A unifying method for the design of algorithms canonizing combinatorial objects

Pascal Schweitzer*
TU Kaiserslautern
schweitzer@cs.uni-kl.de

Daniel Wiebking
RWTH Aachen University
wiebking@informatik.rwth-aachen.de

We devise a unified framework for the design of canonization algorithms. Using hereditarily finite sets, we define a general notion of combinatorial objects that includes graphs, hypergraphs, relational structures, codes, permutation groups, tree decompositions, and so on.

Our approach allows for a systematic transfer of the techniques that have been developed for isomorphism testing to canonization. We use it to design a canonization algorithm for combinatorial objects in general. This result gives new fastest canonization algorithms with an asymptotic running time matching the best known isomorphism algorithm for the following types of objects: hypergraphs, hypergraphs of bounded color class size, permutation groups (up to permutational isomorphism) and codes that are explicitly given (up to code equivalence).

1 Introduction

The problem of computing a canonical form of a graph can be seen as the task to compute a standard representative of the graph up to isomorphism. Specifically, given an input graph G, a graph G' isomorphic to G is to be computed such that the output graph G' depends only on the isomorphism class of G and not on the graph G itself. The problem is closely related to the graph isomorphism problem, which reduces to the task of computing a canonical form: for two given input graphs, we compute their canonical forms and check whether the canonical forms are equal (rather than isomorphic).

In practice, a canonization algorithm is often preferable to an isomorphism test, as it allows each graph to be treated separately, rather than having to compare graphs pairwise. For example, when looking up a molecule in a chemical database, we do not wish to compare the molecule individually to every graph that has been stored in the system.

^{*}The research leading to these results has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 820148).

While various computational problems related to symmetries of graphs are polynomial-time equivalent to the isomorphism problem, for example the computation of the automorphism group of a graph or the computation of the orbit partition [Mat79], it is unknown whether or not canonization reduces to isomorphism in polynomial time.

It is usually not very difficult to turn combinatorial isomorphism tests into canonization algorithms, sometimes the algorithms are canonization algorithms in the first place. However, there are several isomorphism testing algorithms for which to date no canonization algorithms with the same asymptotic running are known.

This seems to be in particular the case for isomorphism algorithms based on group theoretic techniques pioneered by Luks [Luk82], who designed a polynomial time isomorphism algorithm for graphs of bounded degree.

Luks's framework and the result for bounded degree graphs were subsequently extended to canonization [BL83]. In that paper, Babai and Luks lay the foundation for canonization techniques using the string canonization problem and algorithmically exploiting cosets. The original technique of Luks also sparked a series of isomorphism algorithms without respective canonization algorithms. For example, Luks presented a $2^{O(|V|)}$ -time isomorphism algorithm for hypergraphs [Luk99], but the best known canonization algorithm has the brute force running time of $|V|^{O(|V|)}$. A similar situation occurs for hypergraphs of bounded rank [BC08]. As pointed out by Codenotti [Cod11] the reason is that these result are based on coset intersection, for which no adequate canonization version is known. Finally, for Babai's quasipolynomial time isomorphism algorithm [Bab16] there was initially no canonization version. However, concurrently to our work, he extended his result to canonization [Bab19]. For results building on his algorithm [GNS18], there are still no known canonization versions. Also for the isomorphism problem for groups, nearly all of the most recent results seem not to provide canonical forms [BCQ12, LW12, RW15, GQ15, GQ17, BMW17].

Our Contribution In this paper, we devise a unified framework for the design of canonization algorithms. To do so, we define, using hereditarily finite sets, a general notion of combinatorial objects that includes graphs, hypergraphs, relational structures, codes, permutation groups, tree decompositions, and more. To this end, we devise for various problems canonization algorithms with an asymptotic running time matching the best isomorphism algorithm. For each of them, no canonization algorithm with such a running time has been known before. Specifically, we obtain canonization algorithms for

- hypergraphs on a vertex set V in time $2^{\mathcal{O}(|V|)}$ matching the hypergraph isomorphism algorithm of Luks [Luk99],
- hypergraphs X = (V, H) of color class size at most k in FPT time $2^{\mathcal{O}(k)}(|V| + |H|)^{\mathcal{O}(1)}$ matching the best isomorphism algorithm of Arvind, Das, Köbler and Toda [ADKT15],
- explicitly given permutation groups Δ (up to permutational isomorphism) on permutation domain V and of order $|\Delta|$ in time $2^{\mathcal{O}(|V|)}|\Delta|^{\mathcal{O}(1)}$ matching the best algorithm for permutational isomorphism of Babai, Codenotti, and Qiao [BCQ12],
- explicitly given codes \mathcal{A} (up to code equivalence) of code word length |V| and code size $|\mathcal{A}|$ in time $2^{\mathcal{O}(|V|)}|\mathcal{A}|^{\mathcal{O}(1)}$ matching the best isomorphism algorithm from [BCGQ11, BCQ12], and
- combinatorial objects over a ground set V in general in time $2^{\mathcal{O}(|V|)}n^{\mathcal{O}(1)}$ where n is the size of the object (formally defined in Section 3).

The new canonization algorithm for hypergraphs above solves an open problem that has been repeatedly stated ([Luk99],[BC08] and [ADKT15]). As the input size of a hypergraph can be as big as $2^{|V|}$, when measured only in the size of the underlying vertex set, the simply exponential running time is optimal. Of course, when measured also in the number of edges, better algorithms with a more refined running time bound might be possible.

For combinatorial objects in general, neither canonization nor isomorphism has been considered before in this generality.

