$, it holds that $v' \in N(w_1)$. This implies that there is no $v' \in C'$ such that $\operatorname{dist}(w_1, v') = 2$ since such a vertex would satisfy $3 = \operatorname{dist}(v, v') > \operatorname{dist}(w_1, v')$. Because w_2 is not a cut vertex (cf. Lemma 3.3), from every $v' \in C'$, there is a path to w_1 that does not contain w_2 . However, this is only possible if there is no vertex $v' \in C'$ such that $\operatorname{dist}(w_1, v') > 1$, in other words: $C' \subseteq N(w_1)$. Since G is regular and $|N(w_1) \setminus C'| \geq 1$, it follows that $\operatorname{deg}(v) \geq |C'| + 1$. But $N(v) \subseteq (C \cup \{w_1\}) \setminus \{v\}$, which implies $\operatorname{deg}(v) \leq |C|$. The combination of both inequalities yields $|C'| + 1 \leq |C|$, which implies $n = 2 + |C| + |C'| \leq 1 + 2|C| \leq n - 1$, a contradiction. So $C_{1,2} = \emptyset$ and by symmetry, it also holds that $C_{2,1} = \emptyset$. But then $C_{2,2} = \emptyset$ by Lemma 3.4.

So $C = C_{1,1}$, which means that $C \subseteq N(w_1) \cap N(w_2)$. In particular, $\deg(w_1) \ge |C| + 1$ since $|N(w_1) \cap C'| \ge 1$. Since G is regular, this implies that $\deg(v) \ge |C| + 1$ for every $v \in C$, which is only possible if $N[v] = C \cup \{w_1, w_2\}$. Because $C \ne \emptyset$, this means that there is a vertex $v \in V(G)$ such that G[N[v]] contains only one non-edge. Now by Condition 1 in Assumption 3.2, this also has to hold for w_1 , and hence, since no vertex in $C \cap N(w_1)$ is adjacent to any vertex in $C' \cap N(w_1)$, it must hold that $\deg(w_1) = 2$. Therefore, by regularity, all vertices in G have degree 2 and thus, being connected, G is a cycle.

Lemma 3.8. G is a cycle.

Proof. It suffices to prove the lemma for the case that G is a graph with a maximum edge set that satisfies Assumption 3.2. Indeed, if G is a cycle, then G has n edges, and the lemma trivially holds for every graph with less edges, since every connected regular graph has at least n edges.

Let $d := \operatorname{dist}(w_1, w_2)$. By Lemmas 3.6 and 3.7, we can assume that $d \ge 3$. Let C be the vertex set of a connected component of $G - w_1 w_2$ of size $|C| \le \frac{n-2}{2}$. Also let $C' := V(G) \setminus (C \cup \{w_1, w_2\})$. For $i, j \ge 1$, let

$$C_{i,j} := \{v \in C \mid \operatorname{dist}(v, w_1) = i \text{ and } \operatorname{dist}(v, w_2) = j\}.$$

By Lemma 3.5, we conclude that $C_{i,j} = \emptyset$ unless $i, j \leq d$. Furthermore, by the definition of d, we have that $C_{i,j} = \emptyset$ unless $i + j \geq d$. This situation is also visualized in Figure 1.

Claim 1.
$$C_{d,d} = C_{d-1,d} = C_{d,d-1} = \emptyset$$
.

Proof. We argue that $C_{d,d} = C_{d-1,d} = \emptyset$. By symmetry, we also obtain that $C_{d,d-1} = \emptyset$.

Suppose towards a contradiction that $C_{d,d} \cup C_{d-1,d} \neq \emptyset$ and pick $v \in C_{\ell,d}$ for some $\ell \in \{d, d-1\}$. Let v_0, \ldots, v_ℓ be a shortest path from $w_1 = v_0$ to $v = v_\ell$. By an easy inductive argument and Lemmas 3.4 and 3.5, it follows that $v_i \in C_{i,d}$ for every $1 \leq i \leq \ell$. In particular, $C_{1,d} \neq \emptyset$.

Now let $v' \in C_{1,d}$ and consider an arbitrary vertex $u \neq v'$ such that $\operatorname{dist}(v', u) < \operatorname{dist}(w_1, u)$ (a possible choice is $u = v_2$, since $d \geq 3$). Then $u \in C$ and $\operatorname{dist}(v', u) \leq d - 1$ by Lemma 3.5. Since $D(v') = D(w_1)$, we conclude that for every vertex $u \neq w_1$ with $\operatorname{dist}(v', u) > \operatorname{dist}(w_1, u)$, it holds that $\operatorname{dist}(w_1, u) \leq d - 1$ (cf. Lemma 3.1). In particular, $\operatorname{dist}(w_1, u) \leq d - 1$ for all $u \in C'$.

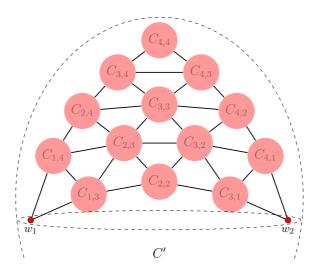


Figure 1: Visualization of the sets $C_{i,j}$ for d=4 in the proof of Lemma 3.8. Each arc between two sets indicates that there may be edges connecting vertices from the two sets.

Overall, this means that, on the one hand, $\operatorname{dist}(w_1, u) \leq d$ for all $u \in V(G)$. On the other hand, there is a $u \in C'$ such that $\operatorname{dist}(w_1, u) \geq 2$ because $d \geq 3$. But then $\operatorname{dist}(v, u) \geq d + 1$ for $v \in C_{d,d} \cup C_{d-1,d}$. So $D(w_1) \neq D(v)$, which is a contradiction.

Claim 2. Let $u, v \in V(G)$ such that dist(u, v) < d. Then there is a unique shortest path from u to v.

Proof. Suppose the statement does not hold and let $\ell < d$ be the minimal number for which the claim is violated. Let $u, v \in V(G)$ be two vertices such that there are two paths of length $\ell = \operatorname{dist}(u,v)$ from u to v. Also let $E' := \{u'v' \mid \chi_G(u,v) = \chi_G(u',v')\}$ and consider the graph $G' := (V(G), E(G) \cup E')$, i.e., the graph obtained from G by inserting all (undirected) edges contained in the set E'. We argue that G' still satisfies Assumption 3.2, which contradicts the edge maximality of G.

First, the coloring χ_G is also a stable coloring for G', which implies that χ_G refines the coloring $\chi_{G'}$. In particular, Condition 1 of Assumption 3.2 is satisfied for the graph G'.

Now let $u'v' \in E'$. Then $\operatorname{dist}(u',v') = \ell$ and there are at least two different walks of length ℓ from u' to v' because the same statement holds for u and v. Due to the minimality of ℓ , the two walks are internally vertex-disjoint paths. If u' and v' lie in different connected components of $G - w_1w_2$, then one of the two paths must pass through w_1 and one through w_2 , forming a cycle of length $2\ell < 2d$. This implies $\operatorname{dist}(w_1, w_2) < d$, a contradiction. Thus, we conclude that there is a connected component with vertex set C of $G - w_1w_2$ such that $u', v' \in C \cup \{w_1, w_2\}$. But this means Condition 2 of Assumption 3.2 is satisfied for the graph G'.

Claim 3. Let $u, v \in V(G)$ such that $\ell := \operatorname{dist}(u, v) < d$. Furthermore, suppose there is a walk $u = u_0, \ldots, u_{\ell+1} = v$ of length $\ell+1$ from u to v. Then there is an $i \in [\ell]$ such that $u_{i-1}u_{i+1} \in E(G)$.

Proof. Suppose the statement does not hold and let $\ell < d$ be the minimal number for which the claim is violated. Let $u, v \in V(G)$ such that $\ell = \operatorname{dist}(u, v)$ and there is a walk $u = u_0, \ldots, u_{\ell+1} = v$

of length $\ell+1$ from u to v such that for all $i \in [\ell]$, it holds that $u_{i-1}u_{i+1} \notin E(G)$. Also, let $E' := \{u'v' \mid \chi_G(u,v) = \chi_G(u',v')\}$ and consider the graph $G' = (V(G), E(G) \cup E')$. Similarly to the previous claim, we argue that G' still satisfies Assumption 3.2, which contradicts the edge maximality of G.

Indeed, by the same argument as in the previous claim, Condition 1 of Assumption 3.2 is satisfied for the graph G'.

Now let $u'v' \in E'$. Then $\operatorname{dist}(u',v') = \ell$ and there is a walk $u' = u'_0, \ldots, u'_{\ell+1} = v'$ of length $\ell+1$ from u' to v' such that for all $i \in [\ell]$, it holds that $u'_{i-1}u'_{i+1} \notin E(G)$. Note that the 2-dimensional WL algorithm can detect whether such a walk exists, since the shortest path is unique by Claim 2 and the algorithm is aware of the number of triangles that share an edge with the shortest path. Due the minimality of ℓ , it holds that the unique shortest path from u' to v' and $u'_0, \ldots, u'_{\ell+1}$ are internally vertex-disjoint. Since $\operatorname{dist}(w_1, w_2) = d$, this implies that there is a connected component of $G - w_1 w_2$ with vertex set C such that $u', v' \in C \cup \{w_1, w_2\}$ (using the same arguments as before). But this again means Condition 2 of Assumption 3.2 is also satisfied for the graph G'.

These claims drastically restrict the structure of the graph G and will allow us to prove that G is a cycle. Intuitively speaking, the claims imply that, when looking towards the connected component G[C] from any of the w_i , the graph has a tree-like structure, i.e., the initial segments of paths up to length d-1 starting in w_i form a tree rooted in w_i .

For $k' \in \{d, \dots, 2d\}$, let

$$C_{k'} \coloneqq \bigcup_{i,j:\ i+j=k'} C_{i,j}.$$

Let $k \in \{d, ..., 2d\}$ be the maximal number such that $C_k \neq \emptyset$. Note that $k \leq 2d - 2$ by Claim 1. First suppose that $k \geq d + 1$.

Claim 4. Let $v \in C_{i,k-i}$ for $k-d+1 \le i \le d-1$. Then $|N(v) \cap (C_{i-1,k-i+1} \cup C_{i-1,k-i})| = 1$ and also $|N(v) \cap (C_{i,k-i-1} \cup C_{i+1,k-i-1})| = 1$.

Proof. This follows directly from Claim 2.

Claim 5. Suppose $C_{i,k-i} \neq \emptyset$ for some $k-d+1 \leq i \leq d-1$. Then G is a cycle.

