Deep Weisfeiler Leman

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We introduce the framework of Deep Weisfeiler Leman algorithms (DeepWL), which allows the design of purely combinatorial graph isomorphism tests that are more powerful than the well-known Weisfeiler-Leman algorithm.

We prove that, as an abstract computational model, polynomial time DeepWL-algorithms have exactly the same expressiveness as the logic Choiceless Polynomial Time (with counting) introduced by Blass, Gurevich, and Shelah (Ann. Pure Appl. Logic., 1999)

It is a well-known open question whether the existence of a polynomial time graph isomorphism test implies the existence of a polynomial time canonisation algorithm. Our main technical result states that for each class of graphs (satisfying some mild closure condition), if there is a polynomial time DeepWL isomorphism test then there is a polynomial canonisation algorithm for this class. This implies that there is also a logic capturing polynomial time on this class.

1. Introduction

The research that lead to this paper grew out of the following seemingly unrelated questions in the context of the graph isomorphism problem.

Question A. Are there efficient combinatorial graph isomorphism algorithms more powerful than the standard Weisfeiler Leman algorithm?

Here we are interested in general purpose isomorphism algorithms and not specialised algorithms for specific graph classes.

Question B. Are there generic methods to construct graph canonisation algorithms from isomorphism algorithms?

This question is also related to an important open problem in descriptive complexity theory, the question of whether there is a logic *capturing* polynomial time. Such a logic would express exactly the properties of graphs that are polynomial-time decidable. It is known that if there is a polynomial time canonisation algorithm for a class of graphs then there is a logic that captures polynomial time on that class. (The converse is unknown.)

Initially, we studied Questions A and B separately, but at some point, we noted an interesting connection, which is based on the empirical observation that typically combinatorial isomorphism algorithms can easily be lifted to canonisation algorithms, whereas for group theoretic algorithms this is not so easy. Before giving any details, let us discuss the two questions individually.

From Weisfeiler Leman to DeepWL

One of the oldest (and most often re-invented) graph isomorphism algorithm is the colour refinement algorithm, which is also known as naive vertex classification or 1-dimensional Weisfeiler-Leman algorithm (1-WL). It iteratively colours the vertices of a graph. Initially, all vertices get the same colour. The initial colouring is repeatedly refined, in the sense that colour classes are split into several classes. In each refinement round, two vertices that still have the same colour get different colours in the refined colouring if they have a different number of neighbours in some colour class of the current colouring. The refinement process stops if no further refinement can be achieved; we call the resulting colouring stable. As such, 1-WL just computes a colouring of the vertices of a graph, but it can be used as an isomorphism test by running it simultaneously on two graphs and comparing the colour histograms. If there is some colour such that the two graphs have a different number of vertices of this colour, we know the graphs are non-isomorphic, and we say that 1-WL distinguishes the two graphs not distinguished by the algorithm. The simplest example is a cycle of length 6 versus two triangles.

In order to design a more powerful isomorphism test, Weisfeiler and Leman [26] proposed a similar iterative colouring procedure for pairs of vertices; this led to what is now known as the classical or 2-dimensional Weisfeiler-Leman algorithm (2-WL). In the initial colouring, the colour of a pair (u, v) indicates whether u and v are equal, adjacent, or distinct and non-adjacent. Then in each refinement round, two pairs (u, v) and (u', v') that still have the same colour a get different colours if for some colours b, c the numbers of vertices w and w' in the configuration shown in Figure 1 are distinct. Again, the refinement process stops if no further refinement can be achieved. The algorithm can easily be adapted to directed graphs, possibly with loops and labelled edges. All we need to do is modify the initial colouring. For example, if we have two edge labels R, S, the initial colouring of 2-WL has twenty different colours encoding the isomorphism types of pairs (u, v), for example, "u = v and there is an R-loop, but no S-loop on u" or " $u \neq v$, there is no edge from u to v, and there is both an R-edge and an S-edge from v to u". Throughout this paper, it will be convenient for us to work with edge-labelled directed graphs, that is, binary relational structures.

When it comes to distinguishing graphs, 2-WL is significantly more powerful than



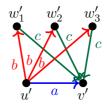


Figure 1: 2-WL differentiates between (u, v) and (u', v') if for some colours b and c there are different numbers of vertices w_i and w'_i , respectively, such that (u, w_i) , (u', w'_i) have colour b and (w_i, v) , (w'_i, v') have colour c.

1-WL, but it is still fairly easy to find non-isomorphic graphs not distinguished by the algorithm. In fact, any two strongly regular graphs with the same parameters are indistinguishable by 2-WL. To further strengthen the algorithm, Babai proposed to colour k-tuples (for an arbitrary k) instead of just pairs of vertices, introducing the k-dimensional Weisfeiler-Leman algorithm (k-WL) (see [7]). For constant k, the algorithm runs in polynomial time, to be precise the result is computable in time $O(n^{k+1}\log n)$. This arguably still simple combinatorial algorithm is quite powerful. It subsumes all natural combinatorial approaches to graph isomorphism testing and, remarkably, also many algebraic and mathematical optimisation approaches (e.g. [1, 2, 5, 22]), with the important exception of the group theoretic approaches introduced by Babai and Luks [3, 4, 20] in the early 1980s.

It is quite difficult to find non-isomorphic graphs not distinguishable by k-WL, even for constant $k \geq 3$. In a seminal paper, Cai, Fürer and Immerman [7] constructed, for every k, a pair G_k, H_k of non-isomorphic graphs of size O(k) that are not distinguished by k-WL. These so-called CFI-graphs encode the solvability of a system of linear equations over a finite field, and all known examples of non-isomorphic graph pairs not distinguished by the Weisfeiler-Leman algorithms are based on variations of this construction. Incidentally, the hardest known instances for practical graph isomorphism tools are based on the same construction [21]. Let us remark that the CFI graphs can easily be distinguished in polynomial time by group theoretic techniques. Indeed, the graphs are 3-regular and thus can be distinguished by Luks's [20] polynomial time isomorphism algorithm for graph classes of bounded degree. But the group theoretic techniques are far more complicated than the simple "local constraint propagation" underlying the Weisfeiler-Leman algorithm.

This brings us to Question A. We start from a different perspective on k-WL: instead of colouring k-tuples, we can think of k-WL as adding all k-tuples of vertices as new elements to our input graph, together with new binary relations encoding the relationship between the tuples and vertices of the original graphs. Then on this extended graph we run 1-WL (or, depending on the details of the construction, 2-WL), and the resulting colours of the k-tuples should correspond to (or subsume) the colours k-WL would assign to these tuples. This correspondence between k-WL on a graph and 1-WL on an extended structure consisting of k-tuples of vertices of the original graph has been known for a while, it may go back to the work of Otto [23]. Here is our new idea: perhaps we do

not need all k-tuples of vertices to distinguish two graphs, but just a few of them. This could arise in a situation where we have two graphs G, H and within them small subsets $S \subseteq V(G), T \subseteq V(H)$ such that the difference between the graphs is confined to the induced subgraphs of these subsets. Then to distinguish the graphs, it suffices to create tuples of elements of these subsets.

Example 1. Let G and H be the graphs obtained by padding the CFI-graphs G_k, H_k with $2^{k \log k}$ isolated vertices, and let $S \subseteq V(G)$ and $T \subseteq V(H)$ be the vertex sets of G_k, H_k within G, H, respectively.

Then $n = |G| = |H| = O(k) + 2^{k \log k}$, and we need (at least) the (k+1)-WL to distinguish G, H, running in time $n^{\Omega(k)} = n^{\Omega(\frac{\log n}{\log \log n})}$. However, to distinguish the graphs, we only need to see all (k+1)-tuples of vertices from the sets S, T, and the number of such tuples is $k^{(k+1)} = O(n)$. Thus if we create only these (k+1)-tuples and then use 1-WL to distinguish the graphs extended by these tuples, we have a polynomial time algorithm.

The example nicely illustrates that it can be beneficial to confine the use of a high-dimensional WL algorithm to a small part of a structure. It allows us to investigate this part to greater depth, using k-WL even for k linear in the size of the relevant part while maintaining an overall polynomial running time. The question is how we find suitable sets S and T on which we focus. We can start from the colour classes of 1-WL on the current structure. Then we can iterate the whole process, that is: we start by running 1-WL on the input graph(s), then choose one or several colours with few elements, add k-tuples of elements of these colours, extend the graph by these tuples and the associated relations, then run 1-WL again, choose new colour classes, add tuples, et cetera. We repeat this procedure as long as our running time permits it. This is the idea of Deep $Weisfeiler\ Leman\ (DeepWL)$, a class of combinatorial algorithms that are based on the same simple combinatorial ideas as Weisfeiler\ Leman, but turn out to be significantly more powerful.

The formal realisation of this idea is subtle and requires some care. Without going into too many details here (see Section 3), let us highlight some of the main points. First of all, since we can iterate the process of tuple creation, it suffices to create pairs; k-tuples can be encoded as nested pairs. Second, it turns out that working with 2-WL instead of 1-WL leads to a much more robust class of algorithms. One intuitive reason for this is that 2-WL (as opposed to 1-WL) allows us to trace connectivity and paths in a graph and thereby allows us to detect if two deeply nested pairs share elements of the input graph. On a technical level, 2-WL allows us to use the language and algebraic theory of coherent configurations [9], which are tightly linked to colourings computed by 2-WL. Moreover, the creation of pairs is particularly natural in combination with 2-WL: we simply pick a colour class of the current colouring (of pairs of elements of the current structure) and then create a new element for each pair of that colour.

A third aspect of the formalisation of DeepWL is less intuitive, but leads to an even more powerful class of algorithms that is also more robust (as Theorem 21 shows). Besides creating pairs of elements, we introduce a second operation for *contracting* con-

nected components of a colour class (or factoring a structure). This allows us to discard irrelevant information and better control the size of the structure we build.

So what is a DeepWL algorithm? Basically, it is a strategy for adaptively choosing a sequence of operations (create elements representing pairs, contract connected components) and the colour classes to which these operations are applied. A run of such an algorithm maintains a growing structure (the original structure plus the newly created elements and relations), but the algorithm has no direct access to the structure. It only gets the information of which colours the 2-WL colouring of the structure computes and how the colour classes relate. This guarantees that a DeepWL algorithm always operates in an isomorphism invariant way: isomorphic input structures lead to exactly the same runs. We introduce DeepWL as a general framework for algorithms operating on graphs (and relational structures), but we are mainly interested in graph isomorphism algorithms that can be implemented in DeepWL. It follows from our results that DeepWL can distinguish all CFI graphs in polynomial time and thus is strictly more powerful than k-WL for any k. (Note that k-WL can be seen as a specific DeepWL algorithm where the strategy is to create all k-tuples.)

Isomorphism Testing, Canonisation, and Descriptive Complexity

The graph isomorphism problem can be seen as the algorithmic problem of deciding whether two different representations of a graph, for example, two different adjacency matrices, actually represent the same graph. One way of solving this problem is to transform arbitrary representations of a graph into a canonical representation. A canonisation algorithm does precisely this. Canonisation is an interesting problem beyond isomorphism testing. For example, if we want to store molecular graphs in a chemical information system, then it is best to store a canonical representation of the molecules.

Formally, a canonical form for a class \mathcal{C} of graphs (which we assume to be closed under isomorphism) is a mapping $\operatorname{Can}: \mathcal{C} \to \mathcal{C}$ such that for all $G \in \mathcal{C}$, the graph $\operatorname{Can}(G)$ is isomorphic to G, and for isomorphic $G, H \in \mathcal{C}$ it holds that $\operatorname{Can}(G) = \operatorname{Can}(H)$. A canonisation algorithm for \mathcal{C} is an algorithm computing a canonical form for \mathcal{C} .

To the best of our knowledge, for all natural classes \mathcal{C} for which a polynomial time isomorphism algorithm is known, a polynomial time canonisation algorithm is also known. For some classes, for example the class of planar graphs or classes of bounded tree width, it was easy to generalise isomorphism testing to canonisation. For other classes, for example all classes of bounded degree, this required considerable additional effort [4]. Question B simply asks if there is a polynomial time reduction from canonisation to isomorphism testing. This is an old question (see, for example, [16]) that may eventually be resolved by a proof that there exists a polynomial time canonisation algorithm for the class of all graphs. But it is conceivable that this question can be resolved without clarifying the complexity status of either isomorphism or canonisation. In any case, it is consistent with current knowledge that there is a polynomial time isomorphism algorithm, but no polynomial time canonisation algorithm for the class of all graphs.

¹We view this as a promise problem, that is, it is irrelevant what the algorithm does on inputs $G \notin \mathcal{C}$.

A pattern that emerged over the years is that it is usually easy to obtain canonisation algorithms from combinatorial isomorphism algorithms and much harder to obtain them from group theoretic isomorphism algorithms. This intuition is supported by the following (folklore) theorem: Let C be a graph class such that k-WL is a complete isomorphism test for C, that is, it distinguishes all non-isomorphic (vertex coloured) graphs in C. Then there is a polynomial time canonisation algorithm for C. (For a proof, see [14].) Interestingly, for some graph classes for which (group theoretic) polynomial time isomorphism tests were known, the first polynomial time canonisation algorithms were obtained by proving that k-WL is a complete isomorphism test for these classes. Examples are classes of bounded rank width [15, 14] and graph classes with excluded minors [24, 12].

As mentioned earlier, a polynomial time canonisation algorithm for a class of graphs yields a logic that captures polynomial time on that class. Arguably the most prominent logic in this context is fixed-point logic with counting (FPC) [18, 10]. FPC captures polynomial time on many natural graph classes, among them all classes with excluded minors [12]. There are deep connections between FPC and the Weisfeiler-Leman algorithm. In particular, for every class C of graphs, isomorphism for graphs from C is expressible in FPC if and only if there is a $k \geq 1$ such that k-WL is a complete isomorphism test for C [23]. A consequence of this is that FPC cannot express isomorphism of the CFI graphs, which implies that the logic does not capture polynomial time on the class of all graphs.

Choiceless polynomial time with counting (CPT) is a richer logic that is strictly more expressive than FPC, but still contained in polynomial time (in the sense that all properties of graphs expressible in CPT are polynomial-time decidable). It was introduced by Blass, Gurevich, and Shelah [6] as a formalisation of "choiceless", that is, isomorphism invariant, polynomial time computations. Dawar, Rossman, and Richerby [8] proved that isomorphism of the CFI graphs is expressible in CPT. It is still an open question if CPT captures polynomial time.

Main Results

Our first main result shows that polynomial time DeepWL algorithms can decide precisely the properties expressible in the logic CPT. Thus DeepWL corresponds to CPT in a similar way as the standard WL-algorithm corresponds to the logic FPC.

Theorem (Theorem 21). A property of graphs is decidable by a polynomial time DeepWL-algorithm if and only if it is expressible in CPT.

Corollary. There is a polynomial time DeepWL algorithm that decides isomorphism of the CFI graphs.

A direct consequence of this result is that DeepWL is strictly more powerful than the standard WL-algorithm. Thus DeepWL provides an answer to Question A: it gives us purely combinatorial isomorphisms tests strictly more powerful than standard WL. Moreover, the logical characterisation in terms of CPT (Theorem 21) shows that the class of polynomial time DeepWL-algorithms is robust and, arguably, natural.

Our second main result addresses Question B. While not fully resolving it, it substantially extends the realm of isomorphism algorithms that can automatically be transformed to canonisation algorithms. A *complete invariant* for a class \mathcal{G} of graphs is a mapping $\mathcal{I}: \mathcal{G} \to \{0,1\}^*$ such that for all $G, H \in \mathcal{G}$ we have $G \cong H$ if and only if $\mathcal{I}(G) = \mathcal{I}(H)$.

Theorem (Theorem 13). Let \mathcal{G} be a class of graphs such that there is a polynomial-time DeepWL-algorithm deciding isomorphism on \mathcal{G} . Then there is a polynomial-time DeepWL-algorithm that computes a complete invariant for \mathcal{G} .

We say that a class \mathcal{G} of (vertex) coloured graphs is closed under colouring if all graphs obtained from a graph in \mathcal{G} by changing the colouring also belong to \mathcal{G} . Isomorphisms between coloured graphs are defined in the usual way such that the colour of each vertex has to be preserved. By a result due to Gurevich [16] relating complete invariants to canonisation, we obtain the following corollary.

Corollary (Corollary 15). Let \mathcal{G} be a class of coloured graphs closed under colouring such that there is a polynomial time DeepWL algorithm deciding isomorphism on \mathcal{G} . Then there is a polynomial time canonisation algorithm for \mathcal{G} .

The rest of this paper is organised as follows. After giving the necessary preliminaries in Section 2, we formally introduce DeepWL in Section 3. In Section 4, we prove that DeepWL is equivalent to a restricted form that we call pure DeepWL. Section 5 is the technical core of the paper. We prove our main technical result about isomorphism testing in DeepWL and canonisation. The difficult part of the proof is a normal form that we obtain for DeepWL-algorithms deciding isomorphism. Finally, in Section 6 we establish the equivalence between DeepWL and CPT. Due to space liminations, we have to defer many of the proofs to a technical appendix.