Our Technique We advocate a clear separation between unordered objects and ordered objects. In our framework, an unordered object is an object over a ground set of a priori indistinguishable vertices. In contrast to this, an ordered object is an object whose underlying vertex set consists of integers which thus carries a natural linear order. It is easily argued, that this induces a polynomial-time computable linear ordering on the class of all ordered objects (see Lemma 1).

For canonization purposes, every unordered object is associated with an isomorphic ordered one, its canonical form, and the ordering of the ordered objects thereby extends to unordered objects. To compute the canonical form, we use the concept of a labeling coset, which is a coset of maps from unordered to ordered objects. A labeling coset can be seen as a form of partial canonization of an unordered object, through which various possible canonical forms have already been ruled out. By representing labeling cosets compactly via generating sets, we can employ the existing extensive library of efficient algorithms dealing with permutation groups.

The fact that the ordered objects are totally ordered allows us to use deterministic subroutines, used in isomorphism tests, on ordered objects in an isomorphism-invariant way. This framework then allows for a systematic transfer of the techniques that have been developed for isomorphism testing to the realm of canonization.

The most important feature of our framework is that it is possible to view these labeling cosets as combinatorial objects themselves. The main technique (see Lemma 9) shows that under mild assumptions it is possible to replace subobjects (such as subgraphs) by their labeling cosets without losing or introducing global symmetries. This paradigm allows for a recursive approach by computing canonical labelings of substructures first, then replacing the substructures by their labeling cosets, and then computing a canonical labeling of a new global object that only consists of the labeling cosets of the substructures rather than the substructures themselves.

For hypergraphs, with a relatively direct application of our framework, we obtain the canonization algorithm mentioned above. However, for the canonization of objects in general the key algorithm handles sets of labeling cosets. As the labeling cosets can describe global interdependencies, our technique of bundling and partitioning for the cosets is significantly more involved and complicated (Section 7).

We also describe a technique of computing a canonical representation of ordered groups which in turn allows us to associate a canonical string (encoding) to every ordered object (see Lemma 22). This complements our framework and allows us to use arbitrary deterministic algorithms for ordered objects as a black box in an isomorphism-invariant way.

Some of the techniques we describe here were used in a weaker, non-generic sense in [GNSW18] to obtain the fastest known canonization algorithm for graphs of bounded tree width. In fact, tree decompositions, nested tree decompositions, and treelike decompositions can also be viewed as combinatorial objects in our framework.

Organization of the Paper The goal of the paper is to compute canonical labelings for arbitrary objects $\mathcal{X} \in \text{Objects}(V)$ formally defined in Section 3. In a bootstrapping manner, we develop canonization algorithms for objects that are more and more complex. Each algorithm uses the previous ones as a black box. In Section 4, we consider two easy cases of canonization in which the object is a pair of atoms. First, we show how to compute a canonical labeling for \mathcal{X} in the case that $\mathcal{X} = (v, \Delta \rho)$ is a pair consisting of a vertex $v \in V$ and a labeling coset $\Delta \rho$. Second, we show how to compute a canonical labeling for \mathcal{X} in the case that $\mathcal{X} = (\Theta \tau, \Delta \rho)$ is a pair of two labeling cosets. In Section 6, we give the canonization algorithm for hypergraphs, which uses the object replacement paradigm explained in Section 5. In Section 7, building on that we show how to compute canonical labelings for \mathcal{X} in the case that $\mathcal{X} = \{\Delta_1 \rho_1, \ldots, \Delta_t \rho_t\}$ is a set of labeling cosets. In Section 8, we bring all our tools together to compute canonical labelings for arbitrary objects $\mathcal{X} \in \text{Objects}(V)$. Finally, in Section 9, we describe the technique of canonical generating sets which allows us to associate a canonical string (encoding) to every ordered object and which (in a certain sense) allows arbitrary deterministic group theoretic algorithms to be used within our framework in an isomorphism-invariant way.

2 Preliminaries

Set Theory For an integer t, we write [t] for $\{1, \ldots, t\}$. For a set S and an integer k, we write $\binom{S}{k}$ for the k-element subsets of S and 2^S for the power set of S.

Group Theory We write composition of functions from left to right, e.g., for two functions $\varphi: V \to V'$ and $\rho: V' \to V''$, we write $\varphi \rho$ for the function that first applies φ and then ρ . For a set V, we write Sym(V) for the symmetric group on V and for an integer t, we write Sym(t) for $\operatorname{Sym}([t])$. By $\operatorname{Stab}_{\Psi}(A) := \{ \psi \in \Psi \mid \psi(a) \in A \text{ for all } a \in A \}$, we denote the setwise stabilizer of $A \subseteq V$ in $\Psi \leq \operatorname{Sym}(V)$. We sometimes also drop the index and write $\operatorname{Stab}(A)$ for $\operatorname{Stab}_{\operatorname{Sym}(V)}(A)$. For a vertex $v \in V$, we write $\operatorname{Stab}_{\Psi}(v)$ for $\operatorname{Stab}_{\Psi}(\{v\})$. We want to extend the definition to tuples (A_1, \ldots, A_t) where $A_i \subseteq V$ and $t \geq 2$. Inductively, we define $\operatorname{Stab}_{\Psi}(A_1, \ldots, A_t)$ as $\operatorname{Stab}_{\operatorname{Stab}_{\Psi}(A_1)}(A_2,\ldots,A_t)$. Note that this way the stabilizer $\operatorname{Stab}_{\Psi}(A_1,\ldots,A_t) = \{\psi \in \Psi \mid$ $\psi(a) \in A_i$ for all $i \in [t]$ and $a \in A_i$ can be computed using an algorithm for the binary stabilizer function Stab_(-) that gets an arbitrary permutation group Ψ and only one set $A \subseteq V$ as an input. A set $A \subseteq V$ is called Ψ -invariant if $\operatorname{Stab}_{\Psi}(A) = \Psi$. For a permutation group $\Psi \leq \operatorname{Sym}(V)$ and a vertex $v \in V$, we write $v^{\Psi} = \{\psi(v) \mid \psi \in \Psi\}$ for the Ψ -orbit of v. The Ψ -orbit partition of V is a partition $V = V_1 \cup \ldots \cup V_t$ such that $v, u \in V_i$ for some $i \in [t]$, if and only if $v^{\Psi} = u^{\Psi}$. A group $\Psi \leq \operatorname{Sym}(V)$ is transitive on a Ψ -invariant set $A \subseteq V$, if A consists of only one Ψ -orbit, i.e., $A = v^{\Psi}$ for some $v \in V$. Slightly abusing terminology, a coset of a set V is a set Λ of bijections from V to a set V' such that $\Lambda = \Delta \rho = \{\delta \rho \mid \delta \in \Delta\}$ for some subgroup $\Delta \leq \operatorname{Sym}(V)$ and a bijection $\rho: V \to V'$.

