

An Upper Bound on the Weisfeiler-Leman Dimension

Thomas Schneider ✉ 

Department of Mathematics, Technische Universität Darmstadt, Germany

Pascal Schweitzer ✉ 

Department of Mathematics, Technische Universität Darmstadt, Germany

Abstract

The Weisfeiler-Leman (WL) algorithms form a family of incomplete approaches to the graph isomorphism problem. They recently found various applications in algorithmic group theory and machine learning. In fact, the algorithms form a parameterized family: for each $k \in \mathbb{N}$ there is a corresponding k -dimensional algorithm WL_k . The algorithms become increasingly powerful with increasing dimension, but at the same time the running time increases. The WL-dimension of a graph G is the smallest $k \in \mathbb{N}$ for which WL_k correctly decides isomorphism between G and every other graph. In some sense, the WL-dimension measures how difficult it is to test isomorphism of one graph to others using a fairly general class of combinatorial algorithms. Nowadays, it is a standard measure in descriptive complexity theory for the structural complexity of a graph.

We prove that the WL-dimension of a graph on n vertices is at most $3/20 \cdot n + o(n) = 0.15 \cdot n + o(n)$.

Reducing the question to coherent configurations, the proof develops various techniques to analyze their structure. This includes sufficient conditions under which a fiber can be restored uniquely up to isomorphism if it is removed, a recursive proof exploiting a degree reduction and treewidth bounds, as well as an exhaustive analysis of interspaces involving small fibers.

As a base case, we also analyze the dimension of coherent configurations with small fiber size and thereby graphs with small color class size.

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1 Introduction

In recent years, the Weisfeiler-Leman (WL) dimension has evolved to become a standard measure for the structural complexity of a graph. Initially coined in the context of isomorphism questions [4, 24, 37], a plethora of equivalent reformulations in seemingly unrelated areas has surfaced (e.g. [2, 3, 7, 9, 10, 19]). The concept in particular has applications in machine learning on graphs (see [32] for a survey).

In its initial formulation, the WL-dimension of a graph G is characterized as the minimum k required so that the k -dimensional WL-algorithm distinguishes G from every non-isomorphic graph. By a central result of Cai, Fürer, and Immerman [7, Theorem 5.2], the dimension



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plus one is also the least number of variables required to identify G in a particular logic (fixed-point logic with counting) and also the number of pebbles required in a particular combinatorial pebble game (the bijective pebble game).

In some sense, the WL-dimension measures how difficult it is to test isomorphism of one graph to others using a fairly general class of combinatorial algorithms. Crucially, isomorphism between graphs of bounded WL-dimension can be decided in polynomial time. More precisely, if the WL-dimension is at most k , then the problem can be solved in time $O(n^{k+1} \log n)$. While group theoretic techniques can circumvent the structural complexity given by high WL-dimension, the currently fastest theoretical algorithm, which runs in quasi-polynomial time [6], nevertheless uses a $O(\log(n))$ -dimensional WL-algorithm as a subroutine.

Many graph classes are known to have bounded WL-dimension (e.g., all classes with an excluded minor [17] and bounded clique width graphs [18]), giving a polynomial time isomorphism algorithm for these classes.

Initial hopes to find a general bound on the WL-dimension of graphs, however, were dispelled by the seminal construction of Cai, Fürer, and Immerman [7] which constructs graphs of order n and WL-dimension $\Omega(n)$.

In this paper we investigate explicit bounds for the WL-dimension. A calculation of the precise constant in [7] yields a lower bound of $0.00465 \cdot n$ as demonstrated in [34, 35]. In a publication independent from ours, Kiefer and Neuen [25] observe a lower bound of $\frac{n}{96} - o(n)$. This constitutes the current best lower bound in the literature and is slightly below the one we state in this paper using essentially the same observations. In [34, 35], an explicit upper bound of $0.5n + 1.5$ follows from upper bounds that apply in a more general context (more specifically from bounds on the “non-counting version” of the WL-algorithm). We previously supervised a Bachelor’s thesis by Simon Lutz at TU Kaiserslautern that shows an upper bound of $\lceil \frac{n}{3} \rceil + 2$. The best currently known upper bound on the WL-dimension of $\lceil \frac{n}{4} \rceil + o(n)$ is proven by Kiefer and Neuen [25] in their mentioned independent work.

Contributions

The main result of this paper establishes an upper bound for the WL-dimension of $0.15 \cdot n + o(n)$ for all n -vertex graphs G . As part of the proof, we also derive an upper bound of $0.05 \cdot n + o(n)$ on the WL-dimension of colored graphs whose color classes all have size at most 7. Possibly more important than the precise value of our bounds are the techniques we develop in the proof, allowing for the analysis of the descriptive complexity of graphs. In brief, they include criteria under which color classes are removable without any effect on the WL-dimension, an analysis of the possible structures joining an arbitrarily color class with a color class of size at most 7, and a general framework to bound the WL-dimension with recursive reductions using potential functions. These techniques are described in more detail below.

As a complementary result, we also observe in this paper that for all orders n there are graphs G with a WL-dimension of at least $0.0105027 \cdot n - o(n)$.

As usual, these upper and lower bounds for the WL-dimension can both be recast in logical terms, bounding the number of variables required for graph identification in fixed point-logic with counting.

Techniques

On a macroscopic scale the idea for the upper bound proof is as follows. To facilitate recursion, we first generalize the problem to vertex- and edge-colored graphs. More specifically, it is sufficient for us to consider vertex- and edge-colored complete graphs that satisfy strong

regularity conditions. In particular, it suffices to consider so-called coherent configurations, which naturally generalize various highly regular graph families, such as strongly regular graphs and distance-regular graphs. They can also be understood as the stable colorings under the 2-dimensional WL-algorithm. By increasing the dimension by at most 2 once, we can at any point in time, even during recursion, assume that all our objects are coherent configurations. In the language of coherent configurations, the notions of vertex color classes translate into so-called *fibers* of the coherent configuration, and we will use terms interchangeably.

The proof strategy is to reduce the number of vertices, with a focus on reducing those contained in large fibers. We repeatedly use individualizations: an individualization artificially assigns a single vertex a different color. The effect on the coherent configuration, when the 2-dimensional WL-algorithm is applied, is that other fibers are split into smaller ones, which simplifies the coherent configuration. A vertex individualization decreases the dimension by at most 1, meaning we can bound the dimension of the configuration without individualization in terms of the dimension of the configuration we obtain after individualization. We use this strategy to argue that, at a sublinear cost regarding the dimension, we can ensure that the maximum color class size is sublinear in the number of vertices.

With small fibers in mind, we investigate situations in which a color class can be removed without decreasing the WL-dimension. We call configurations *critical* if no fiber can be removed this way. Fibers of size at most 3, which we call *tiny*, can always be removed. For fibers that are not tiny, we develop a technique to determine from the combinatorial structure that a fiber is *restorable* and thus can be removed. Formally, the technique is based on extendability of automorphisms of induced subconfigurations.

Our base case of the recursion is the situation in which all fibers have size at most 7. We call such fibers *small*. We analyze the structure of the configurations that small fibers can induce, as well as the possible connections between small fibers. These connections are called *interspaces*. The *quotient graph* captures the structural information given by fibers and interspaces. The vertices of the quotient graph are the vertex color classes (i.e. fibers). Two of these vertices are connected by an edge if the corresponding color classes are not homogeneously connected, that is, if the interspace is not trivial. Intuitively this means that there is some form of structural dependence between the color classes. For example, the connected components of the quotient graph can be treated separately when determining the WL-dimension, since they are structurally independent.

Several reductions lead us to a quotient graph of maximum degree at most 3. This means that every color class is non-trivially connected to at most 3 other color classes. At this point we can use bounds on the treewidth for cubic graphs to bound the WL-dimension. Overall we show that a coherent configuration with fiber size at most 7 has WL-dimension at most $0.05 \cdot n + o(n)$.

For the general recursion we also need to understand the possible interspaces between small and large fibers. We define a specific potential function that measures the progress we make towards the base case. It gives us the possibility of trading individualizations for a reduction of the potential. We then define a sequence of *local reductions* that, for various subconfigurations and types of interspace, provide a positive trade-off. We can thus inductively assume that these subconfigurations and interspaces are not present in our configuration.

