A REFINED ANALYSIS OF WEISFEILER-LEMAN LOWER BOUNDS

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ABSTRACT

In this thesis, we analyse the lower bound on the iteration number of the k-dimensional Weisfeiler-Leman algorithm (k-WL) given by Grohe et al. (FOCS 2023) and extend their result to show that the maximal iteration number of k-WL on graphs is in $\Omega\left(\frac{n^{k/2}}{2^k k^{k-1}}\right)$. We establish asymptotically tight bounds on the smallest cylindrical grid and show that the lower bound persists at least $\Omega\left(n^{k/4}\right)$ even if we let k grow with n. We also show a non-trivial relation between n and k such that the maximal iteration number of k-WL on graphs of size n is in $\Omega\left(n^{k/2-o(1)}\right)$. Finally, we analyse the robustness of the construction.

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violets are blue,
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CONTENTS

1 INTRODUCTION

The *Weisfeiler-Leman algorithm* (WL) is a combinatorial algorithm on graphs (or other relational structures) with applications in various fields of computer science. It classifies graphs based on their structure and is particularly useful (and extensively used) as a subroutine for graph-isomorphism tests, most notably in the quasi-polynomial isomorphism test by Babai [2]. To be more specific, the *k-dimensional Weisfeiler-Leman algorithm* (k-WL) iteratively colours k-tuples of vertices of the input graph such that "similar" tuples get the same colour. A natural question is how strong the algorithm is and how many iterations of colour refinement are needed to reach a stable colouring.

As the dimension k gets larger, the algorithm becomes strictly more powerful. This was proven by Cai et al. [5], providing (for every k and every n) two non-isomorphic graphs of size $\Theta(n)$ that are indistinguishable by k-WL. This implies that there is no k such that k-WL would serve as a complete isomorphism test. In fact, they proved that for two given graphs of size n, a dimension of size $\Theta(n)$ would be needed to distinguish them.

Although k-WL does not identify all graphs up to isomorphism, it might still be useful to identify all graphs in a particular class of graphs, that is to ask if k-WL can distinguish a particular graph from any other graph. For example, Kiefer et al. [15] proved that 3-WL can identify any graph in the class of planar graphs.

One can think of k-WL in multiple ways. It is known that the expressivity of the algorithm is precisely described by the k-variable fragment of the *counting logic* $\mathbf{C}_{k+1}$. There is also an Ehrenfeucht-Fraïssé-like game (sometimes called the *bijective k-pebble game*), where the winning strategies determine the distinguishability of the input graphs by k-WL. It is not difficult to prove that the number of rounds k-WL needs to reach a stable colouring is closely connected to the quantifier depth of the $\mathbf{C}_{k+1}$ formulae and, simultaneously, the number of rounds in the bijective k-pebble game.

Grohe et al. [11] found an upper bound on the iteration number for general relational structures of arity at most k, namely that k-WL stabilises after at most $\mathcal{O}(kn^{k-1}\log n)$ steps, and complemented this result by showing a lower bound of $n^{\Omega(k)}$. The authors achieved the upper bound by generalising the result in [16], namely by translating the colourings to semisimple algebras and bounding the number of them in an increasing chain. The lower bound is achieved by constructing a pair of structures distinguishable by some k-WL and taking a higher dimension, which still requires a linear number of steps, and compressing some vertices while preserving the iteration number.

The lower bound was later improved in [12], where the authors found (for each fixed $k \geqslant 3$) graphs which need $\Omega(n^{k/2})$ refinement steps to reach a stable colouring. The authors show this on a compressed CFI graph of a *cylindrical grid*. However, the lower bound presented in [11] is more robust – it shows that even k'-WL for $k' > k$ needs $n^{\Omega(k)}$ rounds for stabilisation (for a large enough n). We do not have such robustness in the construction from [12]. In fact, already $(3k)$-WL needs only a logarithmic number of rounds to stabilise.

CONTRIBUTIONS OF THE THESIS

The lower bound in [12] assumes that the dimension k is a constant. One of the main aims of the thesis is to analyse this lower bound more precisely, try to find the concrete dependence on k and conclude when exactly we still get similar lower bounds, even if the k may depend on n.

We restate the proof of the lower bound given in [12], and we enhance [12, Lemma 16] and [12, Theorem 30] by analysis under the condition that k is not a constant. Furthermore, we give some new insights into the proofs of [12, Lemma 25] and [12, Lemma 26].

Using this analysis, we show the lower bound $\Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right)$ on the iteration number of k-WL algorithm. Also, we show that the construction only works if $n \in \Omega\left(k^4 (\ln k)^2\right)$. Using the results, we find that we have the lower bound $\Omega\left(n^{k/4}\right)$ even if we let k grow with n. We conclude our analysis with the statement that the maximal iteration number of k-WL on graphs of size $\Omega\left((2k)^{k^{1+\delta}}\right)$ is in $\Omega\left(n^{k/2-\varepsilon}\right)$ for any $\varepsilon > 0$ and $\delta > 0$. These results can be found in Section 5.2.

We also prove the following non-trivial lemma from the field of analytic number theory, which turns out to be crucial for our analysis: If w is the smallest integer such that there are at least k pairwise coprime integers between $w/2$ and w, then

$$(1 - o(1)) k \ln k < w < (2 + o(1)) k \ln k.$$

A second goal of this thesis is to show how robust the lower bound given in [12] is, meaning if a higher-dimensional WL algorithm still needs many rounds to stabilise on the construction given for a smaller dimension. In Section 5.4, we give strategies for the cops in the compressed d-Cops and Robber game for $2k + 1 \leqslant d \leqslant 3k$ and prove that $3k - 2j$ cops can catch the robber in $\mathcal{O}\left(w^{j+1}\right)$ rounds for $j < \frac{k-1}{2}$.

2 PRELIMINARIES AND NOTATION

In this chapter, we define coloured graphs and first-order logic (with counting). These two notions will be crucial for us in the following text, however, the concrete details of the definitions may not be necessary for understanding.

2.1 GRAPHS

Definition 2.1. An **(undirected, coloured) graph** G is a tuple (V, E, ζ) containing a finite set of vertices V, a set of edges $E \subseteq \binom{V}{2}$, and a colouring function $\zeta : V \to C$, where C is some set of colours.

If we want to refer to the vertices, edges, or the colouring function of a particular graph, we use the notation $V(G), E(G), \zeta(G), C(G)$ for the vertices, edges, the colouring function, or the colours set of the graph G, respectively.

Furthermore, let $X \subseteq V(G)$ be a subset of the vertex set of G. We define the **induced subgraph** $G[X]$ **of** G as the graph with the vertex set X and the edge set $(X \times X) \cap E(G)$.

We denote the neighbours of a vertex v in the graph G by $N_G(v)$. If the graph G is clear from the context, we omit the index and denote the neighbours by $N(v)$.

Remark. Note that in other literature, the term *graph* is used for an object with vertices and edges. Regarding the nature of this thesis, we have decided to omit the word *coloured*, since nearly all graphs appearing in this thesis are coloured. If we do not specify the colouring explicitly and it is not clear from the context, we consider the uniform colouring on the graph (that is, the colouring that assigns each vertex the same colour).

Definition 2.2. For graphs G, H and subsets $X \subseteq V(G), Y \subseteq V(H)$, we define a **partial isomorphism** $X \to Y$ as an isomorphism of the induced subgraphs $G[X]$ and $H[Y]$).

Definition 2.3. Let ζ be a colouring function of a graph G. A **partition induced by** ζ, denoted by $V/_\zeta$, is the partition of the set V with respect to ζ, that is,

$$V/_\zeta = \Big\{ \{w \in V \mid \zeta(v) = \zeta(w)\} \mid v \in V \Big\}.$$

We say that the colouring ζ **refines** the colouring ξ, denoted by $\zeta \preccurlyeq \xi$, if for all $v, w \in V$, $\zeta(v) = \zeta(w)$ implies $\xi(v) = \xi(w)$. If ζ refines ξ and ξ refines ζ at the same time, we denote this by $\zeta \equiv \xi$.

2.2 FIRST-ORDER LOGIC WITH COUNTING

Let us fix a countable set of variables $\mathcal{X}$. We usually assume that $x, y, z, x_n, \ldots$ are all elements of $\mathcal{X}$.

Definition 2.4. Let τ be a set of relational and function symbols. The set $\mathcal{T}^\tau$ of τ-terms over $\mathcal{X}$ is defined inductively as follows.

- All variables are τ-terms, i. e., $\mathcal{X} \subseteq \mathcal{T}^\tau$.
- If $t_1, \ldots t_n \in \mathcal{T}^\tau$ are terms and $f \in \tau$ is an n-ary relational symbol, then $ft_1 \ldots t_n \in \mathcal{T}^\tau$ is a term.

Furthermore, we define the set of **atomic first-order logic formulae (with equality)** At^τ inductively as follows.

- If $t_1, t_2 \in \mathcal{T}^\tau$ are terms, then $t_1 = t_2 \in \mathrm{At}^\tau$ is an atomic formula.
- If $t_1, \ldots, t_n \in \mathcal{T}^\tau$ are terms and $R \in \tau$ is an n-ary relational symbol, then $Rt_1 \ldots t_n \in \mathrm{At}^\tau$ is an atomic formula.

Lastly, we define the set of **first-order logic formulae (with equality) $\mathbf{FO}^\tau$** inductively as follows.

- $\mathrm{At}^\tau \subseteq \mathbf{FO}^\tau$, that is, all atomic formulae are first-order logic formulae.
- If $\varphi, \psi \in \mathbf{FO}^\tau$ are formulae, then $(\varphi \wedge \psi), (\varphi \vee \psi), \neg\varphi \in \mathbf{FO}^\tau$ are formulae.
- $\varphi \in \mathbf{FO}^\tau$ and $x \in \mathcal{X}$ is a variable, then $\exists x\varphi, \forall x\varphi \in \mathbf{FO}^\tau$ are formulae.

If τ is not important or it is clear from the context, we also omit the index τ.found

We say that **the free variables of the formula φ are** $x_1, \ldots, x_n$, denoted by $\mathrm{Free}(\varphi) = \{x_1, \ldots, x_n\}$, if

- φ is an atomic formula, x_i occurs in the formula for all i, and φ does not contain any other variables,
- $\varphi \in \{(\psi_1 \wedge \psi_2), (\psi_1 \vee \psi_2)\}$ and
$$\mathrm{Free}(\psi_1) \cup \mathrm{Free}(\psi_2) = \{x_1, \ldots, x_n\},$$
- $\varphi \in \{\exists x\psi, \forall x\psi\}$ and $\mathrm{Free}(\psi) = \{x, x_1, \ldots, x_n\}$, or
- $\varphi = \neg\psi$ and $\mathrm{Free}(\psi) = \{x_1, \ldots, x_n\}$.

To emphasize that the variables of the formula φ are $x_1, \ldots x_n$, we write $\varphi(x_1, \ldots, x_n)$ instead of φ. If $\mathrm{Free}(\varphi) = \emptyset$, we call the formula φ a **sentence**.

Definition 2.5. A **τ-structure** $\mathfrak{A}$ (for a set τ of relational and function symbols) is a collection of

- a non-empty set A, called the universe of $\mathfrak{A}$,
- an interpretation of all relational symbols in τ, that is, for each n-ary relational symbol $R \in \tau$, the structure contains an n-ary relation $R^{\mathfrak{A}} \subseteq A^n$, and
- an interpretation of all function symbols in τ, that is, for each n-ary function symbol $f \in \tau$, the structure contains an n-ary function $f^{\mathfrak{A}} : A^n \to A$.

We say that the τ-structure $\mathfrak{A}$ is **relational** if τ does not contain any function symbols. If all symbols in τ have arity at most n, we say that the structure **has arity at most** n.

Definition 2.6. A **τ-interpretation** (for a set of relational and function symbols) is a pair $\mathfrak{I} = (\mathfrak{A}, \beta)$ of a τ-structure $\mathfrak{A}$ and a mapping $\beta : X \to A$ for $X \subseteq \mathcal{X}$.

For a term t, the τ-interpretation $(\mathfrak{A}, \beta)$ assigns the term t a value $[\![t]\!]^{\mathfrak{I}} \in A$ inductively as follows.

- For each $x \in X$, $[\![x]\!]^{\mathfrak{I}} = \beta(x)$, and
- for $t = fx_1 \dots x_n$, $[\![t]\!]^{\mathfrak{I}} = f^{\mathfrak{A}}([\![t_1]\!]^{\mathfrak{I}}, \dots, [\![t_n]\!]^{\mathfrak{I}})$.

Furthermore, for an atomic formula φ, the τ-interpretation $(\mathfrak{A}, \beta)$ assigns the formula φ a value $[\![\varphi]\!]^{\mathfrak{I}} \in \{0, 1\}$ inductively as follows.

- $[\![t_1 = t_2]\!]^{\mathfrak{I}} = \begin{cases} 1 & \text{if } [\![t_1]\!]^{\mathfrak{I}} = [\![t_2]\!]^{\mathfrak{I}}, \\ 0 & \text{otherwise.} \end{cases}$
- $[\![Rt_1 \dots t_n]\!]^{\mathfrak{I}} = \begin{cases} 1 & \text{if } ([\![t_1]\!]^{\mathfrak{I}}, \dots [\![t_n]\!]^{\mathfrak{I}}) \in R^{\mathfrak{A}}, \\ 0 & \text{otherwise.} \end{cases}$

Lastly, for a formula φ, the τ-interpretation $(\mathfrak{A}, \beta)$ assigns the formula φ a value $[\![\varphi]\!]^{\mathfrak{I}} \in \{0, 1\}$ inductively as follows.

- $[\![\neg\varphi]\!]^{\mathfrak{I}} = 1 - [\![\varphi]\!]^{\mathfrak{I}}$,
- $[\![\varphi \wedge \psi]\!]^{\mathfrak{I}} = \min([\![\varphi]\!]^{\mathfrak{I}}, [\![\psi]\!]^{\mathfrak{I}})$,
- $[\![\varphi \vee \psi]\!]^{\mathfrak{I}} = \max([\![\varphi]\!]^{\mathfrak{I}}, [\![\psi]\!]^{\mathfrak{I}})$,
- $[\![\exists x\varphi]\!]^{\mathfrak{I}} = \max_{a \in A}([\![\varphi]\!]^{\mathfrak{I}[x/a]})$,
- $[\![\forall x\varphi]\!]^{\mathfrak{I}} = \min_{a \in A}([\![\varphi]\!]^{\mathfrak{I}[x/a]})$,

where $\mathfrak{I}[x/a]$ denotes the interpretation $(\mathfrak{A}, \beta[x/a])$, where $\beta[x/a]$ is defined as $\beta[x/a](y) = \beta(y)$ for all $y \neq x$ and $\beta[x/a](x) = a$.

If $[\![\varphi]\!]^{\mathfrak{I}} = 1$, we say that $\mathfrak{I} = (\mathfrak{A}, \beta)$ is a model of φ, also denoted by $(\mathfrak{A}, \beta) \models \varphi$.

Definition 2.7. First-order logic with counting (or the **counting logic**), denoted by **C** is an extension of the first-order logic by counting quantifiers $\exists^{\geqslant n}$ for all $n \in \mathbb{N}$. More precisely, the set $\mathbf{C}^\tau$ is defined inductively in the same way as $\mathbf{FO}^\tau$, but we add the rule

- If $\varphi \in \mathbf{C}^\tau$ is a formula, then $\exists^{\geqslant n} x\varphi \in \mathbf{C}^\tau$ is a formula.

Suppose an interpretation $\mathfrak{I} = (\mathfrak{A}, \beta)$ and a formula $\varphi \in \mathbf{C}^\tau$. Then the evaluation $[\![\varphi]\!]^{\mathfrak{I}}$ is defined in the same way as in first-order logic, but we add the rule

$$[\![\exists^{\geqslant n} x\varphi(x, \overline{y})]\!]^{\mathfrak{I}} = [\![\exists x_1 \ldots \exists x_n \Big(\bigwedge_{1 \leqslant i < j \leqslant n} (x_i \neq x_j) \wedge \bigwedge_{1 \leqslant i \leqslant n} \varphi(x_i, \overline{y}) \Big)]\!]^{\mathfrak{I}}$$

Definition 2.8. The **quantifier-rank of a formula** φ $\mathrm{qr}(\varphi)$ is defined as follows.