Proof. Pick i with $k-d+1 \le i \le d-1$ such that $C_{i,k-i} \ne \emptyset$ and let $v \in C_{i,k-i}$. By Claim 4 and the maximality of k, we get that $|N(v) \setminus C_{i,k-i}| = 2$. If |N(v)| = 2, then we are done (recall that G is regular and connected). So suppose there is a $u \in N(v) \cap C_{i,k-i}$. Then, using Claim 3, it is not hard to see that $N(u) \setminus C_{i,k-i} = N(v) \setminus C_{i,k-i}$ (observe that i < d and k-i < d). Now let A be the vertex set of the connected component containing v in the graph $G[C_{i,k-i}]$. Then G[A] is a clique. Indeed, for every pair $u, u' \in A$, there are at least two paths of length 2 from u to u', since $N(u) \setminus C_{i,k-i} = N(u') \setminus C_{i,k-i}$. Thus, $uu' \in E(G)$ by Claim 2. But now G[N[v]] contains at most one non-edge, namely between the vertices in $N(v) \setminus C_{i,k-i}$. So the same has to be true for w_1 , which implies that $\deg(w_1) = 2$.

Hence, we can assume that $C_{i,k-i} = \emptyset$ for all $k - d + 1 \le i \le d - 1$. Since $C_k \ne \emptyset$, this means that $C_{d,k-d} \ne \emptyset$ or $C_{k-d,d} \ne \emptyset$. Without loss of generality, assume that $C_{k-d,d} \ne \emptyset$. Note that k - d < d.

Let $v \in C_{k-d,d}$. Let $w \in N(v)$ such that $\operatorname{dist}(w_1, w) = k - d - 1$. Note that $w \in C_{k-d-1,d}$ (when k = d + 1, then $w = w_1$). Also, observe that $|N(v) \cap C_{k-d-1,d}| = 1$ by Claim 2. Let A be the vertex set of the connected component in $G[C_{k-d,d}]$ containing v. Let $u, u' \in A$ such that $uu' \in E(G)$. Then $N(u) \cap C_{k-d-1,d} = N(u') \cap C_{k-d-1,d}$ by Claim 3. So $N(u) \cap C_{k-d-1,d} = \{w\}$ for every $u \in A$. Also G[A] forms a clique, since there is a unique shortest path between pairs of vertices at distance 2 by Claim 2. So $G[A \cup \{w\}]$ forms a clique. Now let $u \in N(v) \setminus (A \cup \{w\})$.

Then $u \in C_{k-d,d-1}$ (recall that $C_{k-d+1,d-1} = \emptyset$). First, $uw \in E(G)$ by Claim 3. Also, $A \subseteq N(u)$, since there is a unique shortest path between pairs of vertices at distance 2 by Claim 2. Finally, let $u' \in N(v) \setminus (A \cup \{w\})$ such that $u \neq u'$. Then $\{v, w\} \subseteq N(u) \cap N(u')$ and hence, $uu' \in E(G)$, again using Claim 2. So overall N[v] forms a clique and thus, the same must hold for $N[w_1]$, which is a contradiction since w_1 belongs to a separator.

In the other case, k = d. Observe that $C_{i,d-i} \neq \emptyset$ for all $1 \leq i \leq d-1$. For two disjoint sets $U, W \subseteq V(G)$, let $G[U, W] := (U \cup W, E(G) \cap (U \times W))$ be the bipartite graph induced by U and W.

Claim 6. $|C_{i,d-i}| = |C_{j,d-j}|$ for all $1 \le i, j \le d-1$. Also, the graph $G[C_{i,d-i}, C_{i+1,d-i-1}]$ is a matching graph (i.e., every vertex in the graph has degree 1) for $1 \le i \le d-1$.

Proof. This follows directly from Claim 2.

Since G is regular, we further conclude that $G[C_{i,d-i}]$ is a complete graph for every i with $1 \le i \le d-1$. Now suppose that $|C_{i,d-i}| \ge 2$ for some (and therefore every) $1 \le i \le d-1$. But then G contains an induced subgraph isomorphic to C_4 , which contradicts Claim 2 (recall that $d \ge 3$). So $|C_{i,d-i}| = 1$ for all $1 \le i \le d-1$ and hence, G is a cycle.

Reformulating the previous lemma, we obtain the following theorem.

Theorem 3.9. Let G be a graph such that $\chi_G(u,u) = \chi_G(v,v)$ for all $u,v \in V(G)$. Then (exactly) one of the following holds:

- 1. G is not connected, or
- 2. G is 3-connected, or
- 3. G is a cycle of length $\ell > 4$.

Note that the complete graphs on 2 and 3 vertices are 3-connected (for other work on the connectivity of relations in association schemes, see e.g. [6, 7, 8, 12]). The theorem also implies that a connected constituent graph of an association scheme is either 3-connected or a cycle. It thus provides a generalization of Kodalen's and Martin's result in [29], where they proved the theorem in case the graph stems from a symmetric association scheme.

4 Two Colors

Recall that our overall goal is to prove that the 2-dimensional WL algorithm assigns special colors to 2-separators in a graph. We will use Lemma 3.8 to prove this in case the tuples (u, u) and (v, v) of a 2-separator $\{u, v\}$ obtain the same color under the 2-dimensional WL algorithm. To treat the much more difficult case that u and v obtain distinct colors, we intend to generalize the results of the previous section to two vertex colors. Maybe somewhat surprisingly, we obtain a similar statement to Lemma 3.8. However, now we require the input graphs to be 2-connected (instead of only being connected). This is a necessary condition, since for example the star graphs $K_{1,n}$ for $n \geq 2$ are neither 3-connected nor cycles but still have only two vertex colors under the 2-dimensional WL algorithm.

The route to proving the statement is similar to the one described in Section 3. Still, two colors allowing for more complexity in the graph structure, the statements and proofs become more involved and additional cases need to be considered. We start by adapting several of the auxiliary lemmas given in the previous section to the setting of two vertex colors.

Lemma 4.1. Let G be a connected graph with n vertices and suppose w_1w_2 is a 2-separator of G. Let C be the vertex set of a connected component of $G - w_1w_2$ such that $|C| \leq \frac{n-2}{2}$ and let $v \in C$. Then there is no $u \in V(G)$ such that

- 1. $\operatorname{dist}(u, v) \leq 2$,
- 2. $\chi_G(u,u) = \chi_G(v,v)$, and
- 3. $dist(u, w_i) \le dist(v, w_i) 2 \text{ for both } i \in \{1, 2\}.$

Proof. The proof is analogous to the one for Lemma 3.4.

Lemma 4.2. Let G = (U, V, E) be a 2-connected bipartite graph with n vertices and the following properties:

- 1. $\chi_G(u,u) = \chi_G(u',u')$ for all $u,u' \in U$,
- 2. $\chi_G(v,v) = \chi_G(v',v')$ for all $v,v' \in V$, and
- 3. G has a 2-separator w_1w_2 with $w_1 \in U$ and $w_2 \in V$.

Let $d := \operatorname{dist}(w_1, w_2)$ and let C be the vertex set of a connected component of $G - w_1 w_2$ of size $|C| \le \frac{n-2}{2}$. Then $\operatorname{dist}(v, w_i) \le d+1$ for all $v \in C$ and $i \in \{1, 2\}$.

Proof. Since G is bipartite, d is odd. By symmetry, it suffices to show the statement for i=2. For $u \in U \cap C$, we prove by induction on $\ell := \operatorname{dist}(u, w_1)$ that $\operatorname{dist}(u, w_2) \leq d$. Then the statement follows, because every $v \in V \cap C$ is connected to some $u \in U \cap C$.

For $\ell = 0$, it holds that $u = w_1$ and $\operatorname{dist}(w_1, w_2) = d$. So suppose the statement holds for all $u \in U \cap C$ such that $\operatorname{dist}(u, w_1) \leq \ell$, and pick $u' \in U \cap C$ with $\operatorname{dist}(u', w_1) = \ell + 2$. Let $u \in U \cap C$ such that $\operatorname{dist}(u, w_1) \leq \ell$ and $\operatorname{dist}(u, u') \leq 2$. Then $\operatorname{dist}(u', w_2) \leq \operatorname{dist}(u, w_2) + 1 \leq d + 1$ by Lemma 4.1 and the induction hypothesis. But since G is bipartite and we know that $u' \in U$ and $w_2 \in V$, we have that $\operatorname{dist}(u', w_2)$ is odd and thus, $\operatorname{dist}(u', w_2) \leq d$.

Lemma 4.3. Let G = (U, V, E) be a 2-connected bipartite graph with n vertices and the following properties:

- 1. $\chi_G(u,u) = \chi_G(u',u')$ for all $u,u' \in U$,
- 2. $\chi_G(v,v) = \chi_G(v',v')$ for all $v,v' \in V$, and
- 3. G has a 2-separator w_1w_2 .

Then $w_1w_2 \notin E(G)$.

Proof. Since G is bipartite and by symmetry, we only need to consider the case that $w_1 \in U$ and $w_2 \in V$. Suppose towards a contradiction that $w_1w_2 \in E(G)$. Let C be the vertex set of a connected component of $G - w_1w_2$ such that $|C| \leq \frac{n-2}{2}$. For $i, j \geq 1$, let

$$C_{i,j} := \{v \in C \mid \operatorname{dist}(v, w_1) = i \text{ and } \operatorname{dist}(v, w_2) = j\}.$$

By Lemma 4.2, we conclude that $C_{i,j}=\emptyset$ unless $(i,j)\in\{(1,1),(1,2),(2,1),(2,2)\}$. Furthermore, $C_{1,1}=C_{2,2}=\emptyset$, since G is bipartite.

Note that $C_{1,2} \cup \{w_2\} \subseteq N(w_1)$. Moreover, since G is 2-connected, w_1 must have a neighbor in $V(G) \setminus (C \cup \{w_1, w_2\})$. Thus $\deg(w_1) \ge |C_{1,2}| + 2$. Let $v \in C_{2,1} \subseteq U$. Then all neighbors of v are contained in $C_{1,2} \cup \{w_2\}$, since $C_{1,1} = C_{2,2} = \emptyset$. Hence, $\deg(v) \le |C_{1,2}| + 1 < \deg(w_1)$, which contradicts Condition 1.

Lemma 4.4. Let G be a graph and suppose there are $c_1 \neq c_2$ such that $\{\chi_G(v,v) \mid v \in V(G)\} = \{c_1, c_2\}$. Let $U := \{u \in V(G) \mid \chi_G(u,u) = c_1\}$ and $V := \{v \in V(G) \mid \chi_G(v,v) = c_2\}$. Also let U_1, \ldots, U_k be the vertex sets of the connected components of G[U] and let V_1, \ldots, V_ℓ be the vertex sets of the connected components of G[V]. Let G' be the graph with $V(G') = \{U_1, \ldots, U_k, V_1, \ldots, V_\ell\}$ and $U_i V_j \in E(G')$ if and only if there are $u \in U_i$, $v \in V_j$ such that $uv \in E(G)$.

Then
$$\chi_{G'}(U_i, U_i) = \chi_{G'}(U_j, U_j)$$
 for all $i, j \in [k]$, and $\chi_{G'}(V_i, V_i) = \chi_{G'}(V_i, V_i)$ for all $i, j \in [\ell]$.