Generating Sets and Polynomial-Time Library For a set $S \subseteq \operatorname{Sym}(V)$, we write $\langle S \rangle$ for the smallest group $\Psi \subseteq \operatorname{Sym}(V)$ for which $S \subseteq \Psi$. In this case, S is called a *generating set* for Ψ . We refer to [Ser03] for the basic theory of handling permutation groups algorithmically. Many tasks can be performed efficiently when a group is given implicitly via a generating set. We list the results we use.

1. Permutation groups and cosets can be represented implicitly via generating sets that can be chosen of size quadratic in |V|.

- 2. The pointwise stabilizer $\operatorname{Stab}_{\Psi}(v)$ of a vertex $v \in V$ in a group $\Psi \leq \operatorname{Sym}(V)$ can be computed with the Schreier-Sims algorithm in time polynomial in |V|.
- 3. A subgroup of a permutation group with polynomial time membership problem can be computed in time polynomial in the index of the subgroup.
- 4. Let $S = \Delta_1 \rho_1, \ldots, \Delta_t \rho_t$ be a sequence of cosets of V. We write $\langle S \rangle$ for the smallest coset Λ such that $\Delta_i \rho_i \subseteq \Lambda$ for all $i \in [t]$. Given a representation for S, the coset $\langle S \rangle$ can be computed in polynomial time. Furthermore, the computation of $\langle S \rangle$ is isomorphism invariant w.r.t. S, i.e., $\varphi^{-1} \langle S \rangle = \langle \varphi^{-1} S \rangle$ for all bijections $\varphi : V \to V'$ (see [GS15, Lemma 9.1]).

3 Combinatorial Objects and Labeling Cosets

Labeling Cosets A labeling coset of V is set of bijective mappings $\Delta \rho = \{\delta \rho \mid \delta \in \Delta\}$, where ρ is a bijection from V to $\{1, \ldots, |V|\}$ and Δ is a subgroup of $\operatorname{Sym}(V)$. Let $\rho : V \to \{1, \ldots, |V|\}$ be a bijection. We write $\operatorname{Label}(V)$ for the labeling coset $\operatorname{Sym}(V)\rho = \{\sigma\rho \mid \sigma \in \operatorname{Sym}(V)\}$. We say that $\Theta\tau$ is a labeling subcoset of a labeling coset $\Delta\rho$, written $\Theta\tau \leq \Delta\rho$, if $\Theta\tau$ is a subset of $\Delta\rho$ and $\Theta\tau$ again forms a labeling coset. For a labeling coset $\Delta\rho \leq \operatorname{Label}(V)$ and a Δ -invariant set $A \subseteq V$, we define the restriction of $\Delta\rho$ to A as $(\Delta\rho)|_A := \{\lambda|_A \mid \lambda \in \Delta\rho\}$. Observe that $(\Delta\rho)|_A$ is not necessarily a labeling coset again since the image of $\widetilde{\lambda} \in (\Delta\rho)|_A$ might be a set of natural numbers different from $\{1, \ldots, |A|\}$. Let κ be the unique bijection from $\rho(A)$ to $\{1, \ldots, |A|\}$ that preserves the standard ordering "<" of natural numbers. We define the induced labeling coset of $\Delta\rho$ on $A \subseteq V$ as $(\Delta\rho)\downarrow_A := (\Delta\rho)|_A\kappa$. Similarly, for a labeling coset $\Theta\tau \leq \operatorname{Label}(A)$, we define the lifted labeling coset of $\Theta\tau$ to $V \supseteq A$ as $(\Theta\tau)\uparrow^V := \{\gamma \in \operatorname{Label}(V) \mid \gamma|_A \in \Theta\tau\}$.

Hereditarily Finite Sets and Combinatorial Objects We inductively define hereditarily finite sets over a ground set V. Each vertex $X \in V$ and each labeling coset $Y = \Delta \rho \leq \text{Label}(V)$ is called an atom and is in particular a hereditarily finite set. Inductively, if X_1, \ldots, X_t are hereditarily finite sets, then $\mathcal{X} = \{X_1, \ldots, X_t\}$ and also $\mathcal{X} = (X_1, \ldots, X_t)$ are hereditarily finite sets where $t \in \mathbb{N} \cup \{0\}$. A (combinatorial) object is a pair (V, \mathcal{X}) where \mathcal{X} is a hereditarily finite set over V. The set of all (combinatorial) objects over V is denoted by Objects(V). In the following, we will usually assume that V is apparent from context and identify \mathcal{X} with the object (V, \mathcal{X}) , not distinguishing between hereditarily finite sets and combinatorial objects.

