Relational Colour Refinement for Non-Relational Signatures

Bachelor's Thesis

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Colour Refinement is an iterative algorithm for graphs that computes a colouring of the vertices, based on the colouring of their direct neighbours. Aside from useful applications in various fields, it is theoretically interesting, due to its characterisations. It was proved that the distinguishing power of Colour Refinement is equivalent to that of counting logic with two variables and to that of counting homomorphisms from trees. Therefore, the question, whether such an algorithm is also possible for extensions of graphs was posed. Recently, Scheidt and Schweikardt defined a Colour Refinement algorithm for relational structures with analogous characterisations. Its distinguishing power is equivalent to that of the guarded fragment of counting logic and to that of counting homomorphisms from α-acyclic relational structures.

In this thesis, we want to present the results of Scheidt and Schweikardt and investigate the robustness of their algorithm and characterisations. Concretely, we consider two possible extensions of the algorithm. One to all structures and one to structures with relations and unary functions. We find a logical characterisation for both approaches, but disprove the existence of a characterisation through homomorphism counting. Furthermore, we discuss for which restrictions on relational structures the characterisation through homomorphism counting remains and present results for two different restrictions.

1 Introduction

The graph isomorphism problem is a very interesting and important problem in both theoretical and applied computer science. The question, whether two graphs are structurally identical comes up in many fields of research. For example, when trying to recognize identical chemical structures for patent verification [17] or finding symmetries for optimising algorithms for problems such as the Boolean Satisfiability problem [14]. Furthermore, the graph isomorphism problem is interesting from a complexity theoretic perspective, as it is a prominent example for a problem, which has not been proven to be either NP-complete or solvable in polynomial time. [2]

One (incomplete) algorithm that is often used in practical isomorphism problem solvers [14] is *Colour Refinement*, short CR, also called the *1-dimensional Weisfeiler-Leman algorithm*. Given two graphs, it can decide, whether they might be isomorphic or whether they are not [4]. Concretely, CR is an iterative algorithm that, in the beginning, assigns every vertex the same colour and in following iterations assigns each one a new colour, based on the colours of its neighbours. This procedure is repeated, until the partition of the vertices induced by the colouring stays the same. We then say that Colour Refinement distinguishes two graphs, if there is some colour that appears differently often in the two graphs. It is easy to see that two isomorphic graphs are not distinguished by Colour Refinement. This is equivalent to the fact that if two graphs get distinguished by Colour Refinement, then they cannot be isomorphic. Furthermore, while it is not possible to infer the opposite direction, that is two non-isomorphic graphs always get distinguished by CR, it was shown by Babai, Erdős and Selkow that almost all graphs get distinguished by it [3]. However, there exist some classes of graphs, that cannot be distinguished by Colour Refinement, for example the classes of regular graphs with the same number of vertices.

Aside from isomorphism testing, Colour Refinement has applications in different fields. Incidentally, the first recorded occurrence of this algorithm appeared in 1965 and dealt with the description of chemical structures [16]. Its significance for computer science has been recognised later by Weisfeiler and Leman in 1968 [20]. One interesting application of Colour Refinement is in the reduction of the dimension of linear programs. By defining a variant of Colour Refinement on matrices which finds a partition of the rows and columns, it is possible to reformulate a linear program with a considerably smaller dimension. This method of first reducing the problem and then solving the reduced instance has been shown to be more performant than the standard way of solving linear programs. [13] Another application can be found in the field of machine learning, more precisely for kernel methods. When fixating a natural number h, it is possible to define a kernel for graphs, by counting the number of vertices that share the same colour for the first h rounds. This Weisfeiler-Leman Graph Kernel has an adequate ability to to classify graphs, while having a significantly better runtime than classical graph kernels. [12]

One importance of CR in theoretical computer science can be seen, when we consider other characterisations of its distinguishing power. Thus, CR can be equivalently characterised by counting homomorphisms from trees and by considering a fragment of counting logic. Due to Dvořák [10] and Dell, Grohe and Rattan [9] we have the following characterisation. Given two graphs G and H, we have that Colour Refinement distinguishes them if, and only if, there is some tree T such that the number of homomorphisms from T to G is different than to H. Such a characterisation can also be done through logic. We define C_2 as the logic that extends first-order logic by counting quantifiers and only uses up to two variables. Then, it was the shown by Cai and Immerman [8] and Immerman and Lander [15] that the following holds: Colour Refinement distinguishes G and H if, and only if, there is a sentence in C_2, which is satisfied by G, but not by H.

From the examples above, it can be seen that while Colour Refinement is a simple procedure, it

can be applied in various situations. This versatility has been one of the reasons for its success and poses the question, whether it could be possible to formulate an analogous procedure for more than graphs. One obvious extension of graphs are hypergraphs. These are structures with a set of vertices and undirected edges between those. However, while the edges of classical graphs connect two vertices, edges of hypergraphs can include an arbitrary number of them. One interesting result due to Böker [5] is an extension of Colour Refinement to hypergraphs, which gives rise to an analogous characterisation through homomorphism counting. Concretely, Colour Refinement for a hypergraph is defined like classical CR on a coloured variant of the incidence graph of it. We then consider connected Berge-acyclic hypergraphs, that is hypergraphs whose incidence graphs are trees. When counting homomorphisms from those to hypergraphs, we get that Colour Refinement distinguishes two hypergraphs G and H if, and only if, there is some connected Berge-acyclic hypergraph B, such that B has a different number of homomorphisms to G than to H. Another result with respect to hypergraphs has been achieved by Scheidt and Schweikardt in [18]. They devised a 2-sorted counting logic called GC^k and proved that two hypergraphs G and H satisfy exactly the same GC^k sentences if, and only if, all hypergraphs with generalised hypertree width k have the same number of homomorphisms to G as to H. For the case where $k = 1$, we then get indistinguishability over the class of all α-acyclic hypergraphs, which is a strictly stronger measure of acyclicity than Berge-acyclicity. Interestingly, we will encounter α-acyclicity and GC^1 in Section 3 for characterising relational structures, instead of hypergraphs. A first effort to extend Colour Refinement to relational structures has been made by Butti and Dalmau in [7]. They also defined Colour Refinement on the incidence graph of a relational structure and proved that this distinguishes two relational structures if, and only if, there is a connected Berge-acyclic relational structure with a different number of homomorphisms to the structures. A more recent result with respect to relational structures has been made by Scheidt and Schweikardt [19]. They defined an extension of Colour Refinement for relational structures, called Relational Colour Refinement, short RCR, which is stronger than the version in [7]. Thus it can distinguish structures that the variant in [7] cannot. Furthermore, they defined the guarded fragment of counting logic $\mathsf{GF}(\mathsf{C})$, and where able to prove that this logic characterises RCR in the same way as C_2 characterises classical CR. Additionally, the aforementioned α-acyclic structures characterise RCR as well. Concretely, we have that two relational structures of the same signature get distinguished by RCR if, and only if, there is an α-acyclic structure of the same signature which has different amounts of homomorphisms to the structures. A deeper discussion of the results from [19] can be found in Section 3.

It can be seen that there exist multiple comprehensive results for relational structures and hypergraphs. Especially the results from [19] seem like a very robust and usable extension for relational structures. Furthermore, we notice that non-relational signatures have not yet been investigated. As many practical and useful structures use non-relational signatures, for example all algebraic structures, we pose the question how robust the results from [19] are, when trying to apply them to structures with (unary) functions. Concretely, we consider two possible ways of how Relational Colour Refinement can be adapted to signatures with functions. For both approaches we investigate, whether they can be characterised by a variant of $\mathsf{GF}(\mathsf{C})$ over signatures with function symbols and by counting homomorphisms from acyclic structures with non-relational signatures. We will see that such a characterisation through logic is in fact possible, while counting homomorphisms from acyclic structures is not. Additionally, we prove another result for the characterisation by counting homomorphisms. We show that while it is not possible to require that the acyclic structure is total, it is possible to require the acyclic structure to be symmetric (given that the two distinguished structures are symmetric as well). Therefore, we get that two symmetric structures are distinguished by RCR if, and only if, there is some symmetric, acyclic

structure with different numbers of homomorphisms to the structures.

The results of this thesis are as follows. We define two variants of RCR for non-relational signatures, called naive RCR and RCR_k for a $k \in \mathbb{N}$, where the latter is only defined for unary functions. Naive RCR encodes n-ary functions f directly as a $(n+1)$-ary relations R_f, such that $(x_1, \ldots, x_n, y) \in R_f$ if, and only if, $f(x_1, \ldots, x_n) = y$. Then normal RCR is applied to the relational structure. RCR_k encodes unary functions f as a family of relations R_{f^1}, R_{f^2}, $\ldots$, where $(x, y) \in R_{f^i}$ if, and only if, $f^i(x) = y$, where $f^i(x)$ is the i-times application of f on x. Furthermore we define $\mathsf{nfGF}(\mathsf{C})$ as the logic that is defined as $\mathsf{GF}(\mathsf{C})$ over non-relational signatures but does not allow the nesting of terms. Additionally we define $\mathsf{GF}(\mathsf{C})_k$ as the logic that is the natural extension of $\mathsf{GF}(\mathsf{C})$ to non-relational signatures but terms are only allowed to have an alternation-depth of function applications of up to k. We further call an encoding of a non-relational structure as a relational one total, if the encoding of every function is defined for every value in the domain of the function and we call the structure functional, if the encoding of every function defines at most one value for every element in the domain of the function. We then achieve the following results.

Theorem 1.1 (Theorem 4.4)**.** *Let σ be a signature and let $\mathfrak{A}$ and $\mathfrak{B}$ be two σ-structures. Naive* RCR *distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ if, and only if, there is a sentence $\varphi \in \mathsf{nfGF}(\mathsf{C})$ of signature σ, such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.*

Theorem 1.2 (Theorem 4.9)**.** *Let σ be a signature that only contains relation symbols and unary function symbols. Let $\mathfrak{A}$ and $\mathfrak{B}$ be two σ-structures and let $k \in \mathbb{N}$.* RCR_k *distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ if, and only if, there is a sentence $\varphi \in \mathsf{GF}(\mathsf{C})_k$ of signature σ, such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.*

Theorem 1.3 (Theorem 4.23)**.** *Two structures $\mathfrak{A}$ and $\mathfrak{B}$ get distinguished by naive* RCR *if, and only if, there exists an acyclic and functional structure that distinguishes the encodings of $\mathfrak{A}$ and $\mathfrak{B}$ by homomorphism counts. Furthermore, there exist structures $\mathfrak{A}$ and $\mathfrak{B}$ that get distinguished by naive* RCR*, but there does not exist an acyclic, functional and total structure that distinguishes the encodings of $\mathfrak{A}$ and $\mathfrak{B}$ by homomorphism counts. Or equivalently, there does not exist a structure of the same signature as $\mathfrak{A}$ and $\mathfrak{B}$, which distinguishes them by homomorphism counts.*

Theorem 1.4 (Theorem 5.3)**.** *Two symmetric, relational structures $\mathfrak{A}$ and $\mathfrak{B}$ get distinguished by* RCR *if, and only if, there is a symmetric, acyclic structure that distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ by number of homomorphism.*

The methods used to achieve these results rely heavily on the proofs from [19]. For the logical characterisation of structures with functions we translate both structures to relational structures and translate any formula to a valid $\mathsf{GF}(\mathsf{C})$-formula over a relational signature. The same is done in reverse. For the characterisation through homomorphism counting, we have two results, see Theorem 1.3. For the first result we present a procedure to iteratively remove collisions of function encodings. This then results in a functional structure. The second result is shown by defining two infinite families of counterexamples.

The structure of this thesis is as follows. We begin by defining notation and fundamental definitions in Section 2. In Section 3 we present and explain the results from [19]. Afterwards, we continue in Section 4 by considering structures with functions, where we will first show the logical characterisation for the two approaches, before then discussing the characterisation through homomorphism counting. Lastly, we discuss the restriction to symmetric structures in Section 5.

2 Preliminaries

Let A be a set. Then $a_1, \dots, a_k \in A$ form a tuple with length k of the form $\mathbf{a} = (a_1, \dots, a_k) \in A^k$ and with $\mathbf{a}_n$ we denote a_n. For any function $f : A \to B$, we write $f(\mathbf{a})$ for $(f(a_1), \dots, f(a_k))$. If π is a permutation, that is $\pi \in \mathcal{S}_k$, where $\mathcal{S}_k$ is the symmetric group for k elements, then $\pi(\mathbf{a})$ means $(a_{\pi(1)}, \dots, a_{\pi(k)})$. For a set A and a $k \in \mathbb{N}$, we write $\binom{A}{k}$, to denote all subsets of A with cardinality of exactly k. Let $\mathbf{a} = (a_1, \dots, a_k) \in A^k$ be a tuple of length k and $b \in A$. Then we write $(\mathbf{a}b) \coloneqq (a_1, \dots, a_k, b)$ for the tuple of length $k+1$ with b added to the end. For a tuple $\mathbf{a} = (a_1, \dots, a_k)$ we write $\mathrm{set}(\mathbf{a}) \coloneqq \{a_1, \dots, a_k\}$ for the set that contains the elements from $\mathbf{a}$. Usually, sets are denoted by uppercase, elements from sets as lowercase, and tuples as boldface and lowercase Latin letters.

By $\mathbb{N}$ we mean the set of natural numbers, including 0, and with $\mathbb{N}_{\geq k}$ for a $k \in \mathbb{N}$, we denote the set $\{k, k+1, \dots\} = \mathbb{N} \setminus \{0, \dots, k\}$. We use $[k]$ for any $k \in \mathbb{N}_{\geq 1}$ to mean $\{1, 2, \dots, k\}$.

A multiset $\mathcal{M}$ is a pair with a set A and a function $\mathrm{mult}_{\mathcal{M}} : A \to \mathbb{N}_{\geq 1}$. This denotes that for every $a \in A$, there are exactly $\mathrm{mult}_{\mathcal{M}}(a)$ many copies in $\mathcal{M}$. We also write multisets as $\{\!\{\dots\}\!\}$. As an example, the multiset $\mathcal{M} = \{\!\{a, b, b\}\!\}$ is equivalent to the set $A = \{a, b\}$, together with the function $\mathrm{mult}_{\mathcal{M}} = \{a \mapsto 1, b \mapsto 2\}$.

A signature is a set of relation and function symbols, paired with an arity for every symbol. We usually write relation symbols as uppercase and function symbols as lowercase letters. For example, $\sigma = \{R/2, T/3, f/3\}$ represents a signature with a relation symbol R of arity 2, a relation symbol T of arity 3 and a function symbol f of arity 3. We call a signature relational, if it only contains relation symbols and binary if it contains only unary and binary symbols. For a function or relation symbol $R \in \sigma$, we write $\mathrm{ar}(R)$ for the arity of R and we define $\mathrm{ar}(\sigma) \coloneqq \max_{R \in \sigma}\{\mathrm{ar}(R)\}$ as the maximal arity that appears in σ. For a signature $\sigma = \{R_1/\mathrm{ar}(R_1), R_2/\mathrm{ar}(R_2), \dots, f_1/\mathrm{ar}(f_1), f_2/\mathrm{ar}(f_2), \dots\}$ we define a σ-structure $\mathfrak{A}$ as a tuple $(A, R_1^{\mathfrak{A}}, R_2^{\mathfrak{A}}, \dots, f_1^{\mathfrak{A}}, f_2^{\mathfrak{A}}, \dots)$ where A, called the universe, is a set of elements and $R_i^{\mathfrak{A}} \subseteq A^{\mathrm{ar}(R_i)}$ is a relation of arity $\mathrm{ar}(R_i)$ and $f_i^{\mathfrak{A}} : A^{\mathrm{ar}(f_i)} \to A$ is a function of arity $\mathrm{ar}(f_i)$. We define $|\mathfrak{A}| = |A|$. A structure is usually written as an uppercase Fraktur letter and its universe is written using the same uppercase Latin letter. For relational structures, we use an uppercase, boldface Latin letter to denote the union of all relations, formally $\bigcup_{R \in \sigma} R$. As an example, $\mathfrak{A}$ is a structure, A is its universe and $\mathbf{A}$ is the union of all relations. A graph G is a pair of a set of vertices, denoted as $V(G)$, and a binary and symmetric relation over that set of vertices, called the edges $E(G)$. If not specified, we only talk about finite signatures and finite universes.

For a graph G, we apply Colour Refinement by inductively defining for every $v \in V(G)$ and every $i \in \mathbb{N}$ a colour $C_i(v)$, using the following method. The initial colouring is defined as $C_0(v) \coloneqq 0$. For $i \in \mathbb{N}$, we define $C_{i+1}(v) \coloneqq (C_i(v), \{\!\{C_i(u) : \{v, u\} \in E(G)\}\!\})$. We say that Colour Refinement distinguishes two graphs G and H, if there is an $i \in \mathbb{N}$, such that

$$\{\!\{C_i(v) : v \in V(G)\}\!\} \neq \{\!\{C_i(u) : u \in V(H)\}\!\}.$$

It is possible to adapt classical Colour Refinement to binary relational structures, by using the unary relations in the initial colouring and annotating neighbours with the binary relations that connect the elements. Let $\sigma = \sigma_1 \dot\cup \sigma_2$, where σ_1 contains only unary and σ_2 contains only binary relations. For a binary relational structure $\mathcal{G}$, write $E(\mathcal{G})$ for $\bigcup_{E \in \sigma_2}\{\{v, w\} : (v, w) \in E^{\mathcal{G}}\}$. Then, for every element $e \in G$ we define

$$\gamma_0(e) \coloneqq (\{C \in \sigma_1 : e \in C^{\mathcal{G}}\}, \{E \in \sigma_2 : (e, e) \in E^{\mathcal{G}}\}).$$

For every $e \in G$, every $i \in \mathbb{N}$ we define

$$\gamma_{i+1}(e) \coloneqq (\gamma_i(e), \{\!\{(\lambda(e, f), \gamma_i(f)) : \{e, f\} \in E(\mathcal{G})\}\!\}),$$

and

$$\lambda(e,f) \coloneqq \{E^+ : E \in \sigma_2, (e,f) \in E^{\mathcal{G}}\} \cup \{E^- : E \in \sigma_2, (f,e) \in E^{\mathcal{G}}\},$$

where we introduce two new symbols E^+ and E^- for every $E \in \sigma_2$. This definition can also be found in [19].

For a signature σ and two σ-structures $\mathfrak{A}$ and $\mathfrak{B}$, we call a function $\varphi : A \to B$ a homomorphism, if:

- For every relation symbol $R \in \sigma$ of arity k and every $(x_1, \dots, x_k) \in R^{\mathfrak{A}}$,

  $$(\varphi(x_1), \dots, \varphi(x_k)) \in R^{\mathfrak{B}}$$

  and

- for every function symbol $f \in \sigma$ of arity k and every $(x_1, \dots, x_k)$,

  $$\varphi(f^{\mathfrak{A}}(x_1, \dots, x_k)) = f^{\mathfrak{B}}(\varphi(x_1), \dots, \varphi(x_k)).$$

We then write $\mathrm{Hom}(\mathfrak{A}, \mathfrak{B})$ for the set of all homomorphisms from $\mathfrak{A}$ to $\mathfrak{B}$ and define $\hom(\mathfrak{A}, \mathfrak{B}) \coloneqq |\mathrm{Hom}(\mathfrak{A}, \mathfrak{B})|$. This applies analogously for relational structures and graphs.

For a $\varphi(x_1, \dots, x_k) \in \mathsf{C}$, or a subset of C, where C is the logic that extends FO with counting quantifiers, we write $\mathfrak{A}, a_1, \dots, a_k \models \varphi(x_1, \dots, x_k)$ to mean $\mathfrak{A} \models \varphi(a_1, \dots, a_k)$. Similarly, for a $\psi(x_1, \dots, x_k, y_1, \dots, y_\ell) \in \mathsf{C}$, we write $\mathfrak{A}, a_1, \dots, a_k, b_1, \dots, b_\ell \models \psi(x_1, \dots, x_k, y_1, \dots, y_\ell)$ for $\mathfrak{A} \models \psi(a_1, \dots, a_k, b_1, \dots, b_\ell)$. We use $\top$ for a formula, which is always satisfied.

3 Relational Colour Refinement

Relational structures are a very important and interesting extension of graphs. They can be found in various situations, for example in relational database theory where they are used to model the structure of databases [1]. In this section we want to look at the Relational Colour Refinement algorithm. It was defined by Scheidt and Schweikardt in [19] as an extension of CR for relational structures. The algorithm is similar to the adaptation of classical CR for binary relational structures and has characterisations analogous to classical CR. Let us begin by defining RCR and applying it to a small example.

3.1 RCR and Binary Relational Structures

The idea of RCR is to apply Colour Refinement on the tuples that appear in a relation. This can then be seen as a binary relational structure, on which the before mentioned Colour Refinement algorithm can be applied. To define RCR, we need the following definitions.