Proof. We prove the following statement for all $W_1, \ldots, W_4 \in V(G')$ by induction on the number of rounds r of the WL algorithm. If $\chi_{G'}^r(W_1, W_2) \neq \chi_{G'}^r(W_3, W_4)$, then

$$\{\chi_G(w_1, w_2) \mid w_1 \in W_1, w_2 \in W_2\} \cap \{\chi_G(w_3, w_4) \mid w_3 \in W_3, w_4 \in W_4\} = \emptyset.$$

First observe that this implies the statement of the lemma when setting $W_1 = W_2 = U_i$ and $W_3 = W_4 = U_j$, and similarly for $W_1 = W_2 = V_i$ and $W_3 = W_4 = V_j$.

For r=0, the statement is simple. Indeed, $\chi_{G'}^r(W_1,W_2) \neq \chi_{G'}^r(W_3,W_4)$ if and only if $W_1W_2 \in E(G)$ and $W_3W_4 \notin E(G)$ (or vice versa), or $W_1=W_2$ and $W_3 \neq W_4$ (or vice versa). In both cases, the statement follows from the fact that the 2-dimensional WL algorithm is aware of the connected components $U_1,\ldots,U_k,V_1,\ldots,V_\ell$.

For the inductive step, suppose $r \geq 0$ and pick four sets $W_1, \ldots, W_4 \in V(G')$ such that $\chi_{G'}^{r+1}(W_1, W_2) \neq \chi_{G'}^{r+1}(W_3, W_4)$. If $\chi_{G'}^r(W_1, W_2) \neq \chi_{G'}^r(W_3, W_4)$, the statement immediately follows from the induction hypothesis. Hence, there are colors c_1 and c_2 such that $|M| \neq |M'|$ where

$$M := \{W' \mid \chi_{G'}^r(W', W_2) = c_1, \chi_{G'}^r(W_1, W') = c_2\}$$

and

$$M' := \{W' \mid \chi_{G'}^r(W', W_4) = c_1, \chi_{G'}^r(W_3, W') = c_2\}.$$

Let $w_i \in W_i$ for $i \in [4]$. It suffices to argue that

$$\{\{(\chi_G(w, w_2), \chi_G(w_1, w)) \mid w \in V(G)\}\} \neq \{\{(\chi_G(w, w_4), \chi_G(w_3, w)) \mid w \in V(G)\}\}.$$

But this follows from the induction hypothesis and that $|M| \neq |M'|$.

Theorem 4.5. Let G be a 2-connected graph with the following properties:

- 1. G has a 2-separator w_1w_2 , and
- 2. for every $v \in V(G)$, there is an $i \in \{1, 2\}$ such that $\chi_G(v, v) = \chi_G(w_i, w_i)$.

Then G is a cycle.

Proof. By Lemma 3.8, we can assume without loss of generality that $\chi_G(w_1, w_1) \neq \chi_G(w_2, w_2)$. The statement is proved by induction on the graph size n. For $n \leq 4$, a simple case analysis among the possible graphs G yields the statement.

So let $n \geq 5$. Again, it suffices to prove the statement for the case that G is an n-vertex graph with a maximum edge set that satisfies the requirements of the lemma. Let

$$U := \{ u \in V(G) \mid \chi_G(u, u) = \chi_G(w_1, w_1) \}$$

and

$$V := \{ v \in V(G) \mid \chi_G(v, v) = \chi_G(w_2, w_2) \}.$$

Let U_1, \ldots, U_k be the vertex sets of the connected components of G[U] and let V_1, \ldots, V_ℓ be the vertex sets of the connected components of G[V]. Without loss of generality, assume that

 $w_1 \in U_1$ and $w_2 \in V_1$. Let C be the vertex set of a connected component of $G - w_1w_2$ with size $|C| \leq \frac{n-2}{2}$. Also, let $C' := V(G) \setminus (C \cup \{w_1, w_2\})$.

Claim 1. Suppose that $C \subseteq U_1 \cup V_1$ or $C' \subseteq U_1 \cup V_1$. Then G is a cycle.

Proof. It is not hard to see that, by reasons of connectivity and since $|U_i| = |U_{i'}|$ and $|V_j| = |V_{j'}|$ for all i, j, it suffices to show that $|U_1| \le 2$ and $|V_1| \le 2$.

Suppose $C \subseteq U_1 \cup V_1$. Then $C \cap (U_1 \cup V_1) \neq \emptyset$. By symmetry, we may assume that there exists a vertex $u_1 \in U_1 \cap C$ with $u_1w_1 \in E(G)$. We first argue that $U_1 \cap C' = \emptyset$. Towards a contradiction, suppose that there exists $u'_1 \in U_1 \cap C'$. Then w_1 is a cut vertex in $G[U_1]$. Since the 2-dimensional WL algorithm distinguishes arcs within connected components from arcs between different connected components, by [27, Corollary 7], all vertices in U_1 must be cut vertices, in addition to $G[U_1]$ being connected. It is easy to see that there is no connected graph in which all vertices are cut vertices. Analogously, we cannot have that both $V_1 \cap C \neq \emptyset$ and $V_1 \cap C' \neq \emptyset$ hold

Thus, $U_1 \cap C' = \emptyset$. First assume that $V_1 \cap C = \emptyset$. In this case, we have $C \cup \{w_1\} = U_1$ and, by regularity, $uw_2 \in E(G)$ for all $u \in U_1$. In particular, every vertex in U has exactly one neighbor in V. However, for w_1 , this neighbor must be distinct from w_2 because it must lie in C'. If $|U_1| \geq 3$, this results in $\chi(w_1, w_1) \neq \chi(u_1, u_1)$, a contradiction.

Now assume that $V_1 \cap C' = \emptyset$. Note that for all $j \neq 1$ and all $v \in V_j$, we have that $u_1 v \notin E(G)$. Thus, $|\{j \mid \exists v \in V_j : u_1 v \in E(G)\}| = 1$ by the connectivity of G. Since $\chi(u_1, u_1) = \chi(u, u)$ for all $u \in U$, every vertex in U has neighbors in exactly one of the sets V_j . Moreover, for all $u \in U_1 \setminus \{w_1\}$, this set is V_1 . However, for $w_1 \in U_1$, it is some $V_j \subseteq C'$. Indeed, since $U_1 \cap C' = \emptyset$, the vertex w_1 is the only candidate in $U \cap (C \cup \{w_1\})$ to be adjacent to a vertex in C'.

Suppose there is another vertex $u_2 \in U_1$ with $w_1 \neq u_2 \neq u_1$. Then for every vertex $v_1 \in V_1$, the colors $\chi(u_1, v_1)$ and $\chi(u_2, v_1)$ encode that there exist vertices $v, v' \in V_1$ (possibly equal) such that $u_1v, u_2v' \in E(G)$. The existence of such a v_1 is thus encoded in $\chi(u_1, u_2)$. However, for w_1 and any other vertex in U_1 , there is no equivalent vertex in V, thus w_1 is not incident to any edge of color $\chi(u_1, u_2)$. Hence, $\chi(u_1, u_1) \neq \chi(w_1, w_1)$, which contradicts the assumptions. Therefore $|U_1| \leq 2$. Analogously, it can be shown that $|V_1| \leq 2$.

The case $C' \subseteq U_1 \cup V_1$ follows by symmetry. Altogether, we can deduce that G has to be a cycle.

So for the rest of the proof, we assume that $C \nsubseteq U_1 \cup V_1$ and $C' \nsubseteq U_1 \cup V_1$. Note that, since we have assumed $w_1 \in U_1$ and $w_2 \in V_1$, this implies that both G[U] and G[V] consist of at least two connected components each (again using the fact that G[U] and G[V] do not contain any cut vertices).

Let G' be the graph with $V(G') = \{U_1, \dots, U_k, V_1, \dots, V_\ell\}$ and $U_iV_j \in E(G')$ if and only if there are $u \in U_i$ and $v \in V_j$ such that $uv \in E(G)$. We argue that G' satisfies the requirements of the lemma. First note that $G' - U_1V_1$ is not connected and hence, $\{U_1, V_1\}$ forms a 2-separator of G'. Also, $\chi_{G'}(U_i, U_i) = \chi_{G'}(U_1, U_1)$ for all $i \in [k]$, and $\chi_{G'}(V_j, V_j) = \chi_{G'}(V_1, V_1)$ for all $j \in [\ell]$ by Lemma 4.4.

Clearly, G' is connected because G is. So it remains to argue that G' is 2-connected. If not, then G' contains a cut vertex. Without loss of generality, assume that U_i for a certain $i \in [k]$ is a cut vertex. Then, since the 2-dimensional WL algorithm recognizes cut vertices ([27, Corollary 7]) and by Lemma 4.4, every vertex U_i with $i \in [k]$ is a cut vertex of G'. Considering the cut tree of G' (i.e., the tree in which every cut vertex and every 2-connected component forms a vertex), it is not hard to see that this implies that every V_j for $j \in [\ell]$ has only one neighbor. But this is only possible if $C \subseteq V_1$ or $C' \subseteq V_1$, and we assumed the contraries of both cases.

Suppose that |V(G')| < |V(G)|. Then, by the induction hypothesis, the graph G' is a cycle.

Thus, every vertex in U is adjacent to vertices in exactly one or two connected components of G[V].

We first consider the subcase that both $C \cap U_1 = \emptyset$ and $C \cap V_1 = \emptyset$ hold.

The vertex w_1 is adjacent to vertices in a connected component with vertex set $V_j \subseteq C$, whereas all vertices $u \in U_1$ with $u \neq w_1$ must be adjacent to the same connected component with vertex set $V_{j'} \subseteq (C' \cup \{w_2\})$. In particular, we have $j \neq j'$. Assuming $|U_1| > 2$, similarly as in the proof of Claim 1, we reach a contradiction considering $\chi(w_1, w_1)$. By symmetry, we cannot have $|V_1| > 2$ either. The subcase that $C' \cap U_1 = \emptyset$ and $C' \cap V_1 = \emptyset$ can be treated analogously.

Thus, suppose without loss of generality that $C \cap U_1 \neq \emptyset$ and $C' \cap V_1 \neq \emptyset$. (The case $C' \cap U_1 \neq \emptyset$ and $C \cap V_1 \neq \emptyset$ follows by symmetry.)

Since we cannot have that $C = U_1 \setminus \{w_1\}$, there must be a connected component with vertex set $V_j \subset C$ for a certain $j \neq 1$ such that for every $u_1 \in U_1 \setminus \{w_1\}$, we have $N(u_1) \cap V \subseteq V_j$. However, all neighbors of w_1 in V are contained in a $V_{j'} \subseteq C' \cup \{w_2\}$. In particular, $j \neq j'$. Again, we reach a contradiction when assuming that $|U_1| > 2$ and, by symmetry, also for the assumption $|V_1| > 2$.

Thus, if |V(G')| < |V(G)|, then G is a cycle.

Now assume |V(G')| = |V(G)|. This means that G is a bipartite graph with bipartition (U, V) and all U_i and all V_j are singletons. From Lemma 4.3, we know $w_1w_2 \notin E(G)$. Let $d := \operatorname{dist}(w_1, w_2)$. Note that d is odd and thus, $d \ge 3$.