To finally reach the base case, we employ a global argument concerning the structure of configurations that avoid the subconfigurations. In more detail, we introduce the concept of a *t-reduced* configuration and show that configurations to which none of the local reductions

are applicable are t -reduced. For reduced structures, the global argument allows us to separate the graph into pieces whose underlying structure either has small treewidth or which consist only of small fibers. Overall this recursive approach proves the main theorem.

The lower bound simply follows straightforwardly by combining three known results on expansion, treewidth, and the CFI-construction in the evident fashion. An intermediate step in that argument is that random cubic graphs asymptotically almost surely have treewidth at least $0.04201 \cdot n$.

Structure

We revisit the most important definitions and concepts in Section 2 and give details on the lower bound in the fairly compact Section 4. The proof of the upper bound, in contrast, turned out to be significantly more involved. A detailed outline of the overall proof, the involved ideas, and the new techniques is given in Section 3. However, it omits some repetitive case distinctions, various tedious calculations, and technical aspects. These can be found in the full version of the paper [36].

Related Work

A concrete classification of graphs with WL-dimension 1 is known [1, 27]. Fuhlbrück, Köbler, and Verbitsky analyze the structure of graphs with WL-dimension 2 [14] and bounded color class size. Some of our structural lemmas can be seen as direct generalizations of results in their paper. A recent generalization of their complexity results regarding the WL-dimension can be found in [30]. We should remark that in the two papers, just like in ours, the CFI-graphs appear innately.

A survey on descriptive complexity in particular with bounds related to the WL-dimension can be found in [35]. The term WL-dimension was coined by Grohe in his monograph [17]. The main result of this monograph implies that for non-trivial minor-closed graphs classes the WL-dimension is bounded. As remarked above, this is also true for graphs of bounded rank-width [18]. Recently, for several graph classes explicit bounds on the dimension have been proven, including planar graphs [26], distance hereditary graphs [16], interval graphs [12], permutation graphs [21], and circulant graphs [38].

Future Work

While our overall approach may very well be used to improve the upper bound even further, it seems that our argument involving interspaces will then produce an ever increasing number of cases. Therefore, to further improve the bounds with our approach, these arguments might need to be automated or structurally simplified.

Having developed various new techniques and a global view to deal with coherent configurations, another pressing questions for us is as follows. The Deep-Weisfeiler-Leman framework is an extension of the WL-algorithm to match choiceless polynomial time [20]. For this extension it is an open problem whether it provides a polynomial-time solution to graph isomorphism. This question in turn has consequences for the quest for a logic capturing polynomial time [31], a central problem in finite model theory. We therefore wonder whether some of our new techniques can be used to provide better insight into Deep-Weisfeiler-Leman.

2 Preliminaries

Given a finite set Ω and a binary relation A , we call the pair (Ω, A) a *(directed) graph* G . We denote the set of all vertices of G by $\Omega(G)$ and the set of all arcs of G by $A(G)$. Two vertices $v, w \in \Omega$ are *adjacent* if $vw \in A$ or $wv \in A$. Given the graph G and a coloring $\chi: A(G) \rightarrow C$, we call (G, χ) a *colored graph*.

For positive integers r, s, t , we denote the disjoint union of r copies of a graph G by rG , write K_s for the complete graph of order s , and refer to the bipartite complete graph between two vertex sets of size s and t by $K_{r,s}$. We refer to the cycle of order n by C_n , and use \vec{C}_n for the directed version. We denote the Paley tournament on 7 vertices by $PT(7)$ and the incidence graph of the Fano plane by $L(\text{FP})$. The graph $Sp_{4,6}$ is the incidence graph of K_4 and $\vec{C}_3[K_2]$ is a \vec{C}_3 in which each vertex is replaced by two isomorphic copies of itself.

An *isomorphism* between graphs G and H is a bijection $\varphi: V(G) \rightarrow V(H)$ which preserves adjacency and non-adjacency, that is, for all $v, w \in \Omega(G)$ we have $vw \in A(G)$ if and only if $\varphi(v)\varphi(w) \in A(H)$. Given two colored graphs (G, χ_G) and (H, χ_H) , an isomorphism φ between G and H is called *color-preserving* if for all $v, w \in \Omega(G)$ we have $\chi_G(vw) = \chi_H(\varphi(v)\varphi(w))$. If there exists a color-preserving isomorphism between G and H , then we call the graphs *isomorphic* and write $G \cong H$.

Weisfeiler-Leman algorithm

Given a positive integer k , the *k-dimensional Weisfeiler-Leman algorithm* $\text{WL}k$ is part of a family of incomplete deciders for the *isomorphism problem*, which, given two uncolored graphs G and H , asks whether $G \cong H$ holds.

In a nutshell, the algorithm colors the k -tuples of vertices of the graphs as follows. Initially it colors each k -tuple depending on the isomorphism type of the graph induced by the tuple. Here the order of the vertices is taken into account. The algorithm then repeatedly refines the coloring by considering the possible tuples and colors one obtains by replacing one of the vertices in the tuple by an arbitrary other vertex. During this process, it bundles pieces of information together when possible.

In more detail, given the colored graph (G, χ) , the algorithm $\text{WL}k$ determines for every tuple $(v_1, \dots, v_k) \in \Omega(G)^k$ an initial coloring $\chi_0^{\text{WL}k}(v_1, \dots, v_k) := (\vartheta(v_1v_1), \vartheta(v_1v_2), \dots, \vartheta(v_kv_k))$ where

$$\vartheta(vw) := \begin{cases} (0, \chi(vw)) & \text{if } v = w, \\ (1, \chi(vw)) & \text{if } v \neq w \text{ and } vw \in A(G), \\ (2, 0) & \text{if } v \neq w \text{ and } vw \notin A(G). \end{cases}$$

Next, it iteratively computes $\chi_{i+1}^{\text{WL}k}(v_1, \dots, v_k)$ defined by

$$(\chi_i^{\text{WL}k}(v_1, \dots, v_k), \{(\chi_i^{\text{WL}k}(w, v_2, \dots, v_k), \dots, \chi_i^{\text{WL}k}(v_1, \dots, v_{k-1}, w)) \mid w \in \Omega(G)\})$$

for all $(v_1, \dots, v_k) \in \Omega(G)^k$. This process stops if $\pi(\chi_i^{\text{WL}k})$ is *stable under* $\text{WL}k$, that is $\pi(\chi_i^{\text{WL}k}) = \pi(\chi_{i+1}^{\text{WL}k})$. For the i at which the process stops, we define $\chi_\infty^{\text{WL}k} := \chi_{i+1}^{\text{WL}k}$.

If the initially given graph is uncolored, we start the algorithm on the monochromatic version of it. The algorithm $\text{WL}k$ *distinguishes* graphs (G, χ_G) and (H, χ_H) if $\{\chi_\infty^{\text{WL}k}(\bar{v}) \mid \bar{v} \in \Omega(G)^k\} \neq \{\chi_\infty^{\text{WL}k}(\bar{v}) \mid \bar{v} \in \Omega(H)^k\}$. The algorithm $\text{WL}k$ *identifies* (G, χ_G) if it distinguishes the graph (G, χ_G) from all non-isomorphic graphs. The *Weisfeiler-Leman dimension* $\text{WLdim}((G, \chi_G))$ of a graph (G, χ_G) is the minimal $k \in \mathbb{N}$ such that $\text{WL}k$ identifies G . Note that for a colored graph (G, χ_G) , the WL-dimension only depends on $\pi(\chi_G)$ and not on χ_G itself.

Coherent configurations

Let Ω be a finite set of vertices and \mathcal{A} a set of binary relations partitioning Ω^2 . Then the pair $\mathfrak{X} = (\Omega, \mathcal{A})$ is called *coherent configuration* if all of the following properties are met:

1. All relations of \mathcal{A} contain either only self-loops (v, v) or only edges between different vertices (v, u) with $v \neq u$.
2. For each relation $A \in \mathcal{A}$, the set \mathcal{A} contains the *transposed* relation $A^* = \{(v, u) \mid (u, v) \in A\}$.
3. For all triples $A, B, T \in \mathcal{A}$, and vertices v, w with $(v, w) \in T$ the number of vertices u with $(v, u) \in A$ and $(u, w) \in B$ depends only on A , B , and T , but not on the choice of v and w .