2. Preliminaries

Binary Relations and Structures

Let R be a binary relation. The domain of R is defined as the set $dom(R) := \{u \mid \exists v \colon (u,v) \in R\}$, and the codomain of R is $codom(R) := \{v \mid \exists u \colon (u,v) \in R\}$. The support of R is $supp(R) := dom(R) \cup codom(R)$. The converse of R is the relation $R^{-1} := \{(v,u) \mid (u,v) \in R\}$. The concatenation of two binary relations R_1, R_2 is the relation $R_1 \circ R_2 := R_1R_2 := \{(u,w) \mid \exists v \colon (u,v) \in R_1 \text{ and } (v,w) \in R_2\}$. Union, intersection and difference between relations are defined in the usual set-theoretic sense. The strongly connected components of a binary relation R are defined in the usual way as inclusionwise maximal sets $S \subseteq dom(R) \cap codom(R)$ such that for all $u,v \in S$ there is an R-path of length at least 1 from u to v. (In particular a singleton set $\{u\}$ can be a strongly connected component only if $(u,u) \in R$.) We write SCC(R) to denote the set of strongly connected components of R. Moreover, we let $R^{scc} := \bigcup_{S \in SCC(R)} S^2$ be the relation describing whether two elements are in the same strongly connected component.

For a set V, the diagonal of V is the relation $\operatorname{diag}(V) := \{(v,v) \mid v \in V\}$. For a relation R we let $R^{\operatorname{diag}} := R \cap \operatorname{diag}(\operatorname{dom}(R))$ be the diagonal elements in R. We call R a diagonal relation if $R = R^{\operatorname{diag}} = \operatorname{diag}(\operatorname{dom}(R))$.

A vocabulary is a finite set τ of binary relation symbols. In some places, we need to specify how relation symbols $R \in \tau$ are represented: we always assume that they are binary strings $R \in \{0,1\}^*$. In particular, this allows us to order the relation symbols lexicographically. Note that the lexicographical order on the relation symbols induces a linear order on each vocabulary τ . This will be important later, because it allows us to represent vocabularies in a canonical way. Let $R_1, \ldots, R_t \in \{0,1\}^*$ be the sequence of all relation symbols in τ according to the lexicographical order. A τ -structure A is a tuple $(V(A), R_1(A), \ldots, R_t(A))$ consisting of a finite set V(A), the vertex set or universe, and a (possibly empty) relation $R(A) \subseteq V(A)^2$ for each relation symbol $R \in \tau$. We view graphs as structures whose vocabulary consist of a single relation symbol E. While we are mainly interested in graphs, to develop our theory it will be necessary to consider general structures. We may see structures as directed graphs with coloured edges; each binary relation symbol corresponds to an edge colour and edges may have multiple colours. Note that we can also simulate unary relations and hence vertex colourings in binary structures A by diagonal relations.

Besides substructures of a structure (obtained by deleting vertices and edges) and restrictions of a structure (obtained by removing entire relations from the structure and the vocabulary), we sometimes need to consider a combination of both. Let A be a τ -structure and let $\widetilde{\tau} \subseteq \tau$ and $\widetilde{V} \subseteq V(A)$. The $\widetilde{\tau}$ -subrestriction of A on \widetilde{V} is the $\widetilde{\tau}$ structure $\widetilde{A} := A[\widetilde{\tau}, \widetilde{V}]$ with universe $V(\widetilde{A}) = \widetilde{V}$ and $E(\widetilde{A}) = E(A) \cap \widetilde{V}^2$ for all $E \in \widetilde{\tau}$. We write $A[\widetilde{V}]$ to denote $A[\tau, \widetilde{V}]$.

The Gaifman graph of a τ structure A is the undirected graph with vertex set V(A) in which two elements v, w are adjacent if they are related by some relation of A, that is, $(v, w) \in R(A)$ or $(w, v) \in R(A)$ for some $R \in \tau$. A structure A is connected if its Gaifman graph is connected.

Isomorphisms between τ -structures are defined as bijective mappings between their universes that preserve all relations. We write $A \cong A'$ to denote that A and A' are isomorphic. Structures of distinct vocabularies are non-isomorphic by definition. A property \mathcal{P} of structures is an isomorphism closed class of structures. If all structures in \mathcal{P} have the same vocabulary τ , then \mathcal{P} is a property of τ -structures. An invariant for a class \mathcal{C} of structures (that we usually assume to be closed under isomorphism) is a mapping \mathcal{I} with domain \mathcal{C} such that $A \cong A' \Longrightarrow \mathcal{I}(A) = \mathcal{I}(A')$. If the converse also holds, that is, $A \cong A' \iff \mathcal{I}(A) = \mathcal{I}(A')$, then \mathcal{I} is a complete invariant for \mathcal{C} . A canonical form is a complete invariant Can whose range also consists of structures from \mathcal{C} and that satisfies $A \cong \operatorname{Can}(A)$ for all A.

When carrying out computations on structures, we need to fix an encoding by binary strings. One way of doing this is to first specify the vocabulary, as a list of binary strings representing the relation symbols, then the universe, also as a list of binary strings representing the elements, and then the actual relations as lists of pairs of strings. The details of this encoding are not important. However, it is important to note that this encoding is *not* canonical: isomorphic structures may end up with different string

encodings. Moreover, the encoding depends on how we represent the elements of the universe by binary strings, implicitly fixing a linear order on the universe. Obviously, the output of an algorithm computing a property or invariant of abstract structures must not depend on this choice.

Coherent Configurations and the Weisfeiler-Leman Algorithm

Let σ be a vocabulary. A coherent σ -configuration C is a σ -structure C with the following properties.

- $\{R(C) \mid R \in \sigma\}$ is a partition of $V(C)^2$. In particular, all relations R(C) must be nonempty.
- For each $R \in \sigma$ the relation R(C) is either a subset of or disjoint from the diagonal diag(V(C)).
- For each $R \in \sigma$ there is an $R^{-1} \in \sigma$ such that $R^{-1}(C) = R(C)^{-1}$.
- For all triples $R_1, R_2, R_3 \in \sigma$ there is a number $q = q(R_1, R_2, R_3) \in \mathbb{N}$ such that for all $(u, v) \in R_1(C)$ there are exactly q elements $w \in V(C)$ such that $(u, w) \in R_2(C)$ and $(w, v) \in R_3(C)$.

The numbers $q(R_1, R_2, R_3)$ are called the *intersection numbers* of C and the function $q: \sigma^3 \to \mathbb{N}$ is called the *intersection function*.

We say that a coherent σ -configuration C is at least as fine as, or refines, a τ -structure A (we write $C \sqsubseteq A$) if V(C) = V(A) and for each $R \in \sigma$ and each $E \in \tau$ it holds that $R(C) \subseteq E(A)$ or $R(C) \subseteq V(A)^2 \setminus E(A)$. Conversely, we say that A is at least as coarse as, or coarsens, C. Two coherent configurations C, C' are equally fine, written $C \equiv C'$, if $C \sqsubseteq C'$ and $C' \sqsubseteq C$. In this case, the coherent structures are equal up to a renaming of the vertices and the relation symbols. We say that a coherent configuration C is a coarsest coherent configuration refining a structure A if $C \sqsubseteq A$ and $C' \sqsubseteq C$ for every coherent configuration C' satisfying $C' \sqsubseteq A$. If both C, C' are coarsest coherent configurations refining A, then $C \equiv C'$.

Theorem 2 ([19, 26]). For every binary structure A there is a coarsest coherent configuration C refining A, and given A it can be computed in polynomial time (time $\mathcal{O}(n^3 \log n)$, to be precise).

A coherently σ -coloured τ -structure is a pair (A,C) consisting of a τ -structure A and a coherent σ -configuration C refining A (and thus it holds V(A) = V(C)). Unless explicitly stated otherwise, we always assume that the vocabulary of A is τ and the vocabulary of C is σ , and we say that the vocabulary of (A,C) is (τ,σ) . We call the relation symbols in σ colours, whereas we keep calling the symbols in τ relation symbols. We usually denote colours (from σ) by R and relation symbols (from τ) by E.

We define the *symbolic subset relation* of a coherently coloured structure (A, C) to be the binary relation $\subseteq_{\sigma,\tau} = \{(R, E) \in \sigma \times \tau \mid R(C) \subseteq E(A)\} \subseteq \sigma \times \tau$. We often omit

the subscripts and just write $R \subseteq E$ instead of $R \subseteq_{\sigma,\tau} E$. The algebraic sketch of a coherently coloured structure (A,C) is the tuple

$$D(A,C) = (\tau, \sigma, \subseteq_{\sigma,\tau}, q)$$

consisting of the vocabularies τ , σ , the symbolic subset relation $\subseteq_{\sigma,\tau}$, and the intersection function $q:\sigma^3\to\mathbb{N}$ of C.

The next lemma says that for all coherently coloured structures (A, C), we can choose a canonical coarsest coherent configuration C(A) in the set $\{C' \mid C' \sqsubseteq A\}$.

Lemma 3. There is a polynomial-time algorithm that, for a given algebraic sketch D(A, C'), computes the algebraic sketch of D(A, C) of a coherently coloured structure (A, C) where C is a canonical coarsest coherent configuration of A.

The assertion that C is canonical means that C = C(A) only depends on A, i.e., for algebraic sketches D(A, C'), D(A, C'') the algorithm has the same output. We also write D(A) to denote the algebraic sketch D(A, C(A)).

In fact, the previous lemma implies that we can choose a string encoding for D(A) = D(A, C(A)) canonically. Formally, this means that we have a function enc mapping each structure A to a binary string $\operatorname{enc}(A)$ representing D(A) such that for isomorphic structures A, A' we have $\operatorname{enc}(D(A)) = \operatorname{enc}(D(A'))$. To obtain a canonical string encoding, we have to explain how to encode algebraic sketches. Algebraic sketches are tuples consisting of sets and relations on binary strings and natural numbers and as such can be encoded by binary strings. We encode the natural numbers using the unary representation. With a unary representation the encoding size of the sketch of a coherently coloured structure (A, C(A)) and the encoding size n := |D(A)| are polynomially bounded in each other. This will be useful later.

3. Deep Weisfeiler Leman

A DeepWL-algorithm is a 2-tape Turing machine M with an additional storage device C_{cc} , called cloud, that maintains a coherently coloured structure (A, C(A)). The machine has a work tape T_{wk} and an *interaction tape* T_{ia} that allows a limited form of interaction with the coherently coloured structure in the cloud C_{cc} .

The input of a DeepWL-algorithm M is a structure A (the vocabulary τ of A does not need to be fixed and can vary across the inputs). For the starting configuration of M on input A, the machine is initialised with the coherently coloured structure (A, C(A)) in the cloud and with the algebraic sketch D(A) = D(A, C(A)) (canonically encoded as a string) on the interaction tape. The work tape is initially empty. The Turing machine never has direct access to the structures in its cloud, but it operates on relation symbols and vocabularies. (Recall our assumption that relation symbols are binary strings.)

The Turing machine works as a standard 2-tape Turing machine. Additionally, there are three particular transitions that can modify the coherently coloured structure in the cloud. For such transitions, the Turing machine writes a relation symbol $X \in \tau \cup \sigma$ or a set of colours $\pi \subseteq \sigma$ on the interaction tape and enters one of the four states q_{addPair} ,

 $q_{\mathtt{contract}}$, $q_{\mathtt{create}}$ and $q_{\mathtt{forget}}$. We say that the Turing machine executes $\mathtt{addPair}(X)$, $\mathtt{contract}(X)$, $\mathtt{create}(\pi)$, $\mathtt{forget}(X)$, respectively. These transitions modify the structure A that is stored in the cloud. In particular, they can create new relations and possibly new elements that are added to the structure.

addPair(X). The state q_{addPair} can be entered while $X \in \tau \cup \sigma$ is written on the interaction tape. If $X = E \in \tau$ is a relation symbol, let P := E(A), otherwise if $X = R \in \sigma$ is a colour, let P := R(C(A)). In this case, the machine will add a fresh vertex to the universe for each of the pairs contained in P. Formally, we update $V(A) \leftarrow V(A) \cup P$ (where \cup denotes the disjoint union operator which we assume to be defined in some formally correct way, but we never worry about the identity (or name) of the elements in the disjoint union). Next, we will create relations that describe how the fresh vertices relate to the old universe. We update $\tau \leftarrow \tau \cup \{E_{\text{left}}, E_{\text{right}}\}$ and define D_X to be the lexicographically first binary string that is not already contained in τ and then we update $\tau \leftarrow \tau \cup \{D_X\}$ again. The relation D_X describes the fresh vertices: $D_X(A) := \text{diag}(P)$. The relations $E_{\text{left}}(A), E_{\text{right}}(A)$ describe how the fresh vertices relate to the old universe: $E_{\text{left}}(A) \leftarrow E_{\text{left}}(A) \cup \{(u, (u, v)) \in V(A)^2 \mid (u, v) \in P\}$ and $E_{\text{right}}(A) \leftarrow E_{\text{right}}(A) \cup \{(v, (u, v)) \in V(A)^2 \mid (u, v) \in P\}$ (in case that $E_{\text{left}}, E_{\text{right}}$ were not already defined, we initialise $E_{\text{left}}(A), E_{\text{right}}(A)$ with the empty set before we take the union).

contract(X). The state $q_{\texttt{contract}}$ can be entered while $X \in \tau \cup \sigma$ is written on the interaction tape. We will define a set $\mathcal{S} := \text{SCC}(U)$ consisting of strongly connected components. If $X = E \in \tau$ is a relation symbol, let $\mathcal{S} := \text{SCC}(E(A))$, otherwise if $X = R \in \sigma$ is a colour, let $\mathcal{S} := \text{SCC}(R(C(A)))$. Let $U := V(A) \setminus \bigcup \mathcal{S}$. Next, we will contract these components: we update $V(A) \leftarrow U \cup \mathcal{S}$. Let D_X be the lexicographically first binary string that is not already contained in τ and update $\tau \leftarrow \tau \cup \{D_X\}$. The relation D_X describes the fresh vertices: $D_X(A) := \text{diag}(\mathcal{S})$. We update the relations for each $E \in \tau$ and set $E(A) \leftarrow (E(A) \cap U^2) \cup \{(u, S) \mid \exists v \in S \in \mathcal{S} : (u, v) \in E(A)\} \cup \{(S, v) \mid \exists u \in S \in \mathcal{S} : (u, v) \in E(A)\}$.

 $\mathtt{create}(\pi)$. The state $q_{\mathtt{create}}$ can be entered while $\pi \subseteq \sigma$ is written on the interaction tape. Let E_{π} be the lexicographically first binary string that is not already contained in τ and then update $\tau := \tau \cup \{E_{\pi}\}$ where $E_{\pi}(A) := \bigcup_{R \in \pi} R(C(A))$.

forget(X). The state $q_{\texttt{forget}}$ is entered while $X = E \in \tau$ is written on the interaction tape. We update $\tau \leftarrow \tau \setminus \{E\}$.

Each of these four transitions therefore modify the structure A in the cloud. After such a transition, the machine recomputes the coarsest coherent configuration C(A) refining A. The coherently coloured structure (A, C(A)) is stored in the cloud and the algebraic sketch D(A) (canonically encoded as a string) is written on the interaction tape.

Let us define the running time of DeepWL-algorithms. Recall that the input of the underlying Turing machine is the algebraic sketch D(A). For the running time we take

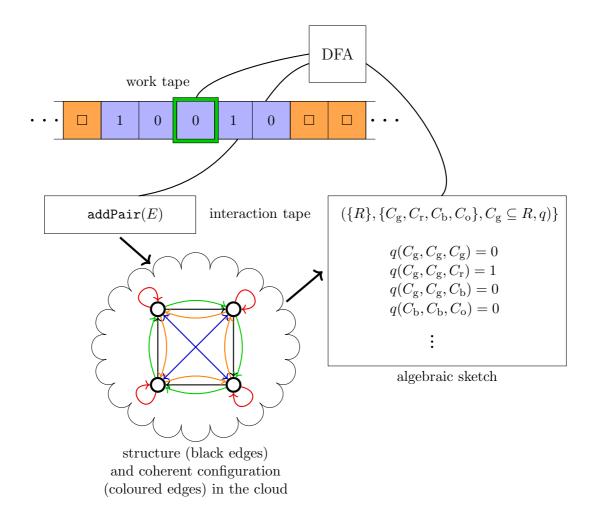


Figure 2: A DeepWL Turing machine

the following costs into account. Each transition taken by the Turing machine counts as one time step. For an input structure A, we take n-many steps into account to write down the initial algebraic sketch D(A) to the tape (where n = |D(A)| is the encoding length of D(A)). Recall, that the intersection numbers are encoded using unary representation and therefore each DeepWL-algorithm needs at least linear time (in |V(A)|). Similar, we also take n'-many steps into to write down the updated algebraic sketch D(A') to the interaction tape (where n' = |D(A')| is the encoding length of D(A')). We say that a DeepWL-algorithm M runs in polynomial time if there is a polynomial p in n = |D(A)| that bounds the running time of M. The definition of polynomial time remains unchanged if we take polynomial costs into account for maintaining the cloud (such as the running time of the Weisfeiler-Leman algorithm).

Isomorphism Invariance

Whenever a DeepWL-computation creates new elements, there is an issue with the identity (or name) of these new elements. This problem is implicit in our usage of the disjoint union operator in the definitions. We do not have to worry about this, because DeepWL-algorithms never have direct access to the structure in the cloud and only depend on its isomorphism types. All we need to make sure is that in every step the newly created elements are distinct from the existing ones.

Since it will be very important throughout the paper, let us state the invariance condition more formally. We define the *internal run* of a DeepWL-algorithm M on input A to be the sequence of configurations of the underlying Turing machine without the content of the cloud. Then the internal run of a DeepWL-algorithm is isomorphism invariant: if A and A' are isomorphic τ -structures, then D(A) = D(A') and therefore the internal run of a DeepWL-algorithm M on input A is identical with the internal run of M on input A'. The contents of the clouds in the computations of M on inputs A and A' may differ, but they are isomorphic in the corresponding steps of the computations.

DeepWL-Decidability and Computability

A DeepWL-algorithm accepts an input if the algorithm halts with 1 written under the head on the work tape. A DeepWL-algorithm decides a property \mathcal{P} of structures if it accepts an input structure A whenever $A \in \mathcal{P}$ and rejects A otherwise. (We do not require that all structures in \mathcal{P} have the same vocabulary.)