Definition 3.1 (Atomic and shared types)**.** Let σ be a relational signature and $\mathfrak{A}$ be a σ-structure. For every $\mathbf{a} \in \mathbf{A}$ we define the atomic type $\operatorname{atp}(\mathbf{a}) \coloneqq \{R \in \sigma : \mathbf{a} \in R\}$ as the set of relations that include $\mathbf{a}$. For every tuple $\mathbf{a} \in \mathbf{A}$ of length n and every tuple $\mathbf{b} \in \mathbf{A}$ of length m we define the shared type $\operatorname{stp}(\mathbf{a}, \mathbf{b}) \coloneqq \{(i, j) \in [n] \times [m] : \mathbf{a}_i = \mathbf{b}_j\}$ as the set of all pairs of indices which denote the elements that appear in both $\mathbf{a}$ and $\mathbf{b}$. As shorthand notation we write $\operatorname{stp}(\mathbf{a})$ for $\operatorname{stp}(\mathbf{a}, \mathbf{a})$.

We can now define Relational Colour Refinement. For every $\mathbf{a} \in \mathbf{A}$ we iteratively construct a colour $\varrho_i(\mathbf{a})$. We begin by defining the initial colour using the atomic and shared type of $\mathbf{a}$ itself. Formally, $\varrho_0(\mathbf{a}) \coloneqq (\operatorname{atp}(\mathbf{a}), \operatorname{stp}(\mathbf{a}))$. For every $i \in \mathbb{N}_{\geq 1}$ the colour $\varrho_i(\mathbf{a})$ is made up of $\varrho_{i-1}(\mathbf{a})$ and the colour of the last round for every tuple that $\mathbf{a}$ shares an element with, in addition to the information which elements are shared. This is formalised as

$$\varrho_{i+1}(\mathbf{a}) \coloneqq (\varrho_i(\mathbf{a}), \{\!\{(\operatorname{stp}(\mathbf{a}, \mathbf{b}), \varrho_i(\mathbf{b})) : \mathbf{b} \in \mathbf{A}, \operatorname{stp}(\mathbf{a}, \mathbf{b}) \neq \emptyset\}\!\}).$$

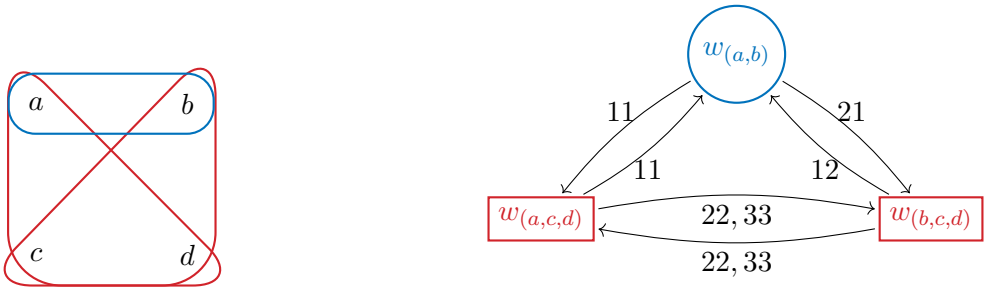
It can easily be verified that if $\varrho_i(\mathbf{a}) \neq \varrho_i(\mathbf{b})$, then $\varrho_{i+1}(\mathbf{a}) \neq \varrho_{i+1}(\mathbf{b})$. The rounds therefore act as a refinement. This also means that there must be a smallest $i_{\mathfrak{A}} \leq \mathbf{A}$, such that for every $\mathbf{a}, \mathbf{b} \in \mathbf{A}$, we have that $\varrho_{i_{\mathfrak{A}}}(\mathbf{a}) = \varrho_{i_{\mathfrak{A}}}(\mathbf{b})$ if, and only if, $\varrho_{i_{\mathfrak{A}}+1}(\mathbf{a}) = \varrho_{i_{\mathfrak{A}}+1}(\mathbf{b})$, we then call this colouring the stable colouring. For a relational structure $\mathfrak{A}$ and $i \in \mathbb{N}$ we define $\mathrm{RC}_i(\mathfrak{A}) \coloneqq \{\varrho_i(\mathbf{a}) : \mathbf{a} \in \mathbf{A}\}$ as the set of colours that get constructed in the i-th round of RCR. Further, for a relational structure $\mathfrak{A}$, a number $i \in \mathbb{N}$ and a colour $c \in \mathrm{RC}_i(\mathfrak{A})$ we write $\operatorname{mult}_{\mathfrak{A}}(c) \coloneqq |\{\mathbf{a} \in \mathbf{A} : \varrho_i(\mathbf{a}) = c\}|$ for the number of occurrences of the colour c. Finally, for two σ-structures $\mathfrak{A}$ and $\mathfrak{B}$ we say that Relational Colour Refinement distinguishes $\mathfrak{A}$ and $\mathfrak{B}$, if there is an $i \leq \max\{i_{\mathfrak{A}}, i_{\mathfrak{B}}\}$ and a colour $c \in \mathrm{RC}_i(\mathfrak{A}) \cup \mathrm{RC}_i(\mathfrak{B})$ such that $\operatorname{mult}_{\mathfrak{A}}(c) \neq \operatorname{mult}_{\mathfrak{B}}(c)$.

When comparing this algorithm with the Colour Refinement algorithm for binary relational structures, we notice similarities. In fact, it is possible to interpret a relational structure as a binary relational structure, on which classical CR can be applied with an equivalent result to RCR on the original structure. For a relational signature σ we define a signature $\widehat{\sigma} \coloneqq \{E_{i,j}/2 : i, j \in [\operatorname{ar}(\sigma)]\} \cup \{U_R/1 : R \in \sigma\}$. For a σ-structure $\mathfrak{A}$, we can now define a binary relational structure $\mathcal{G}_{\mathfrak{A}}$ of signature $\widehat{\sigma}$. The universe of $\mathcal{G}_{\mathfrak{A}}$ is defined as $V(\mathcal{G}_{\mathfrak{A}}) = \{w_{\mathbf{a}} : \mathbf{a} \in \mathbf{A}\}$. In words, we create a new element $w_{\mathbf{a}}$ for every tuple $\mathbf{a} \in \mathbf{A}$. The relations are then defined as follows. For $R \in \sigma$ we set

$$U_R^{\mathcal{G}_{\mathfrak{A}}} \coloneqq \{w_{\mathbf{a}} : \mathbf{a} \in R\}$$

and for $i, j \in [\operatorname{ar}(\sigma)]$ we set

$$E_{i,j}^{\mathcal{G}_{\mathfrak{A}}} \coloneqq \{(w_{\mathbf{a}}, w_{\mathbf{b}}) : (i, j) \in \operatorname{stp}(\mathbf{a}, \mathbf{b})\}.$$



(a) The structure $\mathfrak{A}$, where the blue edge represents R and the red edges represent T.

(b) The binary relational structure $\mathcal{G}_{\mathfrak{A}}$, where the blue circle represents U_R and the red rectangles represent U_T.

Figure 1: A relational structure $\mathfrak{A}$ of signature $\sigma = \{R/2, T/3\}$ and the binary relational structure $\mathcal{G}_{\mathfrak{A}}$ that encodes it.

It was then proved by Scheidt and Schweikardt [19] that, when identifying $\mathbf{a}$ with $w_{\mathbf{a}}$ for every $\mathbf{a} \in \mathbf{A}$, Colour Refinement on $\mathcal{G}_{\mathfrak{A}}$ is equivalent, or rather induces the same partition of the tuples in every round, as Relational Colour Refinement on $\mathfrak{A}$.

3.1.1 An Example for Relational Colour Refinement

We want to illustrate this with a small example. We choose the signature $\sigma = \{R/2, T/3\}$ and a σ-structure $\mathfrak{A} = (A, R^{\mathfrak{A}}, T^{\mathfrak{A}})$ with $A = \{a, b, c, d\}$, $R^{\mathfrak{A}} = \{(a, b)\}$ and $T^{\mathfrak{A}} = \{(a, c, d), (b, c, d)\}$. A graphical representation can be found in Figure 1a. When applying the transformation described above, we get the signature $\widehat{\sigma} = \{E_{(i,j)} : i, j \in [3]\} \cup \{U_T, U_R\}$. The complete definition of $\mathcal{G}_{\mathfrak{A}}$ can be seen in Figure 1b, where an edge with the label ij from element a to b represents a tuple $(a, b) \in E_{i,j}^{\mathcal{G}_{\mathfrak{A}}}$, shared edges are contracted and self-loops are omitted.

We now want to apply RCR on $\mathfrak{A}$ and then classical CR on $\mathcal{G}_{\mathfrak{A}}$. By this we will see that both algorithms generate the same partition of elements. By the definition, it is obvious that $\varrho_0((a, b)) = (\{R\}, \{(1, 1), (2, 2)\})$ and $\varrho_0((a, c, d)) = \varrho_0((b, c, d)) = (\{T\}, \{(1, 1), (2, 2), (3, 3)\})$. Thus (a, b) already has a different colour from the other two tuples. In the next step (a, c, d) and (b, c, d) will also receive different colours. Concretely,

$$\begin{aligned}\varrho_1((a,c,d)) = (\varrho_0((a,c,d)), \{\!\{&(\{(1,1)\}, \varrho_0((a,b))),\\ &(\{(2,2),(3,3)\}, \varrho_0((b,c,d))),\\ &(\{(1,1),(2,2),(3,3)\}, \varrho_0((a,c,d)))\}\!\})\end{aligned}$$

and

$$\begin{aligned}\varrho_1((b,c,d)) = (\varrho_0((b,c,d)), \{\!\{&(\{(1,2)\}, \varrho_0((a,b))),\\ &(\{(2,2),(3,3)\}, \varrho_0((a,c,d))),\\ &(\{(1,1),(2,2),(3,3)\}, \varrho_0((b,c,d)))\}\!\}).\end{aligned}$$

It can thus be seen that $\varrho_1((a, c, d)) \neq \varrho_1((b, c, d))$. The algorithm has now found a stable colouring, as all elements have a distinct colour.

We will now get the same results when applying classical Colour Refinement to $\mathcal{G}_{\mathfrak{A}}$. Similarly to RCR, we have $\gamma_0(w_{(a,b)}) = (\{U_R\}, \{E_{1,1}, E_{2,2}\})$ and $\gamma_0(w_{(a,c,d)}) = \gamma_0(w_{(b,c,d)}) = (\{U_T\}, \{E_{1,1}, E_{2,2}, E_{3,3}\})$.

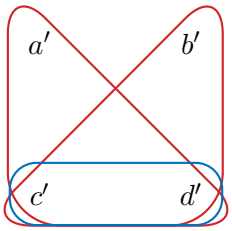


Figure 2: The σ-structure $\mathfrak{B}$ that gets distinguished by RCR from $\mathfrak{A}$.

As before, $w_{(a,c,d)}$ and $w_{(b,c,d)}$ share the initial colour, while $w_{(a,b)}$ has a distinct one. For the second round we now get

$$\begin{aligned}\gamma_1(w_{(a,c,d)}) = (\gamma_0(w_{(a,c,d)}), \{\!\{&(\{E^+_{1,1}, E^-_{1,1}\}, \gamma_0(w_{(a,b)})),\\ &(\{E^+_{2,2}, E^+_{3,3}, E^-_{2,2}, E^-_{3,3}\}, \gamma_0(w_{(b,c,d)})),\\ &(\{E^+_{1,1}, E^+_{2,2}, E^+_{3,3}, E^-_{1,1}, E^-_{2,2}, E^-_{3,3}\}, \gamma_0(w_{(a,c,d)}))\}\!\})\end{aligned}$$

and

$$\begin{aligned}\gamma_1(w_{(b,c,d)}) = (\gamma_0(w_{(b,c,d)}), \{\!\{&(\{E^+_{1,2}, E^-_{2,1}\}, \gamma_0(w_{(a,b)})),\\ &(\{E^+_{2,2}, E^+_{3,3}, E^-_{2,2}, E^-_{3,3}\}, \gamma_0(w_{(a,c,d)})),\\ &(\{E^+_{1,1}, E^+_{2,2}, E^+_{3,3}, E^-_{1,1}, E^-_{2,2}, E^-_{3,3}\}, \gamma_0(w_{(b,c,d)}))\}\!\}).\end{aligned}$$

Again, $\gamma_1(w_{(a,c,d)}) \neq \gamma_1(w_{(b,c,d)})$ and a stable colouring has been found. We see that both procedures act equivalently, which is what was proved by Scheidt and Schweikardt.

Let us now look at an example where RCR distinguishes two structures. For this, consider the σ-structure $\mathfrak{B} = (B, R^{\mathfrak{B}}, T^{\mathfrak{B}})$ with $B = (a', b', c', d')$, $R^{\mathfrak{B}} = \{(c', d')\}$ and $T^{\mathfrak{B}} = \{(a', c', d'), (b', c', d')\}$, which can be seen in Figure 2. It can easily be seen that every colour appears exactly as often in the colouring of the tuples of $\mathfrak{A}$ as of $\mathfrak{B}$. Thus RCR cannot distinguish the structures in round 0. However, the colour $\gamma_1((a, c, d)) \in \mathrm{RC}_1(\mathfrak{A})$ cannot appear in the colouring of $\mathfrak{B}$. This is because for all triples $(x, y, z) \in T^{\mathfrak{B}}$, there does not exist a pair $(x', y') \in R^{\mathfrak{B}}$, such that $x = x'$. Therefore $\mathrm{mult}_{\mathfrak{A}}(\gamma_1((a, c, d))) = 1 \neq 0 = \mathrm{mult}_{\mathfrak{B}}(\gamma_1((a, c, d)))$ and RCR distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ in round 1.

In their paper, Scheidt and Schweikardt consider a larger example, which is an extension of the classical non-distinguishable example for Colour Refinement. They use a signature with a binary relation and a relation of arity 6. The example is then comprised of the structure $\mathfrak{A}_1$ with one 6-cycle and the structure $\mathfrak{A}_2$ with two 3-cycles. Without the 6-ary relation the structure would be a regular graph and therefore could not be distinguished by Colour Refinement. Because of that, the 6-ary relation includes one tuple, containing all 6 elements. With this change, the structures can be distinguished by RCR, which is discussed in [19].

Furthermore, Scheidt and Schweikardt investigate other, seemingly simpler, possible variants of Colour Refinement which use the Gaifman-Graph and Incidence-Graph of a relational structure. However, these variants are not able to distinguish $\mathfrak{A}_1$ and $\mathfrak{A}_2$, which is why they are disregarded in favour of RCR.

3.2 Logical Characterisation of RCR

Classical Colour Refinement gets characterised by counting logic with up to two variables, also called C_2. This means that two graphs G and H get distinguished by Colour Refinement if, and

only if, there is a sentence $\varphi \in \mathsf{C}_2$, such that $G \models \varphi$ and $H \not\models \varphi$ [8, 15]. Similarly, Relational Colour Refinement is characterised by the guarded fragment of counting logic, in short $\mathsf{GF}(\mathsf{C})$. This logic restricts first-order logic with counting quantifiers in the same way, as the guarded fragment of first-order logic GF restricts FO. An investigation of this notion of guards can be found in [11]. The guarded fragment drops the bound on the number of variables, but adds the restriction that quantifiers need be relativised by an atomic formula.

Definition 3.2 (The guarded fragment of counting logic)**.** For a relational signature σ, we define the class $\mathsf{GF}(\mathsf{C})$ over σ and for a formula $\varphi \in \mathsf{GF}(\mathsf{C})$ the set of variables $\mathrm{free}(\varphi)$ inductively, using the following rules:

1. Let $R \in \sigma$ with $\ell = \mathrm{ar}(R)$ and let $x_1, \ldots, x_\ell$ be variables. Then $R(x_1, \ldots, x_\ell) \in \mathsf{GF}(\mathsf{C})$ and $\mathrm{free}(R(x_1, \ldots, x_\ell)) = \{x_1, \ldots, x_\ell\}$.
2. Let x and y be two variables. Then $x = y \in \mathsf{GF}(\mathsf{C})$ and $\mathrm{free}(x = y) = \{x, y\}$.
3. Let $\varphi \in \mathsf{GF}(\mathsf{C})$. Then $(\neg\varphi) \in \mathsf{GF}(\mathsf{C})$ and $\mathrm{free}((\neg\varphi)) = \mathrm{free}(\varphi)$.
4. Let $\varphi, \psi, \in \mathsf{GF}(\mathsf{C})$. Then $(\varphi \wedge \psi) \in \mathsf{GF}(\mathsf{C})$ and $\mathrm{free}((\varphi \wedge \psi)) = \mathrm{free}(\varphi) \cup \mathrm{free}(\psi)$.
5. For a formula built using Rule *1.* or *2.* Δ and a $\varphi \in \mathsf{GF}(\mathsf{C})$, we call Δ a guard for φ, if $\mathrm{free}(\Delta) \supseteq \mathrm{free}(\varphi)$. Let $\Delta, \varphi \in \mathsf{GF}(\mathsf{C})$, where Δ is a guard for φ, let $\mathbf{v}$ be a tuple of variables with $\mathrm{set}(\mathbf{v}) \subseteq \mathrm{free}(\Delta)$ and let $n \in \mathbb{N}_{\geq 1}$. Then $\exists^{\geq n}\mathbf{v}.(\Delta \wedge \varphi) \in \mathsf{GF}(\mathsf{C})$ and $\mathrm{free}(\exists^{\geq n}\mathbf{v}.(\Delta \wedge \varphi)) = \mathrm{free}(\Delta) \setminus \mathrm{set}(\mathbf{v})$.

Formulae that are built using Rules *1.* and *2.* are called atomic formulae, we omit parenthesises in the usual way and use $\exists^{=n}\mathbf{v}.(\Delta \wedge \varphi)$ as shorthand notation for $\exists^{\geq n}\mathbf{v}.(\Delta \wedge \varphi) \wedge \neg\exists^{\geq n+1}\mathbf{v}.(\Delta \wedge \varphi)$.

The semantics of this logic are analogous to classical counting logic, see for example [8], and also are concretely defined in [19].

When comparing $\mathsf{GF}(\mathsf{C})$ with the logic GC^1, see [18], we notice that they seem very similar. A guard in $\mathsf{GF}(\mathsf{C})$ uses only one edge, since atomic formulae are either equalities or relations. This is similar to the one available edge variable in GC^1, over which a guard is defined.

Using a pebble game for $\mathsf{GF}(\mathsf{C})$, called the Guarded-Game, Scheidt and Schweikardt proved the following theorem:

Theorem 3.3 (Theorem B from [19])**.** *Let σ be a relational signature and let $\mathfrak{A}$ and $\mathfrak{B}$ be σ-structures. Then the three following statements are equivalent:*

1. *Relational Colour Refinement distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*
2. *There exists a sentence $\varphi \in \mathsf{GF}(\mathsf{C})$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.*
3. *Spoiler wins the Guarded-Game on $\mathfrak{A}$ and $\mathfrak{B}$.*

Let us again consider the structures from Figures 1a and 2. In the preceding section we used the colour $\varrho_1((a, c, d))$ to distinguish $\mathfrak{A}$ and $\mathfrak{B}$, as it does not appear in the colouring of $\mathfrak{B}$. More precisely, there does not exist a tuple of length 3 in $\mathfrak{B}$, which is in the relation T and its first element is in the relation R with another element. This can be formalised using the formula

$$\varphi_1 \coloneqq \exists^{\geq 1}(x, y, z).\left(T(x, y, z) \wedge \exists^{\geq 1}(y).\,(R(x, y))\right).$$

It is easy to see that $\mathfrak{A} \models \varphi_1$ and $\mathfrak{B} \not\models \varphi_1$.

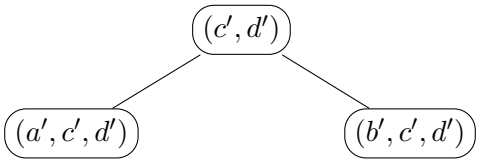


Figure 3: A join-tree for the structure $\mathfrak{B}$ from Figure 2

3.3 Characterising RCR by Homomorphism Counting

Another way to characterise classical CR is to count homomorphisms from trees. Due to [10] and [9] it is known that Colour Refinement distinguishes two graphs G and H if, and only if, there is a tree T, such that $\hom(T, G) \neq \hom(T, H)$. Again, there is an analogous characterisation for Relational Colour Refinement. One obstacle in defining such a characterisation is finding a class that generalises trees for relational structures. As a tree is a connected, acyclic graph, we have to find a fitting notion of acyclicity for relational structures. It can be seen, for example in [6], that there are multiple such definitions for hypergraphs, which can be applied to relational structures as well. When considering the results from [18] and that GC^1 seems very similar to $\mathsf{GF}(\mathsf{C})$, it appears that hypergraphs of generalised hypertree width of 1, or equivalently α-acyclic hypergraphs, may be a possible candidate. This is in fact the case. Let us therefore define α-acyclic structures, which will just be called acyclic structures in the following.