We say that an object is *ordered* if the ground set V is a linearly ordered set. An object is *unordered* if V is an (unordered) set. The linearly ordered ground sets considered in this paper are always subsets of \mathbb{N} with their standard ordering "<". Additionally, we will never consider partially ordered sets in which some but not all elements of V are in \mathbb{N} .

The expressiveness of the object formalism is quite extensive. In particular, we can view graphs G = (V, E) with $E \subseteq \binom{V}{2}$, hypergraphs X = (V, H) with $H \subseteq 2^V$, and relational structures $Y = (V, R_1, \ldots, R_t)$ with $R_i \subseteq V^{k_i}$ as unordered objects (over V). A function $f: V \to V'$ can be encoded as a set of pairs $\{(v, f(v)) \mid v \in V\}$ and is thus an object. Note that a labeling coset could in principle also be represented as a set of maps, and thus as an object in which all atoms are of the type $X \in V$. However, we want to succinctly represent labeling cosets via generating sets rather than as a set of labelings. This is precisely the reason why we model them as a second kind of atom.

Applying Functions to Unordered Objects Let V and V' be ground sets where V is unordered and V' is either unordered or ordered. Let $\mu: V \to V'$ be a bijection. For an object $\mathcal{X} \in \mathrm{Objects}(V)$, the image of \mathcal{X} under μ , written \mathcal{X}^{μ} , is an object over V' defined as follows. For a vertex $X = v \in V$, we define $X^{\mu} := \mu(v)$. For a labeling coset $Y = \Delta \rho \leq \mathrm{Label}(V)$, we define $Y^{\mu} = (\Delta \rho)^{\mu} := \mu^{-1} \Delta \rho$. Inductively, for an object $\mathcal{X} = \{X_1, \dots, X_t\}$, we define $\mathcal{X}^{\mu} := \{X_1^{\mu}, \dots, X_t^{\mu}\}$. Analogously, for an object $\mathcal{X} = (X_1, \dots, X_t)$, we define $\mathcal{X}^{\mu} := (X_1^{\mu}, \dots, X_t^{\mu})$. For example, the image of a graph G = (V, E) under μ is a graph $G^{\mu} = (V', E^{\mu})$ that has an edge $\{\mu(v), \mu(u)\}$, if and only if G has the edge $\{v, u\}$.

Automorphisms of Unordered Objects Two unordered objects $\mathcal{X} \in \text{Objects}(V)$ and $\mathcal{X}' \in \text{Objects}(V')$ are isomorphic, written $\mathcal{X} \cong \mathcal{X}'$, if there is a bijection $\varphi : V \to V'$ such that $\mathcal{X}^{\varphi} = \mathcal{X}'$. In this case, φ is called an isomorphism. The set of all isomorphisms from \mathcal{X} to \mathcal{X}' is denoted by $\text{Iso}(\mathcal{X}; \mathcal{X}')$. Note that we defined isomorphism only for unordered objects¹. The automorphism group of an unordered object \mathcal{X} , written $\text{Aut}(\mathcal{X})$, consists of those $\sigma \in \text{Sym}(V)$ for which $\mathcal{X}^{\sigma} = \mathcal{X}$. For unordered objects, the automorphism group $\text{Aut}(\mathcal{X})$ often has a natural meaning, e.g., $\text{Aut}((\Theta\tau, \Delta\rho)) = \Theta\cap\Delta$ and $\text{Aut}((A, \Delta\rho)) = \text{Stab}_{\Delta}(A)$ where $A \subseteq V$ and $\Theta\tau, \Delta\rho \leq \text{Label}(V)$. The set Iso(V; V') simply consists of all bijections from V to V'. However, instead of talking about bijections, we use the notation Iso(V; V') to indicate and stress that both V and V' are unordered sets and that for every object \mathcal{X} , every map $\varphi \in \text{Iso}(V; V')$ is an isomorphism from \mathcal{X} to \mathcal{X}^{φ} .

Canonical Forms of Unordered Objects A canonical form is a function CF that assigns each unordered object $\mathcal{X} \in \text{Objects}(V)$ an ordered object $\text{CF}(\mathcal{X}) \in \text{Objects}(\{1, \dots, |V|\})$ such that:

(CF1) $\mathcal{X} \cong \mathcal{Y}$ implies $CF(\mathcal{X}) = CF(\mathcal{Y})$ for all objects \mathcal{X}, \mathcal{Y} , and

(CF2)
$$CF(\mathcal{X}) = \mathcal{X}^{\lambda}$$
 for some $\lambda \in Label(V)$.

Condition (CF1) is called *isomorphism invariance* and is equivalent to $CF(\mathcal{X}) = CF(\mathcal{X}^{\varphi})$ for all $\varphi \in Iso(V; V')$ ². Intuitively, Condition (CF2) means that \mathcal{X} and $CF(\mathcal{X})$ are isomorphic if we would forget about the linear ordering of the ground set of $CF(\mathcal{X})$.