A DeepWL-algorithm computes a function $\mathcal{I}: \mathcal{A} \to \{0,1\}^*$ for a class \mathcal{A} of structures if on input $A \in \mathcal{A}$ it stops with $\mathcal{I}(A) \in \{0,1\}^*$ on the work tape. Observe that if $\mathcal{I}: \mathcal{A} \to \{0,1\}^*$ is DeepWL-computable then it is an invariant, that is, if $A, A' \in \mathcal{A}$ are isomorphic then $\mathcal{I}(A) = \mathcal{I}(A')$.

Let \mathcal{E} be a function that maps each structure A to a binary relation $\mathcal{E}(A)$ over V(A). A DeepWL-algorithm computes \mathcal{E} if on input $A \in \mathcal{A}$ it stops with a coherently σ' -coloured τ' -structure (A', C(A')) and the encoding of a relation symbol $E' \in \tau'$ on the work tape such that $E'(A') = \mathcal{E}(A)$.

Let \mathcal{S} be a function that maps each structure A to a subset $\mathcal{S}(A) \subseteq V(A)$. A DeepWL-algorithm computes \mathcal{S} if it computes $\mathcal{E}(A) := \operatorname{diag}(\mathcal{S}(A))$.

Basic DeepWL-computable functions

In the following three lemmas, we collect a few basic properties and functions that are DeepWL-computable.

Lemma 4. Let $E_1, E_2 \in \{0, 1\}^*$ be two relation symbols. Then the following functions on the class of all τ -structures with $E_1, E_2 \in \tau$ are DeepWL-computable in polynomial time.

1.
$$\mathcal{E}_{\cup}(A) := E_1(A) \cup E_2(A)$$
.

2.
$$\mathcal{E}_{\cap}(A) := E_1(A) \cap E_2(A)$$
.

```
3. \mathcal{E}_{\backslash}(A) := E_1(A) \backslash E_2(A).
```

4.
$$\mathcal{E}_{\text{diag}}(A) := \text{diag}(V(A)).$$

5.
$$\mathcal{E}_{-1}(A) := E_1(A)^{-1}$$
.

6.
$$\mathcal{E}_{0}(A) := E_{1}(A) \circ E_{2}(A)$$
.

7.
$$\mathcal{E}_{\mathrm{scc}}(A) := E_1(A)^{\mathrm{scc}}$$
.

Moreover, all the above functions are computable by polynomial-time DeepWL-algorithms that do not add any new vertices to the structure.

Lemma 5. Let $E_1, E_2 \in \{0,1\}^*$ be two relation symbols. Then the following properties of τ -structures with $E_1, E_2 \in \tau$ are DeepWL-decidable in polynomial time.

1.
$$\mathcal{P}_{\subset} := \{ A \mid E_1(A) \subseteq E_2(A) \} \text{ and } \mathcal{P}_{=} := \{ A \mid E_1(A) = E_2(A) \}.$$

2.
$$\mathcal{P}_{\parallel < \parallel} := \{A \mid |E_1(A)| \le |E_2(A)|\} \text{ and } \mathcal{P}_{\parallel = \parallel} := \{A \mid |E_1(A)| = |E_2(A)|\}.$$

Moreover, all the above properties are decidable by polynomial-time DeepWL-algorithms that do not add any new vertices to the structure.

Lemma 6. Let $E \in \{0,1\}^*$ be a relation symbol. Then the following functions S on the class of all τ -structures with $E \in \tau$ are DeepWL-computable in polynomial time.

- 1. S(A) := dom(E(A)).
- 2. $S(A) := \operatorname{codom}(E(A))$.
- 3. $S(A) := \sup(E(A))$.

Moreover, all the above functions are computable by polynomial-time DeepWL-algorithms that do not add any new vertices to the structure.

4. Pure Deep Weisfeiler Leman

A DeepWL-algorithm is called *pure* if the algorithm executes $\mathtt{addPair}(R)$ and $\mathtt{contract}(R)$ only for colours $R \in \sigma$ and not for relation symbols $E \in \tau$. It is sometimes convenient to only consider pure DeepWL-algorithms, and it is an indication of the robustness of the definition that every DeepWL-algorithm is equivalent to a pure one.

Theorem 7. Let \mathcal{E} be a function that assigns each structure A a relation $\mathcal{E}(A)$ and that is DeepWL-computable in polynomial time. Then there is a pure DeepWL-algorithm that computes \mathcal{E} in polynomial-time. (The same holds for functions $\mathcal{I}: \mathcal{A} \to \{0,1\}^*$ and properties $\mathcal{P}: \mathcal{A} \to \{0,1\}$.)

5. Normalised Deep Weisfeiler Leman

This section focuses on DeepWL-algorithms M that decide isomorphism on a class C. There are actually two natural ways of using DeepWL to decide isomorphism.

The first is the obvious one if we take DeepWL as a computation model: an isomorphism test implemented in DeepWL takes the disjoint union of two structures as its input and then decides if they are isomorphic. For simplicity, we assume that the two structures are connected; we can always achieve this by adding a new relation that relates all elements of the respective structures. The disjoint union of two τ -structures A_1 and A_2 is the τ -structure $A := A_1 \uplus A_2$ with universe $V(A) = V(A_1) \cup V(A_2)$ and relations $E(A) = E(A_1) \cup E(A_2)$ for $E \in \tau$. A DeepWL-isomorphism test takes the disjoint union $A_1 \uplus A_2$ of two connected τ -structures as its input and decides the property of the two components of its input structure being isomorphic. We say that a DeepWL-algorithm decides isomorphism on a class $\mathcal C$ of structures if it correctly decides isomorphism for structures $A_1, A_2 \in \mathcal C$.

The second way of using DeepWL to decide isomorphism is inspired by the way the classical Weisfeiler-Leman algorithm is used to decide isomorphism: the WL algorithm is said to distinguish two structures A_1 and A_2 if the algebraic sketches $D(A_1)$ and $D(A_2)$ are distinct. Note that this is an incomplete isomorphism test, because two structures may have the same algebraic sketch even though they are non-isomorphic. Generalising this notion, we say that a DeepWL-algorithm distinguishes two τ -structures A_1 and A_2 if on input A_i the algorithm halts with coherently coloured structure $(A_i', C(A_i'))$ in the cloud such that $D(A_1') \neq D(A_2')$. (Note that here the algorithm only takes a single structure as its input.) If A_1 and A_2 are isomorphic, it can never happen that a DeepWL-algorithm distinguishes them, because DeepWL-computations are isomorphism invariant. However, as for the classical Weisfeiler-Leman algorithm, there may be non-isomorphic structures not distinguished by the algorithm. We say that a DeepWL-algorithm is a distinguisher for a class $\mathcal C$ of structures if it distinguishes all non-isomorphic structures $A_1, A_2 \in \mathcal C$.

In this section, we shall prove that for each class \mathcal{C} of structures, there is a polynomial-time DeepWL-algorithm deciding isomorphism on \mathcal{C} if and only if there is a polynomial-time DeepWL-algorithm that is a distinguisher for \mathcal{C} (Theorem 13). Thus the two concepts we just defined agree. This is a nontrivial theorem that is an important step towards a central goal of the paper: to turn isomorphism testing algorithms into canonisation algorithms (Question B). The reason why the equivalence between isomorphism test and distinguisher is important is that a canonisation algorithm, just like a distinguisher, only works on one input structure, whereas an isomorphism test works on two structures simultaneously. In fact, this issue lies at the heart of the isomorphism versus canonisation problem. So, in order to modify a DeepWL-isomorphism test we first have to decouple the computations on the two structures from each other, that is, transform an isomorphism test into a distinguisher.

The main technical complication in doing so is that a DeepWL-algorithm working on the disjoint union of two graphs can create pairs with endpoints in each of the structures and then create pairs of such pairs and so on, which makes an association of the created objects with one of the structures impossible. We will call algorithms that avoid such constructions normalised. The largest part of this section is devoted to a proof that it suffices to consider normalised algorithms.

We say that $v \in V(A_1 \uplus A_2)$ belongs to A_i if $v \in V(A_i)$ for $i \in \{1,2\}$. We consider structures A that are iteratively obtained from $A_1 \uplus A_2$ by applying the DeepWL-algorithm M. Inductively, if M adds a pair (u,v) to the universe where both u,v belong the same structure A_i , then we say that the fresh vertex (u,v) belongs to A_i for $i \in \{1,2\}$. Analogously, if M contracts a component $S \in SCC(R(C(A)))$ where all vertices in S belong to the same structure A_i , then we say that the fresh vertex S belongs to A_i for $i \in \{1,2\}$. We define $\mathcal{V}_i(A) := \{v \in V(A) \mid v \text{ belongs to } A_i\}$ for both $i \in \{1,2\}$. The vertices $\mathcal{V}_{\text{plain}}(A) := \mathcal{V}_1(A) \cup \mathcal{V}_2(A)$ are called plain. The edges $\mathcal{E}_{\text{plain}}(A) := \mathcal{V}_1(A)^2 \cup \mathcal{V}_2(A)^2$ are called plain. The edges $\mathcal{E}_{\text{cross}}(A) := \{(v_i, v_j) \mid v_i \in \mathcal{V}_i(A), v_j \in \mathcal{V}_j(A), i \neq j \in \{1,2\}\}$ are called crossing. We write σ_{cross} , to denote the set of colours $R \in \sigma$ such that $R(C(A)) \subseteq \mathcal{E}_{\text{cross}}(A)$. Analogously, we define σ_{plain} . Note that it might be the case, that a relation is neither a subset of $\mathcal{E}_{\text{plain}}(A)$ nor $\mathcal{E}_{\text{cross}}(A)$. In such a case, the relation is neither plain nor crossing. The goal is to avoid the construction of such relations.

A DeepWL-algorithm M that decides isomorphism on a class \mathcal{C} is called *normalised* if at any point in time $V(A) = \mathcal{V}_{\text{plain}}(A)$ and A consists of exactly two connected components $(\mathcal{V}_1(A) \text{ and } \mathcal{V}_2(A))$. We also say that a structure A is *normalised* if it is obtained from a normalised DeepWL-algorithm.

Since a normalised structure A consists of exactly two connected components during the entire run, its holds that $\sigma = \sigma_{\text{plain}} \cup \sigma_{\text{cross}}$ for vocabulary of the coherent configuration C(A). Moreover, $\mathcal{E}_{\text{plain}}$ and $\mathcal{E}_{\text{cross}}$ are DeepWL-computable functions since a DeepWL-algorithm can detect whether a colour belongs to edges between the same and between distinct connected components. Since all relation symbols are plain, we can see A as a disjoint union of its subrestrictions $A[\mathcal{V}_1(A)]$ and $A[\mathcal{V}_2(A)]$. The following lemma gives a connection between the coherent configuration C(A) and its subrestrictions.

Lemma 8. Let A be a τ -structure that is normalised. Let $\sigma_i \subseteq \sigma$ be the set of colours R such that $R(C(A)) \cap \mathcal{V}_i(A)^2 \neq \emptyset$. Let $A_i := A[\mathcal{V}_i(A)]$ be the τ -subrestriction, and let $C_i := C(A)[\sigma_i, \mathcal{V}_i(A)]$ be the σ_i -subrestriction, for $i \in \{1, 2\}$.

- 1. It holds $\sigma = (\sigma_1 \cup \sigma_2) \cup \sigma_{\text{cross}}$ and for each $R \in \sigma_{\text{cross}}$, there are diagonal colours $R_1 \in \sigma_1, R_2 \in \sigma_2$ such that $R(C(A)) = \{(v_1, v_2) \in \mathcal{E}_{\text{cross}}(A) \mid v_i \in \text{supp}(R_i(C))\}$,
- (A_i, C_i) is again a coherently coloured structure.
 Moreover, given the set {D(A₁, C₁), D(A₂, C₂)}, the algebraic sketch D(A) can be computed in polynomial time,
- 3. The coherent configurations C_i and $C(A_i)$ are equally fine (i.e., $C_i \equiv C(A_i)$). Moreover, when given the set $\{D(A_1), D(A_2)\}$, the set $\{D(A_1, C_1), D(A_2, C_2)\}$ can be computed in polynomial time.

By A_R , we denote the structure that is obtained from A by executing contract(R) for some colour $R \in \sigma$. The next lemma tells us that, given D(A), the algebraic sketch

 $D(A_R)$ can be computed (by a Turing machine). In this sense, the contraction of strongly connected components does not lead to new information. However, it can still be useful, since it shrinks the size of the universe which might help to ensure a polynomial bound on the universe size.

Lemma 9. Let A be a τ -structure.

- 1. There is a polynomial-time algorithm that for a given algebraic sketch D(A) and a given colour $R \in \sigma$, computes the algebraic sketch $D(A_R)$.
- 2. The coherent configuration $C(A)[V(A) \setminus \bigcup S]$ refines $C(A_R)[V(A_R) \setminus S]$ where S := SCC(R(A)).

The next lemma is of a similar flavour. It states that we do not get any information if we apply $\mathtt{addPair}(R)$ to a coherently coloured structure that is normalised where $R \in \sigma_{\mathrm{cross}}$. By A^R , we denote the structure that is obtained from A by executing $\mathtt{addPair}(R)$ for a colour $R \in \sigma$ with $R \subseteq \mathcal{E}_{\mathrm{cross}}(A)$. More generally, we write A^ω to denote the structure that is obtained from A by executing $\mathtt{addPair}(R)$ for all colours $R \in \omega \subseteq \sigma$.

Lemma 10. Let A be a τ -structure that is normalised and let $\omega \subseteq \sigma_{cross}$ be a set of crossing colours.

- 1. There is a polynomial-time algorithm that for a given algebraic sketch D(A) and a given ω , computes the algebraic sketch $D(A^{\omega})$.
- 2. The coherent configurations C(A) and $C(A^{\omega})[V(A)]$ are equally fine (i.e., $C(A) \equiv C(A^{\omega})[V(A)]$).

Towards showing that all DeepWL-algorithm can be assumed to be normalised we take an intermediate step of algorithms that are almost normalised.

Almost Normalised DeepWL

In the following, let M be a DeepWL-algorithm that decides isomorphism on \mathcal{C} . If M adds a pair $v = (v_1, v_2)$ to the universe where $(v_1, v_2) \in \mathcal{E}_{cross}(A)$, then that fresh vertex v is called a *crossing* pair. The set of crossing vertices is denoted by $\mathcal{V}_{cross}(A)$. Let $\mathcal{V}_{pair}(A)$ denote the set of all pair-vertices (created by adding pairs).

A DeepWL-algorithm M that decides isomorphism on a class \mathcal{C} is called almost normalised if each created pair-vertex is either plain or crossing, i.e., at every point in time $\mathcal{V}_{\text{pair}}(A) \subseteq \mathcal{V}_{\text{plain}}(A) \cup \mathcal{V}_{\text{cross}}(A)$. Furthermore, we require for forget(E)-executions that $E \notin \{E_{\text{left}}, E_{\text{right}}\} \cup \tau$. This additional requirement ensures that $\mathcal{E}_{\text{plain}}, \mathcal{E}_{\text{cross}}, \mathcal{V}_{\text{plain}}, \mathcal{V}_{\text{cross}}$ are DeepWL-computable functions.

We say that a structure A is almost normalised if it is computed by an almost normalised DeepWL-algorithm.

Lemma 11. Assume that isomorphism on some class C is DeepWL-decidable in polynomial time. Then, isomorphism on C is decidable by an almost normalised DeepWL-algorithm in polynomial time.

The proof of the lemma shows how to simulate a DeepWL-algorithm \widehat{M} with an almost normalised algorithm M. While technically quite involved, the idea behind it is simple. To simulate \widehat{M} , we need to guarantee that all vertices that are created are actually crossing or plain, that is, they are formed from pairs of plain vertices. For this, we continuously guarantee that for each vertex v created so far, there are two unique plain vertices $p_{\text{le}}(v)$, $p_{\text{ri}}(v)$ that are only associated with v. Instead of creating a new pair (v, v') for two arbitrary vertices we will then create the pair $(p_{\text{le}}(v), p_{\text{ri}}(v'))$ instead. The crucial point is that this way the new vertex is still plain or crossing because $p_{\text{le}}(v)$ and $p_{\text{ri}}(v)$ are plain.

There is a second less severe issue that we need to take care of, namely vertices that are crossing could lose this property if the two plain end-points of which they are the crossing pair are contracted away. For this reason we copy vertices and use the originals when applying addPair-operations. We use copies to create pairs but only ever contract originals, which resolves the second issue. For details we refer to Appendix D.

Lemma 12. Assume that isomorphism on some class C is DeepWL-decidable in polynomial time. Then, isomorphism on C is decidable by a normalised DeepWL-algorithm in polynomial time.

Similarly to the previous lemma, the proof of this lemma shows how to simulate a DeepWL -algorithm that is almost normalised with a normalised DeepWL -algorithm. The crucial insight here is Lemma 10 which essentially says that we do not need to execute an $\mathsf{addPair}(R)$ -operation when the relation R is crossing, since we can compute the algebraic sketch of the result without modifying the contents of the cloud. One might be worried that we cannot continue to simulate the algorithm because the structure in the cloud was not modified, but Lemma 10 Part 2 shows that the coherent configuration does not become finer by any of the $\mathsf{addPair}$ -operations we only simulate. A similar statement holds for contractions by Lemma 9 Part 2. Again we refer to Appendix D for details.

Theorem 13. Let C be a class of τ -structures. The following statements are equivalent.

- 1. Isomorphism on C is DeepWL-decidable in polynomial time.
- 2. Some complete invariant on C is DeepWL-computable in polynomial time.
- 3. There is a DeepWL-distinguisher for C that runs in polynomial time.