Definition 3.4 (Acyclic structures)**.** Let σ be a relational signature and let $\mathfrak{C}$ be a σ-structure. A join-tree J for $\mathfrak{C}$ is a tree with a vertex for every tuple in $\mathfrak{C}$, thus $V(J) = \mathbf{C}$, which fulfils the join-tree-property: For any $c \in C$, the set $\{\mathbf{c} \in V(J) : c \in \mathrm{set}(\mathbf{c})\}$ induces a connected subgraph of J. This induced subgraph is also a tree and will be denoted as J_c. Finally, we call a structure acyclic, if it has a join-tree.

There are multiple equivalent characterisations for this notion of acyclicity which can be found in [6]. Recall the definition for homomorphisms between structures and the definitions of Hom and hom. This then leads us to another main result from [19].

Theorem 3.5 (Theorem A from [19])**.** *Let σ be a relational signature and let $\mathfrak{A}$ and $\mathfrak{B}$ be σ-structures. Then the two following statements are equivalent:*

1. *Relational Colour Refinement distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*
2. *There exists an acyclic σ-structure $\mathfrak{C}$, such that* $\hom(\mathfrak{C}, \mathfrak{A}) \neq \hom(\mathfrak{C}, \mathfrak{B})$.

We again want to consider the structures from Figures 1a and 2 for a simple example. The structure $\mathfrak{B}$ is acyclic. This can be seen from its join tree depicted in Figure 3. Now consider the homomorphisms from $\mathfrak{B}$. The identity is always a homomorphism, therefore $\hom(\mathfrak{B}, \mathfrak{B}) \geq 1$. However, a homomorphism from $\mathfrak{B}$ to $\mathfrak{A}$ cannot exist. Consider $(c', d') \in R^{\mathfrak{B}}$ and that (a, b) is the only tuple in $R^{\mathfrak{A}}$. We therefore would have to map c' to a and d' to b. But now consider the tuple $(a', c', d') \in T^{\mathfrak{B}}$ and let x be the element that a' gets mapped to. Then (x, a, b) must be in $T^{\mathfrak{A}}$. But there is no such tuple in $\mathfrak{A}$, independently of x. Therefore there cannot exist a homomorphism from $\mathfrak{B}$ to $\mathfrak{A}$, thus $\hom(\mathfrak{B}, \mathfrak{A}) = 0 \neq \hom(\mathfrak{B}, \mathfrak{B})$ and $\mathfrak{B}$ is an acyclic structure that distinguishes $\mathfrak{B}$ and $\mathfrak{A}$ by homomorphism counts.

4 Relational Colour Refinement for Structures With Functions

Many interesting structures use functions. For example all algebraic signatures include function symbols for addition and multiplication. As Colour Refinement and variants of it have shown to be very useful in multiple applications, a similar method for structures with functions seems desirable. This section aims to apply the results from [19], which were discussed in the previous section, to such classes of structures. We will define two different approaches for a Colour Refinement algorithm. Both will encode non-relational structures and non-relational signatures as relational structures and relational signatures, respectively. The already discussed Relational Colour Refinement can then be applied on these structures. We study, whether the non-relational signatures can also be used in the characterisations. Concretely, can we use functions in the formulae which form the logic that characterises the algorithms, if such a logic exists? To what extend can these functions be used and what restrictions apply? The same will be done for the characterisation by homomorphism counting. Can we use the encodings to define acyclic, non-relational structures, and can the classes of those characterise the algorithms by homomorphism counting? We will begin by defining both approaches and comparing them with a simple example. Afterwards we will look at the logical characterisation and end with the characterisation by homomorphism counting.

4.1 Naive Encoding of Functions

The simplest form to encode a non-relational structure as a relational one, is to interpret functions directly as relations. For a non-relational signature σ, we define a relational signature σ'. For every relation symbol $R \in \sigma$, we introduce a relation symbol $R \in \sigma'$ of the same arity and for every function symbol $f \in \sigma$ of arity k, we introduce a relational symbol $R_f \in \sigma'$ of arity $k+1$. Semantically, a structure $\mathfrak{A}$ of signature σ can then be encoded as a structure $\mathfrak{A}'$ of signature σ' with the same universe as $\mathfrak{A}$. For every relational symbol $R \in \sigma$ we set $R^{\mathfrak{A}'} = R^{\mathfrak{A}}$ and for every function symbol $f \in \sigma$ of arity k there exists a relation symbol $R_f \in \sigma'$ and we set $R_f^{\mathfrak{A}} = \{(\mathbf{x}y) : f^{\mathfrak{A}}(\mathbf{x}) = y\}$ where $\mathbf{x}$ is a tuple of length k.

This procedure encodes a non-relational structure as a relational one, on which Relational Colour Refinement can be performed. We say that the Naive Relational Colour Refinement (nRCR) distinguishes two structures $\mathfrak{A}$ and $\mathfrak{B}$ if, and only if, RCR distinguishes their naive encodings $\mathfrak{A}'$ and $\mathfrak{B}'$. However, this results in a relatively weak logical characterisation, that does not allow nesting of terms, namely the nesting-free-fragment of $\mathsf{GF}(\mathsf{C})$, which we will discuss later.

4.2 Using the Transitive Expansion

As a first remark we note that we only consider unary functions for this algorithm. The key idea will be, to encode a function f as a family of relations, which then can capture the notion of nesting function applications. However, a bound on the alternation of different function symbols is necessary to ensure that the expanded signature is still finite, thus we will fixate a maximal alternation depth when discussing our new variant of RCR. Let us concretely define, how we expand the signature.

Definition 4.1 (Transitive expansion)**.** Let $\sigma = \sigma_{\text{Rel}} \dot\cup \sigma_{\text{Func}}$ be a signature with relation symbols σ_{Rel} and unary function symbols σ_{Func} and let $\mathfrak{A}$ be a structure of signature σ with $|\mathfrak{A}| = n$. For readability, we define the family of sets of alternations of function applications $\text{Alters}_n^0(\sigma) \coloneqq \{\text{id}\}$

and

$$\begin{aligned}\mathrm{Alters}_n^k(\sigma) \coloneqq \mathrm{Alters}_n^{k-1}(\sigma) \cup \{f_1^{m_1} f_2^{m_2} \dots f_k^{m_k} : & f_1, f_2, \dots, f_k \in \sigma_{\mathrm{Func}} \\ & \wedge \forall i \in [k] \,.\, m_i \in [n] \\ & \wedge \forall i \in [k-1] \,.\, f_i \neq f_{i+1}\}.\end{aligned}$$

We will now fixate an arbitrary $k \in \mathbb{N}$, which will be our bound on the alternation depth and will define a new signature $\widetilde{\sigma}$ as well as a structure $\widetilde{\mathfrak{A}}$ of said signature, which will be the transitive expansion with alternation depth k of $\mathfrak{A}$. For $\alpha, \beta, \alpha_1, \dots, \alpha_\ell \in \mathrm{Alters}_n^k(\sigma)$ and an $R \in \sigma_{\mathrm{Rel}}$ of arity ℓ, we define the binary relation

$$\mathrm{Eq}_{\alpha,\beta}^{\widetilde{\mathfrak{A}}} \coloneqq \{(a,b) : \alpha^{\mathfrak{A}}(a) = \beta^{\mathfrak{A}}(b)\},$$

and the relation of arity ℓ

$$R_{\alpha_1,\dots,\alpha_\ell}^{\widetilde{\mathfrak{A}}} \coloneqq \{(a_1, \dots, a_\ell) : (\alpha_1^{\mathfrak{A}}(a_1), \dots, \alpha_\ell^{\mathfrak{A}}(a_\ell)) \in R^{\mathfrak{A}}\}.$$

We now define the transitive expansion with alternation depth k signature $\widetilde{\sigma}$, where

$$\begin{aligned}\widetilde{\sigma} \coloneqq \quad & \{\mathrm{Eq}_{\alpha,\beta}/2 : \alpha, \beta \in \mathrm{Alters}_n^k(\sigma)\} \\ & \dot{\cup}\, \{R_{\alpha_1,\dots,\alpha_\ell}/\ell : R \in \sigma_{\mathrm{Rel}}, \mathrm{ar}(R) = \ell \text{ and } \alpha_1, \dots, \alpha_\ell \in \mathrm{Alters}_n^k(\sigma)\}.\end{aligned}$$

Since the following content will heavily depend on this construction, let us consider an example. We define the signature $\sigma = \{R, f, g\}$ where R is a unary relation symbol and f and g are unary function symbols. Now consider a σ structure $\mathfrak{A} = (A, \sigma)$ with $A = \{a, b\}$, $R^{\mathfrak{A}} = \{a\}$, $f^{\mathfrak{A}} = \{a \mapsto b, b \mapsto a\}$ and $g^{\mathfrak{A}} = \{a \mapsto a, b \mapsto b\}$. A graphical representation of $\mathfrak{A}$ can be found in Figure 4a. For the sake of simplicity, we will define the transitive expansion with alternation depth 1 and because $|\mathfrak{A}| = 2$ we will use $\mathrm{Alters}_2^1(\sigma)$ to do so. We see that $\mathrm{Alters}_2^1(\sigma) = \{\mathrm{id}, f, f^2, g, g^2\}$ and as such

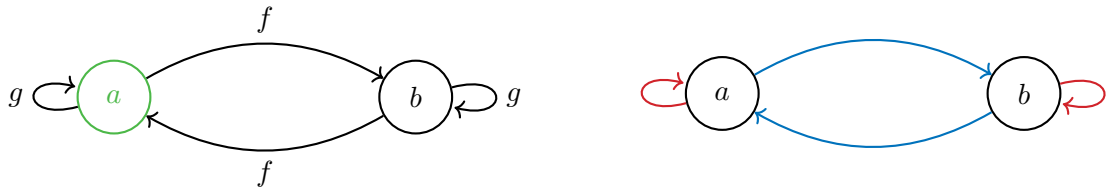
$$\widetilde{\sigma} = \{R_{\mathrm{id}}, R_f, R_{f^2}, R_g, R_{g^2}, \mathrm{Eq}_{\mathrm{id},\mathrm{id}}, \mathrm{Eq}_{\mathrm{id},f}, \mathrm{Eq}_{\mathrm{id},f^2}, \dots, \mathrm{Eq}_{g^2,g^2}\}.$$

Because of the relatively large size of $\widetilde{\sigma}$, we will only give the formal definitions for a few relations, while the rest of the relations in $\widetilde{\mathfrak{A}}$ can be seen in Figure 4b. We find that $R_{\mathrm{id}}^{\widetilde{\mathfrak{A}}} = R_{f^2}^{\widetilde{\mathfrak{A}}} = R_g^{\widetilde{\mathfrak{A}}} = R_{g^2}^{\widetilde{\mathfrak{A}}} = \{a\}$ and that $R_f^{\widetilde{\mathfrak{A}}} = \{b\}$. Additionally, $\mathrm{Eq}_{g,\mathrm{id}}^{\widetilde{\mathfrak{A}}} = \mathrm{Eq}_{g^2,\mathrm{id}}^{\widetilde{\mathfrak{A}}} = \{(a,a),(b,b)\} = \mathrm{Eq}_{\alpha,\alpha}^{\widetilde{\mathfrak{A}}}$ for all $\alpha \in \mathrm{Alters}_2^1(\sigma)$. To give another example, we have $\mathrm{Eq}_{g,f}^{\widetilde{\mathfrak{A}}} = \mathrm{Eq}_{g^2,f}^{\widetilde{\mathfrak{A}}} = \{(a,b),(b,a)\}$. The definitions of all $\mathrm{Eq}_{\alpha,\beta}^{\widetilde{\mathfrak{A}}}$ can be found in Figure 4b.

We can now define RCR for signatures that include unary function symbols.

Definition 4.2 (RCR for structures with unary functions)**.** Let σ be a signature and let $\mathfrak{A}$ and $\mathfrak{B}$ be σ-structures. We say that $\mathfrak{A}$ and $\mathfrak{B}$ are being distinguished by RCR with alternation depth k (RCR_k), if $|\mathfrak{A}| \neq |\mathfrak{B}|$ or the transitive expansions with alternation depth k, $\widetilde{\mathfrak{A}}$ and $\widetilde{\mathfrak{B}}$, are being distinguished by RCR.

Just like nRCR, this algorithm allows for a logical characterisation, which will be investigated later.



(a) The structure $\mathfrak{A}$. Green states represent $R^{\mathfrak{A}}$.

(b) The structure $\widetilde{\mathfrak{A}}$.

Figure 4: Graphical descriptions of $\mathfrak{A}$ and $\widetilde{\mathfrak{A}}$. The blue transitions represent the relations $\mathrm{Eq}_{\alpha,\beta}$ with $(\alpha,\beta) \in \{(\mathrm{id}, f), (f, \mathrm{id}), (f, f^2), (f, g), (f, g^2), (f^2, f), (g, f), (g^2, f)\}$, while the red transitions represent all other binary relations.

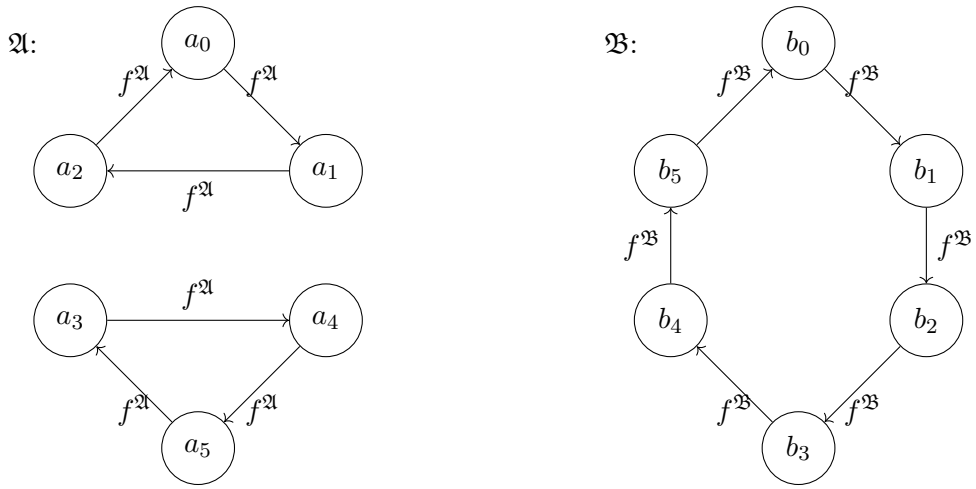


Figure 5: Two $\{f/1\}$-structures $\mathfrak{A}$ and $\mathfrak{B}$ which are not distinguished by naive RCR, but by RCR_k.

4.3 Naive RCR versus RCR_k

We first want to discuss both of the given definitions and will see that RCR_k is the stronger algorithm. Consider the two structures $\mathfrak{A}$ and $\mathfrak{B}$ of signature $\sigma = \{f/1\}$ which can be seen in Figure 5. Formally they are defined as $\mathfrak{A} = (A, f^{\mathfrak{A}})$ and $\mathfrak{B} = (B, f^{\mathfrak{B}})$ where

$$\begin{aligned} A =& \{a_0, a_1, a_2, a_3, a_4, a_5\}, & B =& \{b_0, b_1, b_2, b_3, b_4, b_5\}, \\ f^{\mathfrak{A}} =& \{a_0 \mapsto a_1, a_1 \mapsto a_2, a_2 \mapsto a_0, \quad \text{and} & f^{\mathfrak{B}} =& \{b_0 \mapsto b_1, b_1 \mapsto b_2, b_2 \mapsto b_3, \\ & a_3 \mapsto a_4, a_4 \mapsto a_5, a_5 \mapsto a_3\} & & b_3 \mapsto b_4, b_4 \mapsto b_5, b_5 \mapsto b_0\}. \end{aligned}$$

When applying nRCR to these structures, we find that they cannot be distinguished. This can also be seen when considering the encodings $\mathfrak{A}'$ and $\mathfrak{B}'$, which represent directed, regular graphs, which also cannot be distinguished by classical Colour Refinement.

We now want to see, whether RCR_1 distinguishes the structures $\mathfrak{A}$ and $\mathfrak{B}$. First we compute $\widetilde{\sigma}$ as $\{\mathrm{Eq}_{f^i,f^j}, \mathrm{Eq}_{f^i,\mathrm{id}}, \mathrm{Eq}_{\mathrm{id},f^j} : 0 < i, j \leq 6\} \cup \{\mathrm{Eq}_{\mathrm{id},\mathrm{id}}\}$. For easier readability, we will only give the definitions for the symbols in $\{\mathrm{Eq}_{f^i,\mathrm{id}} : 0 < i \leq n\}$. We find that

$$\mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^i,\mathrm{id}} = \{(a_j, a_{(j+i) \bmod 3}), (a_{j+3}, a_{((j+i) \bmod 3)+3}) : j \in \{0,1,2\}\}$$

and

$$\mathrm{Eq}^{\widetilde{\mathfrak{B}}}_{f^i,\mathrm{id}} = \{(a_j, a_{j+i \bmod 6}) : j \in \{0,\ldots,5\}\}.$$

By using [19], we know that RCR distinguishes $\widetilde{\mathfrak{A}}$ and $\widetilde{\mathfrak{B}}$ if, and only if, there is a formula $\widetilde{\varphi} \in \mathsf{GF}(\mathsf{C})$ of signature $\widetilde{\sigma}$ that distinguishes them. Notice that $\mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^1,\mathrm{id}} = \mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^4,\mathrm{id}}$, $\mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^2,\mathrm{id}} = \mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^5,\mathrm{id}}$ and $\mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^3,\mathrm{id}} = \mathrm{Eq}^{\widetilde{\mathfrak{A}}}_{f^6,\mathrm{id}}$, while only $\mathrm{Eq}^{\widetilde{\mathfrak{B}}}_{f^0,\mathrm{id}} = \mathrm{Eq}^{\widetilde{\mathfrak{B}}}_{f^6,\mathrm{id}}$. Therefore the sentence

$$\exists^{\geq 6}(x,y)\,.\,\Big(\mathrm{Eq}_{f^1,\mathrm{id}}(x,y) \wedge \mathrm{Eq}_{f^4,\mathrm{id}}(x,y)\Big) \in \mathsf{GF}(\mathsf{C})$$

is satisfied by $\widetilde{\mathfrak{A}}$, but not $\widetilde{\mathfrak{B}}$. We can easily derive another formula $\varphi' \in \mathsf{GF}(\mathsf{C})$ to distinguish the transitive expansions, for example $\exists^{\geq 1} x\,.\,\mathrm{Eq}_{f^3,\mathrm{id}}(x,x)$, which expresses the existence of a 3-cycle. We see that RCR_k distinguishes structures that cannot be distinguished by nRCR.

4.4 Characterisation through Logic

In this section we will discuss, how the above approaches of Colour Refinement for non-relational signatures can be characterised by logic. We will see that for both cases we obtain a logic which extends the given definition of $\mathsf{GF}(\mathsf{C})$, see Definition 3.2, but restricts the usage of functions inside of terms.

4.4.1 Characterising Naive RCR Using Logic

The nRCR algorithm will be characterised by the nesting free guarded fragment of counting logic $\mathsf{nfGF}(\mathsf{C})$. This logic forbids the nesting of functions and only allows the usage of them as $f(\mathbf{x}) = y$. This way, a function symbol acts like a relation symbol, which is analogous to the encoding used for nRCR. This leads to the characterisation of nRCR by $\mathsf{nfGF}(\mathsf{C})$, which we will be proved in the following theorem.

Definition 4.3 ($\mathsf{nfGF}(\mathsf{C})$)**.** Consider the definition of $\mathsf{GF}(\mathsf{C})$ given in Definition 3.2. We obtain the nesting-free fragment, by allowing $f(\mathbf{x}) = y$ as a further atomic formula. Concretely, for relation symbols R of arity k and function symbols f of arity ℓ, we only allow atomic formulae of the form $R(x_1,\ldots,x_k)$, $x = y$ and $f(x_1,\ldots,x_\ell) = y$. The remaining definitions stay the same.

We now show that nRCR and $\mathsf{nfGF}(\mathsf{C})$ can distinguish exactly the same structures.

Theorem 4.4. *Let $\mathfrak{A}$ and $\mathfrak{B}$ be two structures of the same signature σ. Then the two following statements are equivalent:*

1. *nRCR distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*
2. *There exists a sentence $\varphi \in \mathsf{nfGF}(\mathsf{C})$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.*

Proof. 1. $\Rightarrow$ 2.: By definition, $\mathfrak{A}$ and $\mathfrak{B}$ are distinguished by nRCR if, and only if, $\mathfrak{A}'$ and $\mathfrak{B}'$ are distinguished by RCR. Using the result of [19], we obtain a sentence $\varphi' \in \mathsf{GF}(\mathsf{C})$ of signature σ' that distinguishes the encoded structures. This formula can then be translated to a formula $\varphi \in \mathsf{nfGF}(\mathsf{C})$ of signature σ, by translating formulae $R_f(x_1,\ldots,x_\ell,y)$ to $f(x_1,\ldots,x_\ell) = y$. From the definitions it can easily be seen that this formula distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.