Canonical Labelings of Unordered Objects A canonical labeling function CL is a function that assigns each unordered object $\mathcal{X} \in \operatorname{Objects}(V)$ a labeling coset $\operatorname{CL}(\mathcal{X}) = \Lambda \leq \operatorname{Label}(V)$ such that:

(CL1)
$$CL(\mathcal{X}) = \varphi CL(\mathcal{X}^{\varphi})$$
 for all $\varphi \in Iso(V; V')$ and,

(CL2)
$$CL(\mathcal{X}) = Aut(\mathcal{X})\pi$$
 for some (and thus for all) $\pi \in CL(\mathcal{X})$.

Again, Condition (CL1) is called *isomorphism invariance*. Note that (CL1) is equivalent to $CL(\mathcal{X})^{\varphi} = CL(\mathcal{X}^{\varphi})$. Roughly speaking, this means that CL is compatible with isomorphisms. More precisely, this means that the following diagram commutes.

¹ If we wanted to have a definition of isomorphisms for objects in general, we should require that an isomorphisms of an object must also preserve the order of the corresponding ground set, which is consistent with the framework.

²If we wanted to define an action of φ on ordered objects, we should define it to act trivially. In that case isomorphism invariance could also be written as $CF(\mathcal{X})^{\varphi} = CF(\mathcal{X}^{\varphi})$, which is more consistent with definitions that follow.

$$\begin{array}{ccc} \mathcal{X} & \stackrel{\varphi}{\longrightarrow} \mathcal{X}^{\varphi} \\ \downarrow_{\mathrm{CL}} & & \downarrow_{\mathrm{CL}} \\ \mathrm{CL}(\mathcal{X}) & \stackrel{\varphi}{\longrightarrow} \mathrm{CL}(\mathcal{X})^{\varphi} \end{array}$$

Condition (CL2) means that \mathcal{X}^{λ} for an arbitrary labeling $\lambda \in CL(\mathcal{X})$ does not depend on the choice of λ .

We give a connection between isomorphisms, canonical forms and canonical labelings. Deciding isomorphism reduces to computing a canonical form. The computation of a canonical form in turn reduces to computing canonical labelings as seen next. We claim that $CF(\mathcal{X}) := \mathcal{X}^{\lambda}$, where $\lambda \in CL(\mathcal{X})$ is an arbitrary labeling, defines a canonical form. First, observe that the canonical form is well defined and does not depend on the choice of $\lambda \in CL(\mathcal{X})$ since (CL2) holds. Next, we check (CF1) and (CF2). Condition (CF2) holds by definition. For (CF1) we need to show that $CF(\mathcal{X}) = CF(\mathcal{X}^{\varphi})$ for all $\varphi \in Iso(V; V')$. Because of (CL1), we have that for all $\lambda \in CL(\mathcal{X})$ there is a $\lambda' \in CL(\mathcal{X}^{\varphi})$ such that $\lambda = \varphi \lambda'$. Therefore, $CF(\mathcal{X}) = X^{\lambda} = (\mathcal{X}^{\varphi})^{\lambda'} = CF(\mathcal{X}^{\varphi})$ which was to show.

The notion of canonical forms and canonical labelings can be defined naturally also for an isomorphism-closed class of objects (e.g., all hypergraphs). In a bootstrapping manner, we will devise canonical labeling algorithms for certain classes of combinatorial objects until we finally give an algorithm for objects in general. We will in each instance state specifically what the requirements of (CL1) and (CL2) are.³

Representation of Objects For an object $\mathcal{X} \in \text{Objects}(V)$, we define the $transitive \ closure$ of \mathcal{X} , written $\text{TClosure}(\mathcal{X})$, as all objects recursively occurring in \mathcal{X} , i.e., $\text{TClosure}(X) \coloneqq \{X\}$ for $X = v \in V$ or $X = \Delta \rho \leq \text{Label}(V)$. And we define $\text{TClosure}(\mathcal{X}) \coloneqq \{\mathcal{X}\} \cup \bigcup_{i \in [t]} \text{TClosure}(X_i)$ for $\mathcal{X} = \{X_1, \dots, X_t\}$ or $\mathcal{X} = \{X_1, \dots, X_t\}$. As mentioned in the preliminaries, we represent labeling cosets efficiently using generating sets. An object itself can be efficiently represented as colored directed acyclic graph over the elements in its transitive closure. With this representation, the input size (i.e., encoding length) of an object \mathcal{X} is polynomial in $|\text{TClosure}(\mathcal{X})| + |V| + t_{\text{max}}$ where t_{max} is the maximal length of a tuple appearing in $\text{TClosure}(\mathcal{X})$.

The Linear Ordering of Ordered Objects In contrast to the previous paragraphs, we will now consider ordered objects where $V \subseteq \mathbb{N}$. Such objects appear in the following context. When evaluating a canonical form, the resulting object is ordered. In order to compare canonical forms, it will be an important task to sort ordered objects in polynomial time. To do so, we define a linear order "<" on objects over the natural numbers. For two natural numbers (atoms) $X, Y \in \mathbb{N}$, we adapt the natural ordering, i.e., X < Y if X < Y. We inductively extend our definition. For two sets $\mathcal{X} = \{X_1, \ldots, X_s\}$ and $\mathcal{Y} = \{Y_1, \ldots, Y_t\}$, we assume that the order "<" is already defined for the elements X_i and Y_j . Then we say $\mathcal{X} < \mathcal{Y}$ if $|\mathcal{X}| < |\mathcal{Y}|$ or if $|\mathcal{X}| = |\mathcal{Y}|$ and the smallest element in $\mathcal{X} \times \mathcal{Y}$ is smaller than the smallest element in $\mathcal{Y} \times \mathcal{X}$. Let $\mathcal{X} = (X_1, \ldots, X_s)$ and $\mathcal{Y} = (Y_1, \ldots, Y_t)$ be two tuples for which "<" is already defined for the entries. We say $\mathcal{X} < \mathcal{Y}$ if s is smaller than t or if s = t and for the smallest $i \in [t]$ for which $X_i \neq Y_i$, we have that $X_i < Y_i$. We extend the order to labelings over natural numbers. For two permutations $\sigma_1, \sigma_2 \in \operatorname{Sym}(\{1, \ldots, |V|\})$ we say $\sigma_1 < \sigma_2$ if there is an $i \in \{1, \ldots, |V|\}$ such that $\sigma_1(i) < \sigma_2(i)$ and $\sigma_1(j) = \sigma_2(j)$ for all $1 \leq j < i$. Last but not least, we extend the definition to labeling cosets $\Delta \rho, \Theta \tau \leq \operatorname{Label}(\{1, \ldots, |V|\})$. We adapt the definition for sets, i.e., $\Delta \rho < \Theta \tau$ if