Proof. To see that 3 implies 1, let M be an distinguisher for C. Given $A = A_1 \uplus A_2$, we simulate the distinguisher on A_1, A_2 in parallel. If the algebraic sketches $D(A_1)$ and $D(A_2)$ are distinct at some point in time, we stop the simulation and reject isomorphism. Otherwise, if the algebraic sketches coincide during the entire run, we accept. Since M is a distinguisher, the structures A_1 and A_2 are isomorphic.

To see that 2 implies 3, let M be a DeepWL-algorithm that computes a complete invariant on \mathcal{C} . Let A_1, A_2 be non-isomorphic. Then the runs ρ_1, ρ_2 of M on inputs A_1, A_2 are distinct. The only way this can happen is that at some point during the

computation the algebraic sketches are distinct. We need to make sure that they remain distinct until the end of the computation. We can achieve this by never executing a forget-operation and by making a copy of the elements that are deleted during a contract-operation before carrying out the contraction. Copying elements can easily be done by applying addPair to the corresponding diagonal colours. Since we never discard elements or relations, once distinct, the algebraic sketches can never become equal again. Of course now we always have a richer structure with a potentially finer coherent configuration in the cloud, but we can still simulate the original computation of M.

It remains to show that 1 implies 2. Let M be a DeepWL-algorithm that decides isomorphism on \mathcal{C} in polynomial-time, i.e., it accepts $A = A_1 \uplus A_2$ if and only if A_1, A_2 are isomorphic. By Lemma 12, there is a normalised DeepWL-algorithm M_{norm} that decides isomorphism on \mathcal{C} . We let $\rho_{\text{norm}}(A) \in \{0,1\}^*$ denote the internal run of the DeepWL-algorithm M_{norm} on input A. We claim that the function $\mathcal{I}(A_1) := \rho_{\text{norm}}(A_1 \uplus A_1)$ defines a complete invariant that is DeepWL-computable in polynomial time. To compute \mathcal{I} with a DeepWL-algorithm, we can easily simulate M_{norm} on input $A_1 \uplus A_1$ and track its internal run. We show that \mathcal{I} defines a complete invariant. Clearly, if A_1 and A_2 are isomorphic, then $\mathcal{I}(A_1) = \mathcal{I}(A_2)$. On the other hand, assume that $\mathcal{I}(A_1) = \mathcal{I}(A_2)$. By definition of \mathcal{I} , we have $I := \rho_{\text{norm}}(A_1 \uplus A_1) = \rho_{\text{norm}}(A_2 \uplus A_2)$. By Lemma 8, we have that $I = \rho_{\text{norm}}(A_1 \uplus A_2)$ since D(A) = D(A') if and only if $D(A[\mathcal{V}_i(A)]) \mid i \in \{1,2\}\} = \{D(A'[\mathcal{V}_i(A')]) \mid i \in \{1,2\}\}$ holds during the entire run. Since I is an accepting run and since M_{norm} decides isomorphism, it follows that A_1, A_2 are isomorphic.

We say that a class \mathcal{G} of vertex-coloured graphs is closed under colouring if all structures obtained from a graph in \mathcal{G} by changing the colouring also belong to \mathcal{G} . Formally, a vertex-coloured graph is a structure A with vocabulary $\tau = \{E, C_1, \ldots, C_t\}$ where E(A) is a binary relation and $C_i(A)$ are diagonal relations (which encode the i-th vertex colour). A class \mathcal{G} is closed under vertex-colouring if for each $\{E, C_1, \ldots, C_t\}$ -structure $A \in \mathcal{G}$ also the $\{E, C'_1, \ldots, C'_s\}$ -structure A' belongs to \mathcal{G} where E(A) = E(A') and $C'_i(A')$ are arbitrary diagonal relations.

Theorem 14 ([16]). Let \mathcal{G} be a class of coloured graphs that is closed under colouring. The following statements are equivalent.

- 1. Some complete invariant on C is computable in polynomial time.
- 2. Some canonical form on C is computable in polynomial time.

This gives us the following corollary.

Corollary 15. Let \mathcal{G} be a class of coloured graphs closed under colouring such that there is a polynomial time DeepWL algorithm deciding isomorphism on \mathcal{G} . Then there is a polynomial time canonisation algorithm for \mathcal{G} .

Remark 16. It can be shown that Corollary 15 also holds for arbitrary time-constructible time bounds of the form $T^{\mathcal{O}(1)}$ where T is at least linear. This can be shown using padding arguments.

6. Equivalence between CPT and DeepWL

In this section, we prove that DeepWL has the same expressiveness as the logic CPT, choiceless polynomial time with counting. As opposed to the previous sections, in this section we use fairly standard techniques from finite model theory. For this reason, and to avoid lengthy definitions, we only describe the high level arguments and omit the technical details.

Let us start with a very brief introduction to CPT, which follows the presentation of [13]. We start by introducing a language that we call BGS (for Blass, Gurevich, Shelah, the authors of the original paper introducing choiceless polynomial time). The syntactical objects of BGS are formulas and terms; the latter play the role of algorithms of DeepWL. Like DeepWL-algorithms, BGS-terms operate on a τ -structure A, the input structure. The terms are interpreted over the hereditarily finite sets over V(A), that is, elements of V(A), sets of elements of V(A), sets of sets of elements, et cetera. We denote the set of all these hereditarily finite sets by HF(A). BGS-formulas are Boolean combinations of formulas $t_1 = t_2$, $t_1 \in t_2$, and $R(t_1, t_2)$, where t_1, t_2 are terms and R is in the vocabulary of the input structure. The formulas $t_1 = t_2$ and $R(t_1, t_2)$ have the obvious meaning, $t_1 \in t_2$ means that $a_1 \in HF(A)$ interpreting t_1 is an element of $a_2 \in \mathrm{HF}(A)$ interpreting t_2 . Ordinary BGS-terms are formed using the binary function symbols Pair, Union, the unary function symbols TheUnique, Card, and the constant symbols Empty and Atoms. The constants are interpreted by the empty set and the set V(A), respectively. (The elements of V(A) are the "atoms" or "urelements" in HF(A).) To define the meaning of the function symbols, let t_1 , t_2 be terms that are interpreted by $a_1, a_2 \in HF(A)$. Then $Pair(t_1, t_2)$ is interpreted by $\{a_1, a_2\}$ and $Union(t_1, t_2)$ is interpreted by $a_1 \cup a_2$, where we treat the union with an atom like the union with the empty set. The Unique (t_1) is interpreted by b if $a_1 = \{b\}$ is a singleton set and by \emptyset otherwise. $Card(t_1)$ is interpreted by the cardinality of a_1 viewed as a von-Neumann ordinal. Besides the ordinary terms, BGS-logic has comprehension terms of the form

$$\{t\colon x\in u\colon \varphi\}. \tag{*}$$

Here t, u are terms, x is a variable that is not free in u, and φ is a formula. To emphasise the role of the variable x, we also write $\{t(x) \colon x \in u \colon \varphi(x)\}$. This term is interpreted by the set of all values t(a), where $a \in \mathrm{HF}(A)$ is an element of the set defined by the term u, and a satisfies the formula $\varphi(x)$. Note that t, u, and φ may have other free variables besides x. The third type of BGS-terms are iteration terms. For every term t that has exactly one free variable x we form a new term t^* . We also write t(x) and $t(x)^*$ to emphasise the role of the free variable x. The term t^* is interpreted by the fixed point of the sequence $t(\emptyset), t(t(\emptyset), t(t(t(\emptyset))), \ldots$, if such a fixed point exists, or by \emptyset if no fixed point exists. The free variables of terms and formulas are defined in the natural way, stipulating that the variable x in a comprehension term of the form (\star) and in an iteration term $t(x)^*$ be bound. As usual, a sentence is a formula without free variables.

CPT is the "polynomial-time fragment" of BGS. To define CPT formally, we restrict the length of iterations to be polynomial in the size of the input structure, and we restrict the number of elements of all sets that appear during the "execution" of a term to be polynomial.

This completes our short description of the syntax and semantics of BGS and CPT. For details, we refer the reader to [13] (or [6, 8] for other, equivalent, presentations of the language).

We say that a property \mathcal{P} of τ -structures is CPT-definable if there is a CPT-sentence φ satisfied precisely by the τ -structures in \mathcal{P} .

Lemma 17. Let \mathcal{P} be a property of τ -structures that is decidable by a polynomial time DeepWL-algorithm. Then \mathcal{P} is CPT-definable.

Proof. We show that we can simulate a polynomial time DeepWL-algorithm in CPT. Formally, for this we have to define a CPT-term that simulates a single computation step and then iterate this term, but we never go to this syntactic level. We only describe the high-level structure of the simulation by explaining how we can simulate the different steps carried out during a DeepWL-computation.

A basic fact that we use in this proof is that CPT is at least as expressive as fixed-point logic with counting FPC [6]. Moreover, we use the Immerman-Vardi Theorem [17, 25] stating that on ordered structures, FPC (even fixed-point logic without counting) can simulate all polynomial time computations.

In our CPT-simulation, we first generate the set N of the first n von-Neumann ordinals, where n is the size of the input structure, together with the natural linear order \leq of these ordinals. We use the ordered domain (N, \leq) to simulate the computation carried out by our DeepWL-algorithm. Since we are considering a polynomial time computation, we can do this in FPC and hence in CPT.

Moreover, during the computation we always maintain a copy of the structure A in the cloud. The elements as well as the relations of A are represented by hereditarily finite sets. To represent pairs of elements, we use the usual von-Neumann encoding of ordered pairs. We can represent the relations of A as sets of pairs, which are again hereditarily finite sets. To maintain the name of a relation, for every relation we create a pair (x,r) consisting of the relation, represented by a set x, and its name r, which is a von-Neumann ordinal whose binary representation is the name of the relation.

Now an addPair step can easily be simulated. For the contract-operation, we note that strongly connected components are definable in fixed-point logic. For create, we use the Union-operation, and forget is trivial.

It remains to explain how we deal with the coherent configurations that the DeepWL-algorithm maintains during its computation. For this, we use the fact that the coarsest coherent configuration of a structure, that is, the ordered partition of the pairs of elements into the colour classes computed by the 2-dimensional Weisfeiler Leman algorithm, is definable in the logic FPC [10, 23]. Thus we can compute the coherent configuration during our simulation, and using the Card-operation we can extract the algebraic sketch. This enables us to simulate all parts of a DeepWL-computation in CPT.

To prove the converse direction that DeepWL can decide all CPT-definable properties, rather than working with CPT directly, we will use the equivalent *interpretation logic*

introduced by Grädel, Pakusa, Schalthöfer and Kaiser [11].

Interpretation logic is based on the logic FO+H, first-order logic with a $H\ddot{a}rtig$ (or equal cardinality) quantifier: the meaning of the formula $Hx.\varphi_1(x).\varphi_2(x)$ is that the number of elements satisfying φ_1 equals the number of elements satisfying φ_2 . Next, we need to define a specific form of syntactical interpretation. A (2-dimensional) $[\tau, \tau']$ -interpretation (over FO+H) is a tuple

$$\mathcal{I} = (\varphi_V(x_1, x_2), \varphi_=((x_1, x_2), (x_1', x_2')), \varphi_E((x_1, x_2), (x_1', x_2'))_{E \in \tau'})$$

of FO+H-formulas. Such an interpretation maps each τ -structure A to a τ' -structure $\mathcal{I}(A)$ defined as follows. Let $V := \{(v_1, v_2) \in V(A)^2 \mid A \models \varphi_V(v_1, v_2)\}$, and let \sim be the finest equivalence relation on V such that $(v_1, v_2) \sim (v_1', v_2')$ for all $(v_1, v_2), (v_1', v_2') \in V$ with $A \models \varphi_=((v_1, v_2), (v_1', v_2'))$. Then the universe of $\mathcal{I}(A)$ is $V/_{\sim}$, and for every relation symbol $E \in \tau'$, the relation $E(\mathcal{I}(A))$ contains all pairs $(a, a') \in (V/_{\sim})^2$ such that there are $(v_1, v_2) \in a$, $(v_1', v_2') \in a'$ with $A \models \varphi_E(v_1, v_2, v_1', v_2')$.

Now we are ready to define interpretation logic IL. An $\mathsf{IL}[\tau]$ -program is a tuple $\Pi = (\mathcal{I}_{\mathsf{init}}, \mathcal{I}_{\mathsf{step}}, \varphi_{\mathsf{halt}}, \varphi_{\mathsf{out}})$ where for some vocabulary τ_{wk} , $\mathcal{I}_{\mathsf{init}}$ is a $[\tau, \tau_{\mathsf{wk}}]$ -interpretation, $\mathcal{I}_{\mathsf{step}}$ is a $[\tau_{\mathsf{wk}}, \tau_{\mathsf{wk}}]$ -interpretation, and φ_{halt} and φ_{out} are τ_{wk} -sentences. Let A be a τ -structure. A τ un of Π on A is a sequence of τ_{wk} -structures A_1, \ldots, A_m where $A_1 := \mathcal{I}_{\mathsf{init}}(A)$ and $A_{i+1} := \mathcal{I}_{\mathsf{step}}(A_i)$ and $A_i \nvDash \varphi_{\mathsf{halt}}$ for all $1 \leq i < m$ and $A_m \vDash \varphi_{\mathsf{halt}}$. The program $\mathsf{accepts}\ A$ if $A_m \vDash \varphi_{\mathsf{out}}$, otherwise it $\mathsf{rejects}$. We say that a program Π $\mathsf{decides}$ a property \mathcal{P} of τ -structures if it accepts an input structure A if $A \in \mathcal{P}$ and rejects A otherwise

We say that a program Π runs in polynomial time if $m + \sum_{1 \leq i \leq m} |V(A_i)|$ is bounded by a polynomial.

Theorem 18 ([11]). For every property \mathcal{P} of τ -structures, the following statements are equivalent.

- 1. P is decidable by a polynomial-time IL-program.
- 2. \mathcal{P} is CPT-definable.

The next lemma states that we can simulate FO+H-formulas in DeepWL.

Lemma 19. Let $\varphi(x_1, x_2)$ be an FO+H[τ]-sentence. Then the function mapping each τ -structure A to the binary relation $\varphi(A) := \{(v_1, v_2) \in V(A)^2 \mid A \models \varphi(x_1, x_2)\}$ is computable by a polynomial time DeepWL-algorithm.

Lemma 20. Let \mathcal{P} be a τ -property of structures that is decidable by a polynomial-time $\mathsf{IL}[\tau]$ -program. Then \mathcal{P} is decidable by a polynomial time DeepWL -algorithm.

Proof. Let $\Pi = (\mathcal{I}_{\text{init}}, \mathcal{I}_{\text{step}}, \varphi_{\text{halt}}, \varphi_{\text{out}})$ be an IL-program that decides \mathcal{P} in polynomial time. We have to simulate the run A_1, \ldots, A_m with a DeepWL-algorithm.

To simulate a single application of $\mathcal{I}_{\text{init}}$ or $\mathcal{I}_{\text{step}}$ applied to a structure A, we proceed as follows: using an addPair-operation, we first compute the extension A' of A by all pairs of elements. Now we can translate the formulas of the interpretation, which have

either 2 or 4 free variables, to formulas with 2 free variables ranging over A'. Then we can apply Lemma 19 to compute the image of the interpretation. Note that to factorise the structure by the equivalence relation \sim , we need to apply a contract-operation.

By repeatedly applying this construction, we can simulate the whole run of Π . To check the halting condition and generate the output, we note that we can formally regard the FO+H-sentences φ_{halt} and φ_{out} as formulas with 2 free dummy variables (these formulas are either satisfied by all pairs of elements or by none). Then we can apply Lemma 19 again.

Theorem 21. For every property \mathcal{P} of τ -structures, the following statements are equivalent.

- 1. \mathcal{P} is decidable by a polynomial-time DeepWL-algorithm.
- 2. \mathcal{P} is CPT-definable.

Proof. We combine Lemma 17, Theorem 18, and Lemma 20.

7. Concluding Remarks

DeepWL is a framework for combinatorial graph isomorphism tests generalising the Weisfeiler Leman algorithm of any dimension. DeepWL is strictly more powerful than Weisfeiler Leman; in particular, it can distinguish the so-called CFI-graphs that are hard examples for Weisfeiler Leman. We show that DeepWL has the same expressivity as the logic CPT (choiceless polynomial time). In some sense, DeepWL can be seen as an isomorphism (or equivalence) test corresponding to CPT in a similar way that Weisfeiler Leman is an isomorphism test corresponding to the logic FPC (fixed-point logic with counting).

The definition of DeepWL is fairly robust, as our result that all DeepWL algorithms are equivalent to more restricted "pure" DeepWL-algorithms shows.

As our main technical result, we prove that if DeepWL decides isomorphism on a class \mathcal{C} of graphs in polynomial time, then \mathcal{C} admits a polynomial time canonisation algorithm, and hence there is a logic capturing polynomial time on \mathcal{C} .

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Appendix

A. Proofs and Details Omitted from Section 2

Proof of Lemma 3. We define a series \leq_0, \leq_1, \ldots of finer and finer total quasiorders of σ .

For each $R \in \sigma$, define $\pi_R := \{E \in \tau \mid R \subseteq_{\sigma,\tau} E\}$. Recall that we assume the relation symbols to be binary strings. Thus the sets π_R are finite sets of binary strings and as such can be ordered lexicographically. We let $R \preceq_0 R'$ if π_R is lexicographically smaller or equal to $\pi_{R'}$. This gives us a total quasiorder. We also write $R \equiv_0 R'$ if $R \preceq_0 R'$ and $R' \preceq_0 R$. The equivalence class of $R \in \sigma$ is denoted by $[R]_0 := \{R' \in \sigma \mid R' \equiv_0 R\}$. Note that the set of equivalence classes $\sigma_0 = \{[R]_0 \mid R \in \sigma\}$ is linearly ordered.