2. $\Rightarrow$ 1.: When considering the definition of $\mathsf{nfGF}(\mathsf{C})$, one can find that the transformation done at the end of the forward direction can be applied in reverse. This then leads to a distinguishing sentence in $\mathsf{GF}(\mathsf{C})$ and with [19] to a distinguishing colouring of the encoded structures, which by definition leads to $\mathfrak{A}$ and $\mathfrak{B}$ being distinguished by nRCR. □

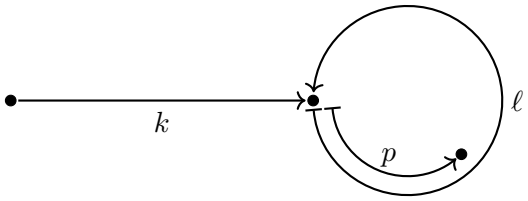


Figure 6: A description of how a path can be decomposed into a cycle, the path to it and a last part of it.

While the above theorem results in a nice characterisation of the naive encoding, the nesting of terms is often very desired when using functions. However, it can be shown that nesting is too powerful for the naive encoding.

For example, consider the structures $\mathfrak{A}$ and $\mathfrak{B}$ from Figure 5 and the formula $\varphi = \exists^{\geq 1} x\,.(f(f(f(x))) = x)$ which utilises term nesting to find a cycle of length three. It is obvious that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$. However, as it was discussed above, one finds that nRCR cannot distinguish the structures. Therefore, term nesting is too powerful for the naive encoding.

4.4.2 Logical Characterisation of RCR_k

A first idea that may come to mind when looking at the definition of the transitive expansion, is to use the classical notion of atomic formulas for guards, fixate a maximal alternation depth for terms and only allow $|\mathfrak{A}|$ applications of the same function symbol in series. Formally, for a function symbol f, a term $s(x)$ and two natural numbers k and m, allow only terms of the form $f^m(s(x))$ where $m \leq |\mathfrak{A}|$ and with only up to k alternations of function applications. However, we prove that we can allow a term $f^m(s(x))$ for an arbitrary $m \in \mathbb{N}$, while the bounded alternation depth is still needed. The reason why this is possible, hinges on the pigeonhole principle. When considering $x, f(x), f^2(x), f^3(x)$ and so forth, until $f^m(x)$, where $m > |\mathfrak{A}|$, there have to be two numbers $i, j \leq |\mathfrak{A}|$, such that $f^i(x) = f^j(x)$. Therefore, we can decompose the path formed by $f^0(x), f^1(x), \ldots, f^m(x)$ into a path to a cycle, the cycle itself, and a last part of that cycle. For the sake of readability, we first want to define the set of all such valid decompositions. Let

$$\begin{aligned}\mathcal{I}(n,m) = \{(k,\ell,p) \in [n]^3 \;:\; & k + p < k + \ell \leq n \wedge \\ & k + r \cdot \ell + p = m \text{ for some } r \in \mathbb{N}\}.\end{aligned}$$

This set will represents all the possible ways, to decompose a path of length m in a structure with n elements into a cycle and the path to and from it. This means, that the triple (k, ℓ, p) will represent a path, that has a beginning part of length k, then a cycle of length ℓ and a last part that consists of the first p elements of that cycle. One can see that in a structure $\mathfrak{A}$ with a unary function f and n elements, any path along of f with length $m > n$ can be decomposed into a triple in the set $\mathcal{I}(n, m)$. A graphical description of such a triple (k, ℓ, p) can be found in Figure 6.

In the beginning we remarked that we have to fixate an alternation depth. This bound can be seen in the definition of the transitive expansion and will be used in the logic that will characterise the Colour Refinement algorithm. Therefore we can only reason about a fragment of $\mathsf{GF}(\mathsf{C})$, where the terms do not alternate too often. This is formally stated in the following definition.

Definition 4.5 (Alternation bounded $\mathsf{GF}(\mathsf{C})$)**.** For a $k \in \mathbb{N}$, we define the fragment of $\mathsf{GF}(\mathsf{C})$ with a bounded alternation depth of k ($\mathsf{GF}(\mathsf{C})_k$) as $\mathsf{GF}(\mathsf{C})$ with the constraint that for all formulae $\varphi \in \mathsf{GF}(\mathsf{C})_k$ of signature σ and every term t that appears in φ, there is an $n \in \mathbb{N}$

and an $\alpha \in \mathrm{Alters}_n^k(\sigma)$ such that $\alpha = t$. Atomic formulae are defined as usual, that is, the formulae $R(t_1(x_1), t_2(x_2), \ldots, t_n(x_n))$ and $t_1(x_1) = t_2(x_2)$ for terms $t_1, t_2, \ldots, t_n$ and variables $x_1, x_2, \ldots, x_n$ are atomic formulae.

With this, we can prove the first result, which allows us to use $f^m(x) = y$ for every $m \in \mathbb{N}$ in a formula.

Lemma 4.6. *Let $\psi(x_1, x_2) \in \mathsf{GF}(\mathsf{C})_1$ be of the form $f^m(x_1) = x_2$. Then there exists a formula $\vartheta(x_1, x_2) \in \mathsf{GF}(\mathsf{C})_1$ such that for any $\mathfrak{A}$ with $|\mathfrak{A}| = n$ it holds*

$$\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2) \text{ if, and only if, } \mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$$

and for any $f^{m'}(x)$ that appears in ϑ we have $m' \leq n$. Furthermore, $\vartheta(x_1, x_2)$ is of the form $\bigvee \Phi(x_1, x_2)$, and if $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$, then there is exactly one $\varphi(x_1, x_2) \in \Phi$, such that $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \varphi(x_1, x_2)$.

Proof. If $m \leq n$, we let $\vartheta \coloneqq \psi$ and the claim follows.

Otherwise, we define

$$\vartheta(x_1, x_2) \coloneqq \bigvee_{(k,\ell,p) \in \mathcal{I}(n,m)} \zeta_{(k,\ell,p)}(x_1, x_2)$$

where

$$\begin{aligned} \zeta_{(k,\ell,p)}(x_1, x_2) \coloneqq & f^{k+p}(x_1) = x_2 \wedge f^k(x_1) = f^{k+\ell}(x_1) \\ & \wedge \mathrm{E}_f^{k,\ell}(x_1) \\ & \wedge \bigwedge_{0 < \ell' < \ell} f^k(x_1) \neq f^{k+\ell'}(x_1) \end{aligned}$$

and for some term $t(x_1)$ we define

$$\mathrm{E}_f^{k,\ell}(t(x_1)) \coloneqq \begin{cases} \top & \text{if } k = 0 \\ f^{k-1}(t(x_1)) \neq f^{k-1+\ell}(t(x_1)) & \text{otherwise.} \end{cases}$$

Due to the definition of $\mathcal{I}(n, m)$, it is obvious that only terms of the form $f^{m'}(x_1)$ with $m' \leq n$ appear. We now proceed with the proof of the equivalence. For the purpose of readability, we will write $f_{\mathfrak{A}}$ instead of $f^{\mathfrak{A}}$.

We will show that if $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$, then $\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2)$. Let $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$. By definition of ϑ, there are $(k, \ell, p) \in \mathcal{I}(n, m)$ with $\mathfrak{A}, a_1, a_2 \models \zeta_{(k,\ell,p)}(x_1, x_2)$. In particular $f_{\mathfrak{A}}^k(a_1) = f_{\mathfrak{A}}^{k+\ell}(a_1)$. It follows that

$$f_{\mathfrak{A}}^k(a_1) = f_{\mathfrak{A}}^{k+\ell}(a_1) = f_{\mathfrak{A}}^{k+2\ell}(a_1) = f_{\mathfrak{A}}^{k+3\ell}(a_1) = \cdots = f_{\mathfrak{A}}^{k+r\cdot\ell}(a_1)$$

for all $r \in \mathbb{N}$. By using the definition of $\mathcal{I}(n, m)$, we get

$$a_2 = f_{\mathfrak{A}}^{k+p}(a_1) = f_{\mathfrak{A}}^{k+r\cdot\ell+p}(a_1) = f_{\mathfrak{A}}^m(a_1)$$

for some $r \in \mathbb{N}$. From this we can deduce that $\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2)$, where $\psi(x_1, x_2)$ has the form $f^m(x_1) = x_2$.

Now we prove that if $\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2)$, then $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$. Let $\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2)$. By assumption $m > n$ and by the pigeonhole principle there have to be distinct i and j such that $f_{\mathfrak{A}}^i(a_1) = f_{\mathfrak{A}}^j(a_1)$. Choose such i, j such that they are lexicographically minimal. Now choose $k \coloneqq i$, $\ell \coloneqq j - i$ and $p \coloneqq (m - i) \bmod (j - i) = (m - i) \bmod \ell$. Obviously $(k, \ell, p) \in \mathcal{I}(n, m)$ and what remains to be shown is that $\mathfrak{A}, a_1, a_2 \models \zeta_{(k,\ell,p)}(x_1, x_2)$. For that, we consider the parts of the conjunction and show for each one that it is satisfied.

- $f^{k+p}(x_1) = x_2$: We use the fact that $a = b \bmod c \Leftrightarrow b = r \cdot c + a$ for some $r \in \mathbb{N}$. Then

$$f_{\mathfrak{A}}^{k+p}(a_1) = f_{\mathfrak{A}}^{i+(m-i)-r\cdot\ell}(a_1) = f_{\mathfrak{A}}^{i+r\cdot\ell+m-i-r\cdot\ell}(a_1) = f_{\mathfrak{A}}^{m}(a_1) = a_2.$$

  Therefore $\mathfrak{A}, a_1, a_2 \models f^{k+p}(x_1) = x_2$.

- $f^{k}(x_1) = f^{k+\ell}(x_1)$: Consider that

$$f_{\mathfrak{A}}^{k}(a_1) = f_{\mathfrak{A}}^{i}(a_1) = f_{\mathfrak{A}}^{j}(a_1) = f_{\mathfrak{A}}^{j+i-i}(a_1) = f_{\mathfrak{A}}^{i+j-i}(a_1) = f_{\mathfrak{A}}^{k+\ell}(a_1).$$

  This leads to $\mathfrak{A}, a_1, a_2 \models f^{k}(x_1) = f^{k+\ell}(x_1)$.

- $\mathrm{E}_f^{k,\ell}(x_1)$: Otherwise $f_{\mathfrak{A}}^{k-1}(a_1) = f_{\mathfrak{A}}^{k-1+\ell}(a)$, but then $(k-1, \ell)$ would be lexicographically smaller than (i, j). Thus $\mathfrak{A}, a_1, a_2 \models \mathrm{E}_f^{k,\ell}(x_1)$.

- The same reasoning applies to $\bigwedge_{0<\ell'<\ell} f^{k}(x_1) \neq f^{k+\ell'}(x_1)$. If it weren't satisfied, there would be a (i, j') with $j' < j$ and $f_{\mathfrak{A}}^{i}(a_1) = f_{\mathfrak{A}}^{j'}(a_1)$ which would be lexicographically smaller than (i, j). It follows that $\mathfrak{A}, a_1, a_2 \models \bigwedge_{0<\ell'<\ell} f^{k}(x_1) \neq f^{k+\ell'}(x_1)$.

Thus we have shown that every subformula of the conjunction, and therefore the formula, is being fulfilled.

Lastly, it remains to prove that if ϑ is satisfied, then there is exactly one $(k, \ell, p) \in \mathcal{I}(n, m)$ such that $\exists^{\geq 1} x_2 \,.\, \zeta_{(k,\ell,p)}(x_1, x_2)$ is fulfilled. We prove this by contradiction. Assume that $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$ and that there are $\zeta_{(k,\ell,p)}(x_1, x_2)$ and $\zeta_{(k',\ell',p')}(x_1, x_2)$ with $(k, \ell, p) \neq (k', \ell', p')$, such that $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \zeta_{(k,\ell,p)}(x_1, x_2)$ and $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \zeta_{(k',\ell',p')}(x_1, x_2)$.

We proceed with a case distinction. Let $k = k'$ and $\ell = \ell'$. Then there are $r, r' \in \mathbb{N}$ such that

$$k + r \cdot \ell + p = k' + r' \cdot \ell' + p' = m.$$

Thus we can infer that $r \cdot \ell + p = r' \cdot \ell' + p'$. By definition of $\mathcal{I}(n, m)$ we know that $p, p' < \ell = \ell'$ and as such

$$r \cdot \ell + p, r' \cdot \ell' + p' \in \{r \cdot \ell, r \cdot \ell + 1, \ldots, r \cdot \ell + (\ell - 1)\}$$

and because p is a non-negative integer, $r = r'$ has to follow and further we get $p = p'$. However this would contradict that $(k, \ell, p) \neq (k', \ell', p')$. Now assume that $k = k'$, $\ell \neq \ell'$ and without loss of generality assume that $\ell < \ell'$. But then $\mathfrak{A}, a_1 \not\models \bigwedge_{0<\hat{\ell}<\ell'} f^{k'}(x_1) \neq f^{k'+\hat{\ell}}(x_1)$, because

$$f_{\mathfrak{A}}^{k'+\ell}(a_1) = f_{\mathfrak{A}}^{k+\ell} = f_{\mathfrak{A}}^{k}(a_1) = f_{\mathfrak{A}}^{k'}(a_1)$$

and $k' + \ell < k' + \ell'$. Thus this cannot be the case as well.

Consider that $k \neq k'$ and without loss of generality assume that $k < k'$. If $\ell = \ell'$, then by the principle of induction, we get that $f_{\mathfrak{A}}^{k}(a_1) = f_{\mathfrak{A}}^{k+\ell}(a_1)$, $f_{\mathfrak{A}}^{k+1}(a_1) = f_{\mathfrak{A}}^{k+1+\ell}(a_1)$ and then $f_{\mathfrak{A}}^{k'}(a_1) = f_{\mathfrak{A}}^{k'+\ell'}(a_1)$. But this contradicts $\mathfrak{A}, a_1 \models \mathrm{E}_f^{k',\ell'}(x_1)$. If $\ell < \ell'$, then

$$f_{\mathfrak{A}}^{k'}(a_1) = f_{\mathfrak{A}}^{k'+(k-k)}(a_1) = f_{\mathfrak{A}}^{k+(k'-k)}(a_1) = f_{\mathfrak{A}}^{k+(k'-k)+\ell}(a_1) = f_{\mathfrak{A}}^{k'+\ell}(a_1),$$

but this again contradicts $\mathfrak{A}, a_1 \models \bigwedge_{0<\hat{\ell}<\ell'} f^{k'}(x_1) \neq f^{k'+\hat{\ell}}(x_1)$. Now assume $\ell' < \ell$. There exists a $t \in \mathbb{N}$, such that

$$k + t \cdot \ell < k' \leq k + (t + 1) \cdot \ell.$$

We now define $r \coloneqq k + (t+1) \cdot \ell - k'$ and get $f_{\mathfrak{A}}^{k'+r}(a_1) = f_{\mathfrak{A}}^{k'+r+\ell'}(a_1)$ and by using $f_{\mathfrak{A}}^{k'+r}(a_1) = f_{\mathfrak{A}}^{k+(t+1)\cdot\ell}(a_1) = f_{\mathfrak{A}}^{k}(a_1)$ it follows that $f_{\mathfrak{A}}^{k}(a_1) = f_{\mathfrak{A}}^{k+\ell'}(a_1)$. This contradicts $\mathfrak{A}, a_1 \models \bigwedge_{0<\hat{\ell}<\ell} f^k(x_1) \neq f^{k+\hat{\ell}}(x_1)$.

One can see that we did not use a_2 in our argumentation. Therefore its value is irrelevant, as long as $\mathfrak{A}, a_1, a_2 \models \vartheta(x_1, x_2)$, which is why we can existentially quantify it in the claim. As all possible cases lead to a contradiction, the first assumption cannot be true and we proved the claim. □

The above proof allows for the translation of a formula $f^m(x) = y$ to a formula $\vartheta(x, y)$ that is equivalent for structures with n elements. A natural extension would be, to allow alternations of functions, for example formulae like $g^m(f^{m'}(x)) = y$. This is also possible and will be proved in the following.

Lemma 4.7. *Let $d \in \mathbb{N}$ and let $\psi(x_1, x_2) \in \mathsf{GF}(\mathsf{C})_d$ be of the form $t(x_1) = x_2$ for a term t. Then there exists a formula $\vartheta_t(x_1, x_2) \in \mathsf{GF}(\mathsf{C})_d$, such that for any structure $\mathfrak{A}$ with $|\mathfrak{A}| = n$ it holds*

$$\mathfrak{A}, a_1, a_2 \models \psi(x_1, x_2) \text{ if, and only if, } \mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2).$$

Furthermore, $\vartheta_t(x_1, x_2)$ is of the form $\bigvee \Phi(x_1, x_2)$ where all $\varphi(x_1, x_2) \in \Phi(x_1, x_2)$ are of the form

$$t'(x_1) = x_2 \wedge \bigwedge \Psi(x_1)$$

for some term $t'(x_1)$, and for every function symbol f there does not appear a term of the form $f^m(s(x))$ where $m > n$. Additionally, if $\mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2)$, then there is exactly one $\varphi \in \Phi$, such that $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \varphi(x_1, x_2)$.

Proof. We prove this via an induction on the term $t(x_1)$.

Base case: If $t(x_1)$ is of the form $f^m(x_1)$ for a unary function symbol f and $m \in \mathbb{N}$, we use the formula constructed in the proof of Lemma 4.6. It can easily be verified that it is in the correct form and from the same proof we get that if the translated formula is fulfilled, exactly one subformula of the disjunction is satisfied.

Inductive step: Assume that $t(x_1)$ is of the form $g^m(s(x_1))$ for a unary function symbol g, a $m \in \mathbb{N}$ and a term $s = f(s'(x))$ where $f \neq g$. By the induction hypothesis, there is a formula $\vartheta_s(x_1, x_2) \in \mathsf{GF}(\mathsf{C})_{d-1}$ of the form $\bigvee \Phi_s(x_1, x_2)$ defined above with $\mathfrak{A}, a_1, a_2 \models s(x_1) = x_2$ if, and only if, $\mathfrak{A}, a_1, a_2 \models \vartheta_s(x_1, x_2)$.

If $m \leq n$, we set $\vartheta_t(x_1, x_2)$ to

$$\bigvee \Phi'(x_1, x_2),$$

where $\Phi'(x_1, x_2) \coloneqq \{g^m(t'(x_1)) = x_2 \wedge \bigwedge \Psi(x_1) : t'(x_1) = x_2 \wedge \bigwedge \Psi(x_1) \in \Phi_s(x_1, x_2)\}$.

If $m > n$, then we set $\vartheta_t(x_1, x_2)$ to

$$\bigvee_{(k,\ell,p) \in \mathcal{I}(n,m)} \bigvee \Phi'_{(k,\ell,p)}(x_1, x_2),$$

where

$$\begin{aligned} \Phi'_{(k,\ell,p)} \coloneqq \{ & g^{k+p}(t'(x_1)) = x_2 \wedge g^k(t'(x_1)) = g^{k+\ell}(t'(x_1)) \\ & \wedge \mathrm{E}_g^{k,\ell}(t'(x_1)) \wedge \bigwedge_{0<\ell'<\ell} g^k(t'(x_1)) \neq g^{k+\ell'}(t'(x_1)) \\ & \wedge \bigwedge \Psi(x_1) : t'(x_1) = x_2 \wedge \bigwedge \Psi(x_1) \in \Phi_s(x_1, x_2)\}. \end{aligned}$$

By using the above definitions, we get $\mathfrak{A}, a_1, a_2 \models s(x_1) = x_2$ if, and only if, $\mathfrak{A}, a_1, a_2 \models \varphi_s(x_1, x_2)$ for some $\varphi_s \in \Phi_s$ where $\varphi_s(x_1, x_2)$ is of the form $t'(x_1) = x_2 \wedge \bigwedge \Psi(x_1)$. Therefore

$$\mathfrak{A}, a_1, a_2 \models s(x_1) = x_2 \text{ if, and only if, } \mathfrak{A}, a_1, a_2 \models t'(x_1) = x_2 \wedge \bigwedge \Psi(x_1). \qquad (\star)$$

We now prove that

$$\mathfrak{A}, a_1, a_2 \models t(x_1) = x_2 \text{ if, and only if, } \mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2).$$

Assume $m \leq n$. Let $\mathfrak{A}, a_1, a_2 \models \vartheta_t$. Then there is some $\varphi(x_1, x_2)$ of the form $g^m(t'(x_1)) = x_2 \wedge \bigwedge \Psi(x_1)$ such that $\mathfrak{A}, a_1, a_2 \models \varphi(x_1, x_2)$. We then get

$$\begin{aligned}
&\mathfrak{A}, a_1, a_2 \models g^m(t'(x_1)) = x_2 \wedge \bigwedge \Psi(x_1) \\
\Leftrightarrow\ &\mathfrak{A}, a_1, a_2, a_3 \models g^m(x_3) = x_2 \wedge t'(x_1) = x_3 \wedge \bigwedge \Psi(x_1) \text{ for some } a_3 \in A \\
\overset{(\star)}{\Leftrightarrow}\ &\mathfrak{A}, a_1, a_2, a_3 \models g^m(x_3) = x_2 \wedge s(x_1) = x_3 \text{ for some } a_3 \in A \\
\Leftrightarrow\ &\mathfrak{A}, a_1, a_2 \models g^m(s(x_1)) = x_2.
\end{aligned}$$

Now let $m > n$. Then there is a

$$\begin{aligned}
\varphi(x_1, x_2) \coloneqq g^{k+p}(t'(x_1)) = x_2 \wedge g^k(t'(x_1)) = g^{k+\ell}(t'(x_1)) \\
\wedge \mathrm{E}_g^{k,\ell}(t'(x_1)) \wedge \bigwedge_{0<\ell'<\ell} g^k(t'(x_1)) \neq g^{k+\ell'}(t'(x_1)) \\
\wedge \bigwedge \Psi(x_1)
\end{aligned}$$

for some $(k, \ell, p) \in \mathcal{I}(n, m)$ with $\mathfrak{A}, a_1, a_2 \models \varphi(x_1, x_2)$. And now

$$\begin{aligned}
&\mathfrak{A}, a_1, a_2 \models \varphi(x_1, x_2) \\
\Leftrightarrow\ &A, a_1, a_2, a_3 \models g^{k+p}(x_3) = x_2 \wedge g^k(x_3) = g^{k+\ell}(x_3) \\
&\qquad \wedge \mathrm{E}_g^{k,\ell}(x_3) \wedge \bigwedge_{0<\ell'<\ell} g^k(x_3) \neq g^{k+\ell'}(x_3) \\
&\qquad \wedge t'(x_1) = x_3 \wedge \bigwedge \Psi(x_1) \text{ for some } a_3 \in A \\
\overset{4.6}{\Leftrightarrow}\ &\mathfrak{A}, a_1, a_2, a_3 \models g^m(x_3) = x_2 \wedge t'(x_1) = x_3 \wedge \bigwedge \Psi(x_1) \text{ for some } a_3 \in A \\
\overset{(\star)}{\Leftrightarrow}\ &\mathfrak{A}, a_1, a_2, a_3 \models g^m(x_3) = x_2 \wedge s(x_1) = x_3 \text{ for some } a_3 \in A \\
\Leftrightarrow\ &\mathfrak{A}, a_1, a_2 \models g^m(s(x_1)) = x_2.
\end{aligned}$$

The other direction follows in both cases, as only equivalent steps have been used and it is obvious that the disjunction of a set is being fulfilled, if a formula of the set is satisfied.