³We remark that in some papers on canonization there is a Condition (CL3) which we do not require in our framework as we see labeling cosets as objects themselves.

 $|\Delta \rho| \leq |\Theta \tau|$ or if $|\Delta \rho| = |\Theta \tau|$ and the smallest element of $\Delta \rho \setminus \Theta \tau$ is smaller than the smallest element of $\Theta \tau \setminus \Delta \rho$. It is known that for two labeling cosets $\Delta \rho, \Theta \tau \leq \text{Label}(\{1, \dots, |V|\})$ given by generating sets, the order " \prec " can be computed in time polynomial in |V| ([GNSW18], Corollary 22). For completeness, we define $X \prec Y \prec \mathcal{X} \prec \mathcal{Y}$ for all integers $X \in \mathbb{N}$, all labeling cosets $Y = \Delta \rho \leq \text{Label}(\{1, \dots, |V|\})$, all tuples \mathcal{X} and all sets \mathcal{Y} . We write $\mathcal{X} \leq \mathcal{Y}$ if $\mathcal{X} = \mathcal{Y}$ or $\mathcal{X} \prec \mathcal{Y}$.

Lemma 1. The ordering "<" on pairs of ordered objects can be computed in polynomial time.

Having defined an ordering for ordered objects that can be efficiently evaluated, we can use it as follows. While we may not be able to distinguish non-isomorphic objects \mathcal{X} and \mathcal{Y} per se, whenever we are given labelings $\lambda \in \mathrm{CL}(\mathcal{X})$ and $\gamma \in \mathrm{CL}(\mathcal{Y})$, we can order the objects by ordering the ordered versions \mathcal{X}^{λ} and \mathcal{Y}^{γ} w.r.t. "<".

4 Canonization of Atoms and Tuples

We are looking for a canonical labeling function for objects \mathcal{X} in the case where the object is a pair of atoms $\mathcal{X} = (v, \Delta \rho)$ consisting of a labeling coset and a distinguished vertex.

Problem 2. Compute a function $\mathrm{CL}_{\mathrm{Point}}$ with the following properties:

```
Input (v, \Delta \rho) \in \text{Objects}(V) where v \in V, \Delta \rho \leq \text{Label}(V) and V is an unordered set.
```

Output A labeling coset $\operatorname{CL}_{\operatorname{Point}}(v, \Delta \rho) = \Lambda \leq \operatorname{Label}(V)$ such that:

(CL1)
$$\operatorname{CL}_{\operatorname{Point}}(v, \Delta \rho) = \varphi \operatorname{CL}_{\operatorname{Point}}(\varphi(v), \varphi^{-1} \Delta \rho) \text{ for all } \varphi \in \operatorname{Iso}(V; V').$$

(CL2)
$$\operatorname{CL}_{\operatorname{Point}}(v, \Delta \rho) = \operatorname{Stab}_{\Delta}(v)\pi$$
 for some (and thus for all) $\pi \in \Lambda$.

The reader may want to take a moment to convince themselves that for input objects $\mathcal{X} = (v, \Delta \rho)$, the conditions (CL1) and (CL2) stated here agree with the condition (CL1) and (CL2) described in the previous section.

Lemma 3. A function CL_{Point} solving Problem 2 can be computed in polynomial time.

Proof. An algorithm for $CL_{Point}(v, \Delta \rho)$:

```
Choose (arbitrarily) \rho^* \in \Delta \rho such that v^{\rho^*} \in \mathbb{N} is minimal.

Set v^{\operatorname{Can}} \coloneqq v^{\rho^*}.

(v^{\operatorname{Can}} is a minimal image of v under \Delta \rho.)

Set \Delta^{\operatorname{Can}} \coloneqq (\Delta \rho)^{\rho}.

Return \Lambda \coloneqq \rho^* \operatorname{Stab}_{\Delta^{\operatorname{Can}}}(v^{\operatorname{Can}}).
```