- $\mathrm{qr}(\varphi) = 0$ if φ does not contain $\exists$ nor $\forall$,
- $\mathrm{qr}(\neg\varphi) = \mathrm{qr}(\varphi)$,
- $\mathrm{qr}(\varphi \circ \psi) = \max(\mathrm{qr}(\varphi), \mathrm{qr}(\psi))$ for $\circ \in \{\vee, \wedge\}$, and
- $\mathrm{qr}(\exists x\varphi) = \mathrm{qr}(\exists^{\geqslant n}\varphi) = \mathrm{qr}(\forall x\varphi) = \mathrm{qr}(\varphi) + 1$ for all $n \in \mathbb{N}$.

Example 2.9. The **C**-formula $\exists^{\geqslant 3} x\, (\forall y\, (x \neq y \to Rxy))$ has quantifier rank 2 and uses 2 variables, whereas the equivalent **FO**-formula

$$\exists x_1 \exists x_2 \exists x_3 \left(\left(\bigwedge_{1 \leqslant i \leqslant 3} \forall y (x_i \neq y \to Rxy) \right) \wedge \bigwedge_{1 \leqslant i < j \leqslant 3} (x_i \neq x_j) \right)$$

has quantifier rank 4 and uses 4 variables.

Definition 2.10. The k**-variable fragment of C**, denoted by $\mathbf{C}_k$ is defined as the set of **C**-formulae that contain at most k variables.

The q**-quantifier-rank fragment of C**, denoted by $\mathbf{C}^{(q)}$ is defined as the set of **C**-formulae with quantifier-rank at most q.

The set $\mathbf{C}_k^{(q)}$ is defined as the set $\mathbf{C}_k \cap \mathbf{C}^{(q)}$.

3 THE WEISFEILER-LEMAN ALGORITHM

The **Weisfeiler-Leman algorithm** (WL) is a combinatorial algorithm that operates on graphs (or other relational structures). The algorithm iteratively colours k-tuples of vertices of the input graph such that "similar" tuples are assigned the same colour. This is known as the **k-dimensional Weisfeiler-Leman algorithm** (k-WL).

To gain a better understanding of the k-dimensional algorithm, we first introduce its "1-dimensional version", which is commonly known as the **colour-refinement algorithm**.

3.1 COLOUR REFINEMENT

The colour refinement (CR) algorithm is a classical technique often used to distinguish non-isomorphic graphs. The original idea was to use it as a machine description for chemical structures. Today, this concept is still used, for instance, by Chemprop ([14]). However, the algorithm quickly became popular in general graph theory.

Essentially, the colour refinement algorithm takes a graph G as input and "encodes" the local neighbourhoods of v in the output colouring of v. More precisely, given a graph $G = (V, E, \zeta)$ and $t \in \mathbb{N}$, we define the colour refinement as follows.[1]

$$\begin{aligned}
\mathrm{cr}^{(0)}(G, v) &= \zeta(v) \\
\mathrm{cr}^{(t+1)}(G, v) &= \Big(\mathrm{cr}^{(t)}(G, v), \{\!\{\mathrm{cr}^{(t)}(w) \mid w \in N(v)\}\!\}\Big)
\end{aligned}$$

We define the colouring $\mathrm{cr}^{(t)}(G)$ as $\mathrm{cr}^{(t)}(G)(v) \coloneqq \mathrm{cr}^{(t)}(G, v)$ for all vertices $v \in V(G)$. For every $t \geqslant 0$, the $(t+1)$-st step refines the (t)-th step, namely $\mathrm{cr}^{(t+1)}(G) \preccurlyeq \mathrm{cr}^{(t)}(G)$ (because the colour of a vertex in round t is "saved" in the round $t+1$ as well). Since the graph is finite, there has to be some t_{max} such that $\mathrm{cr}^{(t_{\max}+1)}(G) \equiv \mathrm{cr}^{(t_{\max})}(G)$. We call $\mathrm{cr}^{(t_{\max})}(G)$ the **stable colouring** and denote this by $\mathrm{cr}^{(\infty)}(G)$.

Example 3.1. Let G be a four-cycle with one additional vertex with an edge to one of the vertices (see Figure 1). The algorithm first distinguishes vertices with respect to their degree, and in the second round, with respect to the degree of the neighbours. The intermediate colourings are depicted in Figure 1.

With the intuition from the previous example, one can easily prove by induction on t that one can think of the colour of vertex v in round t as an unravelling of the graph from v of depth t. (See Figure 2.)

We say that CR **distinguishes** G and H if the graphs get different colourings by the algorithm, that is, $\mathrm{cr}^{(\infty)}(G) \neq \mathrm{cr}^{(\infty)}(H)$. We also say

1 A **multiset** A over a domain U is a mapping $A : U \to \mathbb{N}$ (representing the multiplicity of each element). We denote a multiset by double curly brackets, e. g. $A = \{\!\{x, x, y\}\!\}$, meaning the mapping $x \mapsto 2$ and $y \mapsto 1$.

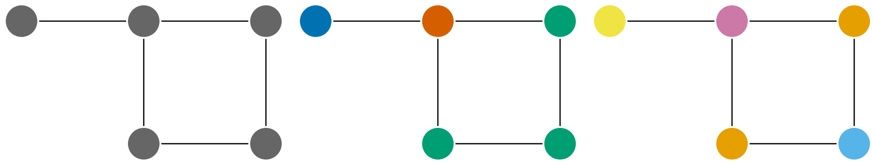

Figure 1: Colourings given by the 0th (left), 1st (center), and 2nd (right) round of the colour refinement algorithm. Note that the first refinement round reflects degrees.

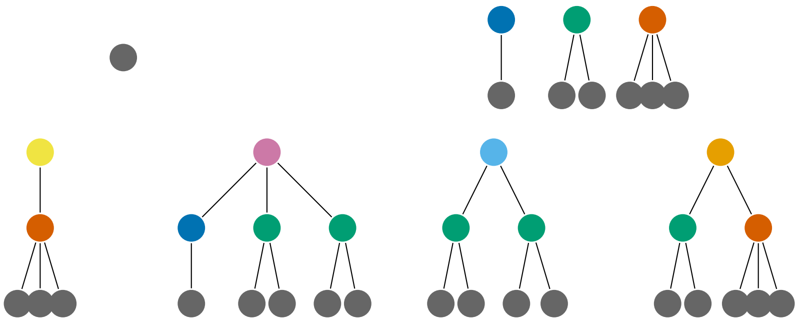

Figure 2: Tree representations of the colours from Example 3.1. The root of a tree is of the colour it represents, and its children are subtrees of neighbours from the previous round.

that CR **identifies** a graph G in a class of graphs $\mathcal{C}$ if CR distinguishes G from all structures $H \in \mathcal{C}$ that are not isomorphic to G.

Colour refinement on its own is in general already a decent heuristic for the graph isomorphism problem. In fact, Babai, Erdős, and Selkow [3] proved that this algorithm identifies almost all graphs (asymptotically). However, the algorithm fails to identify graphs from important classes of graphs, for example, the class of d-regular graphs with n vertices. A precise characterisation and an algorithm[2] to determine if a graph is identifiable by the colour refinement can be found in [1].

For more information about the Colour refinement algorithm, we encourage the reader to visit [10].

3.2 HIGHER DIMENSIONS

A stronger and in a sense similar algorithm to CR was developed by Weisfeiler and Leman in [19], the so-called *classical* Weisfeiler-Leman algorithm. A higher dimensional version (k-WL for every dimension $k \geqslant 1$) for graphs was then developed by Babai and Mathon (see [5]).

There is a subtle difference between the CR algorithm and 1-WL, but this will not be important for us, so we consider them to be "the same" (for details, see [9]). We will define a version of the k-WL algorithm that applies to any relational structure of arity at most k (similarly as in [11]).

Let us first describe the **atomic type** $\mathrm{atp}_k(\mathfrak{A}, \mathbf{v})$ of a tuple $\mathbf{v} \in V(\mathfrak{A})^k$ in a structure $\mathfrak{A}$. We need to encode this tuple in a way such that

2 their algorithm runs in time $\mathcal{O}((n+m)\log n)$, where n is the number of vertices and m is the number of edges

$\mathrm{atp}_k(\mathfrak{A}, \mathbf{v}) = \mathrm{atp}_k(\mathfrak{A}, \mathbf{w})$ if and only if $v_i \mapsto w_i$ is a partial isomorphism. (Note that the ordering and the multiplicity of the elements in the tuple are important here.) There are multiple ways to do this, and the concrete way will not be necessary for this text. (In the case of graphs $\mathfrak{A} = G = (V, E, \zeta)$, for example, one can create a binary string of length $2\binom{k}{2} + k|C(G)|$, which for $1 \leqslant i < j \leqslant k$ has two entries indicating whether $v_i = v_j$ and whether $(v_i, v_j) \in E$ and furthermore, for each $1 \leqslant i \leqslant k$ has $|C(G)|$ entries indicating which colour the vertex v_i has.)

The algorithm colours k-tuples of vertices of a structure $\mathfrak{A}$ as follows. For any tuple of elements $\mathbf{v} \in V(\mathfrak{A})^k$ and $t \in \mathbb{N}$, we let

$$\begin{aligned} \mathrm{wl}_k^{(0)}(\mathfrak{A}, \mathbf{v}) &= \mathrm{atp}_k(\mathfrak{A}, \mathbf{v}), \\ \mathrm{wl}_k^{(t+1)}(\mathfrak{A}, \mathbf{v}) &= \big(\mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v}), M\big), \end{aligned}$$

where

$$\begin{aligned} M = \Bigg\{\!\!\Bigg\{ \Bigg(\mathrm{atp}_{k+1}(\mathfrak{A}, \mathbf{v}w), & \mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v}[w/1]), \\ & \mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v}[w/2]), \\ & \quad \vdots \\ & \mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v}[w/k]) \Bigg) \;\Bigg|\; w \in V(\mathfrak{A}) \Bigg\}\!\!\Bigg\}. \end{aligned}$$

Here, we use the following notation. If $\mathbf{v} = (v_1, \dots, v_k)$ is a k-tuple, then we denote $(v_1, \dots, v_{i-1}, w, v_{i+1}, \dots, v_k)$ by $\mathbf{v}[w/i]$ and the tuple $(v_1, \dots, v_k, w)$ by $\mathbf{v}w$.

Similarly, as in the case of colour refinement, we define the colouring $\mathrm{wl}_k^{(t)}(\mathfrak{A})$ by $\mathrm{wl}_k^{(t)}(\mathfrak{A})(\mathbf{v}) := \mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v})$ for all $\mathbf{v} \in V(\mathfrak{A})^k$. Again, there must be some $t_{\max} < n^k$ with $\mathrm{wl}_k^{(t_{\max})}(\mathfrak{A}) \equiv \mathrm{wl}_k^{(t_{\max}+1)}(\mathfrak{A})$, then we call the colouring $\mathrm{wl}_k^{(\infty)}(\mathfrak{A}) := \mathrm{wl}_k^{(t_{\max})}(\mathfrak{A})$ the **k-stable colouring**.

Similarly, as before, we say that k-WL **distinguishes** $\mathfrak{A}$ and $\mathfrak{B}$ if the structures get different colourings, that is, $\mathrm{wl}_k^{(\infty)}(\mathfrak{A}) \neq \mathrm{wl}_k^{(\infty)}(\mathfrak{B})$. We also say that k-WL **identifies** a structure $\mathfrak{A}$ in a class of structures $\mathcal{C}$ if k-WL distinguishes $\mathfrak{A}$ from all structures $\mathfrak{B} \in \mathcal{C}$ that are not isomorphic to $\mathfrak{A}$.

With the dimension k getting larger, the algorithm becomes strictly stronger in distinguishing non-isomorphic graphs. However, Cai et al. [5] proved that there is no dimension k such that k-WL would serve as a complete isomorphism test. That is the content of the following theorem.

Theorem 3.2 ([5])**.** For any $k \in \mathbb{N}$, there is a pair of non-isomorphic graphs G_k, H_k, both having $\mathcal{O}(k)$ vertices, that are not distinguishable by k-WL.

In a sense, this means that to identify all graphs of size n, we would need to run $\Theta(n)$-WL.

3.3 RELATED TOPICS

3.3.1 *WL dimension*

Let $\mathcal{C}$ be a non-empty class of graphs. We say that $\mathcal{C}$ **has the WL dimension** k, if for all two non-isomorphic graphs graphs $G, H \in \mathcal{C}$, the k-WL distinguishes G and H (that is, $\mathrm{wl}_k^{(\infty)}(G) \neq \mathrm{wl}_k^{(\infty)}(H)$), but for no $k' < k$, k'-WL would distinguish the graphs G, H. Should there be no such k, we say that the WL dimension is ∞.

Observe that the class of all graphs has the WL dimension ∞ (this follows from Theorem 3.2). Other classes of graphs have been inspected, for example, Grohe [7] proved that any class with an excluded minor has a finite WL dimension. Kiefer et al. [15] then determined the WL-dimension of the class of planar graphs to be at most 3.

3.3.2 *Graph neural networks*

The Weisfeiler-Leman algorithm also finds applications in machine learning. The 1-WL algorithm is very closely related to **graph neural networks** (GNN); namely, a GNN layer is more-or-less one refinement step of 1-WL where we aggregate and combine the colours of the neighbours of a particular vertex. This correspondence led to so-called **higher-order GNNs**, first introduced in [17], which resemble the higher dimensional WL algorithm.

4 OTHER SHADES OF k-WL

Over the past decades, a handful of other constructions in some sense equivalent to the k-WL algorithm have been found. In this chapter, we present some of these that were used to lower bound the iteration number of the k-WL algorithm. The first two sections present the connections to the k-variable counting logic $\mathbf{C}_k$ and the bijective k-pebble game, which are both equivalent to the $(k-1)$-WL algorithm in the sense of expressivity. The latter three sections define "special" structures on which k-WL possesses correspondences to other games (like the Cops and Robber game or the k-pebble game[1]).

4.1 COUNTING LOGIC

Cai et al. [5] showed that k-WL for graphs has the same expressive power as the counting logic with $k+1$ variables $\mathbf{C}_{k+1}$ (see Definition 2.7). This result was then extended for all relational structures (see, e.g., [8])

Theorem 4.1. Let $k \geqslant 2$ and let $\mathfrak{A}$ and $\mathfrak{B}$ be relational structures of arity at most k and suppose $\mathbf{v} \in V(\mathfrak{A})^k$ and $\mathbf{w} \in V(\mathfrak{B})^k$. Then for every $t \geqslant 0$, the following are equivalent:

- $\mathrm{wl}_k^{(t)}(\mathfrak{A}, \mathbf{v}) \neq \mathrm{wl}_k^{(t)}(\mathfrak{B}, \mathbf{w})$
- There is a formula $\varphi(\mathbf{x}) \in \mathbf{C}_{k+1}^{(t)}$ with $\mathfrak{A} \models \varphi(\mathbf{v})$ and $\mathfrak{B} \not\models \varphi(\mathbf{w})$.

Corollary 4.2. Let $k \geqslant 2$ and let $\mathfrak{A}$ and $\mathfrak{B}$ be relational structures of arity at most k.

If there is a sentence $\varphi \in \mathbf{C}_{k+1}^{(t)}$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$, then k-WL distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ after at most t refinement rounds.

If k-WL distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ after t rounds, then there is a sentence $\varphi \in \mathbf{C}_{k+1}^{(t+k)}$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.

Remark. Note that in Corollary 4.2, we do not have the particular tuples $\mathbf{v}$ and $\mathbf{w}$. While the WL algorithm can "use the information from these tuples" already after the first round, the counting logic needs to "quantify those elements first". This is more or less the reason we get the quantifier rank $t+k$ in the second direction of Corollary 4.2.