Lastly, we show that if $\mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2)$, then there is exactly one $\varphi \in \Phi$, such that $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \varphi(x_1, x_2)$. As in the proof of Lemma 4.6, we are going to use a proof by contradiction. If $m \leq n$, assume that $\mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2)$ and that there are $\varphi_1, \varphi_2 \in \Phi'(x_1, x_2)$ with $\varphi_1 \neq \varphi_2$, $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 . \varphi_1(x_1, x_2)$ and $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 . \varphi_2(x_1, x_2)$. It is easy to see that

$$\mathfrak{A}, a_1, a_2, a_3 \models g^m(t_1'(x_1)) = x_2 \wedge \bigwedge \Psi_1(x_1) \wedge g^m(t_2'(x_1)) = x_3 \wedge \bigwedge \Psi_2(x_1)$$

for some $a_2, a_3 \in A$, which is equivalent to

$$\begin{aligned}
\mathfrak{A}, a_1, a_2, a_3, a_4, a_5 \models \quad & g^m(x_4) = x_2 \wedge t_1'(x_1) = x_4 \wedge \bigwedge \Psi_1(x_1) \\
& \wedge g^m(x_5) = x_3 \wedge t_2'(x_1) = x_4 \wedge \bigwedge \Psi_2(x_1)
\end{aligned}$$

for some $a_4, a_5 \in A$. However, $t'_1(x_1) = x_2 \wedge \bigwedge \Psi_1(x_1), t'_2(x_1) = x_s \wedge \bigwedge \Psi_2(x_1) \in \Phi_s$ and thus there would be two different $\psi_1(x_1, x_2), \psi_2(x_1, x_2) \in \Phi_s$ such that $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \psi_1(x_1, x_2)$ and $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \psi_2(x_1, x_2)$. But this contradicts the induction hypothesis that Φ_s conforms to the properties stated in the lemma.

If $m > n$, we again assume that $\mathfrak{A}, a_1, a_2 \models \vartheta_t(x_1, x_2)$ and that there are $\varphi_1(x_1, x_2) \in \Phi'_{(k,\ell,p)}(x_1, x_2)$ and $\varphi_2(x_1, x_2) \in \Phi'_{(k',\ell',p')}(x_1, x_2)$ with $\varphi_1 \neq \varphi_2$, $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \varphi_1(x_1, x_2)$ and $\mathfrak{A}, a_1 \models \exists^{\geq 1} x_2 \,.\, \varphi_2(x_1, x_2)$. If $(k, \ell, p) = (k', \ell', p')$, then by looking at the structure of the formulae and by substituting terms and variables like in the first case, we again find that

$$\mathfrak{A}, a_1, a_2, a_3 \models t'_1(x_1) = x_2 \wedge \bigwedge \Psi_1(x_1) \wedge t'_2(x_1) = x_3 \wedge \bigwedge \Psi_2(x_1),$$

where $t'_1(x_1) = x_2 \wedge \bigwedge \Psi_1(x_1), t'_2(x_1) = x_2 \wedge \bigwedge \Psi_2(x_1) \in \Phi_s$. By using the same arguments as before, we arrive at a contradiction. If $(k, \ell, p) \neq (k', \ell', p')$ and there are no such formulae from Φ_s, then, using the same arguments as in the analogous proof in Lemma 4.6, we also get that not both φ_1 and φ_2 can be satisfied. As such, the assumption must be false and we have finished the proof. □

Finally, we want to be able to use terms inside relations. This is also possible and will be shown in the following lemma.

Lemma 4.8. *Let $d \in \mathbb{N}$ and $\psi(x_1, \ldots, x_m) = R(t_1(x_1), \ldots, t_m(x_m)) \in \mathsf{GF}(\mathsf{C})_d$ be an atomic formula. Then there exists a formula $\vartheta_\psi \in \mathsf{GF}(\mathsf{C})_d$, such that for any given structure (of fitting signature) $\mathfrak{A}$ with $|\mathfrak{A}| = n$ it holds*

$$\mathfrak{A}, a_1, \ldots, a_m \models \psi(x_1, \ldots, x_m) \text{ if, and only if, } \mathfrak{A}, a_1, \ldots, a_m \models \vartheta_\psi(x_1, \ldots, x_m).$$

Furthermore, $\vartheta_\psi(x_1, \ldots, x_m)$ is of the form $\bigvee \Phi(x_1, \ldots, x_m)$ where all $\varphi \in \Phi$ are of the form

$$R(t'_1(x_1), \ldots, t'_m(x_m)) \wedge \bigwedge \Psi_1(x_1) \wedge \cdots \wedge \bigwedge \Psi_m(x_m),$$

and for every $f^m(s(x))$ that appear in ϑ_ψ, where f is a unary function symbol and s is a term we have $m \leq n$. Additionally, if $\mathfrak{A}, a_1, \ldots, a_m \models \vartheta_\psi(x_1, \ldots, x_m)$, then there exists exactly one $\varphi(x_1, \ldots, x_m) \in \Phi(x_1, \ldots, x_m)$, such that $\mathfrak{A}, a_1, \ldots, a_m \models \varphi(x_1, \ldots, x_m)$.

Proof. Let $\mathfrak{A}, a_1, \ldots, a_m \models \psi(x_1, \ldots, x_m)$. This is equivalent to

$$\mathfrak{A}, a_1, \ldots, a_m, b_1, \ldots, b_m \models R(y_1, \ldots, y_m) \wedge t_1(x_1) = y_1 \wedge \cdots \wedge t_m(x_m) = y_m$$

for some $b_1, \ldots, b_m \in A$. By applying the previous lemma, we get the equivalent statement

$$\begin{aligned} \mathfrak{A}, a_1, \ldots, a_m, b_1, \ldots, b_m \models R(y_1, \ldots, y_m) \wedge & \bigvee_{i_1} \left(t'_{1,i_1}(x_1) = y_1 \wedge \bigwedge \Psi_{1,i_1}(x_1) \right) \\ & \wedge \ldots \\ & \wedge \bigvee_{i_m} \left(t'_{m,i_m}(x_m) = y_m \wedge \bigwedge \Psi_{m,i_m}(x_m) \right). \end{aligned}$$

Through distributive law of propositional logic we get

$$\begin{aligned} \mathfrak{A}, a_1, \ldots, a_m, b_1, \ldots, b_m \models \bigvee_{i_1} \cdots \bigvee_{i_m} (R(y_1, \ldots, y_m) \wedge & \, t'_{1,i_1}(x_1) = y_1 \wedge \bigwedge \Psi_{1,i_1}(x_1) \\ & \wedge \ldots \\ & \wedge t'_{m,i_m}(x_m) = y_m \wedge \bigwedge \Psi_{m,i_m}(x_m)). \end{aligned} \tag{$\triangle$}$$

Finally, we can resubstitute variables and get

$$\begin{aligned}\mathfrak{A}, a_1, \dots, a_m \models \bigvee_{i_1} \cdots \bigvee_{i_m} (R(t'_{1,i_1}(x_1), \dots, t'_{m,i_m}(x_m)) \\ \wedge \bigwedge \Psi_{1,i_1}(x_1) \\ \wedge \dots \\ \wedge \bigwedge \Psi_{m,i_m}(x_m) =: \vartheta_\psi(x_1, \dots, x_m).\end{aligned}$$

One can see that ϑ_ψ is of the correct form. The equality follows from the fact that only equivalences have been used to derive ϑ_ψ from ψ.

Lastly, we prove that if ϑ_ψ is satisfied, there is exactly one formula of the disjunction that is satisfied. For this, consider the equivalent formula from ($\triangle$). Assume that $\mathfrak{A}, a_1, \dots, a_m \models \vartheta_\psi$ and that there are two subformulae φ_1 and φ_2 of the formula in ($\triangle$), where φ_1 is of the form

$$\begin{aligned}R(y_1, \dots, y_m) \wedge t'_{1,i_1}(x_1) = y_1 \wedge \bigwedge \Psi_{1,i_1}(x_1) \\ \wedge \dots \\ \wedge t'_{m,i_m}(x_m) = y_m \wedge \bigwedge \Psi_{m,i_m}(x_m)\end{aligned}$$

and φ_2 is of the form

$$\begin{aligned}R(y_1, \dots, y_m) \wedge s'_{1,i_1}(x_1) = y_1 \wedge \bigwedge \Psi'_{1,i_1}(x_1) \\ \wedge \dots \\ \wedge s'_{m,i_m}(x_m) = y_m \wedge \bigwedge \Psi'_{m,i_m}(x_m),\end{aligned}$$

such that $\varphi_1 \neq \varphi_2$, $\mathfrak{A}, a_1, \dots, a_m, b_1, \dots, b_m \models \varphi_1$ and $\mathfrak{A}, a_1, \dots, a_m, b_1, \dots, b_m \models \varphi_2$. As $\varphi_1 \neq \varphi_2$, there must be a j such that ψ_1 is of the form $t'_{j,i_j}(x_j) = y_j \wedge \bigwedge \Psi_{j,i_j}(x_j)$, ψ_2 is of the form $s'_{j,i_j}(x_j) = y_j \wedge \bigwedge \Psi'_{j,i_j}(x_j)$ and $\psi_1 \neq \psi_2$. From the construction of the formula we know, that there is a term t_j, a formula ϑ_{t_j} of the form $\bigvee \Phi_{t_j}$ and $\psi_1, \psi_2 \in \Phi_{t_j}$. However, $\mathfrak{A}, a_j \models \exists^{\geq 1} y_j \,.\, \psi_1(x_j, y_j)$ and $\mathfrak{A}, a_j \models \exists^{\geq 1} y_j \,.\, \psi_2(x_j, y_j)$ would contradict the claim that has been proved in Lemma 4.7. □

This lemma also allows the usage of term equations, that is of formulae $t(x_1) = s(x_2)$ for terms t and s, as the equation symbol can be understood as a binary relation, written in infix notation. To illustrate how this translation works, let us consider the formula ψ of the form $g^4(f^3(x)) = y$ for a structure with 2 elements as an example. In the construction of the proof, we inductively translate the inner terms and as such get for the formula $f^3(x) = y$, the formula φ of the form

$$\bigvee_{(k,\ell,p) \in \mathcal{I}(2,3)} \left(f^{k+p}(x) = y \wedge f^k(x) = f^{k+\ell}(x) \wedge \mathrm{E}_f^{k,l}(x) \wedge \bigwedge_{\hat{\ell} < \ell} f^k(x) \neq f^{k+\hat{\ell}}(x) \right)$$

and with $\mathcal{I}(2,3) = \{(0,2,1), (1,1,0), (0,1,0)\}$ we get that φ equals

$$\begin{aligned}&\Big(f(x) = y \wedge x = f^2(x) \wedge x \neq f(x)\Big) \\ \vee &\Big(f(x) = y \wedge f(x) = f^2(x) \wedge x \neq f(x)\Big) \\ \vee &\Big(x = y \wedge x = f(x) \wedge \top\Big)\,.\end{aligned}$$

Now we can construct ϑ_ψ from ψ. From the proof, we know that ϑ_ψ is of the form

$$\bigvee_{(k',\ell',p')\in\mathcal{I}(2,4)} \bigvee_{(k,\ell,p)\in\mathcal{I}(2,3)} \Big(g^{k'+p'}(f^{k+p}(x)) = y \wedge g^{k'}(f^{k+p}(x)) = g^{k'+\ell'}(f^{k+p}(x)) \\ \mathrm{E}_f^{k',\ell'}(f^{k+p}(x)) \wedge \bigwedge_{0<\hat{\ell}<\ell'} g^{k'}(f^{k+p}(x)) \neq g^{k'+\hat{\ell}}(f^{k+p}(x)) \\ f^k(x) = f^{k+l}(x) \wedge \mathrm{E}_f^{k,\ell}(x) \wedge \bigwedge_{0<\hat{\ell}<\ell} f^k(x) \neq f^{k+\hat{\ell}}(x)\Big)$$

and with $\mathcal{I}(2,4) = \{(1,1,0),(0,1,0),(0,2,0)\}$ we can analogously find ϑ_ψ.

This now allows us to prove the logical characterisation of our Colour Refinement Algorithm.

Theorem 4.9. *Let $\mathfrak{A}$ and $\mathfrak{B}$ be two structures of the same signature σ and let $k \in \mathbb{N}$. Then the two following statements are equivalent:*

1. RCR_k *distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*
2. *There exists a sentence $\varphi \in \mathsf{GF}(\mathsf{C})_k$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$.*

Proof. We prove that *1.* implies *2.*. Let $\mathfrak{A}$ and $\mathfrak{B}$ be distinguished by RCR_k. If their universes have different cardinalities, assume without loss of generality that

$$|\mathfrak{A}| = n > n' = |\mathfrak{B}|.$$

Then define $\varphi_{\geq n} \coloneqq \exists^{\geq n} x.\top \in \mathsf{GF}(\mathsf{C})_k$, which obviously distinguishes the structures.

Now assume $|\mathfrak{A}| = |\mathfrak{B}| = n$. By definition, RCR distinguishes $\widetilde{\mathfrak{A}}$ and $\widetilde{\mathfrak{B}}$. When using the proof from [19], we obtain a formula $\widetilde{\varphi} \in \mathsf{GF}(\mathsf{C})$ of signature $\widetilde{\sigma}$ that distinguishes the expansions. This formula $\widetilde{\varphi}$ can then be translated to a formula $\varphi \in \mathsf{GF}(\mathsf{C})_k$ of signature σ. Replace every atomic subformula $\mathrm{Eq}_{\alpha,\beta}(x,y)$, where $\alpha,\beta \in \mathrm{Alters}_n^k(\sigma)$, by the formula $\alpha(x) = \beta(y)$. Similarly, replace every atomic subformula $R_{\alpha_1,\ldots,\alpha_\ell}(x_1,\ldots,x_\ell)$ by the formula $R(\alpha_1(x_1),\ldots,\alpha_\ell(x_\ell))$. Obviously, if a structure's expansion satisfied $\widetilde{\varphi}$, it also satisfies φ and vice versa. Therefore, we get a formula $\varphi \in \mathsf{GF}(\mathsf{C})_k$ that distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.

Now we prove that *2.* implies *1.*. If $|\mathfrak{A}| \neq |\mathfrak{B}|$, assume without loss of generality that $|\mathfrak{A}| > |\mathfrak{B}|$. Then $\mathfrak{A}$ and $\mathfrak{B}$ are being distinguished by $\mathsf{GF}(\mathsf{C})_k$, for example by the formula $\varphi_{\geq|\mathfrak{A}|}$ and by definition, they are also distinguished by RCR. Now assume $|\mathfrak{A}| = |\mathfrak{B}| = n$ again. Let $\varphi \in \mathsf{GF}(\mathsf{C})_k$ such that $\mathfrak{A} \models \varphi$ and $\mathfrak{B} \not\models \varphi$. Using Lemma 4.8 we can obtain a formula ϑ_ψ for every atomic subformula ψ of φ which is equivalent to ψ for structures with n elements. With this, we can construct an equivalent formula $\varphi' \in \mathsf{GF}(\mathsf{C})_k$ of signature σ, which then allows us, to easily translate it to $\widetilde{\sigma}$. We will construct this formula φ' inductively and directly prove the equivalence.

Claim 4.10. *The two formulae φ and φ' are equivalent.*

Proof. **Base cases:** If φ is an atomic formula, that is, either a term equivalence or a relation, then set φ' to ϑ_φ. The equivalence follows directly from the above Lemmas 4.7 and 4.8.

Inductive cases: In the cases where φ is of the form $\neg\vartheta$ or $\vartheta_1 \wedge \vartheta_2$ and by induction hypothesis we have translations ϑ', ϑ_1' and ϑ_2', we set φ' to $\neg\vartheta'$ or $\vartheta_1' \wedge \vartheta_2'$, respectively. The claim follows directly using the induction hypothesis.

Let φ be of the form $\exists^{\geq\ell}\mathbf{v}.(\Delta \wedge \vartheta)$. In addition to translating Δ and ϑ to ϑ_Δ and ϑ', respectively, we also will need to transform the formula, so that it still is a valid formula in $\mathsf{GF}(\mathsf{C})_k$. When

looking at the possible translations from the atomic formula $\Delta(x_1, \dots, x_m)$, we see that it must be of the form $\bigvee_{i\in[o]}(\Delta'_i(x_1, \dots, x_m) \wedge \bigwedge \Psi_i(x_1, \dots, x_m))$. When considering the transformed formula

$$\exists^{\geq \ell}\mathbf{v}\,.\left(\bigvee_{i\in[o]}\left(\Delta'_i \wedge \bigwedge \Psi_i\right) \wedge \vartheta'\right),$$

we then will distribute ϑ' over the disjunction and thus define

$$\psi \coloneqq \exists^{\geq \ell}\mathbf{v}\,.\left(\bigvee_{i\in[o]}\left(\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta'\right)\right)$$

In the following we prove the equivalence of φ and ψ. Let $\mathfrak{A} \models \varphi$. This means there are at least ℓ tuples $\mathbf{a} \in A$, such that $(\mathfrak{A}, \mathbf{a}) \models \Delta(\mathbf{v}) \wedge \vartheta(\mathbf{v})$. Using the induction hypothesis we get that this is equivalent to $(\mathfrak{A}, \mathbf{a}) \models \bigvee(\Delta' \wedge \bigwedge \Psi) \wedge \vartheta'$, which, using the distributive law of propositional logic, is equivalent to $(\mathfrak{A}, \mathbf{a}) \models \bigvee(\Delta' \wedge \bigwedge \Psi \wedge \vartheta')$. Therefore the number of tuples that satisfy $\Delta \wedge \vartheta$ must be the same as for $\bigvee(\Delta' \wedge \bigwedge \Psi \wedge \vartheta')$ and $\mathfrak{A} \models \exists^{\geq \ell}\mathbf{v}\,.\bigvee(\Delta' \wedge \bigwedge \Psi \wedge \vartheta')$ follows. The converse can be shown using the same arguments in reverse order.

However, we are not finished, because $\psi \notin \mathsf{GF}(\mathsf{C})_k$. We will solve this, by considering all possible segmentations of the disjunction. Informally, for $o, \ell \in \mathbb{N}$ we define $\mathrm{Parts}(o, \ell)$ as the set of all multisets with exactly ℓ elements of $[o]$, respecting their multiplicity. We then define φ' as

$$\bigvee_{(M,\mathrm{mult}_M)\in\mathrm{Parts}(o,\ell)} \bigwedge_{i\in M} \exists^{\geq \mathrm{mult}_M(i)}\mathbf{v}\,.(\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta')$$

and will prove the equivalence between ψ and φ' in the following.