Claim 2. Let $u, v \in V(G)$ such that dist(u, v) < d. Then there is a unique shortest path from u to v.

Proof. Suppose the statement does not hold and let $\ell < d$ be the minimal number for which the claim is violated. Let $u, v \in V(G)$ be two vertices such that there are two paths of length $\ell = \operatorname{dist}(u, v)$ from u to v. Also, let $E' := \{u'v' \mid \chi_G(u, v) = \chi_G(u', v')\}$ and consider the graph $G' = (V(G), E(G) \cup E')$. We argue that G' still satisfies the assumptions of the theorem, which contradicts the edge maximality of G.

First, the coloring χ_G is also a stable coloring for G', which implies that χ_G refines the coloring $\chi_{G'}$. In particular, for every $v \in V(G)$, there is an $i \in \{1, 2\}$ such that $\chi_G(v, v) = \chi_G(w_i, w_i)$.

Now let $u'v' \in E'$. Then $\operatorname{dist}(u',v') = \ell$ and there are at least two different walks of length ℓ from u' to v', because the same statement holds for u and v. Due to the minimality of ℓ , the two walks are vertex-disjoint paths. If u' and v' lie in different connected components of $G - w_1w_2$, then one of the two paths must pass through w_1 and one through w_2 , forming a cycle of length $2\ell < 2d$. This implies $\operatorname{dist}(w_1, w_2) < d$, a contradiction. Thus, we conclude that there is a connected component C of $G - w_1w_2$ such that $u', v' \in C \cup \{w_1, w_2\}$. But this means that w_1w_2 is also a 2-separator of the graph G'.

For $i, j \geq 1$, let

$$C_{i,j} := \{v \in C \mid \operatorname{dist}(v, w_1) = i \text{ and } \operatorname{dist}(v, w_2) = j\}.$$

By Lemma 4.2, we conclude that $C_{i,j} = \emptyset$ unless $i, j \leq d+1$. Furthermore, by the definition of d, it holds that $C_{i,j} = \emptyset$ unless $i + j \geq d$. Since G is bipartite, we know $C_{i,j} = \emptyset$ whenever i + j is even.

Claim 3. Suppose $d \geq 7$. Then G is a cycle.

Proof. We argue that deg(u) = 2 for every $u \in U$. Analogously, one can prove that deg(v) = 2 for every $v \in V$, which together means that G is a cycle.

First suppose that $C_{4,d-4} \neq \emptyset$ and let $u \in C_{4,d-4}$. Note that $u \in U$, since 4 is even. Then $N(u) \subseteq C_{3,d-3} \cup C_{5,d-5} \cup C_{5,d-3}$. Moreover, $|N(u) \cap (C_{3,d-3} \cup C_{5,d-5})| = 2$, otherwise there would

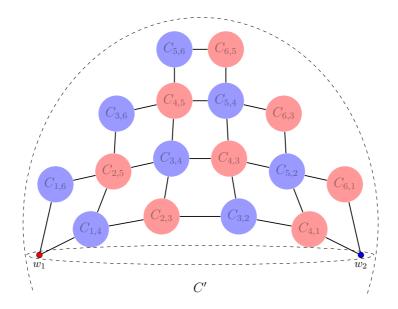


Figure 2: Visualization of the set $C_{i,j}$ for d=5 in the proof of Theorem 4.5. Each edge between two sets indicates that there may be edges connecting vertices from the two sets.

be two shortest paths from u to w_1 or two shortest paths from u to w_2 , contradicting Claim 2. Now suppose towards a contradiction that $\deg(u)>2$. Then there is a $v\in N(u)\cap C_{5,d-3}$. We have that $N(v)\subseteq C_{4,d-4}\cup C_{4,d-2}\cup C_{6,d-4}\cup C_{6,d-2}$. Using Claim 2, we conclude that $|N(v)\cap (C_{4,d-4}\cup C_{4,d-2})|\leq 1$ and $|N(v)\cap (C_{4,d-4}\cup C_{6,d-4})|\leq 1$. Since $\deg(v)\geq 2$ and $u\in N(v)\cap C_{4,d-4}\neq\emptyset$, it follows that $N(v)\cap C_{6,d-2}\neq\emptyset$. But this contradicts Lemma 4.1. So $\deg(u)=2$.

Now suppose $C_{4,d-4} = \emptyset$ and hence, $C_{i,d-i} = \emptyset$ for all $1 \le i \le d-1$. Since $N(w_1) \cap C = C_{1,d-1} \cup C_{1,d+1}$, we conclude that $C_{1,d+1} \ne \emptyset$ and hence, $C_{i,d+2-i} \ne \emptyset$ for all $1 \le i \le d+1$.

So pick $u \in C_{4,d-2}$. Then $N(u) \subseteq C_{3,d-1} \cup C_{5,d-3} \cup C_{5,d-1}$. Again, $|N(u) \cap (C_{3,d-1} \cup C_{5,d-3})| = 2$, using Claim 2. Suppose towards a contradiction that $\deg(u) > 2$. Then there is a vertex $v \in N(u) \cap C_{5,d-1}$. We have that $N(v) \subseteq C_{4,d-2} \cup C_{4,d} \cup C_{6,d-2} \cup C_{6,d}$. By Claim 2, we conclude that $|N(v) \cap (C_{4,d-2} \cup C_{4,d})| \le 1$ and $|N(v) \cap (C_{4,d-2} \cup C_{6,d-2})| \le 1$. Since $\deg(v) \ge 2$, it follows that $N(v) \cap C_{6,d} \ne \emptyset$. As before, this contradicts Lemma 4.1.

Claim 4. Suppose d = 5. Then G is a cycle.

Proof. Again, it suffices to show $\deg(u)=2$ for every $u\in U$, since showing $\deg(v)=2$ for every $v\in V$ works analogously. If $C_{2,3}\neq\emptyset$, we can argue similarly as in the proof of Claim 3 that there are a vertex $u\in C_{2,3}$ and a vertex $v\in N(u)\cap C_{3,4}$ with $N(v)\cap C_{4,5}\neq\emptyset$, which contradicts Lemma 4.1.

Thus, we can assume that $C_{2,3} = \emptyset$. Hence, we have $C_{i,d-i} = \emptyset$ for all $1 \le i \le 4$ and therefore $C_{1,6} \ne \emptyset$ and $C_{i,7-i} \ne \emptyset$ for all $1 \le i \le 6$. Analogously as in the proof of Claim 3, there are vertices $u \in C_{4,3}$ and $v \in N(u) \cap C_{5,4}$, supposing $\deg(u) > 2$. We have $N(v) \subseteq C_{4,3} \cup C_{4,5} \cup C_{6,3} \cup C_{6,5}$. By Claim 2, we have $|N(v) \cap (C_{4,3} \cup C_{6,3})| \le 1$. We would like to apply the same argument to $N(v) \cap (C_{4,3} \cup C_{4,5})$. However, since $\operatorname{dist}(v, w_1) = 5 = d$, we cannot apply Claim 2 immediately. Still, note that the shortest path from w_1 to w_2 with all internal vertices in C has length 7.

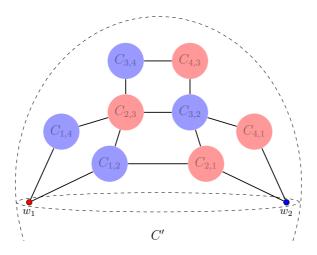


Figure 3: Visualization of the set $C_{i,j}$ for d=3 in the proof of Theorem 4.5. Each edge between two sets indicates that there may be edges connecting vertices from the two sets.

Therefore, analogously as in the proof of Claim 2, using the edge maximality of G, we can show that there cannot be cycles of length at most 10 in G and that thus, there must be a unique shortest path from v to w_1 . In particular, this implies that $|N(v) \cap (C_{4,3} \cup C_{4,5})| \leq 1$. We can conclude the proof analogously as the one for Claim 3.

Claim 5. Suppose d=3. Then G is a cycle.

Proof. First observe that all vertices of C must be contained in one of the sets $C_{i,j}$ with $(i,j) \in \{(1,2),(2,1),(1,4),(2,3),(3,2),(4,1),(3,4),(4,3)\}.$

If w_2 has only one neighbor v in C', then $\{w_1, v\}$ is a unicolored 2-separator. Consider the graph \widehat{G} with vertex set U and an edge between every pair of vertices u and v if there is a path from u to v of length 2 (i.e., via a vertex in V) in G. Since the 2-dimensional WL algorithm implicitly detects such paths, we can apply Theorem 3.9. It is easy to see that \widehat{G} is connected and not 3-connected. Thus, it must be a cycle. In particular, every vertex in \widehat{G} has degree 2. Therefore, the position of each vertex in V is uniquely determined: the graph G is a subdivision of \widehat{G} . Thus, G is a cycle.

Now assume

$$\deg(w_2) > |N(w_2) \cap C'| \ge 2. \tag{1}$$

First suppose $C_{1,2} \neq \emptyset$ and, equivalently, $C_{2,1} \neq \emptyset$. For every vertex $u \in C_{2,1}$ we have $N(u) \subseteq C_{1,2} \cup C_{3,2} \cup \{w_2\}$. By Claim 2, it holds that $|N(u) \cap C_{1,2}| = 1$. Thus, since $uw_2 \in E(G)$, we have $|N(u) \cap C_{3,2}| = r_U - 2$, where $r_U = \deg(u) = \deg(w_1)$. Furthermore, again by Claim 2, for $u' \in C_{2,1}$ with $u' \neq u$, we have $N(u) \cap N(u') = \{w_2\}$ and thus, $|N(C_{2,1}) \cap C_{3,2}| = |C_{2,1}| \cdot (r_U - 2)$. Furthermore, by a similar reasoning, $|N(C_{4,1}) \cap C_{3,2}| = |C_{4,1}| \cdot (r_U - 1)$. Every vertex in $C_{3,2}$ has distance 2 to w_2 and thus has a neighbor in $C_{2,1} \cup C_{4,1}$. Note that $N(w_2) \cap C = C_{2,1} \cup C_{4,1}$. Now since, by Claim 2, we have $(N(C_{2,1}) \cap N(C_{4,1})) \setminus \{w_2\} = \emptyset$, we obtain that $|C_{3,2}| = |C_{2,1}| \cdot (r_U - 2) + |C_{4,1}| \cdot (r_U - 1) < (|C_{2,1}| + |C_{4,1}|) \cdot (r_U - 1) \leq (r_V - 2) \cdot (r_U - 1)$ by (1), where $r_V = \deg(w_2)$. Let $v \in C_{1,2}$. Similarly as above, $|N(v) \cap C_{2,3}| = r_V - 2$. Furthermore, for every vertex $u \in N(v) \cap C_{2,3}$, by Claim 2 and Lemma 4.1, we have $N(u) \subseteq C_{1,2} \cup C_{3,2}$ and $|N(u) \cap C_{1,2}| = 1$.