4.2 BIJECTIVE k-PEBBLE GAME

Let $k \in \mathbb{N}$. The **bijective r-round k-pebble game** is played between two players, Spoiler and Duplicator, on two graphs G, H. We have a pair of pebbles p_i, q_i for every $1 \leqslant i \leqslant k$, where the pebbles p_i

1 Not to confuse with the *bijective* k-pebble game.

can be placed on $V(G)$ and q_i on $V(H)$. We say that a **position** in the game is a pair $\mathbf{u} = (u_1, \dots, u_l) \in V(G)^l, \mathbf{v} = (v_1, \dots, v_l) \in V(H)^l$ for some $l \leqslant k$, where corresponding pebbles are placed on u_i and v_i for every $1 \leqslant i \leqslant l$.

If $|V(G)| \neq |V(H)|$, then Spoiler wins immediately. The pebbles are initially placed beside the graphs. A round of the game is played as follows:

1. Spoiler picks up a pair of pebbles p_i, q_i.
2. Duplicator chooses a bijection $h : V(G) \to V(H)$.
3. Spoiler chooses a vertex $u \in V(G)$ and places p_i on u in G and q_i on $h(u)$ in H.

If the position $\mathbf{u}, \mathbf{v}$ does not induce a partial isomorphism[2] after r rounds, we say that Spoiler wins in r rounds. (If the graphs have some additional structure, like, for example, equivalence relation on the vertex set, the partial isomorphism has to preserve this as well.) Otherwise, we say that Duplicator wins in r rounds. Spoiler wins a play if Spoiler wins after some round, and Duplicator wins otherwise (when Spoiler does not win in any round). Spoiler (respectively, Duplicator) has a winning strategy (in r rounds) if they can force a win (in r rounds) interdependently of the moves of the other player. We write $G, \mathbf{u} \simeq_k^r H, \mathbf{v}$ if Duplicator has a winning strategy from position $\mathbf{u}, \mathbf{v}$ in r rounds, or $G \simeq_k^r H$ if Duplicator has a winning strategy from the initial position. When considering the game without a fixed number of rounds, we write $G \simeq_k H$ if Duplicator has a winning strategy.

Example 4.3. Let G and H be the graphs depicted in Figure 3. These graphs are not isomorphic and Spoiler has a winning strategy in the bijective 3-pebble game on those graphs. One of the possible strategies looks as follows.

The pebble pair (p_1, q_1) is picked up. Duplicator chooses a bijection $h_1 : V(G) \to V(H)$ and Spoiler places the pebbles on the vertex 2 in G and on the vertex $h_1(2)$ in H. Let us consider the following possibilities.

- If $h_1(2) = 2$, then we will use the fact that 2 lies on a triangle in G, but not in H. No matter which bijections Duplicator chooses, in the next two rounds, Spoiler chooses the vertices 3 and 5 in G and the corresponding vertices $h_2(3)$ and $h_3(5)$ in H (h_2 and h_3 are the bijections Duplicator chose in the second and the third round). Now the vertices $2, 3, 5$ form a triangle in G, but there is no triangle in H that would contain 2.

- If $h_1(2) \neq 2$, we will use the fact that there is a path of length exactly 1 from the vertex 2 in G, but this does not happen in any other vertex in H. No matter what Duplicator chooses, Spoiler chooses the vertex 1 in G and the corresponding vertex $h_2(1)$ in H. If $h_1(2)$ and $h_2(1)$ do not have an edge in H, then Spoiler

2 that is, if the mapping $u_i \mapsto v_i$ is not a partial isomorphism

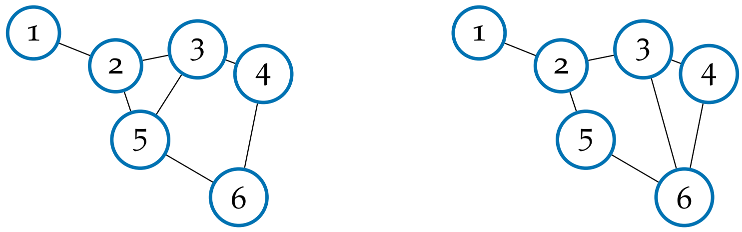

Figure 3: Graph G (left) and graph H (right) from Example 4.3

wins, otherwise there is a vertex $w \in H$ such that $h_1(2), h_2(1), w$ is a path of length 3. Spoiler can now choose the vertex $h_3^{-1}(w)$ in G and w in H and win.[3]

Lemma 4.4 ([13, Proposition 2.3])**.** Let $k \geqslant 2$, let G and H be graphs, $\mathbf{u} \in V(G)^k$, $\mathbf{v} \in V(H)^k$ and $r \in \mathbb{N}$. Then the following are equivalent.

- $G, \mathbf{u} \not\simeq_k^r H, \mathbf{v}$, that is, Spoiler has a winning strategy in the bijective r-round k-pebble game on G and H from position $\mathbf{u}, \mathbf{v}$.
- There is a formula $\varphi(\mathbf{x}) \in \mathbf{C}_k^{(q)}$ with $G \models \varphi(\mathbf{u})$ and $H \not\models \varphi(\mathbf{v})$.

Lemma 4.4 relates the game to the expressive power of k-WL via Corollary 4.2. This is summarised in the following corollary.

Corollary 4.5. Let $k \geqslant 2$, let G, H be graphs, let $\mathbf{u} \in V(G)^k, \mathbf{v} \in V(H)^k$, and let $r \in \mathbb{N}$. Then

$$G, \mathbf{u} \not\simeq_{k+1}^r H, \mathbf{v} \quad \text{if and only if} \quad \mathrm{wl}_k^{(r)}(G, \mathbf{u}) \neq \mathrm{wl}_k^{(r)}(H, \mathbf{v}).$$

Furthermore, $G \not\simeq_{k+1} H$ if and only if k-WL distinguishes G and H, and the required round number of Spoiler and the iteration number of k-WL differ by at most k.

We will need this corollary also in the case that the graphs possess an equivalence relation on the vertex set. If the partial isomorphisms preserve this (as above), the lemma remains true, as stated in [12].

Example 4.3 (continued)*.* Note that Spoiler had a winning strategy in 3 rounds. One can check that the 2-WL distinguishes the graphs after the first round. Note that the required number of rounds is not equal, but it differs by at most 2, as the lemma states.

4.3 CFI GRAPHS, COPS, AND ROBBERS

4.3.1 *CFI construction*

Let G be a connected and ordered graph and define a colouring on G such that every vertex has a unique colour. We refer to the vertices

3 Note that *there is* a path of length 3 in G that contains the vertex 2, however, the winning condition does not state that the sets should be isomorphic, but we indeed need the mapping that maps the vertex under the pebble p_i to the vertex under the pebble q_i to be a partial isomorphism.

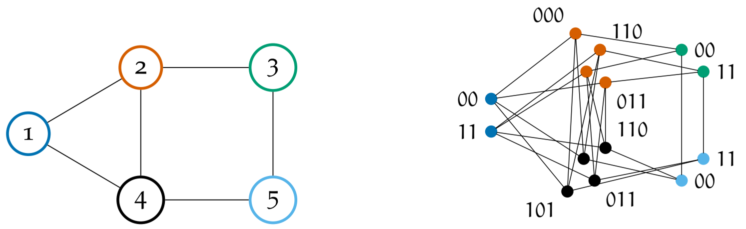

Figure 4: Graph G (left) and the graph $\mathrm{CFI}(G, f)$ (right) from Example 4.6 for f being the constant 0 function.

Figure 5: The edge $\{2, 3\}$ from Example 4.6 when it is not twisted (left) and when it is twisted (right).

and edges of G as **base vertices** and **base edges**, respectively. Furthermore, let $f : E \to \mathbb{F}_2$ be an arbitrary function. If $f(e) = 1$ for an edge $e \in E$, we say that the edge e is **twisted**. If $g : E \to \mathbb{F}_2$ is another function, we say that e **is twisted with respect to** f, g, if $f(e) \neq g(e)$. We define the graph $\mathrm{CFI}(G, f)$ as follows. For any base vertex u of degree d, we have pairs $(u, \mathbf{a})$ for all d-tuples $\mathbf{a} = (a_1, \dots, a_d) \in \mathbb{F}_2^d$ such that $\sum \mathbf{a} = a_1 + a_2 + \ldots + a_d = 0$. We call u **the origin of** $(u, \mathbf{a})$. Vertices inherit the colour of their origin, and we call the vertices of the same origin **a gadget**. Since every vertex of the base graph has a unique colour, the vertices of each gadget form a colour class of the CFI graph.

Suppose that in the base graph, v is the i-th neighbour of w and w is the j-th neighbour of v in the base graph (with respect to the ordering of G). Then we add an edge between $(v, \mathbf{a})$ and $(w, \mathbf{b})$ if and only if $a_i + b_j = f(\{v, w\})$ (where a_i is the i-th entry of $\mathbf{a}$ and b_j is the j-th entry of $\mathbf{b}$). Note that this adds two complete bipartite graphs between the gadgets of v and w.

Example 4.6. An example of graph G and the graph $\mathrm{CFI}(G, f)$ for a constant 0 function f is depicted in Figure 4. Note that between any two colour classes of $\mathrm{CFI}(G, f)$, we can find two disjoint complete bipartite graphs. For example, the edge $\{2, 3\}$ gave rise to the complete bipartite graphs induced by the sets $\{(2, 000), (2, 101), (3, 00)\}$ and $\{(2, 110), (2, 011), (3, 11)\}$. Note that twisting this edge (setting $f(e) = 1$) would give rise to the bipartite graphs induced by the sets $\{(2, 000), (2, 101), (3, 11)\}$ and $\{(2, 110), (2, 011), (3, 00)\}$ (it "exchanges one side of the bipartite graph"). See Figure 5.

4.3.2 *Cops and robber game*

Let us introduce the k-**Cops and Robber game**. The game is played on a graph G between k cooperating cops and one robber. Initially, the robber is placed on some edge of G and the cops are placed beside the

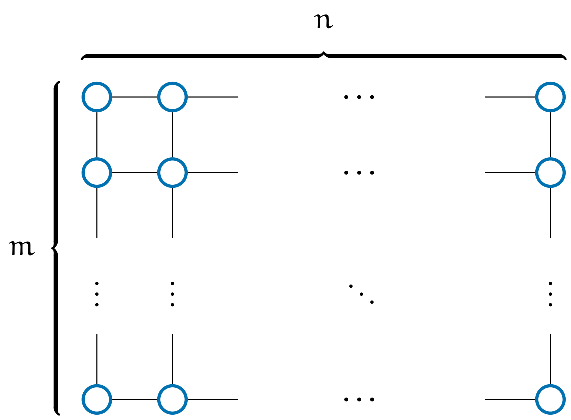

Figure 6: The $m \times n$ grid graph.

graph (if G does not have any edges, the robber loses immediately). A round is played as follows.

1. One cop is picked up, and a destination $v \in V(G)$ for the cop is selected.
2. The robber moves to an edge that is reachable from the robber's position using only edges that are not adjacent to a vertex occupied by a cop.
3. The cop that was picked up in 1. is placed on v.

If cops are placed on both endpoints of the edge the robber is currently on, we say that the robber is caught. If the robber is caught after at most r rounds, we say that the cops win the play in r rounds, otherwise, we say that the robber wins the play in r rounds. If one party can force a win after r rounds, we say that the party **has a winning strategy** in r rounds.

Similarly, as in [12], we consider here a slightly different version of the game than usual in the literature – normally, the robber is placed on a vertex as well and is caught when a cop occupies the same vertex. However, the games are equivalent, and the presented version is more suitable for us here.

Remark. The game is known to capture the so-called **tree-width** of the graph it is played on. Namely, the cop player has a winning strategy in the k-Cop and Robber game if and only if the tree-width of the underlying graph is at most $k-1$. However, this will not be interesting for us, as we will be interested rather in the number of rounds the robber can survive without being caught.

Example 4.7. Let G be an $m \times n$ grid for $m \leqslant n$ (see Figure 6). We need at least $m+1$ cops to catch the robber on G. Suppose we have only m cops. Then after a cop is picked up, there must be a row that is not occupied by any cop and hence the robber can in any round flee to safety. We leave it for the reader to find a strategy for the cops to catch the robber if $m+1$ cops are available.

4.3.3 *The correspondence*

The following two lemmas show us the correspondence between the k-Cops and robber game played on G and the bijective k-pebble game played on two non-isomorphic CFI graphs with base graph G.

Lemma 4.8 ([12, Lemma 5])**.** Let $k \geqslant 2$, G be an ordered base graph and $f, g : E(G) \to \mathbb{F}_2$. If the robber has a winning strategy in the r-round k-Cops and Robber game played on G, then Duplicator has a winning strategy in the r-round bijective k-pebble game played on $\mathrm{CFI}(G, f)$ and $\mathrm{CFI}(G, g)$.

Lemma 4.9 ([12, Lemma 6])**.** Let $k \geqslant 2$, G be an ordered base graph and let $f, g : E(G) \to \mathbb{F}_2$ twist an odd number of edges. If the cops have a winning strategy in the k-Cops and Robber game, then Spoiler has a winning strategy in the bijective k-pebble game when played on $\mathrm{CFI}(G, f)$ and $\mathrm{CFI}(G, g)$.

4.4 COMPRESSING CFI GRAPHS

Let $\equiv$ be an equivalence relation on a set V and let $W \subseteq V$. We define

$$w/_{\equiv} \coloneqq \{v \in V \mid v \equiv w\}, \text{ and}$$
$$W/_{\equiv} \coloneqq \bigcup_{w \in W} w/_{\equiv}.$$

Definition 4.10. An equivalence relation $\equiv$ on the set $V(G)$ is called a G**-compression** if every $\equiv$-equivalence class only contains pairwise non-adjacent vertices of the same degree.

If $\equiv$ is a G-compression, it induces an equivalence relation, denoted also by $\equiv$, on $\mathrm{CFI}(G, f)$ as follows: $(u, \mathbf{a}) \equiv (v, \mathbf{b})$ if and only if $u \equiv v$ and $\mathbf{a} = \mathbf{b}$. We aim to factor the graph $\mathrm{CFI}(G, f)$ by $\equiv$. For this, we need to require that f respects the relation $\equiv$ in the following sense.

Definition 4.11. A function $f : E(G) \to \mathbb{F}_2$ is called $\equiv$**-compressible** if, for every pair of edges $\{u, v\}, \{u', v'\}$, if $u \equiv u'$ and $v \equiv v'$ then $f(\{u, v\}) = f(\{u', v'\})$.

Definition 4.12. Let $\equiv$ be a G-compression and let $f : E(G) \to \mathbb{F}_2$ be a $\equiv$-compressible function.

- The graph $(\mathrm{CFI}(G, f), \equiv)$, the **precompressed CFI graph for** G**,** $\equiv$ **and** f, is the graph $\mathrm{CFI}(G, f)$ extended by the equivalence relation $\equiv$.
- The graph $\mathrm{CFI}(G, f)/_{\equiv}$ is the graph obtained by factoring the graph $\mathrm{CFI}(G, f)$ by $\equiv$, that is, the vertices are the equivalence classes $u/_{\equiv} = \{w \in V(\mathrm{CFI}(G, f)) \mid w \equiv v\}$ and there are $u' \equiv u$ and $v' \equiv v$ such that there is an edge between u' and v' in $\mathrm{CFI}(G, f)$.

Definition 4.13. A set $T \subseteq \{(u,v),(v,u) \mid \{u,v\} \in E(G)\}$ is called a G**-twisting** if, for every $u \in V(G)$, the set $T \cap (\{u\} \times V(G))$ is of even size. The twisting T

- **twists** an edge $\{u,v\} \in E(G)$ if the set T contains exactly one of (u,v) and (v,u), and
- **fixes** a vertex $u \in V(G)$ if $T \cap \{u\} \times V = \emptyset$.

Let $\equiv$ be a G-compression. The twisting T is called $\equiv$**-compressible** if for every $u \equiv u' \in V(G)$ of degree d, and for every $1 \leqslant i \leqslant d$ we have $(u, v_i) \in T$ if and only if $(u', v'_i) \in T$, where v_i is the i-th neighbour of u and v'_i is the i-th neighbour of u'.