Inductively, for each $R \in \sigma$, we define

$$\pi_{R,i+1} := \{ ([R_2]_i, [R_3]_i, \sum_{\substack{R'_2 \in [R_2]_i, R'_3 \in [R_3]_i}} q(R, R'_2, R'_3)) \mid R_2, R_3 \in \sigma \}.$$

Since the set of equivalence classes and the set of natural numbers are both linearly ordered sets, one can define a linear order also on the triples ($[R_2]_i$, $[R_3]_i$, q) contained in the sets $\pi_{R,i+1}$. We let $R \leq_{i+1} R'$ if $\pi_{R,i+1}$ is smaller or equal to $\pi_{R',i+1}$, i.e., it holds $|\pi_{R,i+1}| < |\pi_{R',i+1}|$ or $\pi_{R,i+1} = \pi_{R',i+1}$, or it holds $\pi_{R,i+1} \neq \pi_{R',i+1}$ and $|\pi_{R,i+1}| = |\pi_{R',i+1}|$ and the smallest triple in $\pi_{R,i+1} \setminus \pi_{R,i+1}$.

Let $m \in \mathbb{N}$ be the smallest number for which $\preceq_m = \preceq_{m+1}$. Now, " \preceq_m " defines a total linear order on the equivalence classes $[R]_m$. We claim that $\sigma_m := \{[R]_m \mid R \in \sigma\}$ with $[R]_m(C') := \bigcup_{R' \in [R]_m} R'(C')$ defines a coherent configuration refining A. Setting

$$q([R_1]_m, [R_2]_m, [R_3]_m) = \sum_{R_2' \in [R_2]_m, R_3' \in [R_3]_m} q(R_1, R_2', R_3')$$

is well defined (since $\leq_m = \leq_{m+1}$) and gives a coherent configuration. It refines A since $\sigma_0 = \{[R]_0 \mid R \in \sigma\}$ with $[R]_0(C') := \bigcup_{R' \in [R]_0} R'(C')$ already refines A by definition.

Next, we use this linear order to define a canonical set of relation symbols σ_A . We define σ_A as the set consisting of the first $|\sigma|$ binary strings that are not already contained in τ (w.r.t. to the lexicographic order on strings).

We have to show that for algebraic sketches D(A, C') and D(A, C''), we obtain the same result. Observe that the equivalence classes $[R]_i$ in each step might depend on the coherent configuration C'. However, it can easily shown by induction that the set of relations $\{\bigcup_{R'\in[R]_i} R'(C') \mid R \in \sigma\}$ does not depend on the choice of the coherent σ -configuration C'.

B. Proofs and Details Omitted from Section 3

Proof of Lemma 4. The DeepWL-algorithm uses the command $create(\pi)$ where π depends on the relation we want to compute. The resulting relation symbol E_{π} is written

to the work tape. The set $\pi \subseteq \sigma$ is specified using the algebraic sketch as follows.

- 1. For \mathcal{E}_{\cup} , let $\pi := \{ R \in \sigma \mid R \subseteq E_1 \text{ or } R \subseteq E_2 \}$.
- 2. For \mathcal{E}_{\cap} , let $\pi := \{ R \in \sigma \mid R \subseteq E_1 \text{ and } R \subseteq E_2 \}$.
- 3. For \mathcal{E}_{\setminus} , let $\pi := \{ R \in \sigma \mid R \subseteq E_1 \text{ and } R \not\subseteq E_2 \}$.
- 4. For $\mathcal{E}_{\text{diag}}$, let $\pi := \{R \in \sigma \mid \forall R', R'' \in \sigma, R' \neq R'' : q(R', R'', R) = 0\}$. We show that $R \in \pi$, if and only if R is a diagonal colour. Suppose $R \in \pi$ and $(u, v) \in R(C)$ and let $R' \in \sigma$ be a colour with $(u, u) \in R'(C)$. By the choice of R', it holds that $q(R, R', R) \geq 1$. Since $R \in \pi$, it holds that R = R' is a diagonal colour. On the other hand, assume that $R \in \sigma$ is a diagonal colour. Let $R', R'' \in \sigma$ be colours with $R \neq R'$. Since R(C), R'(C) are disjoint, it holds that q(R', R'', R) = 0. Hence, $R \in \pi$.
- 5. For \mathcal{E}_{-1} , let $\pi:=\{R\in\sigma\mid\exists R_1\in\sigma,R_1\subseteq E_1\exists R_2\in\sigma,R_2\text{ diagonal}:\ q(R_2,R_1,R)\geq 1\}$ (a DeepWL-algorithm can decide whether a colour $R\in\sigma$ is diagonal using 4). We show that $R\in\pi$, if and only if $R(C)\subseteq E_1(A)^{-1}$. Assume that $R\in\pi$. Equivalently, this means that there is a colour $R_1\in\sigma$ with $R_1\subseteq E_1$ and a diagonal colour $R_2\in\sigma$ such that $q(R_2,R_1,R)\geq 1$. This means that for all $(u,u)\in R_2$ there is a $w\in V(C)$ such that $(u,w)\in R_1(C)\subseteq E_1(A)$ and $(w,u)\in R(C)$. Therefore, $R(C)\cap E_1(A)^{-1}\neq\emptyset$. Since (A,C) is a coherently coloured structure, this is equivalent to $R(C)\subseteq E_1(A)^{-1}$. Conversely, if $R(C)\subseteq E_1(A)^{-1}$ and $(u,v)\in R(C)$ then choose R_2 so that it contains (v,v) and R_1 so that it contains (v,u), then $R_1\subseteq E_1$ and R_2 is diagonal and $q(R_2,R_1,R)\geq 1$ to see that $R\in\pi$.
 - 6. For \mathcal{E}_{\circ} , let $\pi := \{ R \in \sigma \mid \exists R_1, R_2 \in \sigma, R_1 \subseteq E_1, R_2 \subseteq E_2 : q(R, R_1, R_2) \ge 1 \}$.
- 7. For \mathcal{E}_{scc} , observe that $E_1(A)^{scc} = E_1(A)^m \cap (E_1(A)^m)^{-1}$ where $E_1(A)^1 := E_1(A)$ and $E_1(A)^{i+1} := E_1(A)^i \cup E_1(A)E_1(A)^i$ and m is the smallest number with $E(A)^{m+1} = E(A)^m$. Using, 1,2,5 and 6, the relation $E_1(A)^{scc}$ can be computed.

Proof of Lemma 5. To evaluate the queries, we use the algebraic sketch as follows.

- 1. Observe that $E_1(A) \subseteq E_2(A)$, if and only if for all $R \in \sigma$ it holds that $R \subseteq E_1$ implies $R \subseteq E_2$. Moreover, $E_1(A) = E_2(A)$, if and only if $E_1(A) \subseteq E_2(A)$ and $E_2(A) \subseteq E_1(A)$.
- 2. We show that the machine M can actually compute the cardinality by using the following formula.

$$\begin{split} |E_1(A)| &= \sum_{\substack{R_1 \in \sigma \\ R_1 \subseteq E_1}} |R_1(C)| \\ \text{where } |R_1(C)| &= \sum_{\substack{R_{\text{diag}} \in \sigma \\ R_{\text{diag}} \text{ diagonal}}} q(R_{\text{diag}}, R_1, R_1^{-1}) \cdot |R_{\text{diag}}(C)| \text{ and } \\ \text{where } |R_{\text{diag}}(C)| &= \sum_{\substack{R_2 \in \sigma \\ R_2(C) = R_{\text{diag}}(C)R_2(C)R_{\text{diag}}(C)}} q(R_{\text{diag}}, R_2, R_2^{-1}). \end{split}$$

We show the correctness. The first equation for $|E_1(A)|$ is correct since $E_1(A)$ is partitioned by the colour classes contained within it. We consider the equation for

 $|R_1(C)|$. Observe that for a fixed vertex $u \in V(C)$ with $(u, u) \in R_{\text{diag}}(C)$ the number $q(R_{\text{diag}}, R_1, R_1^{-1})$ counts the number of outgoing edges $(u, v) \in R_1(C)$. Therefore, $q(R_{\text{diag}}, R_1, R_1^{-1}) \cdot |R_{\text{diag}}(A)|$ is the number of edges $(u, v) \in R_1(C)$ where $u \in V(C)$ is some vertex with $(u, u) \in R_{\text{diag}}(C)$. Summing up over $R_{\text{diag}} \in \sigma$ removes the dependency of $R_{\text{diag}} \in \sigma$. Last but not least, consider the cardinality $|R_{\text{diag}}(A)|$. For a fixed vertex $u \in V(C)$ with $(u, u) \in R_{\text{diag}}(C)$, the sum counts the number of vertices (u, v) with $(v, v) \in R_{\text{diag}}(C)$. This is simply the number of vertices $v \in V(C)$ with $(v, v) \in R_{\text{diag}}(C)$, which in turn is equal to $|R_{\text{diag}}(C)|$.

Proof of Lemma 6. The DeepWL-algorithm for each function uses the $create(\pi)$ for a set $\pi \subseteq \sigma$ defined as follows.

- 1. We define $\pi := \{R \in \sigma \mid R \text{ diagonal such that } |R(C) \circ E(A)| \geq 1\}$. We prove the correctness. Assume that for $R \in \sigma$ it holds $R(C) \subseteq \text{diag}(\text{dom}(E(A)))$. Then, $R \in \pi$. On the other hand, if $R \in \pi$ then $R(C) \cap \text{diag}(\text{dom}(E(A))) \neq \emptyset$. Since (A, C) is a coherently coloured structure, it follows that $R(C) \subseteq \text{diag}(\text{dom}(E(A)))$.
- 2. Observe that $\operatorname{codom}(E(A)) = \operatorname{dom}(E(A)^{-1})$. Using 1 and Lemma 4 Part 5, we conclude that $\operatorname{codom}(E(A))$ is DeepWL-computable.
- 3 Observe that $\operatorname{supp}(E(A)) = \operatorname{dom}(E(A)) \cup \operatorname{codom}(E(A))$ and that unions are DeepWL-computable by Lemma 4.1,

C. Proofs and Details Omitted from Section 4

Let (A, C) be a coherently σ -coloured τ -structure. A set $U \subseteq V(A)$ is called *colour-aligned* if for each diagonal colour $R \in \sigma$ the support $\operatorname{supp}(R(C))$ is either a subset or is disjoint from U. A colour-aligned set $U \subseteq V(A)$ is called *homogeneous* if there is a diagonal colour $R \in \sigma$ such that $U = \operatorname{supp}(R(C))$. Observe that a DeepWL-algorithm can decide whether $\operatorname{dom}(X(A))$, $\operatorname{codom}(X(A))$ and $\operatorname{supp}(X(A))$ are homogeneous for a given symbol $X \in \sigma \cup \tau$. A colour-aligned set $U \subseteq V(A)$ is called *discrete* if for all $u \neq v \in U$ there are diagonal colours $R_u \neq R_v \in \sigma$ such that $(u, u) \in R_u(C)$, $(v, v) \in R_v(C)$.

A coherent configuration C is called *homogeneous* if the universe V(C) is homogeneous and is called *discrete* if the universe V(C) is discrete.

Recall the definition of *subrestrictions* from the preliminaries. The next lemma tells us that we can compute the algebraic sketch for a subrestriction.

Lemma 22. There is a polynomial-time algorithm that for a given algebraic sketch D(A) and a given subset $\tilde{\tau} \subseteq \tau$ and diagonal relation symbol $E_U \in \tau$, computes the algebraic sketch $D(A[\tilde{\tau}, U])$ where $U := \sup(E_U(A))$.

Proof. Let $\widetilde{A} := A[\widetilde{\tau}, U]$. It suffices to show that we can compute $D(\widetilde{A}, \widetilde{C})$ for some coherently coloured structure $(\widetilde{A}, \widetilde{C})$. Then, by Lemma 3, we can also compute $D(\widetilde{A}) = D(\widetilde{A}, C(\widetilde{A}))$. We define the algebraic sketch of $(\widetilde{A}, \widetilde{C})$ as $(\widetilde{\tau}, \widetilde{\sigma}, \subseteq_{\widetilde{\sigma}, \widetilde{\tau}}, \widetilde{q})$ where $\widetilde{\sigma} := \{R \in \sigma \mid \sup(R(C)) \subseteq U\}$ and where $\subseteq_{\widetilde{\sigma}, \widetilde{\tau}}$ and \widetilde{q} are the restrictions of $\subseteq_{\sigma, \tau}$ and q to $\widetilde{\tau} \times \widetilde{\sigma}$ and $\widetilde{\sigma}^3$, respectively.

Proof of Theorem 7. Let \widehat{M} be polynomial-time DeepWL-algorithm that computes \mathcal{E} . We will give a pure DeepWL-algorithm M that computes \mathcal{E} . Let $D(\widehat{A}) = (\widehat{\tau}, \widehat{\sigma}, \subseteq_{\widehat{\sigma}, \widehat{\tau}}, \widehat{q})$ be the algebraic sketch maintained by \widehat{M} . Analogously, we let $D(A) = (\tau, \sigma, \subseteq_{\sigma, \tau}, q)$ be the algebraic sketch maintained by the pure DeepWL-algorithm M. Furthermore suppose $(\widehat{A}_1, C(\widehat{A}_1)), \ldots, (\widehat{A}_m, C(\widehat{A}_m))$ is the sequence of coherently $\widehat{\sigma}_i$ -coloured $\widehat{\tau}_i$ -structures in the cloud of the machine \widehat{M} until the machine eventually halts.

We say that our DeepWL-algorithm M successfully simulates the t-th step for $t \leq m$ if

- 1. the machine M maintains a subset $\omega \subseteq \tau$ and a diagonal relation $E_U \in \tau$ with $U := \operatorname{supp}(E_U(A))$ such that $A[\omega, U]$ is isomorphic to \widehat{A}_t up to renaming relation symbols, that is, there is a bijective function $\varphi : V(A[\omega, U]) \to V(\widehat{A}_t)$ and a one-to-one correspondence between the relation symbols $E \in \omega$ and relation symbols $\widehat{E} \in \widehat{\tau}_t$, i.e., $E(A)^{\varphi} = \widehat{E}(\widehat{A}_t)$ (the machine also maintains this one-to-one correspondence between the vocabularies),
- 2. $|V(A)| \leq \sum_{i \leq t} |V(\widehat{A}_i)|$

When the algorithm M starts, it holds $A = \widehat{A}_1$. Then, we create a diagonal relation symbol $E_U \in \tau$ with $E_U(A) = \operatorname{diag}(V(A))$. Now, the machine M already successfully simulates the first step with $\omega := \tau \setminus \{E_U\}$.

So assume that M successfully simulates the t-th step. We need to explain how to simulate step t+1. By Lemma 22, we can compute $D(A[\omega,U])=D(\widehat{A}_t)$ and therefore we can track the internal run of \widehat{M} until the machine makes an execution of addPair or contract. Assume that the parameter of addPair or contract is a colour $\widehat{R} \in \widehat{\sigma}_t$. By deleting all relation symbols in $\tau \setminus (\omega \cup E_U)$, we can assume that there is a colour $R \in \sigma$ with $R(C(A))^{\varphi} = \widehat{R}(C(\widehat{A}_t))$. Then, the machine M can execute addPair(R) or contract(R) to simulate the next step. So assume that addPair(R) or contract(R) is executed by R where R in this case, our DeepWL-algorithm R finds a relation symbol R in that corresponds to R is a simple the one-to-one correspondence from 1. Depending on whether the execution adds pairs or contracts components we do the following.

Case 1: \widehat{M} executes addPair(\widehat{E}).

Let $E \in \tau$ be the relation symbol corresponding to $\widehat{E} \in \widehat{\tau}_t$. If $E(A) = \emptyset$, then we are done and simulated also the (t+1)-th step. Otherwise, let $R_1 \in \sigma$ be a colour such that $R_1(C) \subseteq E(A)$. A pure DeepWL-algorithm can determine such a colour from the algebraic sketch D(A). The pure DeepWL-algorithm executes $\operatorname{addPair}(R_1)$. Then, it creates a relation symbol $E_2 \in \tau$ such that $E_2(A) := E(A) \setminus R_1(C)$. The algorithm executes $\operatorname{addPair}(E_2)$ recursively. And continues until $E_m(A) = \emptyset$ for some $m \in \mathbb{N}$. Then it creates a relation symbol D_E such that $D_E(A) = D_{R_1}(A) \cup \ldots \cup D_{R_{m-1}}(A)$. We define $\omega := \omega \cup \{E_{\operatorname{left}}, E_{\operatorname{right}}, D_E\}$ and create a relation symbol $E'_U \in \tau$ with $E'_U(A) = E_U(A) \cup D_E(A)$ (which we use in place of E_U).

We claim that M simulates the (t+1)-th step. We extend the bijection $\varphi: V(A[\omega,U]) \to V(\widehat{A}_{t+1})$ by matching the freshly added pairs. The relation symbols $E_{\text{left}}, E_{\text{right}} \in \tau$ correspond to the relation symbols $E_{\text{left}}, E_{\text{right}} \in \widehat{\tau}_{t+1}$. The number of freshly added vertices

is bounded by $|V(\widehat{A}_{t+1})|$ and therefore we maintain $|V(A)| \leq |V(\widehat{A}_{t+1})| + \sum_{i \leq t} |V(\widehat{A}_i)| = \sum_{i \leq t+1} |V(\widehat{A}_i)|$.

Case 2: \widehat{M} executes $contract(\widehat{E})$.