Let $\mathfrak{A} \models \psi$. Then there are ℓ different tuples $\mathbf{a}$, such that $\mathfrak{A}, \mathbf{a} \models \bigvee_{i\in[o]}(\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta')$. From the above lemmas we know that for every such tuple, there is exactly one i such that $\mathfrak{A}, \mathbf{a} \models \Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta'$. Now construct a multiset (M, mult_M) with exactly these i that are being satisfied and with the multiplicity of the amount of tuples satisfying them. One can see that $(M, \mathrm{mult}_M) \in \mathrm{Parts}(o, \ell)$ and that

$$\mathfrak{A} \models \bigwedge_{i\in M} \exists^{\geq \mathrm{mult}_M(i)}\mathbf{v}\,.(\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta').$$

It directly follows that $\mathfrak{A} \models \varphi'$.

Let $\mathfrak{A} \models \varphi'$. Then there exists a multiset $(M, \mathrm{mult}_M) \in \mathrm{Parts}(o, \ell)$, such that

$$\mathfrak{A} \models \bigwedge_{i\in M} \exists^{\geq \mathrm{mult}_M(i)}\mathbf{v}\,.(\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta').$$

We know that for an $\mathbf{a}$ with $\mathfrak{A}, \mathbf{a} \models (\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta')$ there does not exist a $j \neq i$, such that $\mathfrak{A}, \mathbf{a} \models (\Delta'_j \wedge \bigwedge \Psi_j \wedge \vartheta')$. From this we can reason that there exist at least ℓ different tuples that fulfil some $\Delta'_i \wedge \bigwedge \Psi_i \wedge \vartheta'$. It now follows that $\mathfrak{A} \models \psi$. We therefore have proved the claim. □

Note that for every term α that appears in φ', it holds that $\alpha \in \mathrm{Alters}^k_n(\sigma)$. This follows from the properties of the translation in Lemma 4.8. Furthermore, for every atomic subformula, we have a corresponding relation symbol in $\widetilde{\sigma}$. With this, we can transform φ' to a formula $\widetilde{\varphi} \in \mathsf{GF}(\mathsf{C})$ of signature $\widetilde{\sigma}$, such that $\mathfrak{A} \models \varphi'$ if, and only if, $\widetilde{\mathfrak{A}} \models \widetilde{\varphi}$, respectively with $\mathfrak{B}$ and $\widetilde{\mathfrak{B}}$.

It can be seen that the only subformulae that need to be changed are atomic. Let ψ be an atomic subformula of φ'. If ψ is a term equation, that is, it is of the form $t(x) = s(y)$, we know

through the construction of φ' and the definition of the transitive expansion, that there are $\alpha, \beta \in \text{Alters}_n^k(\sigma)$ with $\alpha = t$ and $\beta = s$. As such, we can replace ψ with $\text{Eq}_{\alpha,\beta}(x, y)$.

If ψ is a relation, that is, it is of the form $R(t_1(x_1), \ldots, t_m(x_m))$, we again have $\alpha_1, \ldots, \alpha_m \in \text{Alters}_n^k(\sigma)$, such that $\alpha_i = t_i$ for all $i \in [m]$. We then can replace ψ with $R_{\alpha_1,\ldots,\alpha_m}(x_1, \ldots, x_m)$. From the semantic definition of the transitive expansion, it can be easily seen that φ' and $\widetilde{\varphi}$ are equivalent for structures with n elements.

With this, we have obtained a formula $\widetilde{\varphi} \in \mathsf{GF}(\mathsf{C})$ of signature $\widetilde{\sigma}$, where $\widetilde{\mathfrak{A}} \models \widetilde{\varphi}$ and $\widetilde{\mathfrak{B}} \not\models \widetilde{\varphi}$. Using [19], we thus know that RCR distinguishes $\widetilde{\mathfrak{A}}$ and $\widetilde{\mathfrak{B}}$ and by definition we can deduce that RCR_k distinguishes $\mathfrak{A}$ and $\mathfrak{B}$. □

We thus can characterise RCR_k with the logic $\mathsf{GF}(\mathsf{C})_k$.

4.5 Characterisation Through Homomorphism Counting

One very interesting property of classical, as well as Relational Colour Refinement is that aside from its logical characterisation, it can be characterised by counting homomorphisms from certain structures. We introduced two possible extensions of Relational Colour Refinement and showed their logical characterisations. We now want to consider, whether those extensions can also be characterised by counting homomorphisms.

In the following we will see that, using the two established approaches, it is in general not possible to find acyclic structures with functions that divide two structures by homomorphism counts. We will concentrate on the encoding defined in Section 4.1, as it is subsumed by the transitive expansion encoding, defined in Section 4.2.

To begin, let us define two concepts for relational structures that encode a non-relational structure.

Definition 4.11 (Total structures)**.** Let $\sigma = \sigma_{\text{Rel}} \dot{\cup} \sigma_{\text{Func}}$ be a signature where σ_{Func} contains exactly all function symbols. Now let σ' be the relational encoding of σ and let $\mathfrak{A}'$ be a σ'-structure. We call $\mathfrak{A}'$ total, if for every $R_f \in \sigma'$ with arity $n+1$, where $f \in \sigma_{\text{Func}}$ has arity n, and every tuple $\mathbf{x}$ of length n, there is a y such that $(\mathbf{x}y) \in R_f^{\mathfrak{A}'}$.

Total structures capture the notion that every relation that encodes a function is defined for the complete domain of the function, or equivalently that functions in structures are total functions and not partial. Another defining aspect of functions of structures is that they valuate to exactly one value. This idea is captured by the following definition.

Definition 4.12 (Functional structures)**.** We define σ, σ' and $\mathfrak{A}'$ exactly as in Definition 4.11. We call $\mathfrak{A}'$ functional, if for every $R_f \in \sigma'$ with arity $n+1$, where $f \in \sigma_{\text{Func}}$ has arity n, if $(\mathbf{x}y) \in R_f^{\mathfrak{A}'}$ there is no $y' \neq y$ such that $(\mathbf{x}y') \in R_f^{\mathfrak{A}'}$.

To continue, we have to define what it means to be acyclic for a structure with functions.

Definition 4.13 (Acyclic, non-relational structures)**.** Let σ be a signature with function symbols and σ' its encoding as it is defined in Section 4.1. Let $\mathfrak{C}$ be a σ-structure and $\mathfrak{C}'$ be its encoding of signature σ'. We then call $\mathfrak{C}$ acyclic, if $\mathfrak{C}'$ is acyclic, with respect to acyclicity as it is defined in Definition 3.4.

We now want to find the equivalence between the existence of an acyclic structure with functions and an encoding of an acyclic structure with the above properties (with respect to homomorphism counting).

Lemma 4.14. *Let σ be a signature with function symbols and σ' be the relational encoding of it. Let $\mathfrak{A}$ and $\mathfrak{B}$ be σ-structures and $\mathfrak{A}'$ and $\mathfrak{B}'$ be their respective encodings of signature σ'. Then the two following statements are equivalent.*

1. *There exists an acyclic structure $\mathfrak{C}$ of signature σ such that* $\hom(\mathfrak{C}, \mathfrak{A}) \neq \hom(\mathfrak{C}, \mathfrak{B})$.
2. *There exists an acyclic, total and functional structure $\mathfrak{C}'$ of signature σ' such that* $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$.

Proof. We begin by proving that *1.* implies *2.*. Let $\mathfrak{C}$ be such a σ-structure. Now let $\mathfrak{C}'$ be its encoding as a σ'-structure. By definition $\mathfrak{C}'$ is acyclic and when considering the definition of the encoding, we find that it also has to be total and functional. We now show that $\mathrm{Hom}(\mathfrak{C}, \mathfrak{A}) = \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$ and $\mathrm{Hom}(\mathfrak{C}, \mathfrak{B}) = \mathrm{Hom}(\mathfrak{C}', \mathfrak{B}')$.

Let $\varphi \in \mathrm{Hom}(\mathfrak{C}, \mathfrak{A})$. We show that $\varphi \in \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$. Let $(\mathbf{x}y) \in R_f^{\mathfrak{C}'}$ for a function symbol $f \in \sigma$. Then by definition of the encoding $f^{\mathfrak{C}}(\mathbf{x}) = y$ and then $f^{\mathfrak{A}}(\varphi(\mathbf{x})) = \varphi(f^{\mathfrak{C}}(\mathbf{x})) = \varphi(y)$. Thus $(\varphi(\mathbf{x})\varphi(y)) \in R_f^{\mathfrak{A}'}$, but this is equivalent to $\varphi(\mathbf{x}y) \in R_f^{\mathfrak{A}'}$. Let $\mathbf{x} \in R^{\mathfrak{C}'}$ where $R \neq R_f$ for all function symbols $f \in \sigma$. Then $R^{\mathfrak{C}'} = R^{\mathfrak{C}}$ and $R^{\mathfrak{A}} = R^{\mathfrak{A}'}$. Therefore, because $\mathbf{x} \in R^{\mathfrak{C}}$, we have $\varphi(\mathbf{x}) \in R^{\mathfrak{A}} = R^{\mathfrak{A}'}$.

Let $\varphi \in \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$. We show that $\varphi \in \mathrm{Hom}(\mathfrak{C}, \mathfrak{A})$. Let $\mathbf{x} \in R^{\mathfrak{C}}$ for a relational symbol R. By the construction of the encoding we know that $R^{\mathfrak{C}} = R^{\mathfrak{C}'}$ and $R^{\mathfrak{A}'} = R^{\mathfrak{A}}$ and with the same argument as before we can conclude that $\varphi(\mathbf{x}) \in R^{\mathfrak{A}}$. Let $\mathbf{x}$ and y be such that $f^{\mathfrak{C}}(\mathbf{x}) = y$. Then by construction we know that $(\mathbf{x}y) \in R_f^{\mathfrak{C}'}$. Because φ is a homomorphism it follows that $\varphi(\mathbf{x}y) \in R_f^{\mathfrak{A}'}$ and because $\mathfrak{A}'$ is also an encoding, we have that $f^{\mathfrak{A}}(\varphi(\mathbf{x})) = \varphi(y) = \varphi(f^{\mathfrak{C}}(\mathbf{x}))$. This was to be shown. $\mathfrak{A}$ and $\mathfrak{A}'$ can be replaced by $\mathfrak{B}$ and $\mathfrak{B}'$, respectively, to get the analogous result for the other structure.

We now show that *2.* implies *1.*. Let $\mathfrak{C}'$ be an acyclic, total and functional σ'-structure. We can now construct a σ-structure $\mathfrak{C}$ by decoding $\mathfrak{C}'$ and will also get that $\mathrm{Hom}(\mathfrak{C}', \mathfrak{A}') = \mathrm{Hom}(\mathfrak{C}, \mathfrak{A})$. For a relation symbol $R \in \sigma$ we can define $R^{\mathfrak{C}} := R^{\mathfrak{C}'}$. For a function symbol $f \in \sigma$ we can define $f^{\mathfrak{C}}$ as follows: Let f be of arity n. Then for all tuples $\mathbf{x}$ of length n, there must be a y such that $(\mathbf{x}y) \in R_f^{\mathfrak{C}'}$ because $\mathfrak{C}'$ is total and there must be exactly one such y because $\mathfrak{C}'$ is functional. Therefore we define $f^{\mathfrak{C}}(\mathbf{x}) = y$. The claim that the sets of homomorphisms are equal can be verified using exactly the same arguments as in the analogous proof of the forward direction. □

We can now continue to put this in relation to the statement regarding RCR. Naive RCR distinguishes two σ-structures $\mathfrak{A}$ and $\mathfrak{B}$ if, and only if, RCR distinguishes the encodings $\mathfrak{A}'$ and $\mathfrak{B}'$ of signature σ'. Due to the results of [19] this is the case if, and only if, there is an acyclic σ'-structure $\mathfrak{C}'$ such that $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$. We would like to achieve the result that this is equivalent to there being an acyclic σ structure that distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ by homomorphism counts (however this will not be the case). By the above lemma, the latter is equivalent to there being an acyclic, total and functional σ'-structure $\mathfrak{C}''$ that distinguishes $\mathfrak{A}'$ and $\mathfrak{B}'$ by homomorphism counts. Our goal will therefore be, to study the relationship between the two following statements.

1. There is an acyclic σ'-structure $\mathfrak{C}'$ such that $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$.
2. There is an acyclic, total and functional σ'-structure $\mathfrak{C}''$ such that $\hom(\mathfrak{C}'', \mathfrak{A}') \neq \hom(\mathfrak{C}'', \mathfrak{B}')$.

It is obvious that *2.* implies *1.*, however the other direction will not hold in general. In fact, we will be able to construct a functional structure from $\mathfrak{C}'$, but totality will not be able to be

constructed. We will in the following prove the former claim and then show the latter claim, using a family of counterexamples.

Lemma 4.15. *Let $\mathfrak{A}$ and $\mathfrak{B}$ be structures of signature σ and let $\mathfrak{A}'$, $\mathfrak{B}'$ and σ' be the respective encodings. If there is an acyclic structure $\mathfrak{C}'$ of signature σ' with $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$, then we can construct a functional, acyclic structure $\mathfrak{C}''$ of signature σ' such that $\hom(\mathfrak{C}'', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{A}')$ and $\hom(\mathfrak{C}'', \mathfrak{B}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$.*

Proof. The proof for the above lemma will work as follows. If $\mathfrak{C}'$ is not functional, then there is a function symbol $f \in \sigma$ and two different tuples with $(\mathbf{x}y), (\mathbf{x}z) \in R_f^{\mathfrak{C}'}$, we call this a collision. We will give a procedure to iteratively remove such collisions. The procedure will reduce the number of elements of $\mathfrak{C}'$ by one, keep the acyclicity property and will result in a structure with the same amount of homomorphisms as $\mathfrak{C}'$ to $\mathfrak{A}'$ and $\mathfrak{B}'$, respectively. Thus, by continuously applying that procedure to all collisions, we will get $\mathfrak{C}''$. The algorithm must terminate, as the number of elements strictly decreases and we only consider finite structures.

The remainder of this proof will be dedicated to describing the procedure and proving the above claims. Assume that there is a function symbol $f \in \sigma$ and two different tuples $(\mathbf{x}y), (\mathbf{x}z) \in R_f^{\mathfrak{C}'}$. Our goal will be to construct a structure $\mathfrak{C}''$ of signature σ' without this particular collision and with the following properties:

a. $|\mathfrak{C}''| = |\mathfrak{C}'| - 1$

b. $\mathfrak{C}''$ is acyclic

c. $\hom(\mathfrak{C}'', \mathfrak{A}') = \hom(\mathfrak{C}', \mathfrak{A}')$ and $\hom(\mathfrak{C}'', \mathfrak{B}') = \hom(\mathfrak{C}', \mathfrak{B}')$.

We define $\mathfrak{C}'' \coloneqq ((C' \setminus \{y, z\}) \cup \{v_{y,z}\}, \sigma)$ and will define the relations using the following function. The function $\chi : \mathbf{C}' \to \mathbf{C}''$ maps tuples of $\mathfrak{C}'$ to tuples of $\mathfrak{C}''$, where y and z are contracted to $v_{y,z}$. Concretely, for an arbitrary tuple $\mathbf{c} \in \mathbf{C}'$ of length k and for every $i \in [k]$, we have

$$\chi(\mathbf{c})_i \coloneqq \begin{cases} \mathbf{c}_i & \text{if } \mathbf{c}_i \notin \{y, z\} \\ v_{y,z} & \text{if } \mathbf{c}_i \in \{y, z\}. \end{cases}$$

Then, for all $R \in \sigma$, we define $R^{\mathfrak{C}''} \coloneqq \{\chi(\mathbf{c}) : \mathbf{c} \in R^{\mathfrak{C}'}\}$. We will now proceed by proving the above properties.

Property a.: This property follows directly from the definition of C''. We have $y \neq z$, $y, z \in C'$ and thus $|C' \setminus \{y, z\}| = |C'| - 2$. Furthermore, we have $v_{y,z} \notin C'$ and therefore $|(C' \setminus \{y, z\}) \cup \{v_{y,z}\}| = |C'| - 1$. This was to be shown.

Property b.: To show that $\mathfrak{C}''$ is acyclic, we first will define an undirected graph J'', will prove that it is connected and cycle free, thus a tree, and that it fulfils the join tree property for $\mathfrak{C}''$. By the assumption we know that $\mathfrak{C}'$ is acyclic and thus has a join tree J'. We further notice that $\mathbf{C}'' = \{\chi(\mathbf{c}) : \mathbf{c} \in \mathbf{C}'\}$. Now we define $V(J'') \coloneqq \mathbf{C}''$ and $E(J'') \coloneqq \{\{\chi(\mathbf{u}), \chi(\mathbf{v})\} : \{\mathbf{u}, \mathbf{v}\} \in E(J')\}$.

Claim 4.16. *J'' is connected.*

Proof. Consider $\mathbf{u}, \mathbf{v} \in V(J'')$. Then there are $\mathbf{a}, \mathbf{b} \in V(J')$, such that $\chi(\mathbf{a}) = \mathbf{u}$ and $\chi(\mathbf{b}) = \mathbf{v}$. By assumption, J' is a tree, so there are $\mathbf{a}_0, \mathbf{a}_1, \ldots, \mathbf{a}_k$ with $\mathbf{a}_0 = \mathbf{a}$, $\mathbf{a}_k = \mathbf{b}$ and $\{\mathbf{a}_{i-1}, \mathbf{a}_i\} \in E(J')$ for all $i \in [k]$. By definition, we have $\chi(\mathbf{a}_0), \chi(\mathbf{a}_1), \ldots, \chi(\mathbf{a}_k) \in V(J'')$ with $\chi(\mathbf{a}_0) = \chi(\mathbf{a}) = \mathbf{u}$, $\chi(\mathbf{a}_k) = \chi(\mathbf{b}) = \mathbf{v}$ and $\{\chi(\mathbf{a}_{i-1}), \chi(\mathbf{a}_i)\} \in E(J'')$ for all $i \in [k]$. Thus $\mathbf{u}$ and $\mathbf{v}$ are connected. □

In the following, for an arbitrary $e \in C'$, we define the set $V_e \coloneqq \{\mathbf{c} \in V(J') : e \in \mathbf{c}\}$. One can see that $V(J'_e) = V_e$, where J'_e is the subgraph of J', induced by all elements containing e.

Claim 4.17. *J'' is cycle-free.*

Proof. Assume that there were $\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k \in V(J'')$ with $\{\mathbf{u}_{i-1}, \mathbf{u}_i\} \in E(J'')$ for all $i \in [k]$ and $\{\mathbf{u}_k, \mathbf{u}_0\} \in E(J'')$. We now define directed edges such that $e_0 = (\mathbf{u}_0, \mathbf{u}_1)$, $e_1 = (\mathbf{u}_1, \mathbf{u}_2)$, $\ldots$, $e_k = (\mathbf{u}_k, \mathbf{u}_0)$, therefore we have $e_i = (\mathbf{u}_i, \mathbf{u}_{i+1 \bmod k})$. For every edge e_i choose two elements $\mathbf{a}_i, \mathbf{b}_i \in V(J')$ such that $\{\mathbf{a}_i, \mathbf{b}_i\} \in E(J')$, $\chi(\mathbf{a}_i) = \mathbf{u}_i$ and $\chi(\mathbf{b}_i) = \mathbf{u}_{i+1 \bmod k}$. These elements must exist by the definition of $E(J'')$.

We now prove that there exists a cycle in J', which would contradict our assumption of J' being a join tree for $\mathfrak{C}'$. To show this, we prove that for all $i \in \{0\} \cup [k]$, the elements $\mathbf{b}_i$ and $\mathbf{a}_{i+1 \bmod k}$ are connected in J'. We see that $\chi(\mathbf{b}_i) = \mathbf{u}_{i+1 \bmod k} = \chi(\mathbf{a}_{i+1 \bmod k})$.

If there is a $c \in \operatorname{set}(\mathbf{u}_{i+1 \bmod k})$ with $c \neq v_{y,z}$, then by definition of χ, we have $c \in \operatorname{set}(\mathbf{b}_i) \cap \operatorname{set}(\mathbf{a}_{i+1 \bmod k})$. Therefore, $\mathbf{b}_i, \mathbf{a}_{i+1 \bmod k} \in V_c$ and because J' is a join tree, $\mathbf{b}_i$ and $\mathbf{a}_{i+1 \bmod k}$ have to be connected.