The last property is the mentioned regularity condition, which we call *coherence*. A graph induced by a basis relation of \mathcal{A} is called a *constituent* of \mathfrak{X} . A basis relation of loops is called a *fiber*, and if a coherent configuration \mathfrak{X} has only one fiber, we call \mathfrak{X} *homogeneous*. Given two fibers R and B , the partition of $R \times B$ according the relations of \mathfrak{X} is called *interspace* $\mathfrak{X}[R, B]$. An interspace is called *homogeneous* if $|\mathfrak{X}[R, B]| = 1$. The overarching connectivity between fibers of \mathfrak{X} is captured by the *quotient graph* $Q(\mathfrak{X})$ of \mathfrak{X} which uses the set of fibers as vertex set and contains an edge between two fibers if they form a non-homogeneous interspace, that is, an interspace containing more than one relation. By $\text{qdeg}(F)$ we denote degree of a fiber F in $Q(\mathfrak{X})$, that is, the number of non-homogeneous interspaces incident with F . A set of fibers is *dominating* if it forms a dominating set in the quotient graph.

The 2-dimensional Weisfeiler-Leman algorithm (WL2) computes the coarsest coherent configuration refining a given configuration. By interpreting edges, non-edges, and self-loops as separate relations, and applying WL2, every graph can be transformed into a coherent configuration. So coherent configurations are stable under WL2, and in fact “stability under WL2” and “coherence” essentially refer to the same concept. We refer to the full version of the paper [36] for further details.

3 Upper Bound

In this section, we outline all steps necessary to prove the mentioned upper bound. While we introduce various new ideas, concepts, and techniques, we omit repetitive case distinctions, various tedious calculations, and some technical aspects in this section.

First, to facilitate recursion, instead of proving our upper bound only for graphs, we generalize the claim to coherent configurations: The coherence condition of coherent configuration generalizes strongly regular graphs to complete directed graphs with multiple binary relations other than self-loops, edges, and non-edges. In fact, while coherent configurations are usually uncolored combinatorial objects, they can be interpreted as colored graphs: an *associated graph* of a coherent configuration \mathfrak{X} is the colored graph $(G_{\mathfrak{X}}, \chi_{\mathfrak{X}})$ where G is the complete graph on $\Omega(\mathfrak{X})$ and the color classes under $\chi_{\mathfrak{X}}$ correspond to basis relations of \mathfrak{X} . We use this interpretation to define the WL-dimension of a coherent configuration by defining $\text{WLdim}(\mathfrak{X}) := \text{WLdim}((G_{\mathfrak{X}}, \chi_{\mathfrak{X}}))$. This leads us to the main theorem of the paper:

► **Theorem 1.** *If \mathfrak{X} is a coherent configuration on n vertices, then $\text{WLdim}(\mathfrak{X}) \leq \frac{3}{20} \cdot n + o(n)$.*

Strategy-wise, the proof of the theorem aims to iteratively reduce the number of vertices or simplify the coherent configuration as follows. For a coherent configuration \mathfrak{X} , we want to bound $\text{WLdim}(\mathfrak{X})$ in terms of $\text{WLdim}(\mathfrak{X}')$ where \mathfrak{X}' has fewer vertices than \mathfrak{X} or is a structurally simpler. Here, for example, \mathfrak{X}' could be obtained from \mathfrak{X} by an individualization followed by the application of WL2. This means that $\text{WLdim}(\mathfrak{X}) \leq \text{WLdim}(\mathfrak{X}') + 1$.

Working towards the goal of simplifying \mathfrak{X} are several types of reductions. In the first, we exploit knowledge on the WL-algorithm to show that certain color classes can be removed without changing the dimension at all. In the second, called *local reductions*, we individualize vertices. As described in the example, this means we artificially assign a new color to a vertex and then reestablish coherence. While each individualization increments our upper bound, we ensure that sufficient progress is made during the reduction progress. We do so by carefully choosing the vertices we individualize. (Formally a potential function argument is used.) Eventually, no further local reduction can be applied.

At the point when no local reductions can be applied, we split the resulting coherent configuration using a global reduction. This way, the configuration is split into multiple independent components. These components are the base cases of our reduction process, and we deal with each component separately. More formally, the overall dimension can be bound in terms of the maximum of the dimensions of the subconfigurations induced by the components.

In all of the reductions, we heavily rely on structural analysis of fibers, interspaces, and their overall connectivity. A criteria often influencing the selection of the reduction is the size of the fiber: in particular, fibers F are differentiated into *tiny* fibers ($|F| < 4$), *small* fibers ($4 \leq |F| \leq 7$), and *large* fibers ($7 < |F|$).

3.1 Criticality and restorability

For the first set of reductions, we employ the concept of a critical configuration:

► **Definition 2.** *We call a coherent configuration critical if its dimension is at least 2 and the removal of any union of fibers causes the WL-dimension to decrease.*

It turns out that a critical coherent configuration cannot decompose into homogeneously connected components, contain tiny fibers (fibers with at most 3 vertices), or contain $cK_{1,d}$ interspaces:

► **Proposition 3.** *Let \mathfrak{X} be a coherent configuration. If \mathfrak{X} is critical, then*

1. *the quotient graph $Q(\mathfrak{X})$ is connected,*
2. *no interspace of \mathfrak{X} contains a constituent isomorphic to $cK_{1,d}$ for $c, d \in \mathbb{N}$,*
3. *no fiber of \mathfrak{X} is tiny,*
4. *no interspace of \mathfrak{X} contains a constituent isomorphic to tC_{2x} for positive integers t, x with x odd, and*
5. *for all induced paths (R, B, Y) in $Q(\mathfrak{X})$ the size of the fiber B is not prime.*

A new technique we develop to deal with fibers that are not tiny is the restorability of fibers: intuitively, when a restorable fiber is removed, there is up to isomorphism a unique way of reinserting the fiber. More formally, we call a union of fibers \mathcal{R} *restorable* if the following holds: All automorphisms of $\mathcal{B} := N(\mathcal{R})$ (so, the union of the neighbors of the fibers in \mathcal{R}) that extend to automorphisms of $\mathfrak{X} - \mathcal{R}$ also extend to automorphisms of $\mathfrak{X}[\mathcal{B} \cup \mathcal{R}]$. We essentially argue that the WL-algorithm, when used as an isomorphism test, is able to deal with $\mathfrak{X} - \mathcal{R}$ and $\mathfrak{X}[\mathcal{B} \cup \mathcal{R}]$ separately. Therefore, the WL-dimension of \mathfrak{X} is the maximum dimension of both subconfigurations $\mathfrak{X} - \mathcal{R}$ and $\mathfrak{X}[\mathcal{B} \cup \mathcal{R}]$. With regard to criticality of \mathfrak{X} , we conclude that $\mathfrak{X} - (\mathcal{R} \cup \mathcal{B})$ must be empty:

► **Proposition 4.** *Let \mathfrak{X} be coherent configuration. If \mathfrak{X} is critical, then every restorable union of fibers is dominating.*

■ **Table 1** Classification of all homogeneous coherent configurations with $4 \leq n \leq 7$.

n	$T(\mathfrak{X})$
4	$(K_4), (C_4, 2K_2), (2K_2, 2K_2, 2K_2), (\vec{C}_4, 2K_2)$
5	$(K_5), (C_5, C_5), (\vec{C}_5, \vec{C}_5),$
6	$(K_6), (2K_3, K_{3,3}), (2\vec{C}_3, K_{3,3}), (3K_2, K_{2,2,2}), (3K_2, \vec{C}_3[K_2]),$ $(C_6, 3K_2, 2K_3), (\vec{C}_6, 2\vec{C}_3, 3K_2), (3K_2, 3K_2, 2\vec{C}_3, 3K_2)$
7	$(K_7), (C_7, C_7, C_7), (PT\mathcal{r}(7)), (\vec{C}_7, \vec{C}_7, \vec{C}_7)$

■ **Table 2** Classification of all interspaces $\mathfrak{X}[R, B]$ between fibers R and B with $4 \leq |R| \leq |B| \leq 7$ in critical coherent configurations.