Lemma 4.14 ([12, Corollary 14])**.** For every $k \geqslant 3$, every $r \in \mathbb{N}$, every G-compression $\equiv$, and every $\equiv$-compressible $f, g : E(G) \to \mathbb{F}_2$, we have that if

$$(\mathrm{CFI}(G,f),\equiv) \simeq_k^r (\mathrm{CFI}(G,g),\equiv) \text{ and } (\mathrm{CFI}(G,f),\equiv) \not\simeq_k^{r+1} (\mathrm{CFI}(G,g),\equiv),$$

then

$$\mathrm{CFI}(G,f)/_{\equiv} \simeq_k^{r-2} \mathrm{CFI}(G,g)/_{\equiv} \text{ and } \mathrm{CFI}(G,f)/_{\equiv} \not\simeq_k^{r+1} \mathrm{CFI}(G,g)/_{\equiv}.$$

Essentially, this means we can study precompressed CFI graphs to obtain lower bounds on the iteration number of k-WL on compressed CFI graphs. For that, we introduce the r**-round compressed** k**-Cops and Robber game**.

The game is played on an ordered base graph G, together with a G-compression $\equiv$. The cops are placed on $\equiv$-equivalence classes of G and the robber is placed on one edge of G. One round of the game looks as follows.

1. One cop is picked up, and a destination $v \in V(G)$ for the cop is selected.
2. The robber moves. To move from the current edge e_1 to another edge e_2, the robber has to provide a $\equiv$-compressible G-twisting that only twists the edges e_1 and e_2 and that fixes every vertex contained in a $\equiv$-equivalence class occupied by a cop.
3. The cop that was picked up in 1. is placed on v.

If the cops occupy the $\equiv$-equivalence classes of both endpoints of the edge the robber is located on, we say that the robber is caught. If the robber is caught after r rounds, then the cops win the r-round compressed k-Cops and Robber game, and otherwise, the robber wins the r-round game. Note that the initial position of the robber may matter to decide who wins in the compressed game.

It turns out that the compressed CFI graphs and the compressed Cops and Robber game possess a similar correspondence as the non-compressed versions.

Lemma 4.15 ([12, Lemma 15])**.** Let $k \geqslant 3$, $\equiv$ be a G-compression, and $f, g : E(G) \to \mathbb{F}_2$ such that there is exactly one twisted edge e with respect to f, g. If the robber has a winning strategy in the r-round compressed k-Cops and Robber game, where the robber is initially placed on e, then $(\mathrm{CFI}(G, f), \equiv) \simeq_k^r (\mathrm{CFI}(G, g), \equiv)$.

4.5 XOR-CONSTRAINTS AND k-PEBBLE GAME

In this section, we present a correspondence between a game on propositional XOR constraints and the k-WL algorithm on a special pair of relational structures. This correspondence was first shown by Berkholz and Nordström ([4]) and it was used by Grohe et al. [11] to show a robust lower bound of $n^{\Omega(k)}$ on the iteration number of k-WL. This topic will not be important in the following text and can be skipped without loss of the flow of the text.

Let V be a finite set. We think of it as a set of variables taking values in $\{0, 1\}$. An **XOR-constraint (over** V**)** is a pair (C, a) where $C \subseteq V$ and $a \in \{0, 1\}$. Let $\mathcal{C}$ be a set of XOR-constraints. We say that $\mathcal{C}$ has arity at most k if for all $(C, a) \in \mathcal{C}$ it holds $|C| \leqslant k$. We also say that a partial assignment $\beta : X \to \{0, 1\}$ with $X \subseteq V$ **violates** an XOR-constraint $(C, a) \in \mathcal{C}$ if $C \subseteq X$ and

$$\sum_{x \in C} \beta(x) \neq a \mod 2.$$

If a partial assignment $\beta : X \to \{0, 1\}$ does not violate (C, a) and $C \subseteq X \subseteq V$ then we say that β **satisfies** (C, a).

Note that $(\emptyset, 0)$ is always satisfied (there is no partial assignment that would violate it) and $(\emptyset, 1)$ is unsatisfiable (every partial assignment violates it).

Example 4.16. Let $V = \{x_1, x_2, x_3\}$ and $\mathcal{C} = \Big\{\big(\{x_1, x_2\}, 0\big), \big(\{x_1, x_3\}, 1\big)\Big\}$. Then $\mathcal{C}$ has arity 2. There are exactly 6 partial assignments that violate $\big(\{x_1, x_2\}, 0\big)$: every violating assignment has to have domain $\{x_1, x_2\} \subseteq X \subseteq V$, that is, either $X = \{x_1, x_2\}$ or $X = \{x_1, x_2, x_3\}$. An assignment $\beta : X \to \{0, 1\}$ violates $\big(\{x_1, x_2\}, 0\big)$ if and only if $\beta(x_1) \neq \beta(x_2)$. Therefore, there are 2 violating assignments in the first case. In the latter case, it does not matter what x_3 is set to, and hence we have the other four violating assignments. We leave it to the reader to check that $\big(\{x_1, x_3\}, 1\big)$ has exactly six violating assignments as well, two of which are also violating for $\big(\{x_1, x_2\}, 0\big)$.

4.5.1 *The game*

We now define the r**-round** k**-pebble game** $\mathcal{G}_k^r(V, \mathcal{C})$. The game has two players called Verifier and Falsifier. The initial position of the game is the empty assignment.

Suppose that $\beta : X \to \{0, 1\}$ is the current position. The next round consists of the following steps.

- Falsifier chooses $x \in V \setminus X$ and $X' \subseteq X$ such that $|X' \cup \{x\}| \leqslant k$.
- Verifier chooses $b \in \{0, 1\}$.
- The game moves to the position $\beta' : X' \cup \{x\} \to \{0, 1\}$, where $\beta'(x') = \beta(x')$ for all $x' \in X'$ and $\beta'(x) = b$.

Falsifier wins a play if within the first r rounds an assignment β violates some XOR-constraint $(C, a) \in \mathcal{C}$. (If $r = 0$, Falsifier wins if $(\emptyset, 1) \in \mathcal{C}$.) We say that Falsifier wins the game $\mathcal{G}_k^r(V, \mathcal{C})$ if Falsifier has a winning strategy for the game. Otherwise, Verifier wins the game. The k-pebble game $\mathcal{G}_k(V, \mathcal{C})$ is played in the same way, but without any restriction on the number of rounds played.

Example 4.16 (continued). Note that Verifier has a winning strategy in the game $\mathcal{G}_2(V, \mathcal{C})$ in our example. In the beginning, the position is $\beta_0 : \emptyset \to \{0, 1\}$. Suppose that Falsifier chooses x_i. Verifier answers with $b = 0$ if $i = 3$ and with $b = 1$ otherwise. One can check that the game cannot come into a position which would violate one of the constraints and hence Verifier always wins. Note that there is another winning strategy for the Verifier; we leave it to the reader to find it.

Example 4.17. It is important to note the winning condition for Verifier is not the satisfiability of the set of constraints as a whole. In fact, only adding one more constraint to the set in Example 4.16 will show us a counterexample to that. Let $V = \{x_1, x_2, x_3\}$ and let

$$\mathcal{C} = \Big\{ \big(\{x_1, x_2\}, 0\big), \big(\{x_1, x_3\}, 1\big), \big(\{x_2, x_3\}, 0\big) \Big\}.$$

There is no assignment $\beta : V \to \{0, 1\}$ that would satisfy all constraints in $\mathcal{C}$ (the first and the third constraint tell us that all three variables have to be set at the same value, but the middle constraint says that x_1 and x_3 have to be set differently). However, the Verifier has a winning strategy in the game $\mathcal{G}_2(V, \mathcal{C})$: every position in the game has domain size at most 2 and Verifier can always choose a value for the new variable such that the only constraint that could be violated is satisfied.

4.5.2 *The structures*

For a set of XOR-constraints (over a set $V = \{x_1, \ldots, x_n\}$) $\mathcal{C}$, we define two relational structures $\mathfrak{A} := \mathfrak{A}(\mathcal{C})$ and $\mathfrak{B} := \mathfrak{B}(\mathcal{C})$ as follows. We set $V(\mathfrak{A}) = V(\mathfrak{B}) := V \times \{0, 1\}$. For each $1 \leqslant i \leqslant n$, we have a unary relation X_i and we set $X_i^{\mathfrak{A}} = X_i^{\mathfrak{B}} := \{(x_i, 0), (x_i, 1)\}$. Lastly, for each $(C, a) \in \mathcal{C}$ with $C = (x_{i_1}, \ldots, x_{i_k})$ we have a k-ary relation $R_{C,a}$ and we set

$$R^{\mathfrak{A}}_{C,a} := \left\{ \Big((x_{i_1}, b_1), \ldots, (x_{i_k}, b_k) \Big) \;\middle|\; b_1, \ldots, b_k \in \{0,1\}, \sum_{j=1}^{k} b_j \equiv 0 \mod 2 \right\},$$

and

$$R^{\mathfrak{B}}_{C,a} := \left\{ \Big((x_{i_1}, b_1), \ldots, (x_{i_k}, b_k) \Big) \;\middle|\; b_1, \ldots, b_k \in \{0,1\}, \sum_{j=1}^{k} b_j \equiv a \mod 2 \right\},$$

We think of the relation $R^{\mathfrak{B}}_{C,a}$ as the set of solutions for the constraint (C, a) and $R^{\mathfrak{A}}_{C,a}$ as the set of solutions for $(C, 0)$.

Example 4.18. Let $\mathcal{C} = \Big\{ \big(\{x_3\}, 1\big), \big(\{x_1, x_2\}, 0\big), \big(\{x_1, x_2, x_3\}, 0\big) \Big\}$ be a set of constraints over the set $V = \{x_1, x_2, x_3\}$. Both structures $\mathfrak{A}$ and $\mathfrak{B}$ have the elements $\{x_1, x_2, x_3\} \times \{0, 1\}$ and the following relations:

$$\begin{aligned}
X_1^{\mathfrak{B}} = X_1^{\mathfrak{A}} &= \big\{(x_1, 0), (x_1, 1)\big\} \\
X_2^{\mathfrak{B}} = X_2^{\mathfrak{A}} &= \big\{(x_2, 0), (x_3, 1)\big\} \\
X_3^{\mathfrak{B}} = X_3^{\mathfrak{A}} &= \big\{(x_3, 0), (x_3, 1)\big\} \\
R^{\mathfrak{B}}_{\{x_3\},1} &= \Big\{(x_3, 1)\Big\} \qquad R^{\mathfrak{A}}_{\{x_3\},1} = \Big\{(x_3, 0)\Big\} \\
R^{\mathfrak{B}}_{\{x_1,x_2\},0} = R^{\mathfrak{A}}_{\{x_1,x_2\},0} &= \Big\{ \big((x_1, 0), (x_2, 0)\big), \big((x_1, 1), (x_2, 1)\big) \Big\} \\
R^{\mathfrak{B}}_{\{x_1,x_2,x_3\},0} = R^{\mathfrak{A}}_{\{x_1,x_2,x_3\},0} &= \Big\{ \big((x_1, 1), (x_2, 1), (x_3, 0)\big), \\
&\qquad \big((x_1, 1), (x_2, 0), (x_3, 1)\big), \\
&\qquad \big((x_1, 0), (x_2, 1), (x_3, 1)\big) \Big\}
\end{aligned}$$

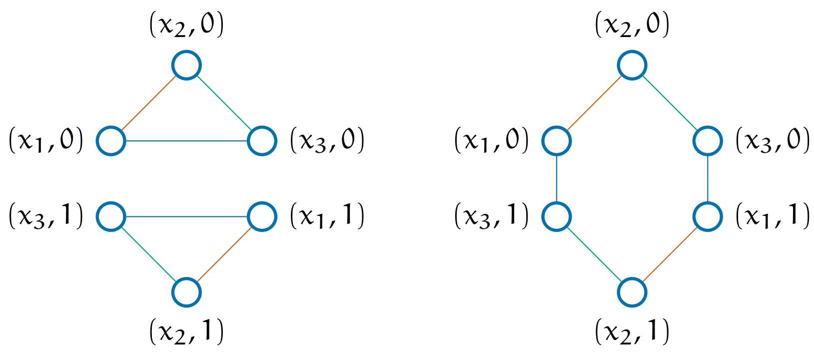

Figure 7: Structures $\mathfrak{A}$ (left) and $\mathfrak{B}$ (right) as defined in Example 4.17. The unary relations are omitted in the figure. The binary relations (for both structures) $R_{\{x_1,x_2\},0}$, $R_{\{x_1,x_3\},1}$, $R_{\{x_2,x_3\},0}$ are depicted by different colours of the edges.

4.5.3 *The correspondence*

Lemma 4.19 ([4, Lemma 2.1]). Let $k, r \in \mathbb{N}$ such that $r > 0$ and $k \geqslant 2$ and let $\mathcal{C}$ be a set of XOR-constraints over a set V of arity at most k. Then the following statements are equivalent.

- Falsifier wins the r-round k-pebble game $\mathcal{G}_k^r(V, \mathcal{C})$.
- There is a sentence $\varphi \in C_k^{(r)}$ such that $\mathfrak{A}(\mathcal{C}) \models \varphi$ and $\mathfrak{B}(\mathcal{C}) \not\models \varphi$.

Example 4.17 (continued). Let us construct the structures for the set of constraints $\mathcal{C}$. In both structures $\mathfrak{A}$ and $\mathfrak{B}$, there are three unary relations $X_i^{\mathfrak{A}} = X_i^{\mathfrak{B}} = \{(x_i, 0), (x_i, 1)\}$ for $i \in \{1, 2, 3\}$. Also, there are three binary relations $R_{\{x_1,x_2\},0}$, $R_{\{x_1,x_3\},1}$, and $R_{\{x_2,x_3\},0}$. We depict these as graphs with differently coloured edges (see Figure 7). These structures are non-isomorphic, however, as written above, Verifier has a winning strategy in the game $\mathcal{G}_2(V, \mathcal{C})$. Similarly, one can check that 1-WL cannot distinguish between the two structures.

Example 4.18 (continued). Note that in the example above, Falsifier has a winning strategy for the game $\mathcal{G}_3^{(3)}(V, \mathcal{C})$. No matter what Verifier chooses, Falsifier can choose x_3, x_1 and x_2 and since x_3 has to be set to 1 and x_1 has to be set to the same value as x_2, an odd number of variables (between x_1, x_2 and x_3) is set to 1 and hence the constraint $(\{x_1, x_2, x_3\}, 0)$ is violated. Hence, Falsifier wins.

Furthermore, consider the sentence

$$\varphi := \exists x \exists y \exists z \Big(X_1 x \wedge X_2 y \wedge X_3 z \\ \wedge R_{\{x_3\},1} z \wedge R_{\{x_1,x_2\},0} xy \wedge R_{\{x_1,x_2,x_3\},0} xyz \Big).$$

We claim that $\mathfrak{A} \models \varphi$ but $\mathfrak{B} \not\models \varphi$. In $\mathfrak{A}$, we can choose the elements $(x_1, 1), (x_2, 1), (x_3, 0)$ for the variables x, y, z, respectively. However, in $\mathfrak{B}$, there are no such elements, essentially by the same reasoning as to why Falsifier wins the game: z has to be set to the element $(x_3, 1)$ and x and y have to be set either to $(x_1, 0), (x_2, 0)$ or $(x_1, 1), (x_2, 1)$ so that $R_{\{x_1,x_2\},0} xy$ is satisfied. However, in both possibilities, $R_{\{x_1,x_2,x_3\},0} xyz$ is not satisfied.

5 REFINED ANALYSIS

In this chapter, we consider the lower bound given in [12]. The original construction considers the dimension k to be fixed. One of our goals is to relax this; when we allow k to grow as some function of n, we want to see if the construction still exists and how large the lower bound will then be. We recall the construction in Section 5.1, restate the results with a special focus on a variable dimension k, and answer these questions in Section 5.2.