Again using Claim 2, every two vertices in $N(v) \cap C_{2,3}$ must have disjoint neighborhoods in $C_{3,2}$. Thus, we obtain that $|C_{3,2}| \ge (r_V - 2)(r_U - 1)$.

Altogether $(r_V-2)(r_U-1) \leq |C_{3,2}| < (r_V-2)(r_U-1)$, which yields a contradiction. Therefore, $C_{1,2} = C_{2,1} = \emptyset$. Hence, it must hold that $C_{1,4} \neq \emptyset$ and consequently, also $C_{i,5-i} \neq \emptyset$ for every $i \in [4]$. Using the same arguments as before, we have $|C_{3,2}| \leq (r_V-2)(r_U-1)$. Every vertex $v' \in C_{3,2}$ has at least one neighbor in the set $C_{4,1}$ and at least one neighbor in $C_{2,3}$. Since for every $u' \in C_{4,3}$, there is a $v' \in C_{3,2} \cap N(u')$, this implies $|C_{4,3}| \leq (r_V-2)(r_U-1)(r_V-2)$.

Let $v \in C_{1,4}$ (recall that $C_{1,4} \neq \emptyset$). Then $|N(v) \cap C_{2,3}| = r_V - 1$ and for every vertex $u' \in N(v) \cap C_{2,3}$, we have by Claim 2 that $|N(u') \cap (C_{3,4} \cup C_{3,2})| = r_U - 1$. Again by Claim 2, for a second vertex $u'' \in N(v) \cap C_{2,3}$ with $u'' \neq u'$, it must hold that

$$N(u') \cap (C_{3,4} \cup C_{3,2}) \cap N(u'') = \emptyset.$$
 (2)

Let $S := N(N(v)) \cap (C_{3,4} \cup C_{3,2})$. Note that the shortest path from w_1 to w_2 with all internal vertices in C has length 5. Therefore, using the edge maximality of G, analogously as in the proof of Claim 2, there cannot be any cycles of length 6 in G. In particular, this implies that for every pair $v', v'' \in S$ with $v' \neq v''$ we have $N(v') \cap N(v'') \cap C_{4,3} = \emptyset$.

Thus, Equation (2) implies that $|C_{4,3}| \ge (r_V - 1)(r_U - 1)(r_V - 2)$, since every vertex in S has at most two neighbors not contained in $C_{4,3}$.

Altogether we obtain $(r_V - 1)(r_U - 1)(r_V - 2) \le |C_{4,3}| \le (r_V - 2)(r_U - 1)(r_V - 2)$, which is a contradiction. This concludes the proof.

5 Detecting Decompositions with Weisfeiler and Leman

In this section, we show that the 2-dimensional WL algorithm implicitly computes the decomposition of a graph into its 3-connected components.

Let S be a set of colors. We say a path u_0, \ldots, u_ℓ avoids S if $\chi_G(u_i, u_i) \notin S$ for every $i \in [\ell-1]$. Note that we impose no restriction on the colors of the endpoints of the path. It is easy to see that, given two vertices $u, v \in V(G)$, the 2-dimensional WL algorithm is aware of whether there is a path from u to v that avoids S.

Lemma 5.1. Let G be a graph and let $X := \{\chi_G(v, v) \mid v \in V(G)\}$. Furthermore, let $S \subseteq X$ and define G[[S]] = (V, E), where $V = \{v \in V(G) \mid \chi_G(v, v) \in S\}$ and

 $E = \{uv \mid there \ is \ a \ path \ from \ u \ to \ v \ in \ G \ that \ avoids \ S\}.$

Then $\chi_{G[[S]]}(u, u) = \chi_{G[[S]]}(v, v)$ for all $u, v \in V$ with $\chi_{G}(u, u) = \chi_{G}(v, v)$.

Proof. It is easy to see that, given two vertices $u, v \in V(G)$, the 2-dimensional WL algorithm detects whether there is a path from u to v that avoids S. Thus, there is a set of colors T such that $uv \in E$ if and only if $\chi_G(u, v) \in T$. Hence, any refinement performed by the 2-dimensional WL algorithm in G[[S]] can also be done in G.

Theorem 5.2. Let G and H be 2-connected graphs and let $w_1, w_2 \in V(G)$ such that w_1w_2 forms a 2-separator in G. Also let $v_1, v_2 \in V(H)$ and suppose $\chi_G(w_1, w_2) = \chi_H(v_1, v_2)$. Then v_1v_2 forms a 2-separator in H.

Proof. Let $S := \{\chi_G(w_1, w_1), \chi_G(w_2, w_2)\}$ and let G' := G[[S]]. Clearly, the graph G' is connected. We argue that G' is 2-connected. Suppose towards a contradiction that there is a separating vertex w in G'. Let C and C' be the vertex sets of two connected components of G' - w. Let

 $v \in C$ and $v' \in C'$. We show that w separates v from v' in G. Towards a contradiction, suppose there is a path P from v to v' in G that does not pass w. Then there is a corresponding path P' in G', which simply skips all inner vertices of P not contained in S. In particular, P' connects v and v', but avoids w. This contradicts w being a cut vertex in G'. Hence, G' is 2-connected.

First suppose that |V(G')| = 2. Let $A := \{v \in V(H) \mid \chi_H(v, v) \in S\}$. Then |A| = 2 and thus $A = \{v_1, v_2\}$. Moreover, H - A is disconnected, since the 2-dimensional WL algorithm detects that $G - w_1w_2$ is disconnected. Hence, v_1v_2 forms a 2-separator in H.

Now assume $|V(G')| \geq 3$ and suppose there is a vertex set C of a connected component of $G - w_1w_2$ such that $V(G') \subseteq C \cup \{w_1, w_2\}$. Let C' be the vertex set of a second connected component of $G - w_1w_2$ and let $v \in C'$. Then w_1 and w_2 are the only vertices with color in S that can be reached from v via a path that avoids S. Hence, using the expressive power of the 2-dimensional WL algorithm, it is not hard to see that there must also be a vertex $u \in V(H)$ such that v_1 and v_2 are the only vertices with color in S that can be reached from u via a path that avoids S. Since $|V(G')| \geq 3$, there is a $u' \in V(H)$ such that $v_1 \neq u' \neq v_2$ and $\chi_H(u', u') \in S$, because in order not to be distinguished, unions of color classes with color in S must have the same cardinality in both graphs. But then v_1v_2 separates u from u' in H and thus, v_1v_2 forms a 2-separator in H.

In the other case, w_1w_2 forms a 2-separator in G'. Hence, G' is a cycle by Lemma 5.1 and Theorem 4.5. Note that $|V(G')| \ge 4$ and $w_1w_2 \notin E(G')$. It follows that H[[S]] is also a cycle, since otherwise, the 2-dimensional WL algorithm would distinguish the graphs. Also, $|V(H[[S]])| \ge 4$ and $v_1v_2 \notin E(H[[S]])$. So v_1v_2 forms a 2-separator in H[[S]] and thus, it also forms a 2-separator in H.

Corollary 5.3. Suppose $k \geq 2$. Let G and H be connected graphs. Assume $\{w_1, \ldots, w_k\} \subseteq V(G)$ is a k-separator in G. Let $\{v_1, \ldots, v_k\} \subseteq V(H)$ and suppose $\chi_{G,k}(w_1, \ldots, w_k) = \chi_{H,k}(v_1, \ldots, v_k)$. Then $\{v_1, \ldots, v_k\}$ forms a k-separator in H.

Proof. First suppose k=2. If G and H are 2-connected, the statement is exactly Theorem 5.2. If either G or H is not 2-connected, then that graph contains a cut vertex, while the other graph does not. By [27, Corollary 7], the presence of the cut vertex is encoded in every vertex color and thus, the multisets $\{\{\chi_G(u,v) \mid u,v \in V(G)\}\}$ and $\{\{\chi_H(u,v) \mid u,v \in V(H)\}\}$ are disjoint. Therefore, the statement trivially holds.

Suppose both G and H are not 2-connected. The statement is obviously true if w_1 or w_2 is a cut vertex in G. If this is not the case, then w_1 and w_2 must lie in a common 2-connected component of G, otherwise they form no 2-separator. By [27, Theorem 6], the same must hold for v_1 and v_2 in H. Furthermore, again by [27, Theorem 6], the 2-dimensional WL algorithm distinguishes arcs from w_1 , w_2 and from v_1 , v_2 to vertices in the same 2-connected component from arcs to other vertices. Thus, the algorithm distinguishes the 2-connected component C_G containing w_1 and w_2 and the 2-connected component C_H containing v_1 and v_2 , respectively, from the remainder of G and G, respectively. Hence, the computed colors in G and G induce a refined partition of the one induced by the colors computed in G and G, respectively. Therefore, (v_1, v_2) and (w_1, w_2) have equal colors in G and G and thus, applying Theorem 5.2, we can deduce that $\{v_1, v_2\}$ forms a 2-separator in G and therefore also in G.

Finally, consider the case k > 2. Let G and H be two graphs and suppose $\{w_1, \ldots, w_{k+1}\} \subseteq V(G)$ is a (k+1)-separator in G. Also let $\{v_1, \ldots, v_{k+1}\} \subseteq V(H)$ and furthermore, suppose that $\chi_{G,k+1}(w_1,\ldots,w_{k+1}) = \chi_{H,k+1}(v_1,\ldots,v_{k+1})$. The claim follows from the observation that we can assume $G - \{w_1,\ldots,w_{k-2}\}$ and $H - \{v_1,\ldots,v_{k-2}\}$ to be connected, that $\{w_{k-1},w_k\}$ forms a 2-separator in the graph $G - \{w_1,\ldots,w_{k-2}\}$, and that it suffices to show the analogous statement for H.

Using the corollary, we can prove a strengthened version of [27, Theorem 13]. Following [27], we say that the k-dimensional WL algorithm determines orbits in a graph class \mathcal{G} if for all arccolored graphs (G, λ) , (G', λ') with $G, G' \in \mathcal{G}$, arc colorings λ , λ' and for all vertices $v \in V(G)$ and $v' \in V(G')$, there exists an isomorphism from (G, λ) to (G', λ') mapping v to v' if and only if $\chi_{G,k}(v,\ldots,v) = \chi_{G',k}(v',\ldots,v')$.

Theorem 5.4. Let \mathcal{G} be a minor-closed graph class and assume $k \geq 2$. Suppose the k-dimensional WL algorithm determines orbits on all arc-colored 3-connected graphs in \mathcal{G} . Then the k-dimensional WL algorithm distinguishes all non-isomorphic graphs in \mathcal{G} .

The proof is very similar to the proof of [27, Theorem 13], building on the improved bound on the dimension of the WL algorithm required to distinguish 2-separators from other pairs of vertices. Thus, we only provide a sketch of the proof here.

Proof sketch. Let G and G' be non-isomorphic graphs in \mathcal{G} and suppose the 2-dimensional WL algorithm determines orbits on all arc-colored 3-connected graphs in \mathcal{G} . To show that G and G' are distinguished, we proceed just as outlined in [27, Section 5], improving the lower bound on the dimension k of the WL algorithm stated there from 3 to 2 using our new results.