(CL1.) Assume for some bijection $\varphi \in \text{Iso}(V; V')$ that we have $\varphi(v), \varphi^{-1}\Delta\rho$ instead of $v, \Delta\rho$ as an input of the algorithm. Observe that $\varphi^{-1}\rho$ is a coset representative of $\varphi^{-1}\Delta\rho = \varphi^{-1}\Delta\varphi(\varphi^{-1}\rho)$. We argue that the algorithm outputs $\varphi^{-1}\Lambda$ instead of Λ . Since $v^{\rho^*} = \varphi(v)^{\varphi^{-1}\rho^*}$, we now obtain $\varphi^{-1}\rho^*\delta^{\text{Can}}$ instead of ρ^* where δ^{Can} is some element in $\text{Stab}_{\Delta^{\text{Can}}}(v^{\text{Can}})$ (the choices for ρ^* vary up to elements in $\text{Stab}_{\Delta^{\text{Can}}}(v^{\text{Can}})$). The computed objects $v^{\text{Can}} = \varphi(v)^{\varphi^{-1}\rho^*\delta^{\text{Can}}}$ and $\Delta^{\text{Can}} = (\varphi^{-1}\Delta\rho)^{\varphi^{-1}\rho}$ remain unchanged. The computed group $\text{Stab}_{\Delta^{\text{Can}}}(v^{\text{Can}})$ remains unchanged. Finally, the algorithm returns $\varphi^{-1}\Lambda$ instead of Λ . This gives $\text{CL}_{\text{Point}}(\varphi(v), \varphi^{-1}\Delta\rho) = \varphi^{-1}\Lambda = \varphi^{-1}\text{CL}_{\text{Point}}(v, \Delta\rho)$ which was to show.

(CL2.) This property holds by construction since $\rho^* \operatorname{Stab}_{\Delta^{\operatorname{Can}}}(v^{\operatorname{Can}}) = \operatorname{Stab}_{\Delta}(v)\rho^*$. (Running time.) The pointwise stabilizer $\operatorname{Stab}_{\Delta^{\operatorname{Can}}}(v^{\operatorname{Can}})$ can be computed with the Schreier-Sims algorithm in polynomial time.

We want to point out here that the Schreier-Sims-algorithm is applied to ordered objects only, and thus we do not need to worry about canonicity of its output.

We continue with the canonization of more interesting objects which we later use as subroutine to canonize pairs of labeling cosets. A (partial) *matching* is a set $M \subseteq V_1 \times V_2$ such that for all $(v_1, v_2), (u_1, u_2) \in M$ with $(v_1, v_2) \neq (u_1, u_2)$, it holds that $v_1 \neq u_1$ and $v_2 \neq u_2$.

Problem 4. Compute a function $\mathrm{CL}_{\mathrm{Match}}$ with the following properties:

Input $(M, \Delta \rho) \in \text{Objects}(V)$ where $M \subseteq V_1 \times V_2$ is a matching, $\Delta \rho \leq \text{Label}(V)$, $\Delta \leq \text{Stab}(V_1, V_2)$ and $V = V_1 \cup V_2$ is an unordered set.

Output A labeling coset $CL_{Match}(M, \Delta \rho) = \Lambda \leq Label(V)$ such that:

- (CL1) $\operatorname{CL}_{\operatorname{Match}}(M, \Delta \rho) = \varphi \operatorname{CL}_{\operatorname{Match}}(M^{\varphi}, \varphi^{-1} \Delta \rho) \text{ for all } \varphi \in \operatorname{Iso}(V; V').$
- (CL2) $\operatorname{CL}_{\operatorname{Match}}(M, \Delta \rho) = (\operatorname{Aut}(M) \cap \Delta)\pi$ for some (and thus for all) $\pi \in \Lambda$.

The reader may again want to take a moment to convince themselves that for input objects $\mathcal{X} = (M, \Delta \rho)$, the Conditions (CL1) and (CL2) stated here agree with Condition (CL1) and (CL2) described in the previous section.

Lemma 5. A function $\operatorname{CL}_{\operatorname{Match}}$ solving Problem 4 can be computed in time $2^{\mathcal{O}(k_2)}|V|^{\mathcal{O}(1)}$ where k_2 is the size of the largest Δ -orbit of $V_2 \subseteq V$.

Proof. For the purpose of recursion, we use an additional input parameter. Specifically, we use a subset $A \subseteq V_2$ such that $M \subseteq V_1 \times A$ and $\Delta \subseteq \operatorname{Stab}(V_1, A)$. Initially, we set $A = V_2$.

An algorithm for $CL_{Match}(M, A, \Delta \rho)$:

```
If |M| = 0: Return \Lambda := \Delta \rho.
```

If |A| = 1: (Because of $|M| \ge 1$, it holds that |M| = 1.) Assume $M = \{(v_1, v_2)\}$.

Return $\Lambda := CL_{Point}(v_1, \Delta \rho)$.

If Δ is intransitive on A:

Partition $A = A_1 \cup A_2$ where A_1 is a Δ -orbit such that A_1^{ρ} is minimal.

(Minimal w.r.t. the order "<" defined in Section 3.)

Partition $M = M_1 \cup M_2$ where $M_i \coloneqq \{(v_1, v_2) \in M \mid v_2 \in A_i\}$ for i = 1, 2.

Compute $\Lambda_1 := \mathrm{CL}_{\mathrm{Match}}(M_1, A_1, \Delta \rho)$ recursively.

Recurse and return $\Lambda_2 := CL_{Match}(M_2, A_2, \Lambda_1)$.

If Δ is transitive on A:

Let $A^{\operatorname{Can}} \coloneqq A^{\rho}$ and $\Delta^{\operatorname{Can}} \coloneqq (\Delta \rho)^{\rho}$.

Partition $A^{\operatorname{Can}} = A_1^{\operatorname{Can}} \cup A_2^{\operatorname{Can}}$ such that $|A_1^{\operatorname{Can}}| = |A_1^{\operatorname{Can}}|/2|$ and A_1^{Can} is minimal.

(Minimal w.r.t. the order "<" defined in Section 3.)