$ R $	$ B $	$T(\mathfrak{X}[R, B])$
4	4	$(C_8, C_8), (2K_{2,2}, 2K_{2,2})$
4	6	$(Sp_{4,6}, Sp_{4,6}), (2K_{2,3}, 2K_{2,3})$
6	6	$(C_{12}, C_{12}, 3K_{2,2}), (2K_{3,3}, 2K_{3,3}), (3K_{2,2}, 3K_{2,2}, 3K_{2,2}), (3K_{2,2}, R \times B - 3K_{2,2})$
7	7	$(L(\text{FP}), R \times B - L(\text{FP}))$

3.2 Interspaces and interspace patterns

We now analyze the structure of interspaces between two fibers at least one of which is small. In a series of publications (see [22] and [23] for example) Miyamoto and Hanaki generated all homogeneous coherent configurations up to order 34. We can observe that the constituents of a homogeneous coherent configuration of order at most 7 uniquely determine the isomorphism type of the configuration. While this does not necessarily hold for homogeneous coherent configurations of larger orders, the observation carries over to coherent subconfigurations induced by small fibers. Table 1 summarizes the classification.

Regarding interspaces, we next introduce a condensed description, which captures sufficient information to uniquely determine the isomorphism type of small coherent configurations: given an interspace $\mathfrak{X}[R, B]$ between two (not necessarily distinct) fibers R and B , define $T(\mathfrak{X}[R, B])$ to be the collection of isomorphism types of the constituents induced by the basis relations A in a $\mathfrak{X}[R, B]$ up to isomorphism (omitting reflexive and transposed basis relations).

First, we use the classification of subconfigurations induced by a small fiber to analyze possible interspaces $\mathfrak{X}[R, B]$ between two small fibers R and B . A (slightly lengthy) case analysis leads to a classification. For critical coherent configurations, it is summarized in Table 2. This classification has the following structural consequence:

► **Proposition 5.** *Let \mathfrak{X} be a critical coherent configuration. If all fibers of \mathfrak{X} are small, then either all fibers have the same size or for all $R \in F(\mathfrak{X})$ we have $|R| \in \{4, 6\}$.*

Our next goal is to describe the possible interspaces between a small fiber S and a fiber L of arbitrary size. Since the large fiber is not bounded in size, there is of course an infinite number of isomorphism types that appear.

Our solution turns out to be rather technical, but the idea is simple. If we forget the structure inside the class L , vertices in L will partition into equivalence class depending on their neighborhood in S (taking colors of arcs into account). We now record the isomorphism

type of the interspace we obtained by just retaining one representative from each class. However, we also capture, for one vertex x of L what structure the neighborhoods with respect to each color induced in S . Due to coherence and the small size of S , this structure is the same (up to isomorphism) for every vertex of L . Because S has size at most 6, it turns out that it is essentially sufficient to check the color degrees of x and which neighborhoods induce monochromatic cliques to capture almost all relevant information. (The reader pressed for time may want to skip the specific details in the rest of this subsection and take Proposition 7 simply as a statement that there is some type of classification of the interspaces.)

To formalize this idea and classify the possible interspaces between a small fiber S and a fiber L of arbitrary size, we introduce a new concept: an *interspace pattern* is a string of information which suffices to characterize the interspace up to a certain equivalence and allows us to extract all combinatorial information relevant for our purposes. The formal definition is slightly technical.

► **Definition 6.** For distinct fibers L, S , the interspace $\mathfrak{X}[L, S]$ has the interspace pattern $(G^1, d_1^1, d_2^1, \dots, d_{t_1}^1; \dots; G^k, d_1^k, d_2^k, \dots, d_{t_k}^k)$ if $\sum_{j=1}^k t_j = |\mathfrak{X}[L, S]| - 1$, there are distinct $A^1, \dots, A^k \in \mathfrak{X}[S]$ such that for each $i \in \{1, \dots, k\}$ the underlying undirected graph of (S, A^i) is isomorphic to G^i , and there are distinct $U_1^i, \dots, U_{t_i}^i \in \mathfrak{X}[L, S]$ such that for all $\ell \in L$ and $j \in \{1, \dots, t_i\}$ the set $\ell U_j^i = \{s \in S \mid \ell s \in U_j^i\}$ induces a d_j^i -clique in the underlying undirected graph of (S, A^i) .

We should emphasize that the sum of the t_i is $|\mathfrak{X}[L, S]| - 1$ and thus we omit exactly one basis relation of the interspaces in the pattern. In fact, in general the missing interspace will not satisfy a clique condition. Also, it is a priori not clear that an interspace always has a pattern of this form we just defined. For $d_j^i = 3$, a refined definition distinguishes two versions of the interspace patterns, which we mark with \dagger and \ddagger . The reader may find more details on interspace patterns in the full version of the paper [36].

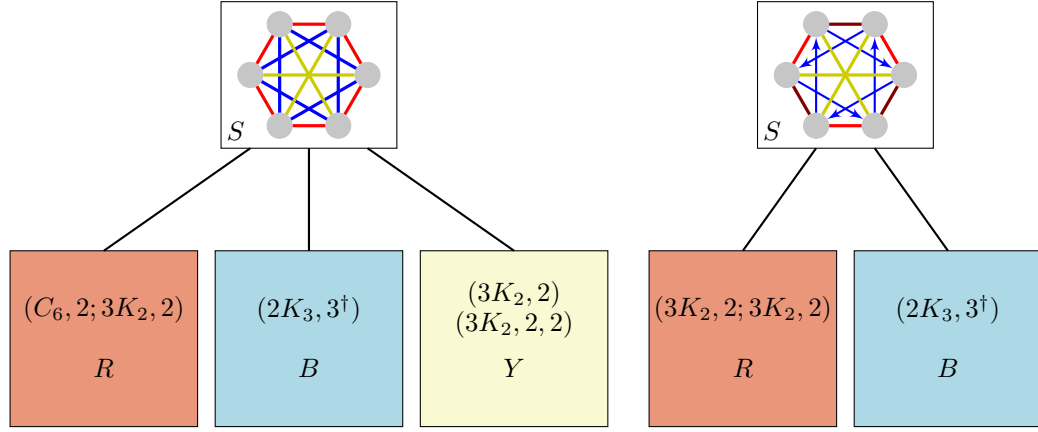
We remark that in our application the small fiber S is restricted to size 4 or 6. (It turns out that we do not need to invoke interspace patterns for fibers of size 5 and 7 since the second set of reductions described further below allows us to deal with them in simpler manner.) A (again slightly lengthy) case distinction iterates through the possible homogeneous coherent configurations introduced by a small fiber S and the possible connections. We obtain the following classification:

► **Proposition 7.** Let \mathfrak{X} be a critical coherent configuration and L, S fibers adjacent in $Q(\mathfrak{X})$. If $|S| \in \{4, 6\}$, then $\mathfrak{X}[L, S]$ has exactly one of the following interspace patterns:

- | | | |
|------------------|-------------------------------|-------------------------------|
| 1. $(K_4, 2)$ | 7. $(3K_2, 2, 2)$ | 13. $(K_6, 3^\dagger)$ |
| 2. $(2K_2, 2)$ | 8. $(C_6, 2; 3K_2, 2)$ | 14. $(K_6, 3^\ddagger)$ |
| 3. $(C_4, 2)$ | 9. $(3K_2, 2; 3K_2, 2)$ | 15. $(2K_3, 3^\dagger)$ |
| 4. $(K_6, 2)$ | 10. $(K_{2,2,2}, 2; 3K_2, 2)$ | 16. $(K_{2,2,2}, 3^\dagger)$ |
| 5. $(K_6, 2, 2)$ | 11. $(K_{3,3}, 2)$ | 17. $(K_{2,2,2}, 3^\ddagger)$ |
| 6. $(3K_2, 2)$ | 12. $(K_{3,3}, 2, 2)$ | |

We would like to emphasize that the size of fiber L is arbitrary. In particular, the results classifies an infinite number of isomorphism types of interspaces into finitely many classes.

► **Proposition 8.** Let \mathfrak{X} be a coherent configuration, and let (R, Y, B) be an induced path in $Q(\mathfrak{X})$. If \mathfrak{X} is critical, then the subconfiguration $\mathfrak{X}[Y]$ does not contain a constituent isomorphic to K_4 or K_6 .



(a) \mathcal{U} contains a basis relation and its transposed basis relation. (b) \mathcal{U} is a union of two basis relations.

■ **Figure 1** Visualisation of the partition of the neighborhood in Proposition 11.

3.3 Exploiting restorability

With the interspace classifications at hand, we examine induced coherent subconfigurations containing a non-dominating small fiber S with regards to criticality. It turns out that certain combinations of interspace patterns occurring simultaneously at one fiber cause S to be restorable. This dictates that certain interspace patterns must appear. It also gives us lower bounds on the number of neighbors certain small fiber S must have.