Namely, we prove the theorem by induction on |V(G)| + |V(G')|. If both of the graphs are 3-connected, the statement follows from the assumptions, since "determines orbits" is a stronger assumption than "distinguishes". If exactly one of the graphs is 3-connected, then exactly one of them has a 2-separator and the statement follows from Corollary 5.3.

Thus, suppose that both graphs are not 3-connected and assume all pairs of arc-colored graphs (H, λ_H) and $(H', \lambda_{H'})$ with |V(H)| + |V(H')| < |V(G)| + |V(G')| are distinguished. By [27, Theorem 5], with \mathcal{G} being the class of graphs containing every graph isomorphic to G, G' or a minor of one of them, it suffices to show the statement for the case that G and G' are 2-connected.

If G and G' do not have the same minimum degree, they are distinguished by their degree sequences. Now first suppose both G and G' have minimum degree at least 3. Then, since (G, λ) and (G', λ') are not isomorphic, we can consider the decompositions of the graphs into their 3-connected components and cut off the leaves of these decompositions maintaining all necessary information in additional colors in the corresponding (former) 2-separators, as described in detail in [27, Section 3]. Then by [27, Lemma 4], the obtained arc-colored graphs $(G_{\perp}, \lambda_{\perp})$ and $(G'_{\perp}, \lambda'_{\perp})$ are non-isomorphic and thus distinguished by the k-dimensional WL-algorithm by induction assumption.

Using Corollary 5.3, we can now proceed just as outlined in the proof of Lemma 17 in [27] to obtain a strengthened version of that lemma and thus show that the vertices in $V(G_{\perp})$ and $V(G'_{\perp})$ have different colors than the vertices in $V(G) \setminus V(G_{\perp})$ and $V(G') \setminus V(G'_{\perp})$.

Showing that the partition of the vertices and arcs induced by the coloring χ_G^k restricted to $V(G_\perp)$ is finer than the partition induced by λ_\perp , i.e., that the WL algorithm implicitly computes λ_\perp , requires some more work, breaking down to strengthening Lemma 18 in [27]. However, since by Corollary 5.3, the k-dimensional WL algorithm assigns vertices belonging to 2-separators special colors, we can easily get rid of the second separator vertex s_2 in the lemma and obtain a strengthened version with colors $\chi_G^k(s_1,v)$ and $\chi_{G'}^k(s_1',v)$ for $k \geq 2$ instead of $\chi_G^k(s_1,s_2,v)$ and $\chi_{G'}^k(s_1',s_2',v)$ for $k \geq 3$.

Thus, since the k-dimensional WL-algorithm distinguishes $(G_{\perp}, \lambda_{\perp})$ from $(G'_{\perp}, \lambda'_{\perp})$, it also distinguishes (G, λ) from (G', λ') .

By [27, Lemma 15], the case that G and G' do not have minimum degree at least 3 reduces to the case of minimum degree at least 3, letting \mathcal{G} be the class of graphs containing every graph isomorphic to G, G' or a minor of one of them.

Thus, since by [27], the WL dimension of the class of planar graphs is 2 or 3, the concrete value only depends on the dimension needed to determine orbits on arc-colored 3-connected planar graphs.

For a graph G and $v_1, v_2, v_3 \in V(G)$, we define $s_G(v_1, v_2, v_3) := |C|$, where C is the vertex set of the connected component of $G-v_1v_2$ that contains v_3 (if $v_3 \in \{v_1, v_2\}$, then $s_G(v_1, v_2, v_3) := 0$).

Theorem 5.5. Let G and H be two 2-connected graphs. Also suppose $v_1, v_2, v_3 \in V(G)$ and $w_1, w_2, w_3 \in V(H)$ such that $\chi_G(v_i, v_j) = \chi_H(w_i, w_j)$ for all $i, j \in \{1, 2, 3\}$. Then $s_G(v_1, v_2, v_3) = s_H(w_1, w_2, w_3)$.

Proof. The statement trivially holds if $v_3 = v_1$ or $v_3 = v_2$. Thus, assume $v_1 \neq v_3 \neq v_2$.

If v_1v_2 is not a 2-separator, the statement follows easily from Theorem 5.2. Thus, we may assume that v_1v_2 and w_1w_2 are 2-separators. Let $S := \{\chi_G(v_1, v_1), \chi_G(v_2, v_2)\}$ and let G' := G[[S]]. As in the proof of Theorem 5.2, the graph G' is 2-connected.

First suppose that |V(G')| = 2. Let $A := \{v \in V(H) \mid \chi_H(v, v) \in S\}$. Then $A = \{w_1, w_2\}$. Moreover, $s_G(v_1, v_2, v_3)$ is the number of vertices that are reachable from v_3 without ever visiting a vertex with a color from S. This is encoded in the color $\chi_G(v_3, v_3)$. Since $\chi_G(v_3, v_3) = \chi_H(w_3, w_3)$, it follows that $s_G(v_1, v_2, v_3) = s_H(w_1, w_2, w_3)$.

Next, suppose there is a vertex set of a connected component C of $G - v_1v_2$ such that $V(G') \subseteq C \cup \{v_1, v_2\}$. If $v_3 \notin C$, then v_1 and v_2 are the only vertices in V(G') that v_3 can reach via paths that avoid S. Also, as before, $s_G(v_1, v_2, v_3)$ is the number of vertices that are reachable from v_3 without ever visiting a vertex with a color in S. The same has to hold for w_1 and w_2 with respect to w_3 , since $\chi_G(v_3, v_3) = \chi_H(w_3, w_3)$. Thus, $s_G(v_1, v_2, v_3) = s_H(w_1, w_2, w_3)$. In the other case, $v_3 \in C$ and $s_G(v_1, v_2, v_3) = |C|$. But $|C| = n - 2 - \sum_{C' \neq C} |C'|$, where C' ranges over all vertex sets of connected components of $G - v_1v_2$. As discussed above, the sizes of these vertex sets C' are encoded in the vertex colors of the graph G and the same is true for H.

Otherwise, v_1v_2 forms a 2-separator in G' and hence, G' is a cycle by Lemma 5.1 and Theorem 4.5. Note that $|V(G')| \geq 4$ and $v_1v_2 \notin E(G')$. It follows that H[[S]] is also a cycle using Lemma 5.1. Also, $|V(H[[S]])| \geq 4$ and $w_1w_2 \notin E(H[[S]])$. Note that every vertex can reach only two vertices in S via paths that avoid S. Thus, the colors $\chi_G(v,v')$ for $vv' \in E(G')$ encode the number of vertices with color not in S for which v and v' are the only vertices reachable via paths that avoid S. Hence, the 2-dimensional WL algorithm implicitly computes the edge-colored cycle G' (and the analogous edge-colored cycle H' for H). Thus, it suffices to consider these two cycles, for which the statement is easy to see.

The last theorem can also be formulated in terms of the expressive power of the 3-variable fragment C^3 of first-order logic with counting quantifiers of the form $\exists^{\geq k} x \varphi(x)$. Indeed, it implies that for all $n, s \in \mathbb{N}$, there is a formula $\varphi_{n,s}(x_1, x_2, x_3) \in \mathsf{C}^3$ such that, for every 2-connected n-vertex graph G and $v_1, v_2, v_3 \in V(G)$, it holds that $G \models \varphi_{n,s}(v_1, v_2, v_3)$ if and only if $s_G(v_1, v_2, v_3) = s$ (for details about the connection between the WL algorithm and counting logics, see e.g. [9, 26]).

6 New Bounds for Graphs of Treewidth k

As an application of the results presented so far, we investigate the WL dimension of graphs of treewidth at most k. Up to this point, the best known upper bound on the WL dimension of such graphs has been k+2, i.e., the (k+2)-dimensional WL algorithm identifies every graph of treewidth at most k [17]. In this chapter, we present new upper and lower bounds.

6.1 Upper Bound

The basic idea for proving a new upper bound is to provide a winning strategy for Spoiler in the corresponding bijective pebble game. Our proof works similarly to the proof that the (k+2)-dimensional WL algorithm identifies every graph of treewidth at most k [17]. The main difference is a much more careful implementation of the general strategy in order to get by with the desired number of pebbles. As a major ingredient, we exploit that separators can be detected using fewer pebbles.

For a (k+1)-tuple $(v_1, \ldots, v_k, v_{k+1})$ of vertices of a graph G, we define $s_G(v_1, \ldots, v_k, v_{k+1}) := |C|$, where C is the vertex set of the unique connected component of $G - \{v_1, \ldots, v_k\}$ such that $v_{k+1} \in C$.

Lemma 6.1. Suppose $k \geq 2$. Let G and H be two graphs and let $v_1, \ldots, v_{k+1} \in V(G)$ and $w_1, \ldots, w_{k+1} \in V(H)$ such that $s_G(v_1, \ldots, v_k, v_{k+1}) \neq s_H(w_1, \ldots, w_k, w_{k+1})$. Then Spoiler wins the game $BP_{k+1}(G, H)$ from the initial position $((v_1, \ldots, v_{k+1}), (w_1, \ldots, w_{k+1}))$.

Proof. It is easy to see that it suffices to prove the statement for the case that the following conditions hold:

- $v_{k+1} \notin \{v_1, \dots, v_k\}$ and $w_{k+1} \notin \{w_1, \dots, w_k\}$, and
- \bullet G and H have the same size and are connected.

Also note that by Corollary 5.3, the graph G is 2-connected if and only if H is 2-connected.

First suppose k=2. Assume the graphs are connected, but not 2-connected. We are going to use the correspondence from Theorem 2.1. The proof basically exploits the fact that the decomposition into 2-connected components has a tree-like structure and that the 2-dimensional WL algorithm recognizes cut vertices (see [27, Corollary 7]), thus being able to "transport information" from one side of a cut vertex to the other. Note that v_i is a cut vertex if and only if w_i is a cut vertex.

First, suppose that exactly one vertex in $\{v_1, v_2\}$ is a cut vertex, say v_1 . Then we can ignore the vertex v_2 and for every v', the color triple formed by $\chi(v_1, v'), \chi(v', v_3)$, and $\chi(v_1, v_3)$ encodes how many vertices are contained in the same connected component of $G - v_1$ as v_3 , using the methods from [27, Theorem 6]. Thus, $\chi(v_1, v_3)$ encodes the size of the connected component of $G - v_1$ that contains v_3 . Also by the above observation, we know whether v_2 is in this connected component or not. Thus, we know the size of the connected component of $G - v_1v_2$ that contains v_3 .

Now assume that both v_1 and v_2 are cut vertices. Then, as above, we can determine whether v_3 lies in the same connected component of $G-v_1$ as v_2 and whether v_3 lies in the same connected component of $G-v_2$ as v_1 , and compute the corresponding sizes. These numbers determine s_G and thus also s_H .