Let $E \in \tau$ be the relation symbol corresponding to $\widehat{E} \in \widehat{\tau}_t$. Using Lemma 4 Part 7, we create a relation symbol $E_{\text{scc}} \in \tau$ with $E_{\text{scc}}(A) = E(A)^{\text{scc}}$ (note that the DeepWL-algorithm from Lemma 4 that creates this symbol is pure).

If all strongly connected components $S \in SCC(E_{scc}(A))$ are discrete (a DeepWL-algorithm can recognise this case from the algebraic sketch), we pick diagonal relation symbols $R_1, \ldots, R_s \in \sigma$ such that $supp(R_1(C)) \cup \ldots \cup supp(R_s(C))$ intersects each $S \in SCC(E_{scc}(A))$ in exactly one vertex. We create a diagonal relation symbol $E_S \in \tau$ such that $E_S(A) = R_1(C) \cup \ldots \cup R_s(C)$. Then $supp(E_S(A)) \cap S$ is a singleton for each $S \in SCC(E(A))$. We want to use this singleton as representation of S. To make this work, we create a relation symbol $E'_U \in \tau$ with $E'_U(A) = (E_U(A) \setminus supp(E_{scc}(A))) \cup E_S(A)$. For each $E \in \omega$ that corresponds to some $\widehat{E} \in \widehat{\tau}_t$, we define a relation symbol $E' \in \tau$ with

$$E'(A) = E'_{U}(A)ZE(A)ZE'_{U}(A)$$

where $Z:=E_{\mathrm{scc}}(A)\cup\mathrm{diag}(V(A))$. We redefine $\omega:=\{E'\in\tau\mid E\in\omega\}$. We claim that our DeepWL-algorithm M simulates the (t+1)-th step. The bijection $\varphi:V(A[\omega,U])\to V(\widehat{A}_{t+1})$ identifies the unique vertex in $S\cap\mathrm{supp}(E_{\mathcal{S}}(A))$ with the vertex $\varphi(S)\in V(\widehat{A}_{t+1})$. Moreover, our DeepWL-algorithm M does not add fresh vertices and therefore

$$|V(A)| \le \sum_{i \le t} |V(\widehat{A}_i)| \le \sum_{i \le t+1} |V(\widehat{A}_i)|.$$

It remains the case, in which there is a strongly connected component $S \in SCC(E_{scc}(A))$ which is not discrete. In this case, our pure DeepWL-algorithm chooses an arbitrary non-diagonal colour $R \in \sigma$ (the lexicographically least, say) with $R(C) \subseteq E_{scc}(A)$ such that supp(R(C)) is homogeneous. Such a colour exists and can be found using the algebraic sketch (in fact, $R \in \sigma$ is the colour of (u, v) for some $u, v \in S$ that have the same colour). Then, it contracts the elements in SCC(R(C)) by applying the contract(R)-instruction. If all strongly connected components of $E_{scc}(A)$ are discrete after this contraction, the algorithm continues with the first case. Otherwise, it iteratively contracts E_{scc} .

To show that the algorithm terminates after polynomially many iterations, we need to show that SCC(R(C)) contains a non-singleton and therefore the number of elements in $E_{scc}(A)$ reduces in each iteration. We claim that for a non-diagonal colour R(C) that has a homogeneous support supp(R(C)) it holds that $R(C)^{scc}$ is also non-diagonal. Since supp(R(C)) is homogeneous, each vertex in R(C) (viewed as a directed graph) has the same in-degree and out-degree. This implies that every edge of R(C) is contained in a cycle. Since R is non-diagonal, there is a pair $(u, v) \in R(C)$ with $u \neq v$, and since (u, v) is contained in a cycle, it is also contained in a strongly connected component. Thus $u \neq v$ belong to the same strongly connected component of R(C) which proves the claim.

Case 3: \widehat{M} executes $create(\widehat{\pi})$.

We define a subset $\pi \subseteq \sigma$ corresponding to $\widehat{\pi} \subseteq \widehat{\sigma}_t$ as follows. By deleting all relation symbols in $\tau \setminus (\omega \cup E_U)$, we can assume that for each colour $\widehat{R} \in \widehat{\sigma}_t$ there is a colour $R \in \sigma$ with $R(C(A))^{\varphi} = \widehat{R}(C(\widehat{A}_t))$. Let $\pi := \{R \in \sigma \mid \widehat{R} \in \widehat{\pi}\}$. We execute $\operatorname{create}(\pi)$ for $\pi \subseteq \sigma$ and update $\omega := \omega \cup \{E_{\pi}\}$.

Case 4: \widehat{M} executes forget(\widehat{E}).

We simply update $\omega := \omega \setminus \{E\}$ for the relation symbol $E \in \tau$ that corresponds to $\widehat{E} \in \widehat{\tau}_t$.

We analyse the total running time of M. Since \widehat{M} is a polynomial-time DeepWL-algorithm the following values are polynomially bounded. The length m of the sequence $\widehat{A}_1, \ldots, \widehat{A}_m$, the size of each universe $V(\widehat{A}_i)$ and the running time of the underlying Turing machine. Therefore, the size of the universe $|V(A)| \leq \sum_{i \leq m} |V(\widehat{A}_i)|$ is polynomially bounded. The pure DeepWL-algorithm M simulates m steps which can each be done in polynomial time.

Remark 23. It can be shown that Theorem 7 also holds for time bounds of the form $T^{\mathcal{O}(1)}$ where T is time-constructible and grows at least linear. For example, quasipolynomial time instead of polynomial time.

D. Proofs and Details Omitted from Section 5

Proof of Lemma 8. 1. We say two crossing colours $R_1, R'_1 \in \sigma_{\text{cross}}$ are equivalent, written $R_1 \sim R'_1$, if $\operatorname{dom}(R_1(A)) = \operatorname{dom}(R'_1(A))$ and $\operatorname{codom}(R_1(A)) = \operatorname{codom}(R'_1(A))$. We denote by $[R_1]_{\sim}$, the equivalence class of R_1 . We will define a structure $[C(A)]_{\sim}$ by taking the union of equivalent colours. More precisely, the structure has the relations $\sigma_1 \cup \sigma_2 \cup [\sigma_{\operatorname{cross}}]_{\sim} \text{ where } [\sigma_{\operatorname{cross}}]_{\sim} := \{ [R_1]_{\sim} \mid R_1 \in \sigma_{\operatorname{cross}} \} \text{ and } [R_1]_{\sim} ([C(A)]_{\sim}) := \{ [R_1]_{\sim} \mid R_1 \in \sigma_{\operatorname{cross}} \}$ $\bigcup_{R_1' \in [R_1]_{\sim}} R_1'(C(A))$. We claim $[C(A)]_{\sim}$ is a coherent configuration. Let (u,v) be a crossing edge with colour $[R_1]_{\sim}$ and let (u, w) be a crossing edge with colour $[R_2]_{\sim}$ and let (w, v) be an edge with colour R_3 . Note that R_3 is plain. Let $Q := \{x \mid (u, x) \text{ has colour } v \in \{x \mid (u, x) \text{$ $[R_2]_{\sim}$ and (x,v) has colour R_3 . We show the number $q=q([R_1]_{\sim},[R_2]_{\sim},R_3):=|Q|$ only depends on $[R_1]_{\sim}$, $[R_2]_{\sim}$, R_3 (and not on (u,v)). Let $Q':=\{x\mid (x,v) \text{ has colour}\}$ R_3 . First we argue that Q=Q'. To see this assume that $x\in Q'$. Then, the colour R^x of (x,x) is the same as the colour R^w of (w,w). Assume that (u,u) has colour $R^u \in \sigma_1 \cup \sigma_2$. We know that (u, w) has colour R_2 . Let R'_2 be the colour of (u, x). We have that $dom(R_2(A)) = dom(R'_2(A))$ since the domains $dom(R_2(A)), dom(R'_2(A))$ are homogeneous sets which intersect non-trivially in u. Moreover, we also have that $\operatorname{codom}(R_2(A)) = \operatorname{supp}(R^w(A)) = \operatorname{supp}(R^x(A)) = \operatorname{codom}(R_2(A)).$ Therefore, $R_2 \sim R_2'$, which implies $x \in Q$. Since Q = Q' and C(A) is a coherent configuration it follows that Q only depends on R_3 . Similarly, the intersection numbers $q([R_1]_{\sim}, R_2, [R_3]_{\sim})$ where R_2 is plain and R_1 and R_3 are crossing only depend on $[R_1]_{\sim}$, R_2 and $[R_3]_{\sim}$. This proves the claim that $[C(A)]_{\sim}$ is a coherent configuration. On the other hand, the coherent configuration $[C(A)]_{\sim}$ still refines A since A has no crossing edges. Therefore, $[C(A)]_{\sim}$ refines C(A). By definition, C(A) also refines $[C(A)]_{\sim}$ and therefore $[C(A)]_{\sim} \equiv C(A)$ which means that each equivalence class is a singleton.

- 2. We explain how D(A) = D(A, C(A)) can be computed for given $D(A_1, C_1), D(A_2, C_2)$. The set of colours is $\sigma = (\sigma_1 \cup \sigma_2) \cup \sigma_{\text{cross}}$. For the symbolic subset relation, we have $R \subseteq_{\sigma,\tau} E$ if and only if $R \subseteq_{\sigma_i,\tau_i} E$ for some $i \in \{1,2\}$. And for the intersection number for $R_1, R_2, R_3 \in \sigma_i, i \in \{1,2\}$ it holds that $q(R_1, R_2, R_3) = q_i(R_1, R_2, R_3)$. In case that $R_j \in \sigma_{\text{cross}}$ for some $j \in \{1,2,3\}$, we can use Part 1 to determine the intersection number $q(R_1, R_2, R_3)$. For example, for $R_1 \in \sigma_1$ and $R_2, R_3 \in \sigma_{\text{cross}}$ we have that $q(R_1, R_2, R_3) = |\operatorname{codom}(R_2(C(A)))| = |\operatorname{dom}(R_3(C(A)))|$.
- 3. Assume for contradiction that there is a coherent configuration C'_i refining A that is coarser than C_i for some $i \in \{1, 2\}$. Without loss of generality we assume that i = 1. Indeed, the previous construction from 2 shows that given the coherently coloured structures $(A_1, C'_1), (A_2, C_2)$, we can define a coherently coloured structure (A, C') where C' is coarser than C(A). This is a contradiction since C(A) is a coarsest coherent configuration.

Proof of Lemma 9. We show 1. For a given algebraic sketch D(A), the algebraic sketch $D(A_R)$ can be computed as follows. By Lemma 3, it suffices to compute an algebraic sketch $D(A_R, C)$ for some coherently coloured structure (A_R, C) (where C refines A_R , but is not necessarily as coarse as possible).

Let C_R be the structure that is obtained from C(A) by contracting the strongly connected components of R(C(A)). The relations $R_1(C_R)$, for $R_1 \in \sigma$, are defined in the usual way. For example, for $S_1, S_2 \in \mathrm{SCC}(R(C(A)))$ we let $(S_1, S_2) \in R_1(C_R)$ if and only if there are $v_1 \in S_1, v_2 \in S_2$ such that $(v_1, v_2) \in R(C(A))$. We define an equivalence relation "~" on σ and say that $R_1 \sim R'_1$ if $R_1(C_R) = R'_1(C_R)$. The key observation is that the equivalence relation can be computed in polynomial time, when the algebraic sketch D(A) = D(A, C(A)) is given (we do not need access to the actual structure C(A)). More precisely, we have $R_1 \sim R'_1$ if and only if $E_V R_1(C(A)) E_V = E_V R'_1(C(A)) E_V$ where $E_V = \mathrm{diag}(V(A) \setminus \mathrm{dom}(R(C(A))^{\mathrm{scc}})) \cup R(C(A))^{\mathrm{scc}}$. Equivalently, $R_1 \sim R'_1$ if and only if $E_V R_1(C(A)) E_V$ and $E_V R'_1(C(A)) E_V$ intersect non-trivially. By $[R_1]_{\sim}$, we denote the equivalence class of the colour $R_1 \in \sigma$. Let $([C]_{\sim})_R$ be the coherent configuration with universe $V(C_R)$ and vocabulary $\sigma_R := \{[R_1]_{\sim} \mid R_1 \in \sigma\}$ and relations $[R_1]_{\sim}(([C]_{\sim})_R) := R_1(C_R)$. We define an algebraic sketch $D(A_R, ([C]_{\sim})_R) = (\tau_R, \sigma_R, \subseteq_{\sigma_R, \tau_R}, q_R)$ as follows. Let $\tau_R := \tau$. We say that

$$[R_1]_{\sim} \subseteq_{\sigma_R, \tau_R} E \text{ if } R'_1 \subseteq_{\sigma, \tau} E \text{ for some } R'_1 \in [R_1].$$

To show the correctness, we show that $[R_1]_{\sim} \subseteq_{\sigma_R,\tau_R} E$, if and only if $R_1(C_R) \subseteq E(A_R)$. Assume that $R'_1 \subseteq_{\sigma,\tau} E$ for some $R'_1 \in [R_1]_{\sim}$. Then $R_1(C_R) = R'_1(C_R) \subseteq E(A_R)$. On the other hand, assume that $R_1(C_R) \subseteq E(A_R)$. Therefore, $E_V R_1(C(A)) E_V$ and E(A) intersect non-trivially. Then, there is a colour $R'_1 \in \sigma$ such that $R'_1(C(A)) \subseteq E_V R_1(C(A)) E_V \cap E(A)$. This implies $E_V R'_1(C(A)) E_V$ and $E_V R_1(C(A)) E_V$ intersect non-trivially and thus $R'_1 \sim R_1$. Therefore, $R'_1 \subseteq_{\sigma,\tau} E$ and thus $[R_1]_{\sim} \subseteq_{\sigma_R,\tau_R} E$. We

define

$$q_R([R_1]_{\sim},[R_2]_{\sim},[R_3]_{\sim}) := \frac{1}{c_{R_2,R_3}} \cdot \sum_{\substack{R_2' \in [R_2]_{\sim}, \\ R_3' \in [R_3]_{\sim}}} q(R_1,R_2',R_3')$$

where we set $c_{R_2,R_3} = 1$ whenever $\operatorname{codom}(R_2(C(A)))$ and $\operatorname{supp}(\operatorname{SCC}(R(C(A))))$ are disjoint and where $c_{R_2,R_3} = |S|$ for some $S \in \operatorname{SCC}(R(C(A)))$ whenever

$$\operatorname{codom}(R_2(C(A))) \subseteq \operatorname{supp}(\operatorname{SCC}(R(C(A)))).$$

This is well-defined since C(A) is a coherent configuration and therefore the sizes of the strongly connected components of R(C(A)) coincide. We show the correctness. Assume that $c_{R_2,R_3} = |S|$ and let $(u,v) \in R_1(C(A))$. The number of vertices $w \in V(A_R)$ with $(u,w) \in [R_2]_{\sim}(C_R)$ and $(w,v) \in [R_3]_{\sim}(C_R)$ is equal to the number of strongly connected components $S \in SCC(R(C(A)))$ for which there are $w \in S, R'_2 \in [R_2]_{\sim}, R'_3 \in [R_3]_{\sim}$ such that $(u,w) \in R'_2(C(A))$ and $(w,v) \in R'_3(C(A))$. Instead of counting strongly connected components $S \in SCC(R(C(A)))$, we count vertices $v \in S \in SCC(R(C(A)))$ and divide the result by |S|.

Proof of Lemma 10. We show Part 1. For a given algebraic sketch D(A), the algebraic sketch $D(A^{\omega}) = (\tau^{\omega}, \sigma^{\omega}, \subseteq_{\sigma^{\omega}, \tau^{\omega}}, q^{\omega})$ is constructed as follows.

$$\tau^{\omega} := (\tau \cup \{E_{\text{left}}, E_{\text{right}}\}) \cup \{D_R \mid R \in \omega\}.$$

First, we describe the coherent configuration C^{ω} of A^{ω} by describing its relations $R(C^{\omega})$ for $R \in \sigma^{\omega}$. Later in the proof, we will express the intersection numbers of C^{ω} in terms of the old intersection numbers. In the following let $v = (v_1, v_2) \in V(A^{\omega})$ be a pair-vertex for a crossing edge. We define $p_i(v) := v_i$ for both $i \in \{1, 2\}$. For a plain vertex $v \in V(A)$, we define $p_i(v) = v$ for both $i \in \{1, 2\}$. For a pair $e = (u, v) \in V(A^{\omega})^2$, let $R_e := \{(R_u, R_{11}, R_{12}, R_{21}, R_{22}, R_v) \in \sigma^6 \mid (p_i(u), p_j(v)) \in R_{ij}(C(A)), i, j \in \{1, 2\}, (p_1(u), p_2(u)) \in R_u(C(A)), (p_1(v), p_2(v)) \in R_v(C(A))\}$. The set R_e can be seen as the isomorphism type of the σ -coloured graph induced on the set V_4 where $V_4 := \{p_1(u), p_2(u), p_1(v), p_2(v)\}$. Define

$$\sigma^{\omega} := \{ R_e \mid e \in V(A^{\omega})^2 \}.$$

The key observation is that V_4 intersects both sets $\mathcal{V}_i(A)$ in at most two vertices. By Lemma 8.1, the colour of crossing edges $\mathcal{E}_{\text{cross}}(A)$ only depends on the diagonal colours of the adjacent vertices. For this reason, the set of colours σ^{ω} only depends on the colouring of pairs which only depends on D(A) and ω (and not on the actual structures A, C(A)). In fact, we can compute σ^{ω} in polynomial time when D(A) and $\omega \subseteq \sigma$ are given.