If $\operatorname{set}(\mathbf{u}_{i+1 \bmod k}) = \{v_{y,z}\}$, we have four possible cases. If $y \in \operatorname{set}(\mathbf{b}_i) \cap \operatorname{set}(\mathbf{a}_{i+1 \bmod k})$ or $z \in \operatorname{set}(\mathbf{b}_i) \cap \operatorname{set}(\mathbf{a}_{i+1 \bmod k})$, then we can do the same as before by setting $c = y$ or $c = z$, respectively. Otherwise we have $y \in \operatorname{set}(\mathbf{b}_i)$ and $z \in \operatorname{set}(\mathbf{a}_{i+1 \bmod k})$, or $z \in \operatorname{set}(\mathbf{b}_i)$ and $y \in \operatorname{set}(\mathbf{a}_{i+1 \bmod k})$. We will only consider the former option, as the latter can be proven analogously. From our beginning assumption we know that $(\mathbf{x}y), (\mathbf{x}z) \in R_f^{\mathfrak{C}'}$. Choose some $x \in \mathbf{x}$, and $(\mathbf{x}y), (\mathbf{x}z) \in V_x$ follows. Furthermore, we have $\mathbf{b}_i, (\mathbf{x}y) \in V_y$ and $\mathbf{a}_{i+1 \bmod k}, (\mathbf{x}z) \in V_z$. Since J' is a join tree, we thus know that $\mathbf{b}_i$ is connected with $(\mathbf{x}y)$, which in turn is connected with $(\mathbf{x}z)$, which is connected with $\mathbf{a}_{i+1 \bmod k}$. Therefore $\mathbf{b}_i$ and $\mathbf{a}_{i+1 \bmod k}$ are connected.

Thus we have found a cycle in J', which is a contradiction to it being a join tree. Therefore our assumption of the existence of the elements $\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k$ has to be false. □

The last missing piece to prove the acyclicity of $\mathfrak{C}''$ is to show that J'' fulfils the join tree property. That is, for any $c \in C''$, the set $\{\mathbf{c} \in V(J'') : c \in \operatorname{set}(\mathbf{c})\}$ induces a connected subgraph of J''.

Claim 4.18. *J'' is a valid join tree.*

Proof. Consider any $c \in C''$ and two elements $\mathbf{u}$ and $\mathbf{v}$ from the set $S \coloneqq \{\mathbf{c} \in V(J'') : c \in \operatorname{set}(\mathbf{c})\}$. We show that there is a path from $\mathbf{u}$ to $\mathbf{v}$ in S. If $c \neq v_{y,z}$, then $c \in C'$, thus consider V_c. By definition there are $\mathbf{a}, \mathbf{b} \in V_c$ such that $\chi(\mathbf{a}) = \mathbf{u}$ and $\chi(\mathbf{b}) = \mathbf{v}$. Because J' is a join tree, V_c must induce a connected subtree. Thus there must be $\mathbf{a}_0, \ldots, \mathbf{a}_k \in V_c$, such that $\mathbf{a}_0 = \mathbf{a}$, $\mathbf{a}_k = \mathbf{b}$ and $\{\mathbf{a}_{i-1}, \mathbf{a}_i\} \in E(J')$ for all $i \in [k]$. By definition, we then get that there must be $\chi(\mathbf{a}_0), \ldots, \chi(\mathbf{a}_k) \in S$ and further $\chi(\mathbf{a}_0) = \chi(\mathbf{a}) = \mathbf{u}$, $\chi(\mathbf{a}_k) = \chi(\mathbf{b}) = \mathbf{v}$ and $\{\chi(\mathbf{a}_{i-1}), \chi(\mathbf{a}_i)\} \in E(J'')$ for all $i \in [k]$. Therefore, $\mathbf{u}$ and $\mathbf{v}$ are connected in S.

If $v = v_{y,z}$, we again define $\mathbf{a}, \mathbf{b} \in V(J')$ such that $\chi(\mathbf{a}) = \mathbf{u}$ and $\chi(\mathbf{b}) = \mathbf{v}$. If $\mathbf{a}, \mathbf{b} \in V_y$ or $\mathbf{a}, \mathbf{b} \in V_z$, then we can proceed exactly as in the former case with $c = y$ or $c = z$, respectively. If that is not the case, then either $\mathbf{a} \in V_y$ and $\mathbf{b} \in V_z$, or the other way round. We will only prove the former case, as the latter case can be proven analogously. Since the following will depend on it, we will now prove that $S = \{\chi(\mathbf{c}) : \mathbf{c} \in V_y\} \cup \{\chi(\mathbf{c}) : \mathbf{c} \in V_z\}$.

$\supseteq$: Let $\mathbf{u} \in \{\chi(\mathbf{c}) : \mathbf{c} \in V_y\} \cup \{\chi(\mathbf{c}) : \mathbf{c} \in V_z\}$. We then get that $\mathbf{u} = \chi(\mathbf{a})$ for an $\mathbf{a} \in V(J')$. From the definition it follows that $y \in \operatorname{set}(\mathbf{a})$ or $z \in \operatorname{set}(\mathbf{a})$ has to hold. Thus we get that $v_{y,z} \in \operatorname{set}(\chi(\mathbf{a})) = \operatorname{set}(\mathbf{u})$ and therefore $\mathbf{u} \in S$.

$\subseteq$: Let $\mathbf{u} \in S$, then $v_{y,z} \in \text{set}(\mathbf{u})$ follows. By definition there must exist an $\mathbf{a} \in V(J')$ such that $\chi(\mathbf{a}) = \mathbf{u}$ and $y \in \text{set}(\mathbf{a})$ or $z \in \text{set}(\mathbf{a})$ has to hold. Thus we get $\chi(\mathbf{a}) = \mathbf{u} \in \{\chi(\mathbf{c}) : \mathbf{c} \in V_y\} \cup \{\chi(\mathbf{c}) : \mathbf{c} \in V_z\}$.

It is obvious that $(\mathbf{x}y) \in V_y$ and $(\mathbf{x}z) \in V_z$. We now get a path in V_y with the elements $\mathbf{a}_0, \ldots, \mathbf{a}_k \in V_y$ such that $\mathbf{a}_0 = \mathbf{a}$, $\mathbf{a}_k = (\mathbf{x}y)$ and $\{\mathbf{a}_{i-1}, \mathbf{a}_i\} \in E(J')$ for all $i \in [k]$. We also get a path in V_z with the elements $\mathbf{b}_0, \ldots, \mathbf{b}_\ell \in V_z$ such that $\mathbf{b}_0 = (\mathbf{x}z)$, $\mathbf{b}_\ell = \mathbf{b}$ and $\{\mathbf{b}_{i-1}, \mathbf{b}_i\} \in E(J')$ for all $i \in [k]$. With the above equation, we have two paths in S: $\chi(\mathbf{a}_0), \ldots, \chi(\mathbf{a}_k)$ and $\chi(\mathbf{b}_0), \ldots, \chi(\mathbf{b}_\ell)$, where $\chi(\mathbf{a}_0) = \mathbf{u}$ and $\chi(\mathbf{b}_\ell) = \mathbf{v}$. However, $\chi(\mathbf{a}_k) = \chi((\mathbf{x}y)) = (\chi(\mathbf{x})v_{y,z}) = \chi((\mathbf{x}z)) = \chi(\mathbf{b}_0)$. Therefore, we get one path from $\mathbf{u}$ to $\mathbf{v}$ in S. □

Property c.: To show that $\hom(\mathfrak{C}'', \mathfrak{A}') = \hom(\mathfrak{C}', \mathfrak{A}')$ and $\hom(\mathfrak{C}'', \mathfrak{B}') = \hom(\mathfrak{C}', \mathfrak{B}')$, we will give a mapping $\pi : \text{Hom}(\mathfrak{C}', \mathfrak{A}') \to \text{Hom}(\mathfrak{C}'', \mathfrak{A}')$ from homomorphisms from $\mathfrak{C}'$ to $\mathfrak{A}'$ to homomorphisms from $\mathfrak{C}''$ to $\mathfrak{A}'$. We will then show that π is a bijection, from which follows that both sets have the same cardinality. This then proves the claim for $\mathfrak{A}'$. For $\mathfrak{B}'$, the proof is completely analogous, which is why it will be omitted. Let $\varphi \in \text{Hom}(\mathfrak{C}', \mathfrak{A}')$. We now define $\varphi' \coloneqq \pi(\varphi)$ as

$$\varphi'(x) \coloneqq \begin{cases} \varphi(x) & \text{if } x \neq v_{y,z} \\ \varphi(y) & \text{if } x = v_{y,z}. \end{cases}$$

In the following we will be using that for any $\varphi \in \text{Hom}(\mathfrak{C}', \mathfrak{A}')$, we have that $\varphi(y) = \varphi(z)$. Otherwise, from $(\mathbf{x}y), (\mathbf{x}z) \in R_f^{\mathfrak{C}'}$, it follows that $(\varphi(\mathbf{x})\varphi(y)), (\varphi(\mathbf{x})\varphi(z)) \in R_f^{\mathfrak{A}'}$ for two different tuples $(\varphi(\mathbf{x})\varphi(y))$ and $(\varphi(\mathbf{x})\varphi(z))$. However, this would contradict that, by definition of the encoding, $\mathfrak{A}'$ is functional.

Claim 4.19. *For all $\varphi \in \text{Hom}(\mathfrak{C}', \mathfrak{A}')$, we have $\pi(\varphi) \in \text{Hom}(\mathfrak{C}'', \mathfrak{A}')$.*

Proof. Let $\varphi \in \text{Hom}(\mathfrak{C}', \mathfrak{A}')$ and $\varphi' \coloneqq \pi(\varphi)$. Consider a relation symbol R and a tuple $\mathbf{c} \in R^{\mathfrak{C}''}$. If $v_{y,z} \notin \text{set}(\mathbf{c})$, then $\chi(\mathbf{c}) = \mathbf{c}$, $\varphi(\mathbf{c}) = \varphi'(\mathbf{c})$ and $\mathbf{c} \in R^{\mathfrak{C}'}$ follows. Then we get $\varphi(\mathbf{c}) \in R^{\mathfrak{A}'}$ and further $\varphi'(\mathbf{c}) \in R^{\mathfrak{A}'}$.

If $v_{y,z} \in \text{set}(\mathbf{c})$, then there exists a $\mathbf{c}' \in R^{\mathfrak{C}'}$ such that $\chi(\mathbf{c}') = \mathbf{c}$. We thus get $\varphi(\mathbf{c}') \in R^{\mathfrak{A}'}$. It holds that $\varphi(\mathbf{c}') = \varphi'(\mathbf{c})$, because for all $x \in \text{set}(\mathbf{c}) \setminus \{v_{y,z}\}$, $\varphi(x) = \varphi'(x)$. For $v_{y,z}$, $\varphi'(v_{y,z}) = \varphi(y) = \varphi(z)$ holds. Therefore, $\varphi'(\mathbf{c}) \in R^{\mathfrak{A}'}$ follows, which was to be shown. □

This shows that π is correctly defined as a mapping between homomorphisms. The two following proofs will show that π is bijective.

Claim 4.20. *π is injective.*

Proof. Let $\varphi_1, \varphi_2 \in \text{Hom}(\mathfrak{C}', \mathfrak{A}')$, $\varphi_1 \neq \varphi_2$ and define $\varphi_1' \coloneqq \pi(\varphi_1)$ and $\varphi_2' \coloneqq \pi(\varphi_2)$. Our goal is to show that $\varphi_1' \neq \varphi_2'$. There has to be a $u \in C'$ such that $\varphi_1(u) \neq \varphi_2(u)$, otherwise they would be the same function. We now have a case distinction.

Case 1: $u \notin \{y, z\}$. Then

$$\varphi_1'(u) = \varphi_1(u) \neq \varphi_2(u) = \varphi_2'(u).$$

Case 2: $u \in \{y, z\}$. Then

$$\varphi_1'(v_{y,z}) = \varphi_1(y) = \varphi_1(z) = \varphi_1(u) \neq \varphi_2(u) = \varphi_2(z) = \varphi_2(y) = \varphi_2'(v_{y,z}).$$

In both cases we have found an element that gets mapped differently, thus $\varphi_1' \neq \varphi_2'$ must follow. □

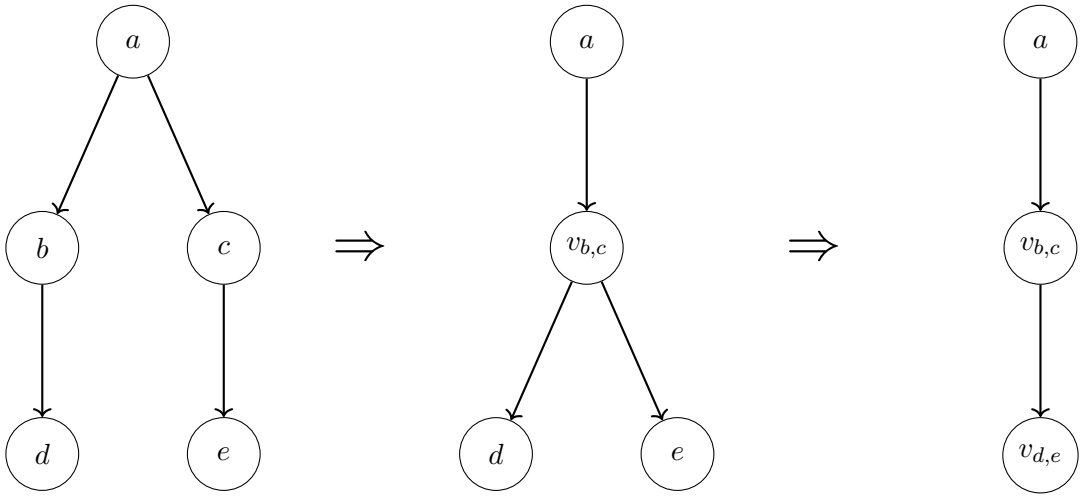


Figure 7: Two successive applications of the procedure described in the proof of Lemma 4.15. The arrows represent a binary relation R_f, which encodes a unary function f.

Claim 4.21. *π is surjective.*

Proof. Let $\varphi' \in \mathrm{Hom}(\mathfrak{C}'', \mathfrak{A}')$. We now construct a $\varphi \in \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$ such that $\pi(\varphi) = \varphi'$. We define

$$\varphi(x) \coloneqq \begin{cases} \varphi'(x) & \text{if } x \notin \{y, z\} \\ \varphi'(v_{y,z}) & \text{if } x \in \{y, z\}. \end{cases}$$

Using that $\psi(y) = \psi(z)$ for all $\psi \in \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$, it can easily be verified that $\pi(\varphi) = \varphi'$. We now only have to show that $\varphi \in \mathrm{Hom}(\mathfrak{C}', \mathfrak{A}')$. Let $\mathbf{c} \in R^{\mathfrak{C}'}$ for a relation symbol R. We now define $\mathbf{c}' = \chi(\mathbf{c})$ and get by construction that $\mathbf{c}' \in R^{\mathfrak{C}''}$. Because we know that φ' is a homomorphism, it follows that $\varphi'(\mathbf{c}') \in R^{\mathfrak{A}'}$. But since $\varphi'(a) = \varphi(a)$ for all $a \notin \{y, z, v_{y,z}\}$ and $\varphi'(v_{y,z}) = \varphi(y) = \varphi(z)$, it follows that $\varphi'(\mathbf{c}') = \varphi(\mathbf{c})$. Therefore $\varphi(\mathbf{c}) \in R^{\mathfrak{A}'}$. □

We now have proved the properties above. Therefore, we showed that it is possible to eliminate collisions, while keeping the number of homomorphisms to $\mathfrak{A}'$ and to $\mathfrak{B}'$ the same, reducing the number of elements by one and still having an acyclic structure. We thus can apply this procedure to any collision, until there are no collisions left, but then the structure is functional. □

From the above lemma it follows that given an acyclic, distinguishing structure, it is possible to construct a new structure, which is also acyclic and distinguishing but in addition also functional. One example how this can be applied can be seen in Figure 7.

Now that we have proved that it is generally possible to enforce a distinguishing, acyclic structure to be functional, we want to proceed by proving that totality cannot be enforced. This proof will work as follows. We will give two families of structures over the signature $\sigma = \{E/2, f/1\}$. Any two elements from these families with the same size can be distinguished by naive RCR, thus there exists an acyclic relational structure that distinguishes their encodings by homomorphism counts. Therefore, the first statement from above is true. However, we will then prove that there cannot be an acyclic and total structure that also distinguishes them by homomorphism counts.

Let $(\mathfrak{A}_i)_{i \in \mathbb{N}_{\geq 4}}$ be a family of σ-structures, defined as $\mathfrak{A}_n = (A_n, \mathrm{E}^{\mathfrak{A}_n}, f^{\mathfrak{A}_n})$, where $A_n = [n]$, $\mathrm{E}^{\mathfrak{A}_n} = \{(i, i+1), (i+1, i) : i \in [n-2]\}$ and $f^{\mathfrak{A}_n} = \{i \mapsto i+1 \bmod n-1 : i \in [n-1]\} \cup \{n \mapsto n-1\}$. Let $(\mathfrak{B}_i)_{i \in \mathbb{N}_{\geq 4}}$ also be a family of σ-structures, defined as $\mathfrak{B}_n = (B_n, \mathrm{E}^{\mathfrak{B}_n}, f^{\mathfrak{B}_n})$, where $B_n = [n]$,

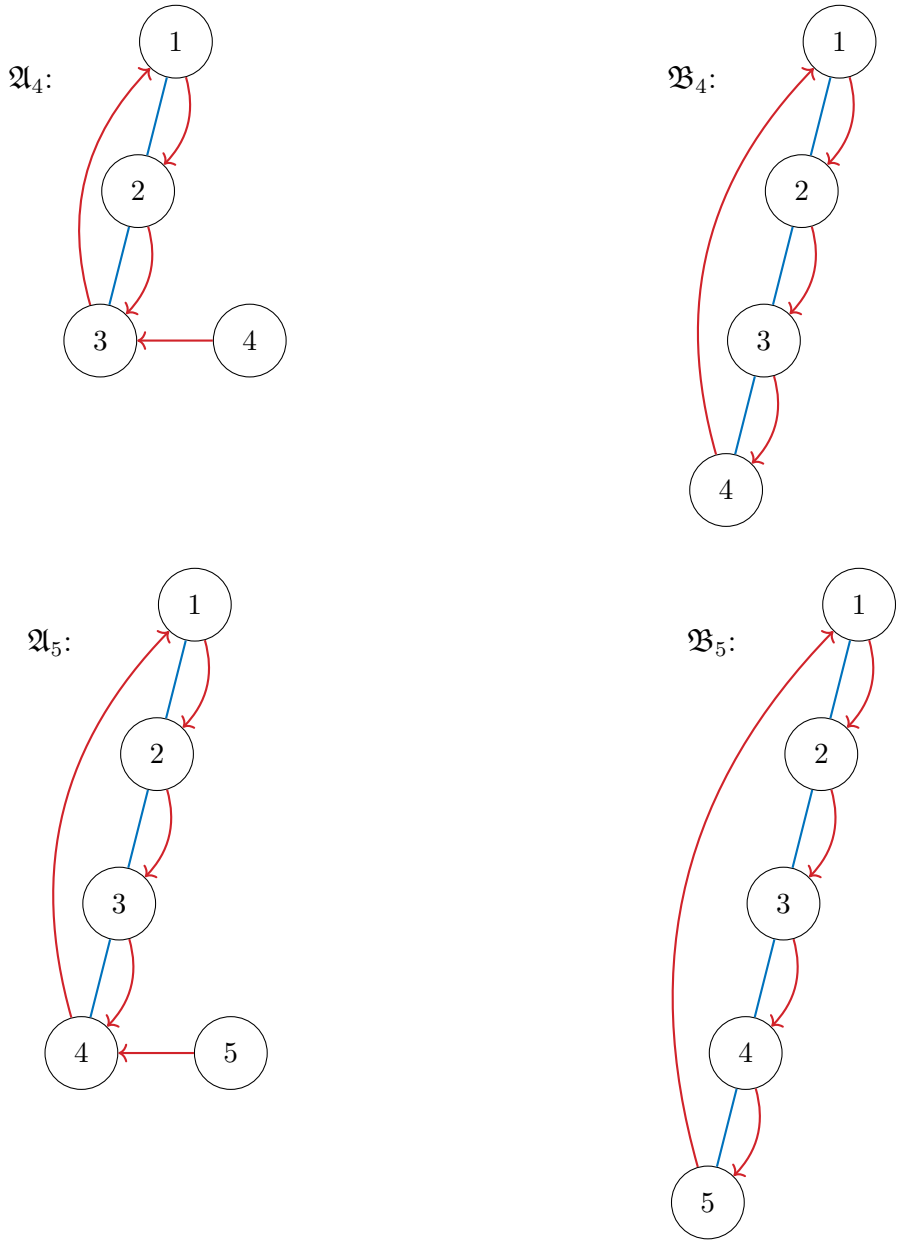


Figure 8: Examples for the structures $\mathfrak{A}_4$, $\mathfrak{A}_5$, $\mathfrak{B}_4$ and $\mathfrak{B}_5$. The blue edges represent the binary relation E, while the red arrows constitute the unary function f.

$\mathrm{E}^{\mathfrak{B}_n} = \{(i, i+1), (i+1, i) : i \in [n-1]\}$ and $f^{\mathfrak{B}_n} = \{i \mapsto i + 1 \bmod n : i \in [n]\}$. Graphical representations for a few examples of these structures can be seen in Figure 8.