Otherwise, neither v_1 nor v_2 is a cut vertex. The only problematic case is that v_1v_2 forms a 2-separator (implying that v_1 and v_2 lie in a common 2-connected component of G). In this case, we can proceed analogously as in the proof of Theorem 5.5.

For the general case, i.e., k > 2, let $\widehat{G} := G - \{v_1, \dots, v_{k-2}\}$ and $\widehat{H} := H - \{v_1, \dots, v_{k-2}\}$. Then $s_{\widehat{G}}(v_{k-1}, v_k, v_{k+1}) \neq s_{\widehat{H}}(w_{k-1}, w_k, w_{k+1})$ and hence, Spoiler wins the game $\mathrm{BP}_3(\widehat{G}, \widehat{H})$ from the initial position $((v_{k-1}, v_k, v_{k+1}), (w_{k-1}, w_k, w_{k+1}))$ by Theorems 2.1 and 5.5. But then Spoiler also wins $\mathrm{BP}_{k+1}(G, H)$ from the initial position $((v_1, \dots, v_{k+1}), (w_1, \dots, w_{k+1}))$ by simply never moving the pebbles $((v_1, \dots, v_{k-2}), (w_1, \dots, w_{k-2}))$.

To build Spoiler's strategy along a given tree decomposition, we use the following characterization of treewidth. Let G be a graph of treewidth k. For a k-separator $S \subseteq V(G)$ and the vertex

set C of a connected component of G-S, we define G(S,C) to be the graph on vertex set $S \cup C$ obtained by inserting a clique between the vertices in S into $G[S \cup C]$.

Lemma 6.2 (Arnborg et al. [1]). Suppose G(S, C) has at least k + 2 vertices. Then G(S, C) has treewidth at most k if and only if there exists $v \in C$ such that for every connected component A of $G[C \setminus \{v\}]$, there is a k-element separator $S_A \subseteq S \cup \{v\}$ such that

- 1. no vertex in A is adjacent to the unique element from $S \setminus S_A$, and
- 2. $G(S_A, V(A))$ has treewidth at most k.

Suppose G(S, C) has treewidth at most k. Let $D_G(S, C)$ denote the set of possible vertices $v \in C$ that satisfy Lemma 6.2.

Theorem 6.3. Suppose $k \geq 2$. Let G be a graph of treewidth at most k. Then the k-dimensional WL algorithm identifies G.

Proof. Let G be a connected graph of treewidth k and suppose H is a second connected graph such that $G \ncong H$. Let (T, β) be a tree decomposition of G of width k. For a k-element separator $S \subseteq V(G)$ and an integer $m \in \mathbb{N}$, we define

 $C_G(S, m) := \{C \subseteq V(G) \mid C \text{ is the vertex set of a connected component of } G - S \text{ of size } m\}.$

Moreover,

$$G(S,m) \coloneqq G \left[S \cup \bigcup_{C \in \mathcal{C}_G(S,m)} C \right].$$

An ordered separator is a tuple $\bar{a}=(a_1,\ldots,a_k)$ such that the underlying set $\{a_1,\ldots,a_k\}$ is a separator. In this proof, slightly abusing notation, we do not distinguish between ordered separators and their underlying unordered separators. For two ordered separators $\bar{a}\in \left(V(G)\right)^k$ and $\bar{b}\in \left(V(H)\right)^k$, we define $m(\bar{a},\bar{b})$ to be the minimal number $m\geq 1$ such that $(G(\bar{a},m),\bar{a})\not\cong (H(\bar{b},m),\bar{b})$. Here, $(G(\bar{a},m),\bar{a})$ denotes the graph $G(\bar{a},m)$ where, additionally, each vertex in \bar{a} is individualized. More formally, it holds that $(G(\bar{a},m),\bar{a})\cong (H(\bar{b},m),\bar{b})$ if there is an isomorphism $\varphi\colon G(\bar{a},m)\cong H(\bar{b},m)$ such that for $\bar{a}=(a_1,\ldots,a_k)$ and $\bar{b}=(b_1,\ldots,b_k)$, it holds that $\varphi(a_i)=b_i$ for all $i\in [k]$.

We now argue that Spoiler wins the game $\mathrm{BP}_{k+1}(G,H)$. Suppose the game is in a position $(\bar{a},\bar{b})\in \left(V(G)\right)^k\times \left(V(H)\right)^k$ where $\bar{a}\supseteq\beta(s)\cap\beta(t)$ for an edge $st\in E(T)$. We shall prove by induction on $m:=m(\bar{a},\bar{b})$ that Spoiler wins the game from the initial position (\bar{a},\bar{b}) . In each case, Spoiler wishes to play another pebble. Let $f\colon V(G)\to V(H)$ be the bijection chosen by Duplicator. Using Lemma 6.1, we can assume that f maps the vertex set of $G(\bar{a},m)$ to the vertex set of $H(\bar{b},m)$. Now let $C\in\mathcal{C}_G(\bar{a},m)$ such that

$$|\{C' \in \mathcal{C}_G(\bar{a}, m) \mid (G(\bar{a}, C'), \bar{a}) \cong (G(\bar{a}, C), \bar{a})\}| > |\{C' \in \mathcal{C}_H(\bar{b}, m) \mid (H(\bar{b}, C'), \bar{b}) \cong (G(\bar{a}, C), \bar{a})\}|.$$

Also let

$$D := \Big\{ v \in D_G(\bar{a}, C') \mid C' \in \mathcal{C}_G(\bar{a}, m) \text{ and } \big(G(\bar{a}, C'), \bar{a} \big) \cong (G(\bar{a}, C), \bar{a}) \Big\}.$$

Then there exists a $v \in D$ such that the following holds for $C_G \in \mathcal{C}_G(\bar{a}, m)$ with $v \in C_G$ and $C_H \in \mathcal{C}_H(\bar{b}, m)$ with $f(v) \in C_H$:

$$(G[C_G \cup \bar{a}], \bar{a}, v) \not\cong (G[C_H \cup \bar{b}], \bar{b}, f(v)). \tag{3}$$

Now Spoiler places pebbles on (v, w) with w = f(v).

For the base case of the induction, suppose m=1. This means $C_G=\{v\}$ and $C_H=\{w\}$ and thus, Spoiler wins immediately. So assume m>1. Let $A_1,\ldots,A_\ell\subseteq C_G$ be the vertex sets of the connected components of $G[C_G\setminus\{v\}]$. Note that $|A_i|\leq m-1$ for every $i\in[\ell]$. Also let $B_1,\ldots,B_{\ell'}\subseteq C_H$ be the vertex sets of the connected components of $H[C_H\setminus\{w\}]$. Due to Equation (3), there is an $A\in\{A_1,\ldots,A_\ell\}$ such that

$$\begin{aligned} & \left| \left\{ i \in [\ell] \, \middle| \, G[A_i \cup \bar{a} \cup \{v\}], \bar{a}, v) \cong G[A \cup \bar{a} \cup \{v\}], \bar{a}, v) \right\} \right| \\ > & \left| \left\{ i \in [\ell'] \, \middle| \, H[B_i \cup \bar{b} \cup \{w\}], \bar{b}, w \right\} \cong G[A \cup \bar{a} \cup \{v\}], \bar{a}, v) \right\} \right|. \end{aligned}$$

We pick such a set $A \in \{A_1, \ldots, A_\ell\}$ with minimal cardinality (i.e., there is no set $A' \in \{A_1, \ldots, A_\ell\}$ strictly smaller than A and satisfying the above condition). Now suppose $\bar{a} = (a_1, \ldots, a_k)$ and $\bar{b} = (b_1, \ldots, b_k)$. Pick $i \in [k]$ such that no vertex in A is adjacent to a_i (cf. Lemma 6.2). Now Spoiler removes the pair of pebbles (a_i, b_i) . Let $\bar{a}' := (a_1, \ldots, a_{i-1}, a_{i+1}, \ldots, a_k, v)$ and $\bar{b}' := (b_1, \ldots, b_{i-1}, b_{i+1}, \ldots, b_k, w)$. Observe that (\bar{a}', \bar{b}') is the current position of the game. Now let m' = |A| < m. Note that $A \in \mathcal{C}_G(\bar{a}', m')$.

Claim 1. $(G(\bar{a}', m'), \bar{a}') \not\cong (H(\bar{b}', m'), \bar{b}')$.

Proof. To prove the claim, it suffices to argue that $|\mathcal{A}| > |\mathcal{B}|$ where

$$\mathcal{A} := \left\{ A' \in \mathcal{C}_G(\bar{a}', m') \mid \left(G(\bar{a}', A'), \bar{a}' \right) \cong \left(G(\bar{a}', A), \bar{a}' \right) \right\}$$

and

$$\mathcal{B} \coloneqq \Big\{ B' \in \mathcal{C}_H(\bar{b}', m') \mid \big(H(\bar{b}', B'), \bar{b}' \big) \cong \big(G(\bar{a}', A), \bar{a}' \big) \Big\}.$$

Let $\mathcal{A}' := \{A' \in \mathcal{A} \mid A' \subseteq C_G\}$ and $\mathcal{A}'' := \mathcal{A} \setminus \mathcal{A}'$. Similarly, define $\mathcal{B}' := \{B' \in \mathcal{B} \mid B' \subseteq C_H\}$ and $\mathcal{B}'' := \mathcal{B} \setminus \mathcal{B}'$. From the definition of the set A, it follows that $|\mathcal{A}'| > |\mathcal{B}'|$. Now define

$$G' \coloneqq G\left[\bar{a} \cup \{v\} \cup \bigcup_{m'' \le m'} \mathcal{C}_G(\bar{a}, m'') \cup \bigcup_{i \in [\ell] \colon |A_i| < m'} A_i\right]$$

and

$$H' := H\left[\bar{b} \cup \{w\} \cup \bigcup_{m'' \le m'} \mathcal{C}_H(\bar{b}, m'') \cup \bigcup_{i \in [\ell'] \colon |B_i| < m'} B_i\right].$$

From the definitions of the number m and the set A, it follows that $(G', \bar{a}, v) \cong (H', \bar{b}, w)$.

Now let $A' \in \mathcal{A}''$ and let C be the vertex set of a connected component of $G - \bar{a}$ such that $C \neq C_G$ and $A' \cap C \neq \emptyset$. Then $C \subseteq A'$, since C is a connected set in the graph $G - \bar{a}'$. Since |A'| = m', this implies $A' \subseteq V(G')$. By the same argument, $B' \subseteq V(H')$ for all $B' \in \mathcal{B}''$. But this means that $|\mathcal{A}''| = |\mathcal{B}''|$ because $(G', \bar{a}, v) \cong (H', \bar{b}, w)$. Overall, this proves the claim.

Since m' < m, Spoiler wins from the initial position (\bar{a}', \bar{b}') by the induction hypothesis. Using the induction principle, this completes the proof.