Assuming that S is a small fiber of size 4 we have the following restrictions.

- **Proposition 9.** *Let \mathfrak{X} be a critical coherent configuration with distinct fibers R, S .*
1. *If $\{S\}$ is non-dominating and $|S| = 4$, then there are two fibers adjacent to S in $Q(\mathfrak{X})$ inducing interspace patterns $(C_4, 2)$ and $(2K_2, 2)$, respectively.*
 2. *If $\{R, S\}$ is non-dominating and $|R| = |S| = 4$, then there is no constituent in the interspace between R and S that is isomorphic to C_8 .*
 3. *If $\{S\}$ is non-dominating and $|S| = 4$, then there are at least 3 fibers adjacent to S in $Q(\mathfrak{X})$.*

We present similar claims for S being a small fiber of size 6. However, since the amount of possible interspace patterns increases, we first examine the case in which all interspace incident to S in $Q(\mathfrak{X})$ have the same interspace pattern. Intuitively, for certain interspace patterns, WL2 captures enough combinatorial information to ensure S is restorable. Overall we obtain the following:

- **Proposition 10.** *Let \mathfrak{X} be a critical coherent configuration with a size 6 fiber S that is not dominating. There is no interspace pattern \mathfrak{P} in the following list such that for all fibers R adjacent to S in $Q(\mathfrak{X})$ the interspace $\mathfrak{X}[R, S]$ has this interspace pattern \mathfrak{P} :*

- | | | |
|------------------------|------------------------|-------------------------|
| 1. $(2K_3, 3^\dagger)$ | 3. $(3K_2, 2, 2)$ | 5. $(3K_2, 2; 3K_2, 2)$ |
| 2. $(3K_2, 2)$ | 4. $(C_6, 2; 3K_2, 2)$ | 6. $(K_{3,3}, 2)$ |

The previous proposition implies that, if fiber S has size 6 and $|T(\mathfrak{X}[S])| = 2$, then there are at least two distinct interspace patterns are incident with S . If, however, $|T(\mathfrak{X}[S])| > 2$, then there is essentially a union of basis relations that induces a graph isomorphic to C_6 . In this case, up to four distinct interspace patterns may occur in the interspaces incident to S in $Q(\mathfrak{X})$. We summarize as follows.

- **Proposition 11.** *Let \mathfrak{X} be a critical coherent configuration, and let R, S be distinct fibers such that $\{R, S\}$ is not dominating, the interspace $\mathfrak{X}[R, S]$ has the interspace pattern $(C_6, 2; 3K_2, 2)$ or $(3K_2, 2; 3K_2, 2)$, and a union \mathcal{U} of basis relations of $\mathfrak{X}[S]$ induce a graph isomorphic to C_6 .*
- *There is a partition \mathcal{P} of the neighborhood of a small fiber S in $Q(\mathfrak{X})$ that is defined by the interspace patterns of the interspace incident to S .*
 - *If R has an arbitrary size, then $\text{qdeg}(S) \geq 2$ (visualized in Figures 1a and 1b).*
 - *If $|R| = 6$, then $\text{qdeg}(S) \geq 3$, the fiber R is unique with respect to S , and three distinct interspace patterns occur (visualized in Figure 1a).*

The proofs of most of these claims follow a similar pattern: we start with an induced coherent subconfigurations consisting of multiple fibers and interspaces with a small non-dominating fiber S (and in rare cases multiple non-dominating fibers).

The homogeneous coherent configuration induced by S together with the interspace patterns with its neighbors determines the structure relevant to us. We introduce *partition structures* to capture this information. It turns out that the automorphisms of the partition structure form a subset of the automorphisms of the fibers neighboring S . We can exploit this fact to prove restorability in various cases.

3.4 First base case: only small fibers

With the preparations complete, we examine the first base case: let \mathfrak{X} be a critical coherent configuration in which all fibers are small. Due to Proposition 5, either all of its fibers have size 5, all of them have size 7, or \mathfrak{X} consists of size 4 and size 6 fibers. In the first two cases, we bound the WL-dimension by a constant due to arguments based on the criticality of \mathfrak{X} .

- **Proposition 12.** *Let \mathfrak{X} be a critical coherent configuration.*

1. *If all fibers of \mathfrak{X} have size 5, then $\text{WLdim}(\mathfrak{X}) \leq 2$.*
2. *If all fibers of \mathfrak{X} have size 7, then $\text{WLdim}(\mathfrak{X}) \leq 3$.*

In the third case, we simplify \mathfrak{X} by individualizing carefully chosen vertices and restoring coherence and criticality afterwards.

- **Proposition 13.** *Let \mathfrak{X} be a critical coherent configuration on n vertices in which fibers all have size 4 or 6 and let S be a fiber of \mathfrak{X} . There is a critical coherent configuration \mathfrak{X}' on n' vertices obtained by individualizing a vertex in \mathfrak{X} and restoring coherence and criticality such that the following holds.*

1. *If $|S| = 4$ and $\text{qdeg}(S) \geq 4$, then $\text{WLdim}(\mathfrak{X}) \leq 1 + \text{WLdim}(\mathfrak{X}')$ and $n' \leq n - 20$.*
2. *If $|S| = 6$ and $\text{qdeg}(S) \geq 3$, then $\text{WLdim}(\mathfrak{X}) \leq 1 + \text{WLdim}(\mathfrak{X}')$ and $n' \leq n - 20$.*

The proof of this proposition heavily relies on Propositions 9 and 11. After their application we are left with simplified critical coherent configuration \mathfrak{X} , whose fibers all have size 4. By Proposition 9, it is essentially a colored CFI-graph and its 3-regular quotient graph $Q(\mathfrak{X})$ takes the role of the base graph. For two such coherent configurations we observe, by Fomin and Hoie's upper bound for the treewidth of cubic graphs [13], there is a winning strategy for $\frac{n'}{6} + o(n')$ cops in the cop-and-robbers game played on their quotient graphs of order n' . We also observe that individualizing a vertex in a fiber R and restoring coherence causes all all vertices of R to become singletons. Combining both observations, we create a winning strategy for spoiler using $\frac{n'}{6} + o(n')$ pebbles in the pebble game played on the simplified coherent configurations.

- **Proposition 14.** *Let \mathfrak{X} be a critical coherent configuration on n vertices such that all fibers S of \mathfrak{X} have size 4 and $\text{qdeg}(S) \leq 3$ and all interspace are either homogeneous or contain a constituent isomorphic to $2K_2$. Then $\text{WLdim}(\mathfrak{X}) \leq \frac{n}{24} + o(n)$.*

We now combine all the three propositions. Note that we can use Proposition 13 inductively. Overall, this establishes an upper bound on the WL-dimension of a critical coherent configuration \mathfrak{X} with fiber size at most 7.

► **Proposition 15.** *If all fibers of a critical coherent configuration \mathfrak{X} on n vertices are small, then $\text{WLdim}(\mathfrak{X}) \leq \frac{n}{20} + o(n)$.*

3.5 Second base case: limited fiber size

In our overall argument, we want to use a bound on the size of the fibers that appear in the coherent configurations. For this purpose we adapt Zemlyachenko's degree reduction technique (see [5]) to coherent configurations. For the cost of a sublinear number of individualizations we obtain a bound d on the degree of all but the largest relation in each interspace and fiber. Using an adaptation of the argument, we exploit the fact that the degree can be bounded with another sublinear number of individualizations to obtain a bound on the fiber size of the resulting coherent configuration of interest:

► **Proposition 16.** *Let \mathfrak{X} be a critical coherent configuration, and $c, d \in \mathbb{N}$. Using $\frac{2n}{d} + \frac{dn}{c}$ individualizations and reestablishing coherence, we obtain a coherent configuration \mathfrak{X}' with a WL-dimension bounded by the dimension of certain of its subconfigurations. These subconfigurations have fiber size at most c and degree at most d .*

Now assume that, in addition to an upper bound $t \in \mathbb{N}$ on the fiber size, the treewidth of $Q(\mathfrak{X})$ is bounded as well. We adapt the strategy of the first base case (by individualizing all vertices of R instead of only one vertex) and obtain the following statement:

► **Proposition 17.** *If \mathfrak{X} is a critical coherent configuration and all fibers of \mathfrak{X} have size at most t , then $\text{WLdim}(\mathfrak{X}) \leq t \cdot \text{tw}(Q(\mathfrak{X}))$, where $\text{tw}(Q(\mathfrak{X}))$ is the treewidth of the quotient graph.*