For every $n \in \mathbb{N}_{\geq 4}$ it is clear that naive RCR distinguishes $\mathfrak{A}_n$ and $\mathfrak{B}_n$. The formula

$$\varphi_n = \exists^{\geq 2\cdot(n-1)}(x, y) \,.\, \mathrm{E}(x, y) \in \mathsf{nfGF}(\mathsf{C})$$

distinguishes $\mathfrak{A}_n$ and $\mathfrak{B}_n$ and using Theorem 4.4, this is equivalent to naive RCR distinguishing $\mathfrak{A}_n$ and $\mathfrak{B}_n$. Therefore, there exists an acyclic structure that distinguishes the encodings by homomorphism counts. It now only remains to show that this structure cannot be total, acyclic

and distinguishing.

Lemma 4.22. *Let $n \in \mathbb{N}_{\geq 4}$ and let $\mathfrak{C}'_n$ be an acyclic σ'-structure that distinguishes $\mathfrak{A}'_n$ and $\mathfrak{B}'_n$ by homomorphism counts. Then $\mathfrak{C}'_n$ cannot be both acyclic and total.*

Proof. Using basic boolean equivalences, we prove the equivalent statement that if $\mathfrak{C}'_n$ is total, than it either is not distinguishing or not acyclic. As such, let $\mathfrak{C}'_n$ be a total σ'-structure.

We observe that if $\mathfrak{C}'_n$ contains R_f-loops, that is an element $x \in C'_n$ such that $(x, x) \in R_f^{\mathfrak{C}'_n}$, then $\mathfrak{C}'_n$ is not distinguishing. In fact, then $\hom(\mathfrak{C}'_n, \mathfrak{A}'_n) = \hom(\mathfrak{C}'_n, \mathfrak{B}'_n) = 0$. If that were not the case, there would exist a homomorphism φ to either $\mathfrak{A}'_n$ or $\mathfrak{B}'_n$. Let $c \in C'_n$ be such that $(c, c) \in R_f^{\mathfrak{C}'_n}$. Then we would have $(\varphi(c), \varphi(c)) \in R_f^{\mathfrak{A}'_n}$ or $(\varphi(c), \varphi(c)) \in R_f^{\mathfrak{B}'_n}$, respectively. But in either structure, there does not exist such a loop.

Using similar arguments, we can reason that if $\mathfrak{C}'_n$ contains R_f-2-cycles, that is two elements c and d such that $(c, d), (d, c) \in R_f^{\mathfrak{C}'_n}$, then $\mathfrak{C}'_n$ cannot be distinguishing, as it does not have any homomorphisms to either $\mathfrak{A}'_n$ or $\mathfrak{B}'_n$. Otherwise, there again would be a homomorphism φ to $\mathfrak{A}'_n$ or $\mathfrak{B}'_n$. Let $c, d \in C'_n$ form such a R_f-2-cycle. Then we would have $(\varphi(c), \varphi(d)), (\varphi(d), \varphi(c)) \in R_f^{\mathfrak{A}'_n}$ or $(\varphi(c), \varphi(d)), (\varphi(d), \varphi(c)) \in R_f^{\mathfrak{B}'_n}$, respectively. But in either structure there does not exist such a 2-cycle.

From the two observations above it follows that if $\mathfrak{C}'_n$ has cardinality 1 or 2, then it cannot be distinguishing, as it is total and therefore would need to contain either R_f-loops or R_f-2-cycles. When now considering that $\mathfrak{C}'_n$ is total, thus for every c there is a d such that $(c, d) \in R_f^{\mathfrak{C}'_n}$, it is obvious that $\mathfrak{C}'_n$ must contain a R_f cycle of size greater than 2. Thus the Gaifman-Graph of $\mathfrak{C}'_n$ is not acyclic. As it can be found in [6] and [19], this is equivalent to $\mathfrak{C}'_n$ itself not being acyclic. So if $\mathfrak{C}'_n$ is total and does not contain R_f-loops and R_f-2-cycles, then it cannot be acyclic. □

We thus have showed that there cannot exist an acyclic and total $\mathfrak{C}'_n$ that distinguishes $\mathfrak{A}'_n$ and $\mathfrak{B}'_n$ by homomorphism counts. However, in Lemma 4.14 we showed that the existence of an acyclic, total and functional $\mathfrak{C}'_n$ that distinguishes $\mathfrak{A}'_n$ and $\mathfrak{B}'_n$ is equivalent to the existence of an acyclic $\mathfrak{C}_n$ that distinguishes $\mathfrak{A}_n$ and $\mathfrak{B}_n$. Since there is no acyclic and total $\mathfrak{C}'_n$, there also is no acyclic, total and functional $\mathfrak{C}''_n$ that distinguishes the encodings, and therefore there is no $\mathfrak{C}_n$ that distinguishes $\mathfrak{A}_n$ and $\mathfrak{B}_n$ by homomorphism counts. The results of this section are summarised in the following theorem.

Theorem 4.23. *Let σ be a signature, let $\mathfrak{A}$ and $\mathfrak{B}$ be two σ-structures and let σ', $\mathfrak{A}'$ and $\mathfrak{B}'$ be their respective encodings. Now consider the following statements:*

1. *Naive Relational Colour Refinement distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*
2. *There exists an acyclic and functional σ'-structure $\mathfrak{C}'$ such that $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$.*
3. *There exists an acyclic σ-structure $\mathfrak{C}$ such that $\hom(\mathfrak{C}, \mathfrak{A}) \neq \hom(\mathfrak{C}, \mathfrak{B})$.*

Then statement 1. is equivalent to statement 2., but while statement 3. implies statement 1., the converse does not hold.

Proof. ***1. is equivalent to 2.*** Naive RCR distinguishes $\mathfrak{A}$ and $\mathfrak{B}$ if, and only if, there is an acyclic σ'-structure $\mathfrak{C}'$ such that $\hom(\mathfrak{C}', \mathfrak{A}') \neq \hom(\mathfrak{C}', \mathfrak{B}')$. Using Lemma 4.15, we then can construct an acyclic and functional σ'-structure that also distinguishes $\mathfrak{A}'$ and $\mathfrak{B}'$ by homomorphism counts. The converse directly follows from the existence of an acyclic σ'-structure that distinguishes $\mathfrak{A}'$ and $\mathfrak{B}'$ by homomorphism counts.

3.* implies *1. The existence of such a σ-structure is, by Lemma 4.14, equivalent to there being an acyclic, total and functional σ'-structure that distinguishes the encodings. Using the results of [19], this implies that RCR distinguishes the encodings and by definition this means that naive RCR distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.

1.* does not imply *3. By Lemma 4.14, Statement *3.* is equivalent to there being an acyclic, total and functional σ'-structure that distinguishes the encodings by homomorphism counts. However as we showed in Lemma 4.22, this is not implied by the existence of an acyclic σ'-structure which distinguishes the encodings. This is however equivalent to statement *1.*. □

We found that naive RCR cannot be characterised by acyclic structures, as the totality of functions inherently results in cycles. When prohibiting loops and 2-cycles, which would not violate the acyclicity, there thus have to be larger cycles which result in the structure not being acyclic. The notion of acyclicity with respect to α-acyclicity and the used encoding is therefore strictly weaker than naive RCR. However, there could be other classes of structures, which characterise naive RCR in the desired way.

5 Relational Colour Refinement for Symmetric Structures

One interesting question that can be posed when looking at the characterisation of RCR through homomorphism counting is, which restrictions to the class of structures can be made. Concretely, which subclass $\mathcal{S}$ of the relational structures can be chosen, such that we get the following equivalence: Two structures $\mathfrak{A}$ and $\mathfrak{B}$ from $\mathcal{S}$ get distinguished by RCR if, and only if, there is an acyclic structure $\mathfrak{C}$ from $\mathcal{S}$ with $\hom(\mathfrak{C},\mathfrak{A}) \neq \hom(\mathfrak{C},\mathfrak{B})$.

This is not possible for the class of total structures, as they are defined in Definition 4.11. Consider the naive encodings of the families from Lemma 4.22. These are distinguished by RCR, but there does not exist an acyclic, total structure, which distinguishes them by homomorphism counts. Another class which can be investigated is the class of symmetric structures.

Definition 5.1 (Symmetric structures)**.** Let σ be a relational signature. A structure $\mathfrak{A}$ of signature σ is a symmetric structure, if for every relation and every tuple in those relations, the order of the elements is irrelevant. This means, that every relation R of arity k is a subset of all possible subsets of A with exactly k elements. Formally, that means

$$R \subseteq \binom{A}{k}.$$

An equivalent characterisation uses the symmetric group $\mathcal{S}_k$. We call a σ-structure $\mathfrak{A}$ symmetric, if for every $R \in \sigma$ of arity k, every k-tuple $\mathbf{x} = (x_1, x_2, \ldots, x_k) \in R^{\mathfrak{A}}$ and every k-permutation $\pi \in \mathcal{S}_k$

$$(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(k)}) \in R^{\mathfrak{A}}.$$

We will prove in the following that the restriction to symmetric structures in indeed possible. However, before we prove this, we have to show a lemma which will be used in the proof. As a reminder on notation, for a k-tuple $\mathbf{x} = (x_1, x_2, \ldots, x_k)$, a homomorphism φ and a permutation π, we write $\varphi(\mathbf{x})$ for $(\varphi(x_1), \varphi(x_2), \ldots, \varphi(x_k))$ and $\pi(\mathbf{x})$ for $(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(k)})$.

Lemma 5.2. *Let $\pi \in \mathcal{S}_k$, φ be a homomorphism, R a relation of arity k and $\mathbf{x} = (x_1, x_2, \ldots, x_k) \in R$. Then $\varphi(\pi(\mathbf{x})) = \pi(\varphi(\mathbf{x}))$.*

Proof. We show that $\varphi(\pi(\mathbf{x}))_i = \pi(\varphi(\mathbf{x}))_i$ for all $i \in [k]$. Note that the definitions of $\varphi(\pi(\mathbf{x}))$ and $\pi(\varphi(\mathbf{x}))$ are

$$\varphi(\pi(\mathbf{x})) = (\varphi(x_{\pi(1)}), \varphi(x_{\pi(2)}), \ldots, \varphi(x_{\pi(k)}))$$

and

$$\pi(\varphi(\mathbf{x})) = (\varphi(\mathbf{x})_{\pi(1)}, \varphi(\mathbf{x})_{\pi(2)}, \ldots, \varphi(\mathbf{x})_{\pi(k)}),$$

respectively. From these, we directly get

$$\varphi(\pi(\mathbf{x}))_i = \varphi(x_{\pi(i)}) = (\varphi(x_1), \varphi(x_2), \ldots, \varphi(x_2))_{\pi(i)} = \varphi(\mathbf{x})_{\pi(i)} = \pi(\varphi(\mathbf{x}))_i.$$

Therefore the lemma must hold. □

We can now prove the main result of this section.

Theorem 5.3. *Let σ be a relational signature and $\mathfrak{A}$ and $\mathfrak{B}$ be two σ-structures. Then the following two statements are equivalent:*

1. RCR *distinguishes $\mathfrak{A}$ and $\mathfrak{B}$.*

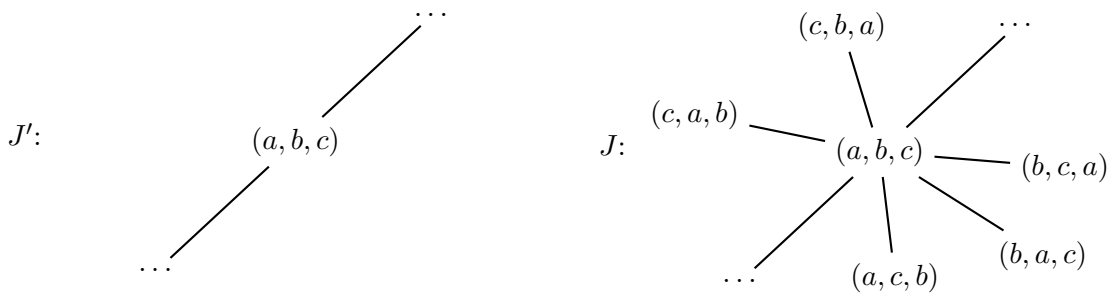


Figure 9: A section from the join tree J' and the join tree J generated from it. We consider a tuple $\mathbf{x} = (a, b, c)$, for which no other permutation appears in $\mathbf{C}'$.

2. There exists an acyclic, symmetric σ structure $\mathfrak{C}$ with $\hom(\mathfrak{C}, \mathfrak{A}) \neq \hom(\mathfrak{C}, \mathfrak{B})$.

Proof. We first prove that *2.* implies *1.* Let $\mathfrak{C}$ be an acyclic, symmetric σ structure with $\hom(\mathfrak{C}, \mathfrak{A}) \neq \hom(\mathfrak{C}, \mathfrak{B})$. As $\mathfrak{C}$ is acyclic, using [19], we get that RCR must distinguish $\mathfrak{A}$ and $\mathfrak{B}$.

We now prove that *1.* implies *2.* Assume that RCR distinguishes $\mathfrak{A}$ and $\mathfrak{B}$. From the results of [19] we know that there exists an acyclic structure $\mathfrak{C}'$ with $\hom(\mathfrak{C}', \mathfrak{A}) \neq \hom(\mathfrak{C}', \mathfrak{B})$. Our goal will be to construct a σ structure $\mathfrak{C}$ from $\mathfrak{C}'$ that is both acyclic and symmetric. Informally, $\mathfrak{C}$ will have the same elements as $\mathfrak{C}'$ and for every tuple that appears in some relation, we will add all possible permutations of that tuple to the relation as well. Formally, we define $\mathfrak{C} \coloneqq (C', \sigma)$ and for all $R \in \sigma$ of arity k, we have

$$R^{\mathfrak{C}} \coloneqq \{(x_{\pi(1)}, x_{\pi(2)}, \dots, x_{\pi(k)}) : \text{for every } (x_1, x_2, \dots, x_k) \in R^{\mathfrak{C}'} \text{ and every } \pi \in \mathcal{S}_k\}.$$

From the second characterisation of symmetric structures given above, it is obvious that $\mathfrak{C}$ is symmetric.

Claim 5.4. *$\mathfrak{C}$ is acyclic.*

Proof. We define a join-tree J for $\mathfrak{C}$. Since $\mathfrak{C}'$ is acyclic, we have a join-tree J' for $\mathfrak{C}'$. From the definition we know that $V(J) = \mathbf{C}$, thus we only have to define the set of edges. Let $\mathbf{x} \in V(J) \setminus V(J')$. From the construction there exists a permutation $\pi_{\mathbf{x}}$, such that $\pi_{\mathbf{x}}(\mathbf{x}) \in V(J')$. We now define $E(J) \coloneqq E(J') \cup \{\{\pi_{\mathbf{x}}(\mathbf{x}), \mathbf{x}\} : \mathbf{x} \in \mathbf{C} \setminus \mathbf{C}'\}$. This construction can be seen in Figure 9.

The connectedness and cycle-freeness follows directly from the fact that J' is a tree. As such, it only remains to show the join-tree property. Consider an arbitrary $v \in C$. Since $C = C'$, it follows that $v \in C'$ and the set of all $\mathbf{x} \in \mathbf{C}'$ with $v \in \text{set}(\mathbf{x})$ induces a connected subgraph in J'. Let $\mathbf{x} \in \mathbf{C} \setminus \mathbf{C}'$ and $v \in \text{set}(\mathbf{x})$. Then $\pi_{\mathbf{x}}(\mathbf{x}) \in \mathbf{C}'$ and $\{\pi_{\mathbf{x}}(\mathbf{x}), \mathbf{x}\} \in E(J)$, thus $\mathbf{x}$ is also connected and the set $\{\mathbf{x} \in V(J) : v \in \text{set}(\mathbf{x})\}$ also induces a connected subgraph. This was to be shown. □

It now remains to prove that $\mathfrak{C}$ also has a different number of homomorphisms to $\mathfrak{A}$, than to $\mathfrak{B}$. In fact, we will show that $\mathfrak{C}$ and $\mathfrak{C}'$ have exactly the same homomorphisms to $\mathfrak{A}$ and $\mathfrak{B}$, respectively. Formally, we will prove that $\text{Hom}(\mathfrak{C}', \mathfrak{A}) = \text{Hom}(\mathfrak{C}, \mathfrak{A})$ and $\text{Hom}(\mathfrak{C}', \mathfrak{B}) = \text{Hom}(\mathfrak{C}, \mathfrak{B})$. However, we will only prove the claim for $\mathfrak{A}$, as the case for $\mathfrak{B}$ can be proven completely analogously.

Let $\varphi \in \text{Hom}(\mathfrak{C}', \mathfrak{A})$. Now consider $\mathbf{x} \in R^{\mathfrak{C}}$ for a $R \in \sigma$ with arity k and we will proceed with a case distinction. If $\mathbf{x} \in \mathbf{C}'$, then we have $\mathbf{x} \in R^{\mathfrak{C}'}$ and by assumption $\varphi(\mathbf{x}) \in R^{\mathfrak{A}}$. If $\mathbf{x} \in \mathbf{C} \setminus \mathbf{C}'$, then there must be a $\pi \in \mathcal{S}_k$, such that $\pi(\mathbf{x}) \in \mathbf{C}'$ and $\pi(\mathbf{x}) \in R^{\mathfrak{C}'}$. Then by assumption, we

get that $\varphi(\pi(\mathbf{x})) \in R^{\mathfrak{A}}$. Using Lemma 5.2, we know that $\varphi(\pi(\mathbf{x})) = \pi(\varphi(\mathbf{x})) \in R^{\mathfrak{A}}$. Now let $\pi' \in \mathcal{S}_k$, such that $\pi' \circ \pi = \mathrm{id} \in \mathcal{S}_k$. As $\mathfrak{A}$ is symmetric, we know that $\pi'(\pi(\varphi(\mathbf{x}))) \in R^{\mathfrak{A}}$ and with $\pi'(\pi(\varphi(\mathbf{x}))) = \varphi(\mathbf{x})$ it follows that $\varphi(\mathbf{x}) \in R^{\mathfrak{A}}$. We therefore have shown that $\varphi \in \mathrm{Hom}(\mathfrak{C}, \mathfrak{A})$.

Now let $\varphi \notin \mathrm{Hom}(\mathfrak{C}', \mathfrak{A})$. Then there is an $R \in \sigma$ of arity k and an $\mathbf{x} \in R^{\mathfrak{C}'}$ with $\varphi(\mathbf{x}) \notin R^{\mathfrak{A}}$. From the definition we get that $\mathbf{x} \in \mathbf{C}$ and thus $\mathbf{x} \in R^{\mathfrak{C}}$ and from the assumption we get that $\varphi(\mathbf{x}) \notin R^{\mathfrak{A}}$. Therefore $\varphi \notin \mathrm{Hom}(\mathfrak{C}, \mathfrak{A})$. □

With this, we have proven that it is possible to only consider symmetric acyclic structures with a different homomorphism counts, when trying to distinguish symmetric structures. Therefore, we can restrict the class of structures to only consider symmetric structures, while retaining the characterisation through homomorphism counting.

6 Conclusion

In this thesis, we presented the results of Scheidt and Schweikardt from [19] and discussed how they can be extended for the use with non-relational signatures. We defined two possible ways on how non-relational structures can be encoded as relational structures and investigated the logical and combinatorial characterisations. Naive Relational Colour Refinement, where a function is directly interpreted as a relation, is characterised by the logic $\mathsf{nfGF}(\mathsf{C})$, which uses function symbols like relation symbols. By using the transitive expansion of a function as its encoding, we can allow arbitrarily many function applications, with a bound on the number of alternations. This notion is captured by the logic $\mathsf{GF}(\mathsf{C})_k$. However, while we find logical characterisations, the characterisation by homomorphism counting is not possible. We showed that the existence of an acyclic, total and functional relational structure that distinguishes two encoded structures by homomorphism counts is equivalent to the existence of a non-relational, acyclic structure that also distinguishes the structures. But while it is possible to construct a functional structure, it is not possible to enforce totality. This then lead us to the question of investigating restrictions of the class of structures and for which restrictions the characterisation by homomorphism counting remains. Aside from the negative result in that regard for total structures, we showed that it is possible to restrict the class to symmetric ones.

There are multiple questions that are still unanswered.

- When characterising RCR_k logically, we were able to show that the number of applications of a single function symbol does not need a bound. The same was not done for the alternation depth. One interesting question would be to investigate, whether it is possible to only consider the transitive expansion up to a certain alternation depth d. Furthermore, would it then be possible to allow any alternation depth in a formula to characterise this algorithm? The result would then be that $\mathsf{GF}(\mathsf{C})$ with the standard definition of atomic formulae would characterise RCR over non-relational structures.

- Our two algorithms operate on different classes of structures. While nRCR is defined for any structure, RCR_k only works for structures over signatures with relation and unary function symbols. It is not clear, whether the used approach can be adapted for functions with arity ≥ 2. However, an iterative colouring algorithm that is stronger than nRCR but still works on any structure is desirable.

- We have considered two possible restrictions on the class of relational structures for the characterisation by homomorphism counting. This poses the question, for which other restrictions this characterisation also holds.

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