6.2 Lower Bound

For the lower bound, we use a construction introduced by Cai, Fürer, and Immerman [9] and start by reviewing it. For a non-empty finite set S, we define the CFI gadget X_S to be the following graph. For each $w \in S$, there are vertices a(w) and b(w), and for every $A \subseteq S$ such that |A| is even, there is a vertex m_A . For every $A \subseteq S$ such that |A| is even, there are edges $\{a(w), m_A\} \in E(X_S)$

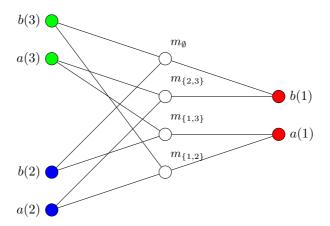


Figure 4: The Cai-Fürer-Immerman gadget X_3 .

for all $w \in A$ and $\{b(w), m_A\} \in E(X_S)$ for all $w \in S \setminus A$. As an example, the graph $X_3 := X_{[3]}$ is depicted in Figure 4. The graph is colored so that $\{m_A \mid A \subseteq S \text{ and } |A| \text{ is even}\}$ forms a color class and so that $\{a(w), b(w)\}$ forms a color class for each w.

Let G be a connected graph of minimum degree 2. For $T \subseteq E(G)$, we define $\mathrm{CFI}_T(G)$ to be the graph obtained from G in the following way. Each $v \in V(G)$ is replaced with a gadget $X_{E(v)}$ where $E(v) \coloneqq \{(v,w) \mid vw \in E(G)\}$ denotes the set of (directed) edges incident to v. Additionally, the following edges are inserted between the gadgets. For every $vw \in E(G) \setminus T$, there are edges from a(v,w) to a(w,v) and from b(v,w) to b(w,v). Also, for every $vw \in T$, there are edges from a(v,w) to b(w,v) and from b(v,w) to a(w,v).

Lemma 6.4 ([9]). Let G be a connected graph of minimum degree 2 and $S, T \subseteq E(G)$. Then $CFI_S(G) \cong CFI_T(G)$ if and only if $|S| \equiv |T| \mod 2$.

Hence, applying the above construction to a specific graph G yields a pair of non-isomorphic graphs $\mathrm{CFI}(G) = \mathrm{CFI}_{\emptyset}(G)$ and $\mathrm{CFI}^{\mathsf{x}}(G) = \mathrm{CFI}_{\{e\}}(G)$ for some $e \in E(G)$.

Theorem 6.5 (Dawar, Richerby [10]). Let G be a connected graph such that $\operatorname{tw}(G) \geq k+1$ and $\operatorname{deg}(v) \geq 2$ for all $v \in V(G)$. Then $\operatorname{CFI}(G) \simeq_k \operatorname{CFI}^{\mathsf{x}}(G)$.

The strategy to obtain a good lower bound is to find graphs G for which we can show a sufficiently good upper bound on the treewidth of $\mathrm{CFI}(G)$ and $\mathrm{CFI}^*(G)$. For $n \geq 2$, let $G_{n,n}$ be the $(n \times n)$ -grid. Moreover, let $G_{n,n}^+$ be the $(n \times n)$ -grid in which each edge is replaced with a path of length 3. Formally, $V(G_{n,n}) = [n] \times [n]$ and $E(G_{n,n}) = \{(i,j)(i',j') \mid (i=i' \wedge |j-j'| = 1) \vee (j=j' \wedge |i-i'| = 1)\}$. Moreover, $V(G_{n,n}^+) = V(G_{n,n}) \cup \{(v,w) \mid vw \in E(G_{n,n})\}$ and $E(G_{n,n}^+) = \{v(v,w) \mid v \in V(G_{n,n}), vw \in E(G_{n,n})\} \cup \{(v,w)(w,v) \mid vw \in E(G_{n,n})\}$.

Lemma 6.6. Let $n \geq 2$. Then there is a tree decomposition (T, β) of $G_{n,n}^+$ of width n + 2 such that

- 1. $|\beta(t) \cap V(G_{n,n})| \leq 1$ for every $t \in V(T)$, and
- 2. if $|\beta(t) \cap V(G_{n,n})| = 1$, then there exists a $v \in V(G_{n,n})$ such that $\beta(t) = E(v) \cup \{v\}$, where $E(v) = \{(v, w) \mid vw \in E(G_{n,n})\}$. In this case, t is a leaf of T and $\beta(s) \cap V(G_{n,n}) = \emptyset$ for the unique $s \in V(T)$ with $st \in E(T)$.

Proof. In order to describe the bags of the tree decomposition, we start by defining several sets $A_{i,j}, B_{i,j}, C_{i,j} \subseteq V(G_{n,n}^+)$ for $i, j \in [n]$. Let

$$\begin{split} A_{i,j} &\coloneqq \ \{((i',j),(i',j+1)) \mid 1 \leq i' \leq i\} \\ & \cup \{((i',j),(i',j-1)) \mid i \leq i' \leq n\} \\ & \cup \{((i,j),(i+1,j)),((i,j),(i-1,j))\}, \\ B_{i,j} &\coloneqq \ \{((i',j),(i',j+1)) \mid 1 \leq i' \leq i\} \\ & \cup \{((i',j),(i',j-1)) \mid i < i' \leq n\} \\ & \cup \{((i,j),(i+1,j)),((i+1,j),(i,j))\}, \\ C_{i,j} &\coloneqq \ \{((i',j),(i',j-1)) \mid 1 \leq i' \leq i\} \\ & \cup \{((i',j-1),(i',j)) \mid i \leq i' \leq n\}. \end{split}$$

(Formally, the sets defined above may also contain elements outside of $V(G_{n,n}^+)$ if some index is not contained in the set [n]. In this case, we simply do not include the corresponding element in the set.) Now define

$$V(T) := \{t_{i,j}^A, t_{i,j}^B, t_{i,j}^C, t_{i,j}^D \mid i, j \in [n]\}.$$

Also set

$$\beta(t_{i,j}^A) := A_{i,j},$$

$$\beta(t_{i,j}^B) := B_{i,j},$$

$$\beta(t_{i,j}^C) := C_{i,j},$$

$$\beta(t_{i,j}^D) := E(i,j) \cup \{(i,j)\}.$$

Observe that each bag contains at most n+3 elements. It remains to define the edges of the tree T. The following edges are added to the set E(T):

- $t_{i,j}^C t_{i+1,j}^C$ for all $i \in [n-1], j \in [n]$,
- $t_{n,i}^C t_{1,i}^A$ for all $j \in [n]$,
- $t_{i,j}^A t_{i,j}^B$ for all $i, j \in [n]$,
- $t_{i,j}^A t_{i,j}^D$ for all $i, j \in [n]$,
- $t_{i,j}^B t_{i+1,j}^A$ for all $i \in [n-1], j \in [n]$, and
- $t_{n,j}^B t_{1,j+1}^C$ for all $j \in [n-1]$.

It can be verified in a straight-forward manner that (T, β) defines a tree decomposition of $G_{n,n}^+$ with the desired properties.

Lemma 6.7. For
$$n \geq 2$$
, it holds that $\operatorname{tw}(\operatorname{CFI}(G_{n,n})) \leq 2n+5$ and $\operatorname{tw}(\operatorname{CFI}(G_{n,n})) \leq 2n+5$.

Proof. We need to define a tree decomposition for the graphs $\mathrm{CFI}(G_{n,n})$ and $\mathrm{CFI}^{\kappa}(G_{n,n})$. Fix $n \geq 2$ and let (T,β) be the tree decomposition described in Lemma 6.6 for the graph $G_{n,n}^+$. Now a tree decomposition (T',β') for the graphs $\mathrm{CFI}(G_{n,n})$ and $\mathrm{CFI}^{\kappa}(G_{n,n})$ can be obtained as follows. For each $t \in V(T)$ such that $\beta(t) \cap V(G_{n,n}) = \emptyset$, it also holds that $t \in V(T')$ and

$$\beta'(t) = \{ a(v, w), b(v, w) \mid (v, w) \in \beta(t) \}.$$

Note that $|\beta'(t)| = 2 \cdot |\beta(t)|$. Also, for $t_1t_2 \in E(T)$ with $\beta(t_i) \cap V(G_{n,n}) = \emptyset$, there is an edge $t_1t_2 \in E(T')$.

Otherwise, $|\beta(t) \cap V(G_{n,n})| = 1$ and $\beta(t) = E(v) \cup \{v\}$ for a certain $v \in V(G_{n,n})$. Also, t is a leaf of T and $\beta(s) \cap V(G_{n,n}) = \emptyset$ for the unique $s \in V(T)$ with $st \in E(T)$. For every $A \subseteq E(v)$ such that |A| is even, there is a vertex $t_A \in V(T')$. We define

$$\beta'(t_A) := \{m_A\} \cup \{a(v, w), b(v, w) \mid vw \in E(G_{n,n})\}.$$

Note that $|\beta'(t_A)| \leq 9$, since $\deg_{G_{n,n}}(v) \leq 4$ for every $v \in V(G_{n,n})$. Also, there are edges $t_A s \in E(T')$ for every $A \subseteq E(v)$ such that |A| is even. It is easy to check that (T', β') is a tree decomposition for the graphs $\mathrm{CFI}(G_{n,n})$ and $\mathrm{CFI}^*(G_{n,n})$. Also,

width
$$(T', \beta') \le \max\{9, 2(\text{width}(T, \beta) + 1)\} - 1 \le \max\{9, 2(n+3)\} - 1 = 2n + 5.$$

Theorem 6.8. For every $k \geq 2$, there are non-isomorphic graphs G_k and H_k of treewidth at most 2k + 7 such that $G_k \simeq_k H_k$.

Proof. Let $G_k := \text{CFI}(G_{k+1,k+1})$ and $H_k := \text{CFI}^{\times}(G_{k+1,k+1})$. Then the statement follows from Theorem 6.5 and Lemma 6.7.

For a graph class \mathcal{C} , denote by $\dim_{\mathsf{WL}}(\mathcal{C})$ the WL dimension of \mathcal{C} , i.e., the minimum $k \in \mathbb{N} \cup \{\infty\}$ such that the k-dimensional WL algorithm identifies every graph $G \in \mathcal{C}$. As a corollary from Theorems 6.3 and 6.8, we obtain the following result.

Corollary 6.9. Let $k \geq 2$. Then $\lceil \frac{k}{2} \rceil - 3 \leq \dim_{\mathsf{WL}}(\mathcal{T}_k) \leq k$, where \mathcal{T}_k denotes the class of graphs of treewidth at most k.

7 Conclusion

We have proved that for $k \geq 2$, the k-dimensional WL algorithm implicitly computes the decomposition of its input graph into its triconnected components. As a by-product, we found that every connected constituent graph of an association scheme is either a cycle or 3-connected.

We have applied this insight to improve on the upper bound on the WL dimension of graphs of bounded treewidth and have also provided a lower bound that is asymptotically only a factor of 2 away from the upper bound.

A natural use case of our results may be determining the WL dimension of certain graph classes that satisfy the requirements of Theorem 5.4. We conjecture that the 2-dimensional WL algorithm identifies every planar graph. Indeed, using the results of this paper, it essentially suffices to show this for triconnected planar graphs.

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