3.6 Local reductions

Our overall goal for local reductions is that after their exhaustive application we obtain a critical coherent configuration structurally similar to the base cases previously discussed. In particular, this means avoiding certain local subconfigurations \mathfrak{S} of \mathfrak{X} , e.g., interspaces between a large and a small fiber having a certain interspace pattern. We individualize t -many vertices and reestablish the coherence and criticality. Most times, this causes the large fibers to split into multiple fibers smaller in size. The result is a critical coherent configuration \mathfrak{X}' which does not contain the unwanted local configuration \mathfrak{S} . While we are one step closer to our goal, there are two challenges we need to address:

1. Since each individualization increases our bound on the WL-dimension, the configuration \mathfrak{X}' must be obtained from \mathfrak{X} in a controlled manner. We must carefully choose the vertices to be individualized and charge the costs of individualizations to the progress we made towards our goal. To this end, we define the potential function τ with $\tau(\mathfrak{X}) := \frac{3n_\ell + n_s - 8k_\ell}{20}$ where parameters n_ℓ , k_ℓ , and n_s of \mathfrak{X} are the number of vertices in large fibers, the number of large fibers, and the number of vertices in small fibers respectively. The progress of a local reduction can be quantified by $\tau(\mathfrak{X}') - \tau(\mathfrak{X})$, and only local reductions where $\tau(\mathfrak{X}) \geq t + \tau(\mathfrak{X}')$ for t individualizations are eligible.
2. While reestablishing the coherence causes fibers contained in \mathfrak{S} to split, other fibers outside of \mathfrak{S} might also be affected. So the resulting coherent configuration \mathfrak{X}' depends on $\mathfrak{X} - \mathfrak{S}$. To dodge this pitfall, we introduce a “monotonization” \tilde{f} of the WL-dimension: it maximizes the WL-dimension over all critical coherent configuration whose potential is smaller or equal to a given one.

While we described the main concepts and ideas for the potential function, the machinery of local reductions has more details and some intricacies are not presented here. For the full picture, we refer the reader to the full version [36]. Nevertheless, we summarize that the local reductions roughly adhere to the following blueprint: if \mathfrak{X} contains \mathfrak{S} , then $\text{WLdim}(\mathfrak{X}) \leq t + \tilde{f}(\tau(\mathfrak{X}) - t')$ where $t' \geq t$. To give a flavor of the reductions let us give an example:

► **Proposition 18.** *Let \mathfrak{X} be a critical coherent configuration with non-dominating fibers L, S . If $\mathfrak{X}[L, S]$ has the interspace pattern $(K_{3,3}, 2)$, then $\text{WLdim}(\mathfrak{X}) \leq 1 + \tilde{f}(\tau(\mathfrak{X}) - 1.1)$.*

In the proof of such local reductions, we often rely on restorability to guarantee lower bounds on the adjacent fibers or the existence of interspace patterns in additional incident interspaces. Let us give another example:

► **Proposition 19.** *Let \mathfrak{X} be a critical coherent configuration, and let R be a fiber of \mathfrak{X} adjacent to at least 3 large fibers in $Q(\mathfrak{X})$. If R is a large fiber, then $\text{WLdim}(\mathfrak{X}) \leq 1 + \tilde{f}(\tau(\mathfrak{X}) - 1)$.*

This proposition allows us to bound the treewidth of certain parts of the quotient graph involving large fibers. In general the use of the reductions allows us to reduce our problem to coherent configurations that do not contain various unwanted subconfigurations. Their structure is restricted and this allows us to employ a global argument.

3.7 Global argument

In a configuration \mathfrak{X} to which no local reduction is applicable, we are guaranteed that certain combinations of interspace patterns involving small fibers do not occur. For example, due to Proposition 18, there is no interspace in \mathfrak{X} that contains the interspace pattern $(K_{3,3}, 2)$.

Using our classification results and restorability, we can ensure additional structural properties. To summarize them, we need to distinguish between two types of small fibers: we call a small fiber R *relevant*, if $|R| \in \{4, 6\}$ and there is a constituent in $\mathfrak{X}[R]$ isomorphic to a clique. It is *irrelevant* otherwise. The following definition and proposition allows us to formally capture the structure additionally guaranteed.

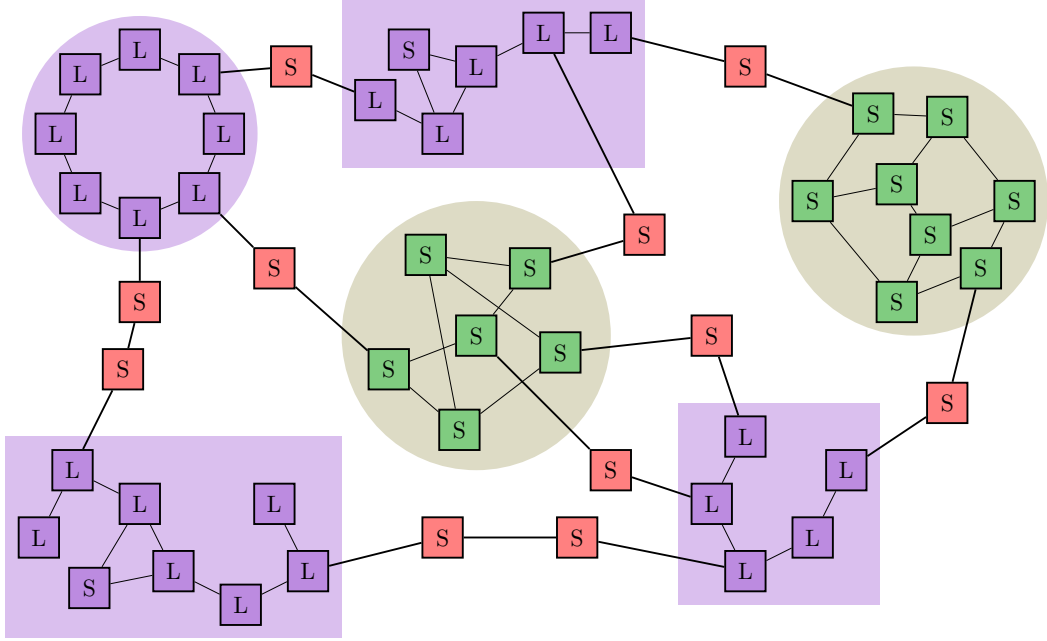
► **Definition 20.** *For $t \in \mathbb{N}$, we call a coherent configuration \mathfrak{X} t -reduced, if it satisfies all of the following properties.*

1. \mathfrak{X} is critical.
2. Every fiber has at most t vertices.
3. All large fibers L have at most two large neighbors.
4. A large fiber has at most one relevant small neighbor.
5. If a relevant small fiber S has a large neighbor, then $\text{qdeg}(S) \leq 2$ and there is a union of basis relation in $\mathfrak{X}[S]$ inducing a graph isomorphic to C_6 .
6. For every $s \in S$ in a relevant small fiber S with three small neighbors, we have that S is discrete in \mathfrak{X}_s .
7. Each relevant small fiber is non-dominating in the quotient graph $Q(\mathfrak{X})$.

► **Proposition 21.** *Let \mathfrak{X} be a critical coherent configuration with fiber size at most t . Then*

- *there is a local reduction which is applicable to \mathfrak{X} ,*
- *$\text{WLdim}(\mathfrak{X})$ is bounded by a constant, or*
- *\mathfrak{X} is t -reduced.*

We need one more structural observation about t -reduced configurations to deal with the irrelevant small fibers.



■ **Figure 2** An example of the quotient graph of a t -reduced critical coherent configuration. The colors represent the following information: ■ large component, ■ small components, ■ fibers of the boundary.

► **Proposition 22.** *Let \mathfrak{X} be a t -reduced coherent configuration. If S is an irrelevant small fiber of \mathfrak{X} , the set of fibers adjacent to S in $Q(\mathfrak{X})$ induces a clique in $Q(\mathfrak{X})$, and S is not adjacent to a relevant small fiber in $Q(\mathfrak{X})$.*

While the notion of t -reduced configuration is defined using local properties, there also are ramifications for the global structure of \mathfrak{X} . In fact, the configuration \mathfrak{X} partitions into large components, small components, and a boundary. Figure 2 visualizes this structure of the quotient graph $Q(\mathfrak{X})$. It is as follows.