The set $R_{(u,v)}$ also encodes whether u is plain since u is plain if and only if $(p_1(u), p_2(u))$ has a plain colour. Similarly, $R_{(u,v)}$ also encodes whether v is plain. Therefore, the following symbolic subset relation is well-defined

$$R_{(u,v)} \subseteq_{\sigma^{\omega},\tau^{\omega}} E$$
 if u,v are plain and $R \subseteq_{\sigma,\tau} E$.

The set $R_{(u,v)}$ also encodes whether $u = p_i(v)$ for some given $i \in \{1,2\}$ since this is the case if and only if $u = p_1(u)$ is plain and $(p_1(u), p_i(v))$ has a diagonal colour. This ensures that the symbolic subset relation for the relation symbols E_{left} , E_{right} , D_R is well-defined.

$$R_{(u,v)} \subseteq_{\sigma^{\omega},\tau^{\omega}} E_{\text{left}}$$
 if u is plain and $v = (u, v_2)$
 $R_{(u,v)} \subseteq_{\sigma^{\omega},\tau^{\omega}} E_{\text{right}}$ if u is plain and $v = (v_1, u)$

Similarly, we have $R_{(u,v)} \subseteq_{\sigma^{\omega},\tau^{\omega}} D_R$ if and only if u = v is not plain and $(p_1(u), p_2(u))$ has colour $R \in \sigma$.

We need to show that C^{ω} indeed defines a coherent configuration. We do this by expressing the intersection numbers recursively. We will observe that they can be expressed using the intersection numbers from D(A). For given $R_{e_1}, R_{e_2}, R_{e_3}$, we assume that $R_{e_1} = R_{(u,v)}, R_{e_2} = R_{(u,w)}, R_{e_3} = R_{(w,v)}$ for some vertex w, otherwise $q^{\omega} = 0$.

Base Case: u, v, w are plain.

$$q^{\omega}(R_{e_1}, R_{e_2}, R_{e_3}) := q(R_1, R_2, R_3)$$

where R_i is defined as colour of $e_i \in R_i(C(A))$ for $i \in \{1, 2, 3\}$.

Case 1: w is not plain (and thus $w = (w_1, w_2)$ a pair-vertex).

$$q^{\omega}(R_{e_1}, R_{e_2}, R_{e_3}) = \prod_{i=1}^{2} q^{\omega}(R_{e_1}, R_{(u, w_i)}, R_{(w_i, v)}).$$

This is well defined since $R_{(u,(w_1,w_2))} = R_{(u',(w'_1,w'_2))}$ implies that $R_{(u,w_i)} = R_{(u',w'_i)}$ and $R_{(w_i,v)} = R_{(w'_i,v)}$ for both $i \in \{1,2\}$. We prove the correctness. Let $Q := \{x \mid R_{(u,x)} = R_{(u,x)} = R_{(u,w)} \text{ and } R_{(x,v)} = R_{(w,v)} \}$ and let $Q_i := \{x_i \mid R_{(u,x_i)} = R_{(u,w_i)} \text{ and } R_{(x_i,v)} = R_{(w_i,v)} \}$ for both $i \in \{1,2\}$. By definition, $q^\omega(R_{e_1},R_{e_2},R_{e_3}) = |Q|$ and $|Q_i| = q^\omega(R_{e_1},R_{(u,w_i)},R_{(w_i,v)})$ for $i \in \{1,2\}$. We claim the function $\varphi(x) := (p_1(x),p_2(x))$ is a bijection from Q to $Q_1 \times Q_2$. The function is obviously injective. We need to show surjectivity. Let $x_1 \in Q_1, x_2 \in Q_2$. By definition, $R_{(u,x_i)} = R_{(u,w_i)}$ and $R_{(x_i,v)} = R_{(w_i,v)}$ for both $i \in \{1,2\}$. In particular, $(p_1(u),x_i)$ has the same colour as $(p_1(u),w_i)$. Since (w_1,w_2) is crossing, exactly one of the edges $(p_1(u),w_i)$ is crossing and therefore also (x_1,x_2) is crossing. Moreover, $R_{(u,x_i)} = R_{(u,w_i)}$ implies that (x_i,x_i) has the same colour as (w_i,w_i) . By Lemma 8.1, we conclude that (x_1,x_2) has same colour as (w_1,w_2) . Since, we added a pair-vertex for the pair (w_1,w_2) and since (x_1,x_2) has the same colour, there exists a pair-vertex $x = (x_1,x_2)$. It follows that $x \in Q$, by the definition of $R_{(u,x)}$ and $R_{(x,v)}$.

Case 2: w is plain, but at least one of u, v is not plain.

Without loss of generality we assume that u is not plain, otherwise we compute the intersection number q^{ω} for the conversed triple $(R_{(v,u)}, R_{(v,w)}, R_{(w,u)})$. So assume $u = (u_1, u_2)$.

$$q^{\omega}(R_{e_1},R_{e_2},R_{e_3}) = q^{\omega}(R_{(u_k,v)},R_{(u_k,w)},R_{(w,v)})$$

where $k \in \{1,2\}$ is chosen such that (u_k, w) has a plain colour. We have to show that q^{ω} is well defined. The value $k \in \{1,2\}$ does not depend on $u, w = p_1(w)$ since

 $R_{(u,w)} = R_{(u',w')}$ implies that $(p_i(u),p_1(w))$ and $(p_i(u'),p_1(w'))$ have the same colour for both $i \in \{1,2\}$. Moreover, $R_{(u_i,v)}$ does not depend on the choice of u,v since $R_{(u,v)} = R_{(u',v')}$ implies that $(p_i(u),v)$ and $(p_i(u'),v')$ have the same colour for both $i \in \{1,2\}$. As above, let $Q = \{x \mid R_{(u,x)} = R_{(u,w)} \text{ and } R_{(x,v)} = R_{(w,v)}\}$. We define $Q' = \{x \mid R_{(u_k,x)} = R_{(u_k,w)} \text{ and } R_{(x,v)} = R_{(u,v)}\}$ for $k \in \{1,2\}$ such that (u_k,w) is plain. We claim that Q = Q'. Let $x \in Q$. Then, $R_{(u,x)} = R_{(u,w)}$ and $R_{(x,v)} = R_{(w,v)}$. Since $R_{(u,x)} = R_{(u,w)}$, it follows that also $R_{(u_i,x)} = R_{(u_i,w)}$ for both $i \in \{1,2\}$. In particular, $R_{(u_k,x)} = R_{(u_k,w)}$ and therefore $x \in Q'$. On the other hand, let $x \in Q'$. Then, $R_{(u_k,x)} = R_{(u_k,w)}$ meaning that (u_k,x) and (u_k,w) have the same colour. By Lemma 8.1, the colour of a crossing edge only depends on the colours of the adjacent vertices and thus $R_{(u,x)} = R_{(u,w)}$. Therefore, $x \in Q$.

Proof of Lemma 11. Let \widehat{M} be a polynomial-time DeepWL-algorithm that decides isomorphism on \mathcal{C} . We will give an almost normalised DeepWL-algorithm M that decides isomorphism on \mathcal{C} in polynomial time. By $D(\widehat{A}) = (\widehat{\tau}, \widehat{\sigma}, \subseteq_{\widehat{\sigma}, \widehat{\tau}}, \widehat{q})$, we denote the algebraic sketch maintained by \widehat{M} . Analogously, we write $D(A) = (\tau, \sigma, \subseteq_{\sigma,\tau}, q)$ to denote the algebraic sketch maintained by the almost normalised DeepWL-algorithm M. We write $(\widehat{A}_1, C(\widehat{A}_1)), \ldots, (\widehat{A}_m, C(\widehat{A}_m))$ to denote the sequence of coherently $\widehat{\sigma}_i$ -coloured $\widehat{\tau}_i$ -structures in the cloud of the machine \widehat{M} until the machine eventually halts.

We say that our DeepWL-algorithm M successfully simulates step t for $t \leq m$ if

- 1. the machine M maintains a subset $\omega \subseteq \tau$ and a diagonal relation symbol $E_U \in \tau$ with $U := \operatorname{supp}(E_U(A))$ such that $A[\omega, U]$ is isomorphic to \widehat{A}_t up to renaming relation symbols, that is, there is a bijective function $\varphi : V(A[\omega, U]) \to V(\widehat{A}_t)$ and a one-to-one correspondence between relation symbol $E \in \omega$ and relation symbols $\widehat{E} \in \widehat{\tau}_t$, i.e., $E(A)^{\varphi} = \widehat{E}(\widehat{A}_t)$ (the machine also maintains this one-to-one correspondence between the vocabularies),
- 2. $|V(A)| \le 160 \sum_{i \le t} |V(\widehat{A}_i)|^4$,
- 3. there is a relation symbol $E_{pa} \in \tau$ such that for each $v \in U$ the set $P_{pa}(v) := \{u \mid (u,v) \in E_{pa}(A)\}$ is a non-empty subset of $\mathcal{V}_{cross}(A) \setminus U$. We require that for all $v \neq v'$ the sets $P_{pa}(v), P_{pa}(v')$ are disjoint. We let $P_{pa} := \bigcup_{v \in U} P_{pa}(v) \subseteq \mathcal{V}_{cross}(A) \setminus U$, and
- 4. there are relation symbols $E_{\rm le}, E_{\rm ri} \in \tau$ such that for each $v \in P_{\rm pa}$ there are two unique vertices $p_{\rm le}(v), p_{\rm ri}(v)$ in $\mathcal{V}_{\rm plain}(A) \setminus U$ with $(p_{\rm le}(v), v) \in E_{\rm le}(A), (p_{\rm ri}(v), v) \in E_{\rm ri}(A)$ (we can think of $E_{\rm le}, E_{\rm ri}$ as $E_{\rm left}, E_{\rm right}$). We require $(p_{\rm le}(v), p_{\rm ri}(v)) \in \mathcal{E}_{\rm cross}(A)$ and that for all $v \neq v'$ that $(p_{\rm le}(v), p_{\rm ri}(v)) \neq (p_{\rm le}(v'), p_{\rm ri}(v'))$,

We explain how to simulate the first step. When the algorithm M starts, it holds that $A = \widehat{A}_1$ and therefore the bound in Property 2 holds. By creating a relation symbol $E_U \in \tau$ with $E_U = \operatorname{diag}(V(A))$, we can assume that Property 1 holds. We need to explain how to ensure Property 3 and 4. We add unique vertices v_1^*, v_2^* to the structures A_1, A_2 which are connected to each vertex in $v_1 \in \mathcal{V}_1(A), v_2 \in \mathcal{V}_2(A)$, respectively. (This

can be done by executing $addPair(E_U)$ and contracting the freshly added pair-vertices belonging to the same structure.) In a next step, we define the crossing relation

$$Z := \{(u, v_i^*) \mid u \in V(A_{3-i}), v_i^* \in \mathcal{V}_i(A)\}.$$

The crossing relation Z is DeepWL-computable, so we can create a relation symbol $E_Z \in \tau$ with $E_Z(A) = Z$. Since each edge in $E_Z(A)$ is crossing, our DeepWL-algorithm is almost normalised. Then, we execute $\mathtt{addPair}(E_Z)$. Next, we can create relation symbols $E_{\mathrm{pa}}, E_{\mathrm{le}}, E_{\mathrm{ri}}$ with the desired properties as follows. We copy each vertex in U by executing $\mathtt{addPair}(E_U)$. Let $\overline{u} = (u,u)$ denote the copy of u. We let $E_{\mathrm{pa}}(A) := \{(u,(u,v_i^*)) \mid u \in V(A_{3-i})\}$. Now, $P_{\mathrm{pa}}(u) = \{(u,v_i^*)\} \subseteq V_{\mathrm{cross}}(A)$, which means that we assign each vertex u a unique singleton set containing one crossing pair-vertex. Furthermore, we define $E_{\mathrm{le}}(A) := \{(\overline{u},(u,v_i^*)) \mid u \in V(A_{3-i})\}$ and $E_{\mathrm{ri}}(A) := \{((v_i^*),(u,v_i^*)) \mid u \in V(A_{3-i})\}$. Now, $p_{\mathrm{le}}((u,v_i^*)) = \overline{u} \in \mathcal{V}_{\mathrm{plain}}(A) \setminus U$ and $p_{\mathrm{ri}}((u,v_i^*)) = v_i^* \in \{v_1^*,v_2^*\} \subseteq \mathcal{V}_{\mathrm{plain}}(A) \setminus U$. This means that we assign each pair-vertex in $(u,v_i^*) \in P_{\mathrm{pa}}$ a pair $((u,u),v_i^*)$ (using the copy \overline{u} instead of u ensures that $p_{\mathrm{ri}}((u,v_i^*))$ is not contained in U). Finally, M simulates the first step successfully.

So assume that M simulates the t-th step. We need to explain how to simulate step t+1. By Lemma 22, we can compute $D(A[\omega,U])=D(\widehat{A}_t)$ and therefore we can track the internal run of \widehat{M} until the machine performs an execution of $\operatorname{addPair}(\widehat{B})$ or $\operatorname{contract}(\widehat{B})$. In this case, our DeepWL-algorithm finds a relation symbol $E \in \tau$ that corresponds to $\widehat{B} \in \widehat{\tau}_t \cup \widehat{\sigma}_t$, i.e., $\widehat{B} = \widehat{E} \in \widehat{\tau}_t$ and $E(A)^{\varphi} = \widehat{E}(\widehat{A}_t)$ or $\widehat{B} = \widehat{R} \in \widehat{\sigma}_t$ and $E(A)^{\varphi} = \widehat{R}(C(\widehat{A}_t))$. In the latter case, the DeepWL-algorithm possibly needs to create such a symbol since the isomorphism from $A[\omega,U]$ to \widehat{A}_t does not ensure that such a symbol already exists (this can be done by Lemma 4). Depending on whether the execution adds pairs or contracts components we do the following.

Case 1: \widehat{M} executes $contract(\widehat{B})$.

Let $E \in \tau$ be the relation symbol corresponding to $\widehat{B} \in \widehat{\tau}_t \cup \widehat{\sigma}_t$. We contract the strongly connected components SCC(E(A)) by executing contract(E). Since contractions are not restricted, the algorithm M remains almost normalised.

We claim that our DeepWL-algorithm M successfully simulates step t+1. We extend the bijection $\varphi: V(A[\omega,U]) \to V(\widehat{A}_{t+1})$ by identifying a vertex $S \in V(A[\omega,U])$ with the vertex $\varphi(S) \in V(\widehat{A}_{t+1})$. Property 3 holds since for each component S we have $P_{\mathrm{pa}}(S) = \bigcup_{v \in S} P_{\mathrm{pa}}(s)$ and the sets $P_{\mathrm{pa}}(S_1), P_{\mathrm{pa}}(S_2)$ are disjoint for distinct/disjoint components S_1, S_2 . Property 4 trivially holds since the vertices and relations in $V(A) \setminus U$ are unaffected by a contraction of a component $S \in \mathrm{SCC}(E(A))$ with $S \subseteq U$.

Case 2: \widehat{M} executes $\mathit{addPair}(\widehat{B})$.

Let $E \in \tau$ be the relation symbol corresponding to $\widehat{B} \in \widehat{\tau}_t \cup \widehat{\sigma}_t$. Let X := dom(E(A)) and Y := codom(E(A)). We assume that X, Y are homogeneous sets (in C(A)), otherwise we can add the pairs step by step as in the proof of Theorem 7. By Lemma 6, the sets X, Y are DeepWL-computable. We define $X_{\text{pa}} := \bigcup_{x \in X} P_{\text{pa}}(x) \subseteq P_{\text{pa}} \subseteq \mathcal{V}_{\text{cross}}(A) \setminus U$ and define $X_{\text{le}} := \{p_{\text{le}}(x) \mid x \in X_{\text{pa}}\} \subseteq \mathcal{V}_{\text{plain}}(A) \setminus U$ and analogously X_{ri} . Analogous, we define $Y_{\text{pa}}, Y_{\text{le}}, Y_{\text{ri}}$.

We can assume that X_{pa} is homogeneous (in C(A)). If this would not be the case, we would pick a homogeneous subset $H \subseteq X_{\mathrm{pa}}$. Since X is homogeneous, the set H intersects $P_{\mathrm{pa}}(x)$ non-trivially for each $x \in X$. Then, we redefine E_{pa} by creating a new relation E'_{pa} in place of E_{pa} with $E'_{\mathrm{pa}}(A) = \{(u,v) \mid u \in H, (u,v) \in E_{\mathrm{pa}}(A)\}$. Now, it holds $P'_{\mathrm{pa}}(x) = P_{\mathrm{pa}}(x) \cap H$ for each $x \in X$. For the same reason, we may assume Y_{pa} to be homogeneous.

As a consequence, also $X_{\rm le}, X_{\rm ri}, Y_{\rm le}, Y_{\rm ri}$ are homogeneous (in C(A)). Assume for contradiction that $v, v' \in X_{\rm le}$ such that (v, v), (v', v') have different colours. Then, let $x, x' \in X_{\rm pa}$ such that $p_{\rm le}(x) = v$ and $p_{\rm le}(x') = v'$. Since C(A) is a coherent configuration, also x, x' have different colours.