We also want to investigate the robustness of the bound, i. e. how many rounds does the d-WL algorithm need to stabilise on the construction for $k < d$. We do not give an explicit answer, but we give some answers about the corresponding Cops and Robber game in Section 5.4.

5.1 THE ORIGINAL CONSTRUCTION

Definition 5.1. A positive even integer w is k**-coprimes-admissible**, if $w \geqslant 2k+2$ and there is a set P of k pairwise coprime integers $p_0, \ldots, p_{k-1}$ with $\frac{w}{2} < p_i \leqslant w$ for all $0 \leqslant i \leqslant k-1$.

Let $k \geqslant 3$ be an integer, let w be some k-coprimes-admissible number and choose a set of k pairwise coprime integers $P = \{p_0, \ldots, p_{k-1}\}$ satisfying the property from Definition 5.1. Let $f(k) = 2k+2$, let $I \coloneqq \{0, 1, \ldots, k-1\}$, and let

$$J \coloneqq \{0, 1, \ldots, \frac{1}{2} \cdot f(k) \cdot p_0 \cdot \ldots \cdot p_{k-1} - 1\}$$
$$J^* \coloneqq \{0, 1, \ldots, f(k) \cdot p_0 \cdot \ldots \cdot p_{k-1} - 1\}.$$

The **cylindrical grid** C_P **with respect to** P is defined as the graph with the vertex set $V(C_P) = I \times J$ and the following edge set: starting with a $I \times J$ grid, they add edges connecting the top and bottom vertex in each column, i. e., the edge $\{(0, j), (k-1, j)\}$ for every $j \in J$. We sometimes say that such a grid was **constructed with respect to** w. Note that there may be multiple grids C_P (for different sets P) constructed with respect to w.

The **cylindrical grid** C_P^* **with respect to** P is defined in the same way as C_P, but on the vertex set $I \times J^*$ and we also connect the first and the last vertex of each row, i. e., we add the edge

$$\big\{(i, 0), (i, \max(J))\big\}$$

for each $i \in I$.

We also look at C_P and C_P^* as ordered base graphs using the lexicographic ordering on $I \times J$ or $I \times J^*$, resp.

In the following, the indices of the numbers $p_0, \ldots, p_{k-1}$ are always taken modulo k, that is, when we write p_i, we mean $p_{i \bmod k}$.

Let us also define equivalence relations $\equiv$ and $\equiv^*$ on the vertex sets $V(C_P)$ and $V(C_P^*)$. In row i, two vertices are only equivalent if their distance is divisible by $f(k) \cdot p_i \cdot p_{i+1}$. We leave the first $f(k) \cdot p_i \cdot p_{i+1}$ vertices and the last $f(k) \cdot p_i \cdot p_{i+1}$ in the row i as singletons and all other vertices are made equivalent by the previous condition. More formally, for $i, i' \in I$ and $j, j' \in J$, we set $(i, j) \equiv (i', j')$ if the following conditions are satisfied.

1. $i = i'$ and $f(k) \cdot p_i \cdot p_{i+1}$ divides $(j' - j)$,
2. $f(k) \cdot p_i \cdot p_{i+1} \leqslant j$ and $j' < \lambda_i \cdot f(k) \cdot p_i \cdot p_{i+1}$,

where λ_i is the largest integer such that $(\lambda_i + 1) \cdot f(k) \cdot p_i \cdot p_{i+1} \leqslant |J|$. We define $(i, j) \equiv^* (i', j')$ if $i = i'$ and $f(k) \cdot p_i \cdot p_{i+1}$ divides $(j' - j)$, that is, only condition 1. (of the definition of $\equiv$) is required. Note that $u \equiv v$ implies $u \equiv^* v$. It is easy to show that $\equiv$ is a C_P-compression (see [12, Lemma 17]).

We restate the following lemma as in [12] when we do not assume that k is a constant.

Lemma 5.2 ([12, Lemma 16, enhanced])**.** The cylindrical grid C_P has width $|J| \in \Omega(\frac{kw^k}{2^k}) \cap \mathcal{O}(kw^k)$ and the compression $\equiv$ has

$$\frac{3}{2}k(k+1)w^2 < n < 8k(k+1)w^2,$$

that is, $n \in \Theta(k^2 w^2)$ many equivalence classes.

Proof. Recall that $|J| = (k+1) \cdot p_0 \cdot \ldots \cdot p_{k-1}$. Since $w/2 < p_i \leqslant w$ for every i, it follows that $|J| \in \Omega(\frac{kw^k}{2^k})$ and $|J| \in \mathcal{O}(kw^k)$.

Consider some row i. Since there are at least $3 \cdot (2k+2) \cdot p_i \cdot p_{i+1}$ and at most $4 \cdot (2k+2) \cdot p_i \cdot p_{i+1}$ equivalence classes, we conclude (by $w/2 < p_i \leqslant w$) that the number of equivalence classes in row i is at least $\frac{3}{2}(k+1)w^2$ and at most $8(k+1)w^2$. Since there are exactly k rows, we obtain that $\frac{3}{2}k(k+1)w^2 < n < 8k(k+1)w^2$ which yields the result. $\square$

From now on, we give only proof sketches for the following statements. For complete proofs, visit [12].

We want to show a strategy for the robber in the $\Omega(w^k)$-round compressed $(k+1)$-Cops and Robber game played on $(C_P, \equiv)$. As stated in Section 4.4, the robber has to provide C_P-twistings to move. We define the following twistings for the robber.

Definition 5.3. Let $W \subseteq V(C_P)$ be a set of vertices. An **end-to-end twisting avoiding** W is a $\equiv$-compressible C_P-twisting that

- twists some edge e_1 in the first column and some edge e_2 of C_P and does not twist any other edge, and
- fixes every vertex in $W/_\equiv$.

We define that equivalence relation $\approx_l$ on $V(C_P^*)$ (and on $V(C_P)$) for $l \geqslant 2$ as follows: if $i, i' \in I$ and $j \leqslant j' \in J^*$, we have

$$(i, j) \approx_l (i', j') \iff i = i' \text{ and } j' - j \text{ is divisible by } l.$$

Definition 5.4. A path $P = (u_1, \dots, u_m)$ is called l-**periodic** if u_1 and u_m are singleton $\equiv$-classes and, for every $i < m$ and every $v \in V(C_P)$ with $v \approx_l u_i$, and $u_i/_\equiv$ and $v/_\equiv$ are not singleton classes, there is a $j < m$ such that $u_j = v$ and $u_{i+1} \approx_l u_{j+1}$. The path induces a twisting $T_P = \{ (u_i, u_{i-1}), (u_i, u_{i+1}) \mid 1 < i < m \}$.

The end-to-end twistings will be useful for the robber. Let us show that the robber can provide l-periodic paths (for some l), and the induced twisting will be $\equiv$-compressible.

Lemma 5.5 ([12, Lemma 20])**.** Let $I' \subseteq I$ and let P be a path in C_P that only uses vertices from rows in I'. Let q be the greatest common divisor of all $f(k)p_ip_{i+1}$ for $i \in I'$. If P is q-periodic, then the induced C_P-twisting T_P is $\equiv$-compressible, twists the edges $\{u_1, u_2\}$ and $\{u_{m-1}, u_m\}$, twists no other edges, and fixes all vertices apart from $u_1, \dots, u_m$.

Proof sketch. The C_P-twisting T_P twists only the edges $\{u_1, u_2\}$ and $\{u_{m-1}, u_m\}$, and fixes all vertices except $u_1, \dots, u_m$ by construction.

Let $(u, v_l) \in T_P$ with v_l being the l-th neighbour of u. We need to show that for all $u' \equiv u$, $(u', v'_l) \in T_P$ (the other direction of the implication in Definition 4.13 is given by symmetry). The idea is that if $u = (s, t)$ and $u' = (s, t')$, we have that $u \approx_q u'$, since q divides $f(k)p_ip_{i+1}$. Because of the lexicographic ordering on the graph C_P, we also have $v_l \approx_q v'_l$. Since $(u, v_l) \in T_P$, we have that there is some j such that $\{u, v_l\} = \{u_j, u_{j+1}\}$. Since P is q-periodic, there is some j' such that $\{u', v'_l\} = \{u_{j'}, u_{j'+1}\}$ and hence $(u', v'_l) \in T_P$. □

Lemma 5.6 ([12, Lemma 21])**.** Let $W \subseteq V(C_P)$ be a set of at most k vertices of C_P such that W is not a pairwise separator. Then there is an end-to-end twisting avoiding W.

Proof sketch. The main idea is that if W is not a pairwise separator, then there is an i such that W is not a pairwise separator for rows i and $i+1$. In these two rows, there is an $f(k)p_{i+1}$-periodic path avoiding W, which then induces the desired twisting. □

Definition 5.7. A set $W \subseteq V(C_P)$ is called a **vertical separator** if in the graph $C_P \setminus W$, the first and the last column are separated. A set $W \subseteq V(C^*_P)$ is called a **toroidal vertical separator** if there is an integer z such that W shifted by z columns in C^*_P, that is, the set $\{ (i, (j+z) \bmod |J^*|) \mid (i,j) \in W \}$, is a vertical separator of C_P.

The following lemma about toroidal vertical separators is straightforward to prove and we omit its proof here.

Lemma 5.8 ([12, Lemma 23])**.** Let $S \subseteq V(C^*_P)$ be a k-vertex toroidal vertical separator. Then

- S contains exactly one vertex per row.
- vertices in consecutive rows are in consecutive columns, i. e., if $(i,j), (i+1, j') \in S$, then $j - j' \in \{-1, 0, 1\}$.
- S spans at most k consecutive columns in C^*_P.

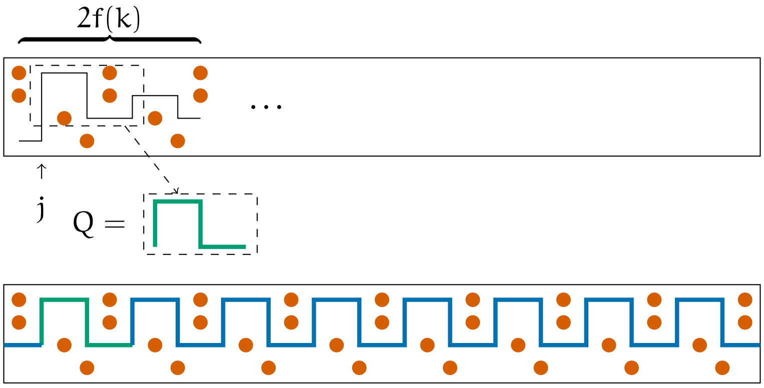

Figure 8: The construction of the twisting obtained in Lemma 5.10. The red vertices represent the set $W/_{\approx}$, and the blue/green path represents the path $\widehat{Q}$.

Definition 5.9. A set $W \subseteq V(C_P)$ is called a **pseudo-separator** is W is a pairwise-separator and $W/_{\approx_{f(k)}}$ is a vertical separator.

Lemma 5.10 ([12, Lemma 25])**.** Let $W \subseteq V(C_P)$ be a set of at most k vertices and assume that W is not a pseudo-separator. Then there is an end-to-end twisting avoiding W.

Proof sketch. If W is not a pairwise-separator, then there is an end-to-end twisting avoiding W by Lemma 5.6. We encourage the reader to follow the rest of the proof with Figure 8.

Otherwise, $W/_{\approx}$ is not a toroidal vertical separator. Then there is a path P from column 1 to column $2f(k)$ avoiding $W/_{\approx}$. There is a column j among the first $f(k)$ columns which does not contain any vertex from $W/_{\approx}$. Let P' be a subpath of P which contains one vertex from the column j, one vertex from the column $j + f(k)$ and otherwise only vertices in the columns between j and $j + f(k)$. Also, extend P' to a path Q by edges in the column j such that Q starts and ends in the same row (this is possible as there is no vertex in $W/_{\approx}$ in column j).

Finally, construct the path $\widehat{Q}$ by shifting Q by multiples of $f(k)$. Then $\widehat{Q}$ is $f(k)$-periodic and induces the desired end-to-end twisting avoiding W (by Lemma 5.5). $\square$

Lemma 5.11 ([12, Lemma 26])**.** Let $W \subseteq V(C_P)$ be set of at most k vertices.

1. There is at most one toroidal vertical separator $S_W \subseteq W/_{\equiv^*}$ of size k (and thus at most one vertical separator of size k).

2. If $W/_{\equiv^*}$ is a toroidal vertical separator, then there is a toroidal vertical separator $S_W \subseteq W/_{\equiv^*}$ of size k.

Proof sketch. Suppose there are two k-vertex toroidal vertical separators $S_W, S'_W \subseteq W/_{\equiv^*}$. Let $(i, t_i) \in S_W$ be the vertex in row i of S_W, and let $(i, t'_i) \in S_W$ be the vertex in row i of S'_W. We first claim that S_W and and S'_W have the same "shape", that is, for all $i \in I$, if $t_i = t_0 + c$ for some $-k \leqslant c \leqslant k$, then $t'_i = t'_0 + c$.

To see this, suppose that $t_i = t_0 + c$ and $t'_i = t'_0 + d$. We know that $(t_i - t'_i) \bmod f(k)p_i p_{i+1} = 0$ (since both vertices are in $W_{\equiv^*}$). Namely, $(c - d) \bmod f(k)p_i p_{i+1} = 0$. However, $-2k \leqslant c - d \leqslant 2k$, and since $f(k) > 2k$, we have that $c = d$.

Now we want to prove that $S_W = S'_W$. For this, look at the first row vertices $(0, t_0)$ and $(0, t'_0)$. For each row $j \in I$, we have that

$$(t_0 - t'_0) \bmod f(k)p_j p_{j+1} = (t_j - t'_j) \bmod f(k)p_j p_{j+1} = 0.$$

Since all p_i are coprime, we have that

$$(t_0 - t'_0) \bmod f(k)p_0 \dots p_{k-1} = 0,$$

which implies $t_0 = t'_0$. Since the choice of t_0 was arbitrary, we have that $t_i = t'_i$ for all $i \in I$ and hence $S_W = S'_W$.

It remains to show the second claim. Let S_W be the minimal toroidal vertical separator in $W/_{\equiv^*}$. If $|S_W| > k$, we have two vertices in the same row, however, since both vertices are in $W/_{\equiv^*}$, they are at least $f(k) = 2k + 2$ apart. But any toroidal vertical separator spans at most k consecutive columns, and hence one of the two vertices can be removed from S_W and we would still have a toroidal vertical separator. That contradicts S_W being minimal. □

Lemma 5.12 ([12, Lemma 27]). Let $W, W' \subseteq V(C_P)$ be some pseudo-separators each of size k such that $|W \cap W'| \geqslant k - 1$, that is, the sets W and W' differ by at most one vertex. Suppose that $W/_{\equiv^*}$ is a toroidal vertical separator. Then

1. $W'/_{\equiv^*}$ contains a k-vertex toroidal vertical separator,
2. the unique k-vertex toroidal vertical separators $S_W \subseteq W/_{\equiv^*}$ and $S_{W'} \subseteq W'/_{\equiv^*}$ satisfy $|S_W \cap S_{W'}| \geqslant k - 1$, that is, they differ by at most one vertex, and
3. every $u \in S_{W'}$ has distance at most 2 to S_W in C^*_P.

Proof sketch. Assume $W/_{\equiv^*} \neq W'/_{\equiv^*}$, let $i \in I$ be the unique row the two sets differ on, and let $S_W \subseteq W/_{\equiv^*}$ be the unique k-vertex toroidal vertical separator. Let $v_i = (i, j_i)$ denote the vertex of S_W in row i.

The set $W'/_{\approx}$ is a set of k-vertex toroidal vertical separators that repeat every $f(k)$ columns since W' is a pseudo-separator. Since all toroidal vertical separators span at most k columns, $S_W \setminus \{v_i\}$ has to be a subset of one of such separators. Hence, there is a vertex $v^*_i = (i, j^*_i) \in W'/_{\approx}$ such that $S_{W'} := (S_W \setminus \{v_i\}) \cup \{v^*_i\}$ is a toroidal vertical separator.