- *Large components* contain at least one large fiber but may also include small fibers. The large fibers in a large component induce either a path or a cycle in $Q(\mathfrak{X})$ since their color degree is at most 2. Further, all small fibers within this component are irrelevant. Due to Proposition 22 and being a suitable clique sum, the treewidth of a large component is at most 3. Since the fiber size of \mathfrak{X} is at most t , the WL-dimension of a large component can be bounded using Proposition 17.
- *Small components* contain only relevant small fibers that have size 4 or 6. Using Proposition 15, an upper bound on their WL-dimension can be established.
- The *boundary* are the inner fibers of an induced path that connects small and large components. All such fibers are relevant small fibers. The ends of the paths are small fibers in small or large components. Further, the paths have length at most 3.

We now aim to separate \mathfrak{X} into the small and large components by individualizing carefully chosen vertices within the paths connecting them. Since the interspaces incident to the fibers of the boundary are guaranteed to have certain interspace patterns, only few individualizations are needed to take care of a path.

► **Proposition 23.** *Let \mathfrak{X} be a t -reduced coherent configuration. Further, let (L, S, L') (respectively (L, S, S', L')) be paths where L, L' are large fibers and S, S' are small ones. There are $|S|/2 - 1$ vertices in S after whose individualization followed by restoration of coherence either vertex sets $L \cup S$ and L' or the vertex sets L and $L' \cup S$ (respectively $L \cup S$ and $S' \cup L'$) are homogeneously connected in the resulting coherent configuration.*

It remains to show that the overall number of individualizations required in the boundary is not too large: due to properties following from \mathfrak{X} being t -reduced, the size of the boundary is bounded by the number of large fibers. This allows us to charge the individualizations to the large components. After some calculations, we bound the costs of the individualizations by $\frac{2}{20}n_\ell$. We thus bound the WL-dimension of t -reduced coherent configuration as follows.

► **Proposition 24.** *If \mathfrak{X} is a t -reduced, critical coherent configuration, then $\text{WLdim}(\mathfrak{X}) \leq \frac{2}{20}n_\ell + \frac{1}{20}n_s + o(n_s) \leq \tau(\mathfrak{X}) + \mathcal{O}(t) + o(n)$.*

3.8 Combining the arguments

When individualizing, generally, the WL-dimension of \mathfrak{X} is bounded from above by the number of individualizations and the WL-dimension of the resulting coherent configuration.

► **Theorem 25.** *Let \mathfrak{X} be a coherent configuration, and let $v_1, \dots, v_\ell \in \Omega(\mathfrak{X})$. Further, let \mathfrak{X}' be the coherent configuration obtained by individualizing v_1, \dots, v_ℓ and restoring coherence. Then $\text{WLdim}(\mathfrak{X}) \leq \ell + \max\{2, \text{WLdim}(\mathfrak{X}')\}$.*

(Here the 2 in the maximum is caused by the (possibly repeated) use of WL2 after individualization). Applying this insight to \mathfrak{X} , we iterate through the different cases of Proposition 21 and count the individualizations used in them:

- We choose t depending on n such that $t(n) \in o(n)$ and $t(n) \in \omega(1)$. By Proposition 16 there are $o(n)$ -many individualizations such that in the resulting coherent configuration \mathfrak{X}' each fiber has size at most t .
- The number of individualizations used in the local reductions to obtain the t -reduced, critical coherent configuration \mathfrak{X}'' is bound by $\tau(\mathfrak{X}') - \tau(\mathfrak{X}'')$.
- Finally, Proposition 24 guarantees that there is a bound on the WL-dimension of the t -reduced, critical coherent configuration \mathfrak{X}'' . We obtain $\text{WLdim}(\mathfrak{X}'') \leq \tau(\mathfrak{X}'') + o(n)$.

Overall, this yields the following:

$$\begin{aligned} \text{WLdim}(\mathfrak{X}) &\leq 2 + \tau(\mathfrak{X}') - \tau(\mathfrak{X}'') + \text{WLdim}(\mathfrak{X}'') + o(n) \leq 2 + \tau(\mathfrak{X}') + o(n) \\ &\leq \frac{3(n_\ell + n_s) - k_\ell}{20} + o(n) \leq \frac{3}{20}n + o(n). \end{aligned}$$

This concludes the proof sketch of the upper bound (Theorem 1).

4 Lower bound

In this section, we assemble several known results to obtain an improved lower bound for the maximum WL-dimension of graphs in terms of their order.

► **Theorem 26.** *A random cubic graph asymptotically almost surely has a treewidth of at least $0.042011151 \cdot n - 1$.*

Proof. By [28] a random cubic graph asymptotically almost surely has vertex expansion (i.e., vertex-isoperimetric number) at least $\alpha \geq 0.144208556$ (this is $A_3(1/2)$ in [28]). This implies that a random cubic graph asymptotically almost surely has treewidth at least $\frac{\alpha}{3(1+\alpha)}n - 1 \geq 0.042011151 \cdot n - 1$ [11, Corollary 7]. ◀

It is well known that cubic graphs of high treewidth yield graphs with high WL-dimension via the CFI-construction. Specifically, we have the following relation.

► **Theorem 27** (Consequence of [8, Theorem 3]). *For a graph G , the CFI-graph $\text{CFI}(G)$ with base graph G satisfies $\text{WLdim}(\text{CFI}(G)) \geq \text{tw}(G)$.*

We remark that there are two versions of the CFI-constructions used in the literature. One, where for cubic graphs each vertex is replaced by a gadget of order 10 and one, where for cubic graphs each vertex is replaced by a gadget of order 4. (See [15, 29, 33] for more information.) These versions are very similar and the theorem, as well as many other theorems, hold for either of them. The difference between the constructions is that the former produces CFI-graphs of order $10|G|$, while the latter produces graphs of order $4|G|$. In the terminology of our current paper, the first version produces coherent configurations with fibers of size 2, so a non-critical configuration. Removal of the tiny fibers yields the other construction.

The two theorems combine as follows.

► **Corollary 28.** *The maximum WL-dimension for graphs of order n is at least $0.0105027 \cdot n - o(n)$.*

In the light of our discussions on configurations with small fiber size we remark that, due to the nature of the CFI-construction, the statement is also true for graphs of color class size 4.

References

- 1 Vikraman Arvind, Johannes Köbler, Gaurav Rattan, and Oleg Verbitsky. Graph isomorphism, color refinement, and compactness. *computational complexity*, 26(3):627–685, 2017. doi:10.1007/s00037-016-0147-6.
- 2 Albert Atserias, Laura Mancinska, David E. Roberson, Robert Sámal, Simone Severini, and Antonios Varvitsiotis. Quantum and non-signalling graph isomorphisms. *Journal of Combinatorial Theory, Series B*, 136:289–328, 2019. doi:10.1016/J.JCTB.2018.11.002.
- 3 Albert Atserias and Elitza N. Maneva. Sherali-adams relaxations and indistinguishability in counting logics. *SIAM Journal on Computing*, 42(1):112–137, 2013. doi:10.1137/120867834.
- 4 László Babai. Lectures on graph isomorphism. Mimeographed lecture notes, Department of Computer Science, University of Toronto, October 1979. Lecture notes.
- 5 László Babai. Moderately exponential bound for graph isomorphism. In *Fundamentals of Computation Theory, FCT’81, Proceedings of the 1981 International FCT-Conference, Szeged, Hungary, August 24-28, 1981*, volume 117 of *Lecture Notes in Computer Science*, pages 34–50. Springer, 1981. doi:10.1007/3-540-10854-8_4.
- 6 László Babai. Graph isomorphism in quasipolynomial time [extended abstract]. In *Proceedings of the 48th Annual ACM SIGACT Symposium on Theory of Computing, STOC 2016, Cambridge, MA, USA, June 18-21, 2016*, pages 684–697. ACM, 2016. doi:10.1145/2897518.2897542.
- 7 Jin-yi Cai, Martin Fürer, and Neil Immerman. An optimal lower bound on the number of variables for graph identification. *Combinatorica*, 12(4):389–410, 1992. doi:10.1007/BF01305232.
- 8 Anuj Dawar and David Richerby. The power of counting logics on restricted classes of finite structures. In *Computer Science Logic, 21st International Workshop, CSL 2007, 16th Annual Conference of the EACSL, Lausanne, Switzerland, September 11-15, 2007, Proceedings*, volume 4646 of *Lecture Notes in Computer Science*, pages 84–98. Springer, 2007. doi:10.1007/978-3-540-74915-8_10.