For $x \in X$ consider the (directed) bipartite graph $L(x) := \{(p_{le}(v), p_{ri}(v)) \mid v \in X\}$ $P_{pa}(x)$ consisting of crossing pairs between $\mathcal{V}_1(A)$ and $\mathcal{V}_2(A)$. We can assume that the maximum out-degree is 1, i.e., for all $(a_{\rm le},a_{\rm ri})\neq(b_{\rm le},b_{\rm ri})\in L(x)$ it holds $a_{\rm le}=$ $b_{\rm le} \implies a_{\rm ri} \neq b_{\rm ri}$. If this would not be the case, then we do the following. We define an equivalence relation " \equiv " on X_{le} . For $c \in X_{ri}$, define $a_{le} \equiv_c b_{le}$ if $(a_{le}, c), (b_{ri}, c) \in L(x)$ for some $x \in X$. We omit the index and say $a_{le} \equiv b_{le}$ if $a_{le} \equiv_c b_{le}$ for some $c \in X_{ri}$. We claim that \equiv_c does not depend on the choice of $c \in X_{ri}$ and therefore \equiv_c equals \equiv . By Lemma 8.3, Lemma 9.2 and Lemma 10.2, imply that $C(A)[\mathcal{V}_i(A)]$ can not be refined by refining $C(A)[V_{3-i}(A)]$. Assume $a_{le} \equiv b_{le}$, we consider the refined structure obtained by individualising the edge (a_{le}, b_{le}) , then the vertices in $W := \{c \in X_{ri} \mid a_{le} \equiv_c b_{le}\}$ have a different colour than vertices in $W \setminus X_{ri}$. Since $W \neq \emptyset$ and X_{ri} is homogeneous, it follows that $W = X_{\rm ri}$. This means $a_{\rm le} \equiv_c b_{\rm le}$ for all $c \in X_{\rm ri}$, which proves the claim. Next, we will add vertices to the universe corresponding to the equivalence classes $[p_{le}(v)]_{\equiv}$. We let $E_{X_{le}}$ be a relation symbol with $E_{X_{le}}(A) = \operatorname{diag}(X_{le})$ and execute addPair $(E_{X_{le}})$. We want to use the equivalence classes $[p_{le}(v)]_{\equiv}$ instead of $p_{le}(v)$ in order to reduce the maximum out-degree. Let $E_{\equiv_{le}}$ be a relation symbol with $E_{\equiv_{le}}(A) = \{((u,u),(v,v)) \mid$ $u \equiv_{\mathrm{le}} v$ and execute contract $(E_{\equiv_{\mathrm{le}}})$. Next, we redefine E_{le} by creating an new relation symbol E'_{le} where we relate $([p_{le}(v)]_{\equiv}, v) \in E'_{le}(A)$ instead of $(p_{le}(v), v)$. Now, the graph $L'(x) = \{([p_{le}(v)]_{\equiv}, p_{ri}(v)) \mid v \in P_{pa}(x)\}$ has the desired properties. With the same argument, we can assume that the in-degree of L(x) is 1 and therefore L(x) is a (directed) matching or a disjoint union of cycles and paths. Indeed, we can assume that L(x) is a (directed) matching, otherwise we do the following. We copy each vertex in X_{le} by executing addPair $(E_{X_{le}})$ for a relation symbol with $E_{X_{le}} = \operatorname{diag}(X_{le})$. Then, we use the copies instead of X_{le} . More precisely, we redefine E_{le} by creating a relation symbol $E'_{le} \in \tau$ with $E'_{le}(A) = \{((u, u), v) \mid (u, v) \in E_{le}(A)\}$. This way, we ensure that X_{le}, X_{ri} are disjoint and thus L(x) is a (directed) matching.

We define a relation Z :=

$$\{(x_i, y_i) \in (X_{le} \cup X_{ri}) \times (Y_{le} \cup Y_{ri}) \mid x_i, y_i \in \mathcal{V}_i(A), i \in \{1, 2\}\}.$$

The relation Z is DeepWL-computable, so we create a relation symbol $E_Z \in \tau$ with $E_Z(A) = Z$.

Next, we define $\mathcal{Z} :=$

$$\{((x_i, y_i), (x_j, y_j)) \in Z^2 \mid x_i \in \mathcal{V}_i(A), x_j \in \mathcal{V}_j(A), i \neq j\}.$$

The relation $\mathcal{Z} \subseteq V(A)^2$ is DeepWL-computable, so we create a relation symbol $E_{\mathcal{Z}} \in \tau$ with $E_{\mathcal{Z}}(A) = \mathcal{Z}$. Moreover, $E_{\mathcal{Z}}(A)$ consists of crossing edges and therefore our DeepWL-algorithm M remains almost normalised. We execute addPair $(E_{\mathcal{Z}})$.

For $v, v' \in X_{pa}$, we say that $v \sim_X v'$ if there is a $x \in X$ such that $v, v' \in P_{pa}(x)$. This defines an equivalence relation since $P_{pa}(x), P_{pa}(x')$ are pairwise disjoint by Property 3. Analogous, we define an equivalence relation for Y_{pa} . Observe that there is a one-to-one correspondence between the equivalence classes of X_{pa} and the set X. We claim that for $x_i \in X_{le}, x_j \in X_{ri}$, there is a unique vertex $v^* =: pair_X\{x_i, x_j\}$ such that $\{p_{le}(v^*), p_{ri}(v^*)\} = \{x_i, x_j\}$. First, we explain why at least one vertex exists and then we explain why it is unique. By definition of X_{le}, X_{ri} there are some vertices $x_i \in X_{le}$ and $x_j \in X_{le}$ for which v^* exists. So assume for contradiction that there is a pair (x_i', x_j') for which such a vertex not exists. Then (x_i', x_j') has a different colour than (x_i, x_j) , contradicting Lemma 8.1. To show uniqueness, we use Property 4 saying that $(p_{le}(v), p_{ri}(v)) \neq (p_{le}(v'), p_{ri}(v'))$ for $v \neq v'$. Moreover, X_{le}, X_{ri} are disjoint and therefore v^* is unique, which proves the claim.

We define an equivalence relation " \sim " on the set $\mathcal Z$ and say that $((x_i,y_i),(x_j,y_j)) \sim ((x_i',y_i'),(x_j',y_j'))$ pair $_X\{x_i,x_j\} \sim_X \operatorname{pair}_X\{x_i',x_j'\}$ and $\operatorname{pair}_Y\{y_i,y_j\} \sim_Y \operatorname{pair}_Y\{y_i',y_j'\}$. Also this equivalence relation is DeepWL-computable, so can create a relation symbol E_{\sim} such that $E_{\sim}(A) = \sim$. We want to add a fresh vertex, for each equivalence class in $[\mathcal Z]_{\sim}$. We create a copy $\mathcal Z'$ of $\mathcal Z$ by executing $\operatorname{addPair}(E_{\mathcal Z})$ again. There is a one-to-one correspondence between elements $((x_i,y_i),(x_j,y_j)) \in \mathcal Z$ and elements $((x_i,y_i),(x_j,y_j))' \in \mathcal Z'$. We contract the equivalence classes in the copy $\mathcal Z'$ by executing $\operatorname{contract}(E_{\sim'})$ where $E_{\sim'}(A) = \{(z_1',z_2') \in \mathcal Z' \times \mathcal Z' \mid z_1 \sim z_2\}$. Clearly, the DeepWL-algorithm M remains almost normalised.

We define a function $\psi: E(A) \to V(A)$ by mapping an pair $e = (\mathtt{pair}_X\{x_i, x_j\}, \mathtt{pair}_Y\{y_i, y_j\}) \in E(A)$ to a vertex $v = \psi(e) \in D_{\mathcal{Z}'}(A)$ that represents the equivalence class $[((x_i, y_i), (x_j, y_j))']_{\sim'}$. By the definition of the equivalence class, this function is injective. We extend E_U and create a relation symbol $E'_U \in \tau$ such that $E'_U(A) = E_U(A) \cup \mathrm{diag}(\mathrm{image}(\psi))$.

Now, we claim that our DeepWL-algorithm M successfully simulates step t+1. We extend the bijection $\varphi: V(A[\omega,U]) \to V(\widehat{A}_{t+1})$ by mapping an equivalence class $v \in V(A)$ to the freshly added vertex $\varphi(\psi^{-1}(v)) \in V(\widehat{A}_{t+1}) \setminus V(\widehat{A}_t)$. We have to explain, how to define $E_{\mathrm{pa}}, E_{\mathrm{le}}, E_{\mathrm{ri}}$ for the fresh vertices $v = [z']_{\sim'}$. We update E_{pa} by setting $E_{\mathrm{pa}}(A) \leftarrow E_{\mathrm{pa}}(A) \cup \{(z, [z']_{\sim'}) \in \mathcal{Z} \times \mathcal{Z}'\}$. To update the relation symbols $E_{\mathrm{le}}, E_{\mathrm{ri}}$, we use the relations E_{left} and E_{right} and update $E_{\mathrm{le}}(A) \leftarrow E_{\mathrm{le}}(A) \cup \{((x_i, y_i), z) \mid z = ((x_i, y_i), (x_j, y_j))\}$ and $E_{\mathrm{ri}}(A) \leftarrow E_{\mathrm{ri}}(A) \cup \{(z, (x_j, y_j)) \mid z = ((x_i, y_i), (x_j, y_j))\}$.

For 2, we have to show that $|V(A)| \leq 160 \sum_{i \leq t+1} |V(\widehat{A}_i)|^4$. The total number of vertices added by M is linearly bounded in $|\mathcal{Z}|$. More precisely, our algorithm M added at most $10|\mathcal{Z}|$ vertices. Clearly, $|V(\widehat{A}_{t+1})| \geq |E(A)| \geq \frac{1}{2}(|X|+|Y|)$ since E(A) is a biregular graph between X and Y. On the other hand, $|\mathcal{Z}| \leq |Z|^2 = (|X_{le}| + |X_{ri}|)^2(|Y_{le}| + |Y_{ri}|)^2$. Since the bipartite graph L(x) between X_{le} and X_{ri} is a (directed) matching, we have $|L(x)| = |X_{le}| = |X_{ri}|$. By Lemma 8.1, the crossing edges between X_{le} and X_{ri} have the same colour and therefore $|X_{le}||X_{ri}| = \sum_{x \in X} |L(x)|$. We conclude $|X_{le}|, |X_{ri}| \leq |X|$ and similar $|Y_{le}|, |Y_{ri}| \leq |Y|$. In total $|\mathcal{Z}| \leq (2|X|)^2(2|Y|)^2 \leq (|X| + |Y|)^4 \leq 16|E(A)|^4 \leq$

 $16|\widehat{A}_{t+1}|^4$. This leads to $|V(A)| \le 10|\mathcal{Z}| + 160 \sum_{i \le t} |V(\widehat{A}_i)|^4 \le 160 \sum_{i \le t+1} |V(\widehat{A}_i)|^4$.

Case 3: \widehat{M} executes create($\widehat{\pi}$).

We simply execute $\mathtt{create}(\pi)$ for some $\pi \subseteq \sigma$ that corresponds to $\widehat{\pi} \subseteq \widehat{\sigma}$. Then, we update $\omega := \omega \cup \{E_{\pi}\}.$

Case 4: \widehat{M} executes forget(\widehat{E}).

We simply update $\omega := \omega \setminus \{E\}$ for some $E \in \tau$ that corresponds to $\widehat{E} \in \widehat{\tau}_t$. The fact, that we do not execute the forget-command ensures that $\mathcal{V}_i(A)$ remains connected for both $i \in \{1,2\}$ (this is required for almost normalised DeepWL-algorithms).

Proof of Lemma 12. Let \widehat{M} be polynomial-time DeepWL-algorithm that decides isomorphism on \mathcal{C} in polynomial time. By Lemma 11, we can assume that \widehat{M} is almost normalised. In fact, the construction from Theorem 7 preserves that the algorithm is almost normalised, so we can assume that \widehat{M} is almost normalised and pure at the same time. We will give a normalised DeepWL-algorithm M that decides isomorphism on \mathcal{C} in polynomial time. By $D(\widehat{A}) = (\widehat{\tau}, \widehat{\sigma}, \subseteq_{\widehat{\sigma}, \widehat{\tau}}, \widehat{q})$, we denote the algebraic sketch maintained by \widehat{M} . Analogously, we write $D(A) = (\tau, \sigma, \subseteq_{\sigma,\tau}, q)$ to denote the algebraic sketch maintained by the normalised DeepWL-algorithm M. We write $(\widehat{A}_1, C(\widehat{A}_1)), \ldots, (\widehat{A}_m, C(\widehat{A}_m))$ to denote the sequence of coherently $\widehat{\sigma}_i$ -coloured $\widehat{\tau}_i$ -structures in the cloud of the machine \widehat{M} until the machine eventually halts.

We say that our DeepWL-algorithm M successfully simulates the t-th step for $t \leq m$ if

- 1. the machine M ensures that the structure A is isomorphic to $\widehat{A}_t[\mathcal{V}_{\text{plain}}(\widehat{A}_t)]$ up to renaming relation symbols, that is, there is a bijective function $\varphi: V(A) \to V(\mathcal{V}_{\text{plain}}(\widehat{A}_t)])$ and a one-to-one correspondence between relation symbol $E \in \tau$ and relation symbols $\widehat{E} \in \widehat{\tau}_t$, i.e., $E(A)^{\varphi} = \widehat{E}(\widehat{A}_t[\mathcal{V}_{\text{plain}}(\widehat{A}_t)])$,
- $2. |V(A)| \le |V(\widehat{A}_t)|,$
- 3. the algebraic sketch $D(\widehat{A}_t)$ is already computed,

When the algorithm M starts, it holds $A = \widehat{A}_1$ and $D(A) = D(\widehat{A}_t)$ therefore M successfully simulates the first step. So assume that M simulates the t-th step.

We need to explain how to simulate step the t+1. Since we already computed $D(\widehat{A}_t)$, we can track the internal run of \widehat{M} until the machine performs an execution of $\operatorname{addPair}(\widehat{R})$, $\operatorname{contract}(\widehat{R})$, $\operatorname{create}(\widehat{\pi})$ or $\operatorname{forget}(\widehat{E})$.

Case 1: \widehat{M} executes $\mathit{addPair}(\widehat{R})$

We have to consider two cases. If $\widehat{R}(C(\widehat{A}_t)) \subseteq \mathcal{E}_{cross}(\widehat{A}_t)$, we do not need to adapt φ . We can compute $D(\widehat{A}_{t+1})$ for given $D(\widehat{A}_t)$ using Lemma 10 Part 1.

If $\widehat{R}(C(\widehat{A}_t)) \subseteq \mathcal{E}_{\text{plain}}(\widehat{A}_t)$, then there is a colour $R \in \tau$ corresponding to $\widehat{R} \in \widehat{\tau}_t$. This follows from the fact that adding pair-vertices for crossing edges and contractions of components in all intermediate steps that were only simulated but truly executed actually do not refine the coherent configuration. This is formally proved in Lemma 10 Part 2 and Lemma 9 Part 2.

We execute addPair(R). Clearly, we maintain Property 1 and 2. To see that we can compute $D(\widehat{A}_{t+1})$ we again invoke Lemma 10 Part 1.

Case 2: \widehat{M} executes $contract(\widehat{R})$.

We can compute $D(\widehat{A}_{t+1})$ for given $D(\widehat{A}_t)$ using Lemma 9.1. To maintain the bijection φ , we need to contract strongly connected components. To do so, we restrict the strongly connected components $S \in SCC(\widehat{R}(C(\widehat{A}_t)))$ to $\mathcal{V}_{plain}(\widehat{A}_t)$ and define $S' := \{S \cap \mathcal{V}_{plain}(\widehat{A}_t) \mid S \in SCC(\widehat{R}(C(\widehat{A}_t)))\}$. We can define a relation symbol $E \in \tau$ such that each $S \in SCC(E(A))$ is mapped to some $\varphi(S) \in S'$. We execute contract(E). Clearly, we maintain Property 1 and 2.

Case 3: \widehat{M} executes $\operatorname{create}(\widehat{\pi})$.

In this case, we create a relation symbol $E_{\pi} \in \tau$ where $E_{\pi}(A)^{\varphi} = E_{\widehat{\pi}}(\widehat{A}_{t+1}) \cap \mathcal{V}_{\text{plain}}(\widehat{A}_{t+1})^2$. To ensure Property 3, we compute $D(\widehat{A}_{t+1})$ for given $D(\widehat{A}_t)$ in polynomial time.

Case 4: \widehat{M} executes $forget(\widehat{E})$.

Let $E \in \tau$ be the relation symbol corresponding to $\widehat{E} \in \widehat{\tau}_t$. We execute forget(E). To ensure Property 3, we compute $D(\widehat{A}_{t+1})$ for given $D(\widehat{A}_t)$ in polynomial time.

E. Proofs and Details Omitted from Section 6

Proof of Lemma 19. Suppose first that the formula $\varphi(x_1, x_2)$ only has 3 (free or bound variables). Then it is equivalent to a formula of the infinitary 3-variable counting logic $\mathsf{C}^3_{\infty\omega}$. It follows from the fact that the 2-dimensional Weisfeiler Leman algorithm decides $\mathsf{C}^3_{\infty\omega}$ -equivalence (due to [7]) that for every τ -structure A the relation $\varphi(A)$ is a union of colours of the coherent configuration C(A). Moreover, given the algebraic sketch D(A) and φ , it can be decided in polynomial time which colour classes these are. That is, given D(A) and φ we can compute in polynomial time a collection of colours $R_1, \ldots, R_m \in \sigma$ such that $\varphi(A) = \bigcup_{i=1}^m R_i(C(A))$ (see [23]). Once we have these colours, we can use the create-operation to compute $\varphi(A)$ in DeepWL.

Now suppose that φ contains k>3 variables. The trick is to first compute the structure A' obtained from A by adding all k-tuples of elements and the projections of the k-tuples to their entries. In DeepWL, we can compute A' by repeated addPair-operations. We can translate $\varphi(x_1, x_2)$ to a formula $\varphi'(x_1', x_2')$ that only uses 3-variables in such a way that $\varphi(A) = \varphi'(A')$. We do this by representing tuples of variables in φ , ranging over elements of V(A), by single variables ranging over tuples in A', and using the two additional variables to decode the tuples. Then we can apply the argument above to A' and φ' .