Certainly, v^*_i has a distance of at most 2 to v_i in the graph C^*_P. We claim that $S_{W'} \subseteq W'/_{\equiv^*}$. We know that $S_W \setminus \{v_i\} \subseteq W'/_{\equiv^*}$ because W and W' differ only in row i. Let $v'_i := (i, j'_i)$ denote the unique vertex from W' in row i.

Note that the sets S_W and $(S_W \setminus \{v_i\}) \cup \{v'_i\}$ contain the same vertex $(i + 1, j_{i+1})$ in row $i + 1$. Hence $j_i = j_{i+1} + c$ and $j'_i = j_{i+1} + d$ for some $c, d \in \{-1, 0, 1\}$ (since both W and W' are pseudo-separators). This implies that

$$(j_i - j'_i) \bmod f(k)p_{i+1} = c - d \in \{-2, \dots, 2\}.$$

Since the sets S_W and $(S_W \setminus \{v_i\}) \cup \{v_i'\}$ also contain the same vertex $(i-1, j_{i-1})$ in row $i-1$, we also have that

$$(j_i - j_i') \bmod f(k)p_i \in \{-2, \dots, 2\},$$

and more strongly we have

$$(j_i - j_i') \bmod f(k)p_i = (j_i - j_i') \bmod f(k)p_{i+1}.$$

Therefore,

$$(j_i - j_i') \bmod f(k)p_i p_{i+1} \in \{-2, \dots, 2\},$$

meaning that there is some vertex $v_i'' = (i, j_i'')$ in row i in $W'/_{\equiv^*}$ with $j_i - j_i'' \in \{-2, \dots, 2\}$.

But now v_i^* and v_i'' are both row i vertices in $W'/_{\approx}$ in a column at most k away from $v_i = (i, j_i)$ in C_P^*. This means $v_i^* = v_i'' \in W'/_{\equiv^*}$ since distinct vertices have to have distance at least $f(k)$. □

Lemma 5.13 ([12, Lemma 28, restated])**.** The robber has a winning strategy in the $|J|/6-(k+2)$-round compressed $(k+1)$-Cops and Robber game played on C_P and $\equiv$ when the robber is initially placed on an edge in the first column.

Proof sketch. One can prove by induction on $r \leqslant |J|/6-(k+2)$ that the robber can maintain two invariants:

- The robber is located among the first $k+2$ or last $k+2$ columns of the cylindrical grid C_P.
- If $W/_{\equiv^*}$ is a toroidal vertical separator, then
  - If the robber is located within the first $k+2$ columns, then the distance between column 1 and the unique k-vertex toroidal vertical separator $S_W \subseteq W/_{\equiv^*}$ is at least $|J|/3-2r$.
  - If the robber is located within the last $k+2$ columns, then the distance between column $|J|$ and the unique k-vertex toroidal vertical separator $S_W \subseteq W/_{\equiv^*}$ is at least $|J|/3-2r$.

The robber can always choose a cop-free column among the first or last $k+2$ columns. (Since there are only $k+1$ cops, such a column exists). Assume by symmetry that the robber stays within the first $k+2$ columns.

Assume that k cops stay on (the equivalence classes of) some vertices in a set W and the new $\equiv$-equivalence class x for one more cop is selected, resulting in a position $X = W \cup \{x\}$.

1. If $W/_{\equiv^*}$ is a toroidal vertical separator, then the robber cannot provide an end-to-end twisting avoiding $W/_{\equiv^*}$ and chooses to stay within the first $k+2$ columns not containing a vertex from X. The robber can move there because the path only uses vertices in singleton $\equiv$-equivalence classes.

   In the next round, a cop is picked up resulting in the position $\widehat{W} \subsetneq X$. We know that W is a pseudo-separator and that in X, there is at most one other k-vertex pseudo-separator.

If such pseudo-separator W' exists, then by Lemma 5.12, the unique k-vertex toroidal vertical separators $S_W \subseteq W/_{\equiv^*}$ and $S_{W'} \subseteq W'/_{\equiv^*}$ differ by at most one vertex and this vertex has distance at most 2 to S_W. Hence the distance between the first column and the k-vertex toroidal vertical separator decreased by at most 2 and hence the second invariant holds.

If there is no such other pseudo-separator, then the k-vertex toroidal vertical separator could not move and the distance could not change.

2. If $W/_{\equiv^*}$ is a pseudo-separator but not a toroidal vertical separator, then, intuitively, the cops do not separate the first and the last column, but we did not define the needed $\equiv$-compressible twisting for the robber. However, by Lemmas 5.11 and 5.12, after picking a cop from position y, $((W \cup \{x\}) \setminus \{y\})/_{\equiv^*}$ cannot be a toroidal vertex separator.

3. Otherwise, $W/_{\equiv^*}$ is not a pseudo-separator. There can be at most one pseudo-separator $W' \subseteq X$.

   If such separator W' exists and $W'/_{\equiv^*}$ is a toroidal vertical separator, then there is a unique k-vertex toroidal separator $S_{W'} \subseteq W'/_{\equiv^*}$ by Lemma 5.11.

   - If the first column has distance at least $|J|/3$ to $S_{W'}$ in C^*_P, then the robber moves to a column among the first $k+2$ columns not containing a vertex of X. If for the resulting position $\widehat{W} \subsetneq X$ (after a cop is picked up), $\widehat{W}/_{\equiv^*}$ is a toroidal vertical separator, then $\widehat{W} = W'$ and the second invariant is satisfied.
   - Otherwise, the last column has distance at least $|J|/3$ to $S_{W'}$ in C^*_P (by construction and Lemma 5.8). By Lemma 5.10, the robber can move via an end-to-end twisting to the last column in C_P and then move to some column among the last $k+2$ columns not containing a vertex of X. In the next round, the robber has a distance of at least $|J|/3$ to $S_{W'}$ and hence the second invariant is satisfied.

   Otherwise, such a separator does not exist, and the resulting position $\widehat{W} \subsetneq X$ (after a cop is picked up) cannot be a toroidal vertical separator.

□

Now, when we have the strategy for the robber, we can use the last lemma of this section to determine the lower bound on the round number of Spoiler in the bijective $(k+1)$-pebble game played on the graphs $\mathrm{CFI}(C_P, f)/_{\equiv}$ and $\mathrm{CFI}(C_P, g)/_{\equiv}$.

Lemma 5.14 ([12, Lemma 29, restated]). Let $f, g : E \to \mathbb{F}_2$ twist a single edge contained in the first column. Spoiler wins the bijective $(k+1)$-pebble game played on $\mathrm{CFI}(C_P, f)/_{\equiv}$ and $\mathrm{CFI}(C_P, g)/_{\equiv}$ but not before $|J|/6 - (k+2)$ many rounds.

Proof sketch. The equivalence relation $\equiv$ is a C_P-compression. Also, the functions f and g are $\equiv$-compressible because, in the first column, all vertices are in singleton $\equiv$-equivalence classes. Spoiler wins the bijective $(k+1)$-pebble game on non-isomorphic CFI graphs over cylindrical grids with k rows. Therefore, Spoiler also wins on the precompressed CFI graphs $(\mathrm{CFI}(C_P, f), \equiv)$ and $(\mathrm{CFI}(C_P, g), \equiv)$ and hence, on the compressed graphs $\mathrm{CFI}(C_P, f)/_\equiv$ and $\mathrm{CFI}(C_P, g)/_\equiv$ by Lemma 4.14.

By Lemma 5.13, the robber wins the $\big(|J|/6 - (k+2)\big)$-round compressed $(k+1)$-Cops and Robber game played on C_P and $\equiv$. Hence, by Lemma 4.15, Duplicator wins the $\big(|J|/6 - (k+2)\big)$-round bijective $(k+1)$-pebble game when played on the precompressed graphs $(\mathrm{CFI}(C_P, f), \equiv)$ and $(\mathrm{CFI}(C_P, g), \equiv)$, and hence, by Lemma 4.14, on the compressed graphs $\mathrm{CFI}(C_P, f)/_\equiv$ and $\mathrm{CFI}(C_P, g)/_\equiv$. $\square$

This leads then to the $\Omega\left(n^{k/2}\right)$ lower bound on the iteration number of k-WL on the graph $\mathrm{CFI}(C_P, f)/_\equiv$ (by Lemma 4.14). We state and enhance the concrete result in the next section as Theorem 5.19.

5.2 THE LOWER BOUND WITH VARIABLE DIMENSION

First, we want to answer the question, for which relations between the dimension and the size we can find such a cylindrical grid. Given a dimension k, we need to find possible k-coprimes-admissible numbers w to construct the graph C_P. Note that there is a graph C_P (for some set of coprimes P of size k) if and only if w is k-coprimes-admissible.

First, let us define $w^*(k)$ as the smallest k-coprimes-admissible number w and let $n^*(k)$ be the size of the smallest cylindrical grid $C_k^* = C_P$ (for some set P of size k) constructed with respect to $w^*(k)$.

We will prove the following number-theoretical lemmas later (see Section 5.3), but let us first explain how they will be helpful.

Lemma 5.15. There is a function $k_1(\varepsilon, \delta)$ such that for every $\varepsilon > 0$, every $\delta > 0$, and every $k \geqslant k_1(\varepsilon, \delta)$,

$$(1-\delta)k\ln k < w^*(k) < (2+\varepsilon)k\ln k.$$

Lemma 5.16. There is a function $k_2(\varepsilon)$ such that for every $\varepsilon > 0$, every $k \geqslant k_2(\varepsilon)$, and every w, if w is a k-coprimes-admissible number, then $(2+\varepsilon)w$ is k-coprimes-admissible.

Corollary 5.17. There is a function $k_3(\varepsilon, \delta)$ such that for every $\varepsilon > 0$, every $\delta > 0$, and every $k \geqslant k_3(\varepsilon, \delta)$,

$$\left(\frac{3}{2} - \delta\right) k^4 (\ln k)^2 < n^*(k) < (32+\varepsilon)k^4(\ln k)^2.$$

Proof. Let $k_1(\varepsilon, \delta)$ be the function from Lemma 5.15. Recall that by Lemma 5.2, we have

$$\frac{3}{2}k(k+1)w^*(k)^2 < n^*(k) < 8k(k+1)w^*(k)^2.$$

Applying the bounds by Lemma 5.15, we get that for all $\varepsilon', \delta' > 0$, and for all $k \geqslant k_1(\varepsilon', \delta')$,

$$\frac{3}{2}(1-\delta')^2 k^4 \ln k < n^*(k) < 8(2+\varepsilon')^2 k^3 (k+1) \ln k.$$

(The lower bound uses the fact that $k < k+1$.) Let $\varepsilon, \delta > 0$. There must be some $k_0(\varepsilon)$ such that for all $k \geqslant k_0(\varepsilon)$,

$$(32+\varepsilon)\frac{k}{k+1} > 32, \tag{$*$}$$

because the left-hand side converges to $32+\varepsilon > 32$ as k approaches ∞. Therefore, we can choose $\varepsilon' > 0$ small enough such that

$$8(2+\varepsilon')^2 < (32+\varepsilon)\frac{k}{k+1}$$

holds for every $k \geqslant k_0(\varepsilon)$, because the right-hand side is larger than 32 by $(*)$ and the left-hand side converges to 32 as ε' approaches 0. Lastly, let $\delta' > 0$ be small enough such that $\frac{3}{2}(1-\delta')^2 > \frac{3}{2} - \delta$. Then we have that for all $k \geqslant k_3(\varepsilon, \delta) := \max\{k_0(\varepsilon), k_1(\varepsilon', \delta')\}$,

$$\left(\frac{3}{2} - \delta\right) k^4 (\ln k)^2 < n^*(k) < (32+\varepsilon) k^4 (\ln k)^2.$$

□

Corollary 5.18. For all $k \geqslant 2$, there is a cylindrical grid C_P (for some P of size k) of size n if and only if $n \in \Omega\left(k^4 (\ln k)^2\right)$.

Proof. Let $k \geqslant 2$ and suppose there is a cylindrical grid C_P (for some P of size k). By definition of $n^*(k)$, the size of C_P has to be at least $n^*(k)$ and it follows directly from Corollary 5.17 that $n^*(k) \in \Theta\left(k^4 (\ln k)^2\right)$ and hence $n \in \Omega\left(k^4 (\ln k)^2\right)$.

Let us prove the other direction. Let $k_2(\varepsilon)$ be the function from Lemma 5.16, let $k \geqslant k_2(0.1)$, and let $n \geqslant n^*(k) \in \Omega\left(k^4 (\ln k)^2\right)$. We claim that for $\varepsilon := 0.1$ there is an $a \in \mathbb{N} \cup \{0\}$ such that

$$\frac{3}{2} k(k+1)\big((2+\varepsilon)^a w^*(k)\big)^2 < n < 8k(k+1)\big((2+\varepsilon)^a w^*(k)\big)^2.$$

This is because these intervals cover all integers $n \geqslant n^*(k)$. To see this, one can easily check that

$$\frac{3}{2} k(k+1)\left(2.1^{a+1} w^*(k)\right)^2 < 8k(k+1)\big(2.1^a w^*(k)\big)^2.$$

(This holds since $\frac{3}{2} \cdot 2.1^2 < 8$.) Now, setting $w := (2+\varepsilon)^a w^*(k)$, we know by Lemma 5.16 (and by a simple inductive argument) that w is k-coprimes-admissible (as $k \geqslant k_2(0.1)$). Therefore, we can construct some cylindrical grid C_P (for some set P of size k) with respect to w. By Lemma 5.2, we have

$$\frac{3}{2} k(k+1)\left((2+\varepsilon)^a w^*(k)\right)^2 < |C_P| < 8k(k+1)\left((2+\varepsilon)^a w^*(k)\right)^2.$$

But then is clearly

$$n < 8k(k+1)\left((2+\varepsilon)^a w^*(k)\right)^2 \leqslant \frac{16}{3}|C_P|, \text{ and}$$

$$n > \frac{3}{2}k(k+1)\left((2+\varepsilon)^a w^*(k)\right)^2 \geqslant \frac{3}{16}|C_P|,$$

and hence $|C_P| \in \Theta(n)$. □

We restate Theorem 30 and its proof from [12], with a special focus on k not being fixed and on the quantification of n.

Theorem 5.19 ([12, Theorem 30, enhanced]).
There is a function $r : \mathbb{N}^2 \to \mathbb{N}$ such that $r(n,k) \in \Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right)$ and, for every integer $k \geqslant 2$ and for every $n \in \Omega\left(k^4(\ln k)^2\right)$, there are graphs G_n, H_n such that

1. $|V(G_n)| = |V(H_n)| \in \Theta(n)$,
2. $G_n \simeq_{k+1}^{r(n,k)-1} H_n$, and
3. $G_n \not\simeq_{k+1}^{r(n,k)} H_n$.

Proof. Let $k \in \mathbb{N}$ and let $n \in \Omega\left(k^4(\ln k)^2\right)$. Set $w := \left\lceil \sqrt{\frac{n}{k^2}} \right\rceil$. By Corollary 5.18, there is a graph C_P for some set P of size k. Let $f, g : E \to \mathbb{F}_2$ twist a single edge contained in the first column of C_P. Consider $G_n := \mathrm{CFI}(C_P, f)/_{\equiv}$ and $H_n := \mathrm{CFI}(C_P, g)/_{\equiv}$. Then $|V(G_n)| = |V(H_n)| \in \Theta(k^2 w^2) = \Theta(n)$ by Lemma 5.2.

By Lemma 5.14, Spoiler wins the bijective $(k+1)$-pebble game played on G_n and H_n. Let $r(n,k)$ denote the minimum number of rounds required by Spoiler to win the bijective $(k+1)$-pebble game played on G_n and H_n. Then $G_n \simeq_{k+1}^{r(n,k)-1} H_n$ and $G_n \not\simeq_{k+1}^{r(n,k)} H_n$ by the definition of $r(n,k)$.