- 9 Holger Dell, Martin Grohe, and Gaurav Rattan. Lovász meets Weisfeiler and Leman. In *45th International Colloquium on Automata, Languages, and Programming, ICALP 2018, July 9-13, 2018, Prague, Czech Republic*, volume 107 of *LIPIcs*, pages 40:1–40:14. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2018. doi:10.4230/LIPICS.ICALP.2018.40.
- 10 Zdenek Dvorák. On recognizing graphs by numbers of homomorphisms. *Journal of Graph Theory*, 64(4):330–342, 2010. doi:10.1002/JGT.20461.
- 11 Zdenek Dvorák and Sergey Norin. Strongly sublinear separators and polynomial expansion. *SIAM Journal on Discrete Mathematics*, 30(2):1095–1101, 2016. doi:10.1137/15M1017569.
- 12 Sergei Evdokimov, Ilia Ponomarenko, and Gottfried Tinhofer. Forestal algebras and algebraic forests (on a new class of weakly compact graphs). *Discrete Mathematics*, 225(1):149–172, 2000. FPSAC’98. doi:10.1016/S0012-365X(00)00152-7.
- 13 Fedor V. Fomin and Kjartan Høie. Pathwidth of cubic graphs and exact algorithms. *Information Processing Letters*, 97(5):191–196, 2006. doi:10.1016/j.ipl.2005.10.012.
- 14 Frank Fuhlbrück, Johannes Köbler, and Oleg Verbitsky. Identifiability of graphs with small color classes by the Weisfeiler-Leman algorithm. *SIAM Journal on Discrete Mathematics*, 35(3):1792–1853, 2021. doi:10.1137/20M1327550.
- 15 Martin Fürer. Weisfeiler-lehman refinement requires at least a linear number of iterations. In *Automata, Languages and Programming, 28th International Colloquium, ICALP 2001, Crete, Greece, July 8-12, 2001, Proceedings*, volume 2076 of *Lecture Notes in Computer Science*, pages 322–333. Springer, 2001. doi:10.1007/3-540-48224-5_27.
- 16 Alexander L. Gavriluk, Roman Nedela, and Ilia Ponomarenko. The Weisfeiler-Leman dimension of distance-hereditary graphs. *Graphs and Combinatorics*, 39(4):84, 2023. doi:10.1007/S00373-023-02683-3.
- 17 Martin Grohe. *Descriptive Complexity, Canonisation, and Definable Graph Structure Theory*, volume 47 of *Lecture Notes in Logic*. Cambridge University Press, 2017. doi:10.1017/9781139028868.
- 18 Martin Grohe and Daniel Neuen. Canonisation and definability for graphs of bounded rank width. *ACM Transactions on Computational Logic*, 24(1):6:1–6:31, 2023. doi:10.1145/3568025.
- 19 Martin Grohe and Martin Otto. Pebble games and linear equations. *The Journal of Symbolic Logic*, 80(3):797–844, 2015. doi:10.1017/JSL.2015.28.
- 20 Martin Grohe, Pascal Schweitzer, and Daniel Wiebking. Deep Weisfeiler Leman. In *Proceedings of the 2021 ACM-SIAM Symposium on Discrete Algorithms, SODA 2021, Virtual Conference, January 10 - 13, 2021*, pages 2600–2614. SIAM, 2021. doi:10.1137/1.9781611976465.154.
- 21 Jin Guo, Alexander L Gavriluk, and Ilia Ponomarenko. On the Weisfeiler-Leman dimension of permutation graphs. *SIAM Journal on Discrete Mathematics*, 38(2):1915–1929, 2024. doi:10.1137/23M1575019.
- 22 Akihito Hanaki and Izumi Miyamoto. Classification of primitive association schemes of order up to 22. *Kyushu Journal of Mathematics*, 54(1):81–86, 2000. doi:10.2206/kyushujm.54.81.
- 23 Akihito Hanaki and Izumi Miyamoto. Classification of association schemes of small order. *Discrete Mathematics*, 264(1-3):75–80, 2003. doi:10.1016/S0012-365X(02)00551-4.
- 24 Neil Immerman and Eric Lander. *Describing Graphs: A First-Order Approach to Graph Canonization*, pages 59–81. Springer New York, New York, NY, 1990. doi:10.1007/978-1-4612-4478-3_5.
- 25 Sandra Kiefer and Daniel Neuen. Bounding the Weisfeiler-Leman dimension via a depth analysis of I/R-trees. In *Proceedings of the 39th Annual ACM/IEEE Symposium on Logic in Computer Science, LICS 2024, Tallinn, Estonia, July 8-11, 2024*, pages 50:1–50:14. ACM, 2024. doi:10.1145/3661814.3662122.
- 26 Sandra Kiefer, Ilia Ponomarenko, and Pascal Schweitzer. The Weisfeiler-Leman dimension of planar graphs is at most 3. *Journal of the ACM*, 66(6):44:1–44:31, 2019. doi:10.1145/3333003.
- 27 Sandra Kiefer, Pascal Schweitzer, and Erkal Selman. Graphs identified by logics with counting. *ACM Transactions on Computational Logic*, 23(1):1:1–1:31, 2022. doi:10.1145/3417515.

- 28 Brett Kolesnik and Nick Wormald. Lower bounds for the isoperimetric numbers of random regular graphs. *SIAM Journal on Discrete Mathematics*, 28(1):553–575, 2014. doi:10.1137/120891265.
- 29 Moritz Lichter. *Continuing the Quest for a Logic Capturing Polynomial Time - Potential, Limitations, and Interplay of Current Approaches*. PhD thesis, Technische Universität Darmstadt, Darmstadt, July 2023. doi:10.26083/tuprints-00024244.
- 30 Moritz Lichter, Simon Raßmann, and Pascal Schweitzer. Computational complexity of the Weisfeiler-Leman dimension. In *33rd EACSL Annual Conference on Computer Science Logic, CSL 2025, February 10-14, 2025, Amsterdam, Netherlands*, volume 326 of *LIPICs*, pages 13:1–13:22. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2025. doi:10.4230/LIPICS.CSL.2025.13.
- 31 Moritz Lichter and Pascal Schweitzer. Choiceless polynomial time with witnessed symmetric choice. *Journal of the ACM*, 71(2):7:1–7:70, 2024. doi:10.1145/3648104.
- 32 Christopher Morris, Yaron Lipman, Haggai Maron, Bastian Rieck, Nils M. Kriege, Martin Grohe, Matthias Fey, and Karsten M. Borgwardt. Weisfeiler and Leman go machine learning: The story so far. *Journal of Machine Learning Research*, 24:1–59, 2023. URL: <http://jmlr.org/papers/v24/22-0240.html>.
- 33 Daniel Neuen and Pascal Schweitzer. Benchmark graphs for practical graph isomorphism. In *25th Annual European Symposium on Algorithms, ESA 2017, September 4-6, 2017, Vienna, Austria*, volume 87 of *LIPICs*, pages 60:1–60:14. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2017. doi:10.4230/LIPICS.ESA.2017.60.
- 34 Oleg Pikhurko, Helmut Veith, and Oleg Verbitsky. The first order definability of graphs: Upper bounds for quantifier depth. *Discrete Applied Mathematics*, 154(17):2511–2529, 2006. doi:10.1016/J.DAM.2006.03.002.
- 35 Oleg Pikhurko and Oleg Verbitsky. Logical complexity of graphs: A survey. In *Model Theoretic Methods in Finite Combinatorics - AMS-ASL Joint Special Session, Washington, DC, USA, January 5-8, 2009*, volume 558 of *Contemporary Mathematics*, pages 129–180. American Mathematical Society, 2009.
- 36 Thomas Schneider and Pascal Schweitzer. An upper bound on the Weisfeiler-Leman dimension. *CoRR*, abs/2403.12581, 2024. doi:10.48550/arXiv.2403.12581.
- 37 Boris Weisfeiler. *On construction and identification of graphs*. Lecture Notes in Mathematics, Vol. 558. Springer-Verlag, Berlin-New York, 1976.
- 38 Yulai Wu and Ilia Ponomarenko. On the Weisfeiler-Leman dimension of circulant graphs, 2024. doi:10.48550/arXiv.2406.15822.