We also know that $r(n,k) \geqslant |J|/6 - (k+2)$ by Lemma 5.14. By Lemma 5.2, we have that

$$r(n,k) \in \Omega\left(\frac{kw^k}{2^k}\right) = \Omega\left(\frac{k\left\lceil\sqrt{\frac{n}{k^2}}\right\rceil^k}{2^k}\right) = \Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right)$$

□

This concludes our result, that the maximum iteration number of k-WL on graphs is in $\Omega(\frac{1}{k^{k-1}2^k} n^{k/2})$.

This leaves us with one more question: do we still get a reasonable lower bound from the construction, even if we define n as a function of k? The answer is summarised in the following proposition.

Proposition 5.20. The iteration number of k-WL on C_P (for some P of size k) of size n is always in $\Omega\left(n^{(k+1)/4}\right) \subseteq \Omega\left(n^{k/4}\right)$, even if n is a function of k.

Proof. Let $r(n,k)$ be the function from Theorem 5.19 and let $k_3(\varepsilon,\delta)$ be the function from Collorary 5.17. We prove that

$$\lim_{k\to\infty} \frac{n^{(k+1)/4}}{n^{k/2}\cdot\frac{1}{2^k k^{k-1}}} = 0,$$

which means that $n^{(k+1)/4} \in \Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right)$ and hence, by Theorem 5.19,

$$r(n,k) \in \Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right) \subseteq \Omega\left(n^{(k+1)/4}\right).$$

Let us prove the previous claim. By Corollary 5.17, we have that $n > k^4(\ln k)^2$ for all $k > k_3(1, \frac{1}{2})$. Therefore,

$$\begin{aligned}
0 &\leqslant \lim_{k\to\infty} \frac{n^{(k+1)/4}}{n^{k/2}\cdot\frac{1}{2^k k^{k-1}}} && \text{the limit is non-negative}\\
&= \lim_{k\to\infty} \frac{2^k k^{k-1}}{n^{(k-1)/4}}\\
&\leqslant \lim_{k\to\infty} \frac{2^k k^{k-1}}{k^{k-1}(\ln k)^{(k-1)/2}} && \text{as } n > k^4(\ln k)^2 \text{ for large } k\\
&= 2\cdot \lim_{k\to\infty} \left(\frac{2}{\sqrt{\ln k}}\right)^{k-1}\\
&= 0 && \text{since } \sqrt{\ln k} > 2 \text{ for } k > 55.
\end{aligned}$$

□

Proposition 5.21. Let $\delta > 0$ and suppose a function

$$h(k) \in \Omega(2^{k^{1+\delta}} k^{(k-1)^{1+\delta}}).$$

For every $\varepsilon > 0$, the maximal iteration number of k-WL on graphs of size $\Theta(h(k))$ is in $\Omega\left(n^{k/2-\varepsilon}\right)$.

Proof. Let $h(k) \geqslant c2^{k^{1+\delta}} k^{(k-1)^{1+\delta}}$ for some $c > 0$ for all sufficiently large k. Since $h(k) \in \Omega\left(k^4(\ln k)^2\right)$, for all $k \geqslant 2$ there is a cylindrical grid C_P (for some P of size k) of size $n \in \Theta(h(k))$ by Corollary 5.18. We claim that

$$\lim_{k\to\infty} \frac{n^{k/2-\varepsilon}}{n^{k/2}\frac{1}{2^k k^{k-1}}} = 0,$$

which proves the proposition, since this means that

$$n^{k/2-\varepsilon} \in \Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right),$$

and hence the iteration number of k-WL on C_P is by Theorem 5.19 in

$$\Omega\left(\frac{1}{2^k k^{k-1}} n^{k/2}\right) \subseteq \Omega\left(n^{k/2-\varepsilon}\right),$$

which implies the statement of the proposition.

Let us prove the previous claim. Note that the following limit is non-negative and that

$$
\begin{aligned}
0 &\leqslant \lim_{k\to\infty} \frac{n^{k/2-\varepsilon}}{n^{k/2 \frac{1}{2^k k^{k-1}}}} \\
&= \lim_{k\to\infty} \frac{2^k k^{k-1}}{n^{\varepsilon}} \\
&\leqslant \lim_{k\to\infty} \frac{2^k k^{k-1}}{c^{\varepsilon} 2^{\varepsilon k^{1+\delta}} k^{\varepsilon (k-1)^{\delta}}} \\
&= c^{-\varepsilon} \lim_{k\to\infty} 2^{k-\varepsilon k^{1+\delta}} \cdot k^{k-1-\varepsilon(k-1)^{1+\delta}} \\
&= 0,
\end{aligned}
$$

where the second inequality comes from $n = h(k) \geqslant c2^{k^{1+\delta}} k^{(k-1)^{1+\delta}}$, and the last equality comes from the following: since $k - \varepsilon k^{1+\delta}$ converges to $-\infty$ (and similarly $k-1-\varepsilon(k-1)^{1+\delta}$), both factors converge to 0.

$\square$

Given a function $h(k)$ representing the size of the graph and k representing the dimension, we have the following hierarchy.

1. If $h(k) \in o(k^4 (\ln k)^2)$, then the construction does not exist. (See Corollary 5.18.)
2. If $h(k) \in \Omega(k^4(\ln k)^2)$, then the construction yields the lower bound $\Omega\left(n^{(k+1)/4}\right) \subseteq \Omega\left(n^{k/4}\right)$ on the iteration number. (See Proposition 5.20.)
3. If $h(k) \in \Omega\left((2k)^{k^{1+\delta}}\right) \subseteq \Omega\left(2^{k^{1+\delta}} k^{(k-1)^{1+\delta}}\right)$ for some $\delta > 0$, then the construction yields the lower bound $\Omega\left(n^{k/2-\varepsilon}\right)$ for an arbitrary $\varepsilon > 0$. (See Proposition 5.21.)

5.3 PROOFS OF LEMMAS 5.15 AND 5.16

We will need the function $F(n,k)$ defined by Erdős and Selfridge ([6]).

Definition 5.22 ([6])**.** Given $n, r \in \mathbb{N}$, we define $F(n,r)$ as the largest number of pairwise coprime integers in the set $\{n, n+1, \dots, n+r\}$.

Observe that w is k-coprimes-admissible if and only if

$$k \leqslant F\left(\frac{w}{2}+1, \frac{w}{2}-1\right),$$

since $F\left(\frac{w}{2}+1, \frac{w}{2}-1\right)$ is the maximal number of pairwise coprime integers between $\frac{w}{2}+1$ and w and we need to find k such integers.

They then investigated the behaviour of the function and were able to prove, that the maximal number of pairwise coprime integers between any $r+1$ consecutive integers grows (with r) asymptotically the same as the number of prime numbers smaller than r. More precisely, they proved the following result.

Lemma 5.23 ([6, discussion after Theorem 1]). For every $\varepsilon > 0$ there is $R_0(\varepsilon)$ such that for all $r \geqslant R_0(\varepsilon)$,

$$\max_n F(n, r) < \left(2 + \varepsilon\right) \frac{r}{\ln r}.$$

Observation 5.24. Let $k \geqslant R_0(\varepsilon)$. If w is k-coprimes-admissible, then

$$k < (2 + \varepsilon) \cdot \frac{\frac{w}{2} - 1}{\ln\left(\frac{w}{2} - 1\right)}.$$

Proof. By Lemma 5.23, we have

$$k \leqslant F\left(\frac{w}{2} + 1, \frac{w}{2} - 1\right) \leqslant \max_n F\left(n, \frac{w}{2} - 1\right) < (2 + \varepsilon) \frac{\frac{w}{2} - 1}{\ln\left(\frac{w}{2} - 1\right)}.$$

□

We will also need bounds on the number of prime numbers in a certain range. Denote by $\pi(n)$ the number of prime numbers smaller or equal to n. We borrow a classical bound from Rosser [18].

Theorem 5.25. ([18]) If $n \geqslant 55$, then

$$\frac{n}{\ln n + 2} < \pi(n) < \frac{n}{\ln n - 4}.$$

Corollary 5.26. Let $n \geqslant 55$. There are at least

$$g(n) := \frac{n(\ln n - 10 - \ln 2)}{(\ln n + \ln 2 + 2)(\ln n - 4)}$$

prime numbers p satisfying $n < p \leqslant 2n$.

Proof. To bound the number of prime numbers between n and $2n$, note that

$$\pi(2n) - \pi(n) > \frac{2n}{\ln(2n) + 2} - \frac{n}{\ln n - 4}.$$

It is straightforward to check that

$$\frac{n}{\ln(2n) + 2} - \frac{n}{\ln n - 4} = \frac{n(\ln n - 10 - \ln 2)}{(\ln n + \ln 2 + 2)(\ln n - 4)}$$

□

In the following, let $e \approx 2.718$ be the Euler's number, the base of the natural logarithm ln.

Remark. Note that $g(n) \leqslant 0$ for $55 < n \leqslant 2e^{10}$.

Proof of Lemma 5.15. First, let us prove the lower bound. We prove that for all $\delta > 0$, there is $c_1(\delta)$ such that for all $k > c_1(\delta)$,

$$(1 - \delta) k \ln k < w^*(k).$$

Let $\delta > 0$. If $\delta \geqslant 1$, then the bound holds immediately. Otherwise, define $c_1(\delta) := \max\left\{e^{\frac{2}{1-\delta}}, R_0(2\delta)\right\}$.

By Observation 5.24, we have that for all $k \geqslant R_0(2\delta)$,

$$k < (2+2\delta) \cdot \frac{\frac{w}{2}-1}{\ln\left(\frac{w}{2}-1\right)}.$$

Suppose for contradiction that $w \leqslant (1-\delta)k\ln k$. Since $\frac{x}{\ln x}$ is increasing for $x \geqslant 3$ and

$$7 < e^2 < k \leqslant \frac{w}{2} - 1 \leqslant \frac{1-\delta}{2}k\ln k - 1 < \frac{1-\delta}{2}k\ln k$$

(recall, that by Definition 5.1, $w \geqslant 2k+2$), we have

$$\begin{aligned} k &< (2+2\delta)\frac{\frac{w}{2}-1}{\ln\left(\frac{w}{2}-1\right)} \\ &< (2+2\delta)\frac{\frac{1-\delta}{2}k\ln k}{\ln\left(\frac{1-\delta}{2}k\ln k\right)} \\ &= (1-\delta^2)\cdot k \cdot \frac{\ln k}{\ln\left(\frac{1-\delta}{2}k\ln k\right)} \\ &< k, \end{aligned}$$

which is a contradiction. (One can check that $\ln k < \ln\left(\frac{(1-\delta)}{2}k\ln k\right)$ for $k \geqslant e^{\frac{2}{1-\delta}}$ and $(1-\delta^2) < 1$.)

Let us move to the proof of the upper bound. We prove that for all $\varepsilon > 0$, there is $c_2(\varepsilon)$ such that for all $k > c_2(\varepsilon)$,

$$w^*(k) < (2+\varepsilon)k\ln k.$$

Let $\varepsilon > 0$ and and let k be large enough (we define $c_2(\varepsilon)$ later). Define $w = (2+\varepsilon)k\ln k$ and let $g(n)$ be the function from Corollary 5.26. It turns out that we can use prime numbers as the numbers $p_0, \ldots, p_{k-1}$ with $\frac{(2+\varepsilon)w}{2} < p_i \leqslant (2+\varepsilon)w$ for all $0 \leqslant i \leqslant k-1$. We show that $g(\frac{w}{2}) \geqslant k$, showing that w is k-coprimes-admissible and since $w^*(k) \leqslant w$, we have the upper bound. Consider

$$\begin{aligned} g\left(\frac{w}{2}\right) &= g\left(\frac{2+\varepsilon}{2}k\ln k\right) \\ &= \frac{\left(\frac{2+\varepsilon}{2}k\ln k\right)\left(\ln\left(\frac{2+\varepsilon}{2}k\ln k\right) - 10 - \ln 2\right)}{\left(\ln\left(\frac{2+\varepsilon}{2}k\ln k\right) + \ln 2 + 2\right)\left(\ln\left(\frac{2+\varepsilon}{2}k\ln k\right) - 4\right)} \\ &= \frac{\frac{2+\varepsilon}{2}k\ln k\left(\ln\left(\frac{2+\varepsilon}{2}\right) + \ln k + \ln\ln k - 10 - \ln 2\right)}{\left(\ln(2+\varepsilon) + \ln k + \ln\ln k + 2\right)\left(\ln\left(\frac{2+\varepsilon}{2}\right) + \ln k + \ln\ln k - 4\right)}. \end{aligned}$$

One can see that $\frac{g(\frac{w}{2})}{k}$ converges to $\frac{2+\varepsilon}{2}$ as k approaches ∞, and hence there is some k_0 with $g\left(\frac{w}{2}\right) > k$ for all $k \geqslant k_0$. Set $c_2(\varepsilon) := k_0$, and we get the upper bound.

For completeness, we define $k_1(\varepsilon, \delta) := \max\{c_1(\delta), c_2(\varepsilon)\}$. Then the claim of the proposition follows. □

Remark. Note that the previous proof shows a slightly stronger statement. Namely, that there is a function $c_2(\varepsilon)$ such that for all $\varepsilon > 0$

and all $k \geqslant c_2(\varepsilon)$, there exists a number $w < (2+\varepsilon)k\ln k$ such that there are k *prime numbers* $p_0, \ldots, p_{k-1}$ such that $w/2 < p_i \leqslant w$ for all $0 \leqslant i \leqslant k-1$.

Proof of Lemma 5.16. Let $\varepsilon > 0$, and let k be large enough (we define the function $k_2(\varepsilon)$ later). Let w be k-coprimes-admissible, then by Observation 5.24, for all $k > R_0\left(\frac{\varepsilon}{2}\right)$,

$$k < \left(2 + \frac{\varepsilon}{2}\right) \frac{\frac{w}{2} - 1}{\ln\left(\frac{w}{2} - 1\right)}.$$

Let $g(n)$ be the function from Corollary 5.26. We show that

$$g\left(\frac{2+\varepsilon}{2}w\right) \geqslant \left(2 + \frac{\varepsilon}{2}\right) \frac{\frac{w}{2} - 1}{\ln\left(\frac{w}{2} - 1\right)} = \left(1 + \frac{\varepsilon}{4}\right) \frac{w-2}{\ln(w-2) - \ln 2},$$

showing that $(2+\varepsilon)w$ is k-coprimes-admissible. Note that

$$\begin{aligned} g\left(\frac{2+\varepsilon}{2}w\right) &= \frac{\left(\frac{2+\varepsilon}{2}w\right)\left(\ln\left(\frac{2+\varepsilon}{2}w\right) - 10 - \ln 2\right)}{\left(\ln\left(\frac{2+\varepsilon}{2}w\right) + \ln 2 + 2\right)\left(\ln\left(\frac{2+\varepsilon}{2}w\right) - 4\right)} \\ &= \frac{\frac{2+\varepsilon}{2}w\left(\ln(2+\varepsilon) + \ln w - 10 - 2\ln 2\right)}{\left(\ln(2+\varepsilon) + \ln w + 2\right)\left(\ln(2+\varepsilon) + \ln w - 4 - \ln 2\right)}. \end{aligned}$$

Also, consider

$$g\left(\frac{2+\varepsilon}{2}w\right) \cdot \frac{\ln(w-2) - \ln 2}{w-2} \geqslant 1 + \frac{\varepsilon}{4}.$$

The left-hand side converges to $1 + \frac{\varepsilon}{2} > 1 + \frac{\varepsilon}{4}$ as w approaches ∞. Therefore, there must be some k_0 such that for all $k \geqslant k_0$ and all $w > 2k+2$ (recall Definition 5.1), the above inequality holds. Then choose $k_2(\varepsilon) \coloneqq \max\left\{R_0\left(\frac{\varepsilon}{2}\right), k_0\right\}$. The proposition follows. $\square$

Remark. Similarly, as before, the proof shows a slightly stronger statement. Namely, that there is a function $k_2(\varepsilon)$ such that for all $\varepsilon > 0$, all $k \geqslant c_2(\varepsilon)$, and all k-coprimes-admissible numbers w, there are k *prime numbers* $p_0, \ldots, p_{k-1}$ such that $\frac{(2+\varepsilon)}{2}w < p_i \leqslant (2+\varepsilon)w$ for all $0 \leqslant i \leqslant k-1$.

5.4 ROBUSTNESS OF THE BOUND

Another question arising from the construction is, whether increasing the dimension still yields a large lower bound on graphs constructed for the smaller dimension.

Let $k \geqslant 3$ and let C_P be a cylindrical grid (for some P of size k) with the equivalence $\equiv$ as defined in Section 5.1. In the following, whenever we say that a cop lands on a vertex v, we mean that the cop lands on the $\equiv$-equivalence class of the vertex v. First, let us prove that the winning strategy for Robber from Lemma 5.13 as shown in [12] is asymptotically tight.

Lemma 5.27. The cops have a winning strategy in the $\mathcal{O}(w^k)$-round compressed $(k+1)$-Cops and Robber game played on C_P and $\equiv$.

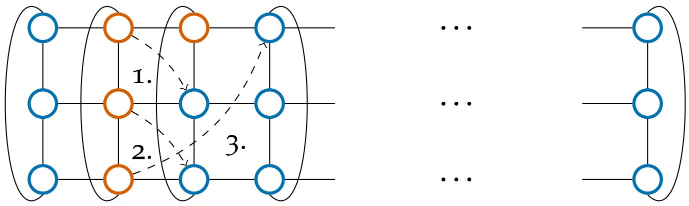

Figure 9: The strategy of the cops in the $3 \times n$ cylindrical grid graph. Here, $j = 1$. The position of the cops is indicated by the red colour and the strategy is sketched by dashed arrows.

Proof. The cops can win like this with a standard strategy on grid graphs. Whenever we say that a cop steps on a vertex, we mean that the cop steps on the equivalence class of the vertex. Furthermore, we only focus on the vertex the cop was said to step on, not on the other vertices (this just makes it harder for the cops to catch the robber).

The cops first land on the first column (i.e. the vertices $(i, 0)$ for all $0 \leqslant i \leqslant k-1$) and the vertex $(0, 1)$. Afterwards, the cop from (i, j) moves to $(i+1, j+1)$ for $i \leftarrow 0, 1, \ldots, k-2$ [1] and (if j is not the last column) the cop from $(k-1, j)$ moves to $(0, j+2)$. This happens for all $j \leftarrow 0, 1, \ldots, |J|-1$. (The strategy is sketched in Figure 9.) Note that at all times, the cops form a vertical separator for C_P and hence the robber has to be either caught or be located to the right of the position of the cops. However, in the end, the cops stay on the last column of C_P and therefore, the robber is caught. Since every node of C_P is visited by some cop exactly once, the number of moves cops needed to catch the robber is exactly $k \cdot |J| \leqslant kw^k \in \mathcal{O}(w^k)$ since k is a constant. □

We now proceed to analyse the winning strategies for the cops on C_P and $\equiv$ in the d-Cops and Robber game for various $d > k$. For $d = 3k$, we can immediately see that the cops can perform a "binary search" and catch the robber in logarithmically many steps.

Lemma 5.28. The cops have a winning strategy in the $\mathcal{O}(\log w)$-round compressed $(3k)$-Cops and Robber game played on C_P and $\equiv$.

Proof. Suppose the cops form two vertical separators on columns j_1 and j_2 where $j_1 < j_2$. We prove by induction on $j_2 - j_1$ that the cops have a winning strategy in $k \cdot \log(j_2 - j_1)$ steps.

If $j_2 - j_1 \leqslant 1$, the robber is already caught (in $k \cdot \log(1) = 0$ steps).

Suppose that for all j_1, j_2 such that $j_2 - j_1 < M$, the cops have a winning strategy in $k \cdot \log(j_2 - j_1)$ steps from the position where the cops stand on the columns j_1 and j_2 and the robber is between the columns j_1 and j_2. The cops choose the column $\left\lfloor \frac{j_1+j_2}{2} \right\rfloor$ and form a vertical separator there. The robber has to decide to either be caught by this separator or choose one side of this separator. If the robber chooses the left (right, resp.) side, the cops from column j_2 (j_1, resp.)

[1] Here, $i \leftarrow 0, 1, \ldots, k-2$ means that it happens for $0, 1, \ldots, k-2$ is this order.

are now free and by the induction hypothesis, the cops can win this new position in $k \cdot \log\left(\left\lfloor \frac{j_1+j_2}{2} \right\rfloor - j_1\right) = k \cdot \log\left(\left\lfloor \frac{j_2-j_1}{2} \right\rfloor\right)$ steps. In total, the number of steps cops needed was

$$\begin{aligned} k + k \cdot \log\left(\left\lfloor \frac{j_2-j_1}{2} \right\rfloor\right) &\leqslant k + k \cdot \log\left(\frac{j_2-j_1}{2}\right) \\ &= k + k \cdot \log(j_2 - j_1) - k \cdot \log 2 \\ &= k \cdot \log(j_2 - j_1), \end{aligned}$$

which was to prove.

Now we set $j_1 = 0$ and $j_2 = |J| - 1$ and let the cops form vertical separators on the columns j_1 and j_2. By the previous, we get that the cops have a winning strategy in the (compressed) $(3k)$-Cops and Robber game in $k \log(j_2 - j_1) = k \log(|J|) \leqslant k^2 \log w \in \mathcal{O}(\log w)$ rounds. □

In the previous, fairly straightforward cases, we actually played the compressed Cops and Robber game as a standard Cops and Robber game. For the following strategies, we will make use of the relation $\equiv$.

Definition 5.29. Let $2 \leqslant j \leqslant k-1$. We call a set $W \subseteq V(C_P)$ of size j a j-**almost separator** if there are $k-j$ vertices $u_1, \dots, u_{k-j} \in V(C_P)$ in rows $j, \dots, k-1$ such that $W \cup \{u_1, \dots, u_{k-j}\}$ forms a column in C_P.

Lemma 5.30. Let $W \subseteq V(C_P)$ be a j-almost separator such that W does not contain any singletons with respect to $\equiv$. Then $W/_\equiv$ contains $\Omega(w^{k-j-1})$ many j-almost separators, and each two of them have distance $f(k)p_0 \dots p_j \in \Theta(w^{j+1})$ or its integer multiple.

Proof. Suppose W contains vertices $(0, t), \dots, (j-1, t)$. Let

$$s := (t \bmod f(k)p_0p_1 \dots p_j) + f(k)p_0p_1 \dots p_j.$$

Note that $s < 2f(k)p_0p_1 \dots p_j)$. As $j \geqslant 2$, the vertex (i, s) is not in a singleton $\equiv$-equivalence class for any $0 \leqslant i < j$. Furthermore, Let $c \geqslant 1$ and consider the sets

$$W_c = \Big\{ (i, s + c \cdot f(k)p_0p_1 \dots p_j) \mid 0 \leqslant i < j \Big\}.$$

If W_c does not contain any vertices from singleton $\equiv$-equivalence classes, then W_c is a j-almost separator. For $c = \frac{1}{2}p_{j+1} \dots p_{k-1} - 3$, we have the set

$$W_c = \Big\{ (i, s + \frac{1}{2}f(k)p_0 \dots p_{k-1} - 3f(k)p_0p_1 \dots p_j) \mid 0 \leqslant i < j \Big\}.$$

Note that

$$\begin{aligned} s + \frac{1}{2}f(k)p_0 \dots p_{k-1} - 3f(k)p_0 \dots p_j & \\ &< \frac{1}{2}f(k)p_0 \dots p_{k-1} - f(k)p_0 \dots p_j, \end{aligned}$$

and since $j \geqslant 2$, the set W_c does not contain any vertices from singleton $\equiv$-equivalence classes (by the construction of C_P). Since W_c for both $c = 1$ and $c = \frac{1}{2}p_{j+1} \dots p_{k-1} - 3$ does not contain any vertices from singleton classes, it follows (by the construction of C_P) that W_c is a j-almost separator for any $1 \leqslant c \leqslant \frac{1}{2}p_{j+1} \dots p_{k-1} - 3$. Therefore, there are at least $\frac{1}{2}p_{j+1} \dots p_{k-1} - 3 \in \Omega(w^{k-j-1})$ such j-almost separators. □

Proposition 5.31. Let $2 \leqslant j \leqslant k-1$ and let $d = \max\{3k-2j, 2k+1\}$. The cops have a winning strategy in the $\mathcal{O}(w^{j+1})$-round compressed d-Cops and Robber game played on C_P and $\equiv$.

Proof. We encourage the reader to follow this proof with Figure 10.

First, we put j cops on the the vertices in $W = \{u_0, \dots, u_j\}$, where $u_i = (i, f(k)w^2)$ for $0 \leqslant i < k-j$.

By Lemma 5.30, there are $\Omega(w^{k-j-1})$ many j-almost separators $S_1, S_2, \dots, S_m$ in $W/_{\equiv}$. We can assume that S_i is located to the left of $S_{i'}$ if and only if $i < i'$.

Now, $k-j$ cops move under S_1 to form a vertical separator. (Now, k cops are placed.) If the robber is not already caught and chooses to stay on the left side, we add one more cop and move as in the standard strategy on grid graphs (similarly as in Lemma 5.27) to the left and catch the robber in $\mathcal{O}(w^2)$ rounds.

Additional $k-j$ cops form a new vertical separator under S_m and similarly, if the robber is not caught and decides to stay on the right side, we can catch the robber in $\mathcal{O}(w^2)$ rounds.

With additional $k-j$ cops, similarly as in Lemma 5.28, we perform a "binary search" to force the robber between some S_i and S_{i+1}. For this, the cops need at most $j \cdot \log P \in \mathcal{O}(\log w)$ rounds. Note that at this point, $3k-2j$ cops are placed.

The robber is now located between some S_i and S_{i+1}. If S_i is in the a-th column, we put $j+1$ cops on $(l, a+1)$ for $0 \leqslant l < j+1$. (Note that now, $2k+1$ cops are placed.) Then move the cop from (l, a) to $(l+1, a+1)$ for all $l \leftarrow j+1, \dots, k-2$. Now move the cop from $(k-1, a)$ to $(0, a+2)$. The k cops located in column $a+1$ and the cop located on $(0, a+2)$ now can perform the standard strategy (similar to the one in Lemma 5.27) and move to the right until they catch the robber or until they touch S_{i+1}, in which case they also catch the robber. By Lemma 5.30, the distance between S_i and S_{i+1} is in $\Theta(w^{j+1})$. Therefore, the cops can catch the robber in $\mathcal{O}(w^{j+1})$ rounds. □

Note that there are two possibilities.

1. If $\frac{k-1}{2} \leqslant j$, then the number of cops $d = 2k+1$ does not depend on j and hence it is better for the cops to take the smallest possible $j = \lceil \frac{k-1}{2} \rceil$ to get the smallest possible round number. Then we see that $2k+1$ cops can win in $\mathcal{O}\left(w^{\lceil \frac{k+1}{2} \rceil}\right)$ rounds.
2. If $j < \frac{k-1}{2}$, then the family of strategies we presented gradually lower the number of rounds with an increasing number of cops.

Table 1 summarises the presented bounds in this section.

d	$k+1$	$2k+1$	$3k-2j$	$3k$
r	$\mathcal{O}\left(w^{k}\right)$	$\mathcal{O}\left(w^{\lceil\frac{k+1}{2}\rceil}\right)$	$\mathcal{O}\left(w^{j+1}\right)$	$\mathcal{O}(\log w)$

Table 1: The cops win in the r-round compressed d-Cops and Robber game on C_P and $\equiv$. The bounds hold for all $1 \leqslant j \leqslant \frac{k-1}{2}$.

Remark. Proposition 5.31 does not necessarily yield an upper bound on the iteration number of d-WL on the cylindrical grid C_P for some $d > k$. Lemma 4.15 only shows that if the robber has a winning strategy in r rounds, then d-WL needs at least r rounds to stabilise. However, the other implication might not hold in general. We have only shown that the robber has no strategy in the compressed d-Cops and Robber games and hence we cannot use this technique to prove a lower bound on the iteration number of d-WL.

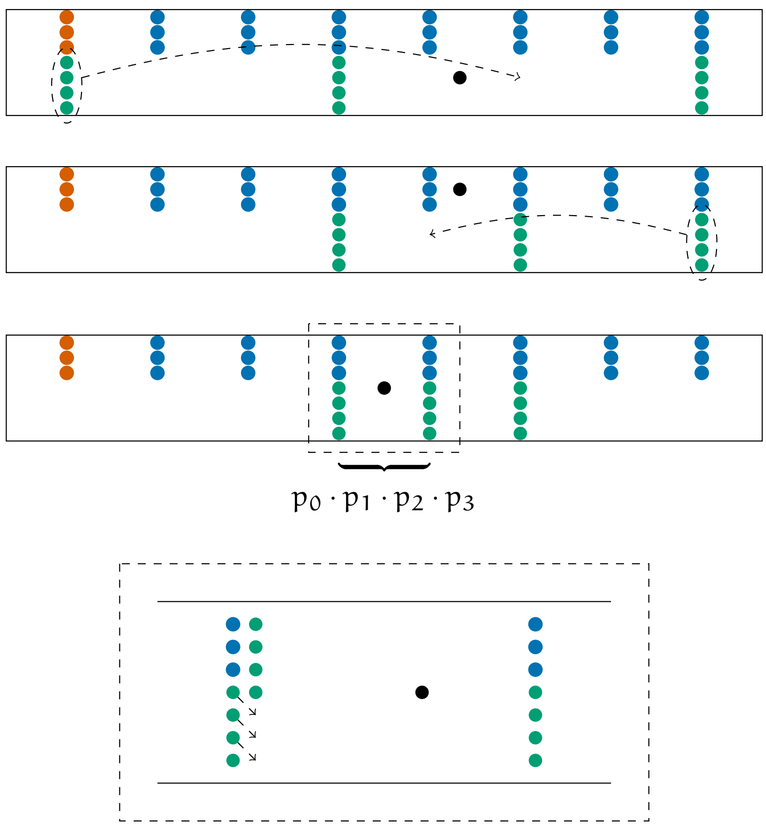

Figure 10: The strategy of the cops presented in Proposition 5.31. The red positions are the vertices we placed the cops on and the blue positions are positions equivalent to those. (In this example, all red and blue positions are occupied by three cops in total.) There is one cop for every green position. For visualisation purposes, the robber is depicted as a black dot, however, note that the robber always stays on some edge. The dotted rectangle is meant to "zoom in" on the second phase of the strategy. In this example, $d = 2k + 1 = 3k - 2j = 15$ cops can to catch the robber (with the strategy from Proposition 5.31 with $j = 3$) on a cylindrical grid graph for $k = 7$ in $\mathcal{O}(w^4)$ rounds.

CONCLUSION

We have analysed the lower bound on the iteration number of k-WL given by Grohe et al. [12] and we gave a new lower bound on the iteration number of k-WL when we do not assume that k is a constant. We also sketched the proof of the lower bound from [12] and gave a few further insights for better understanding.

Furthermore, we showed for which relations between n and k the construction exists, and even if we take the smallest possible size n, the lower bound decreases only by a square root. Furthermore, we gave relations between n and k for which the lower bound decreases insignificantly.

We also analysed the robustness of the construction, i. e. how many rounds does the d-WL algorithm need to stabilise on the construction for $k < d$. We did not give an explicit answer, but we gave strategies for the cops in the compressed d-Cops and Robber game for the number of cops $2k + 1 \leqslant d \leqslant 3k$.

We conclude the text with a few open problems regarding the analysis of the construction, that may be interesting to investigate.

- Proposition 5.21 gives a particular relation between the size n and the dimension k. How does the lower bound look like, if a function $h(k)$ representing the size n does not satisfy the assumptions of Proposition 5.21?
- Given k and some cylindrical grid C_P for some P of size k, is it possible to give lower bounds on the iteration number of d-WL on C_P for $d > k$?
- We only analysed the robustness of the construction given in [12] and did not provide any lower bounds. Can we answer the previous question if we alter the construction of the graph C_P?
- What happens when we do not fix the dimension k in the robustness analysis?

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