Compute $\Psi^{\operatorname{Can}} := \operatorname{Stab}_{\Lambda \operatorname{Can}}(A_1^{\operatorname{Can}}, A_2^{\operatorname{Can}}).$

(The group can be computed using a membership test as stated in the preliminaries.)

Decompose $\Delta^{\operatorname{Can}}$ into left cosets of $\Psi^{\operatorname{Can}}$ and write $\Delta^{\operatorname{Can}} = \bigcup_{i \in [s]} \delta_i^{\operatorname{Can}} \Psi^{\operatorname{Can}}$.

Compute $\Delta_i \rho_i := \mathrm{CL}_{\mathrm{Match}}(M, A, \rho \delta_i^{\mathrm{Can}} \Psi^{\mathrm{Can}})$ for each $i \in [s]$ recursively.

Rename the indices in [s] such that:

 $(M,\Delta\rho)^{\rho_1} = \ldots = (M,\Delta\rho)^{\rho_r} < (M,\Delta\rho)^{\rho_{r+1}} \leq \ldots \leq (M,\Delta\rho)^{\rho_s}.$

Return $\Lambda := \langle \Delta_1 \rho_1, \dots, \Delta_r \rho_r \rangle$.

(This is the smallest coset containing these cosets as defined in the preliminaries.)

(CL1.) Assume we have M^{φ} , A^{φ} , $\varphi^{-1}\Delta\rho$ instead of M, A, $\Delta\rho$ as an input. Observe that $\varphi^{-1}\rho$ is a coset representative for $\varphi^{-1}\Delta\rho$. We show that the algorithm outputs $\varphi^{-1}\Lambda$ instead of Λ .

In the base case |M| = 0, we return $\varphi^{-1}\Delta\rho$ instead of $\Delta\rho$.

Now, consider the case |A| = 1. We obtain $\varphi(v_1)$ and $\varphi(v_2)$ instead of v_1 and v_2 , respectively. By (CL1) of CL_{Point} , we return $\varphi^{-1}\Lambda$ instead of Λ .

In the intransitive case, we obtain $A^{\varphi} = A_1^{\varphi} \cup A_2^{\varphi}$ as a partition since $A_1^{\rho} = A_1^{\varphi\varphi^{-1}\rho}$. By induction, we obtain $\varphi^{-1}\Lambda_1$ instead of Λ_1 . Again, by induction, we return $\varphi^{-1}\Lambda_2$ instead of Λ_2 . In the transitive case, observe that A^{Can} and $\Delta^{\operatorname{Can}}$ remain unchanged since $A^{\varphi\varphi^{-1}\rho} = A^{\rho}$ and $(\varphi^{-1}\Delta\rho)^{\varphi^{-1}\rho} = (\Delta\rho)^{\rho}$. Therefore, we still obtain $A^{\operatorname{Can}} = A_1^{\operatorname{Can}} \cup A_2^{\operatorname{Can}}$ and also $\Psi^{\operatorname{Can}}$. We obtain cosets $\varphi^{-1}\rho\delta_i^{\operatorname{Can}}\Psi^{\operatorname{Can}}$ instead of $\rho\delta_j^{\operatorname{Can}}\Psi^{\operatorname{Can}}$ since the indexing is arbitrary. The calls we do now are of the form $\operatorname{CL}_{\operatorname{Match}}(M^{\varphi}, A^{\varphi}, \varphi^{-1}\delta_i^{\operatorname{Can}}\Psi^{\operatorname{Can}})$ instead of $\operatorname{CL}_{\operatorname{Match}}(M, A, \delta_j^{\operatorname{Can}}\Psi^{\operatorname{Can}})$. By induction, we get $\varphi^{-1}\Delta_i\rho_i$ instead of $\Delta_j\rho_j$. We obtain $\varphi^{-1}\rho_i$ instead of ρ_j . But since $(M, \Delta\rho)^{\rho_i} = (M^{\varphi}, \varphi^{-1}\Delta\rho)^{\varphi^{-1}\rho_i}$ we get the same ordered sequence. The computation of Λ is isomorphism invariant and therefore we return $\varphi^{-1}\Lambda$ instead of Λ .

(CL2.) In the Case that $M = \emptyset$, it holds $\operatorname{Aut}(M) \cap \Delta = \Delta$.

In Case |A| = 1 and thus |M| = 1, it holds that $\operatorname{Aut}(M) \cap \Delta$ is actually equal to $\operatorname{Stab}_{\Delta}(v_1)$ since $\{v_2\} = A$ is already stabilized by Δ .

For the intransitive case, we have $\Lambda_1 = (\operatorname{Aut}(M_1) \cap \Delta)\pi_1$ for some $\pi_1 \in \Lambda_1$ by induction. Again, by induction, the returned coset is $\Lambda_2 = (\operatorname{Aut}(M_2) \cap \operatorname{Aut}(M_1) \cap \Delta)\pi_2$ for some $\pi_2 \in \Lambda_2$. Since (M_1, M_2) is a Δ -invariant *ordered* partition of M, it holds that $\Lambda_2 = (\operatorname{Aut}(M) \cap \Delta)\pi_2$.

For the transitive case, observe that (CL1) of $\operatorname{CL}_{\operatorname{Match}}$ implies $(\operatorname{Aut}(M) \cap \Delta)\pi \subseteq \Lambda$ for some $\pi \in \Lambda$. Next, we show the reversed inclusion $\Lambda \subseteq (\operatorname{Aut}(M) \cap \Delta)\pi$. We need to show that $\rho_i \rho_j^{-1}$ is an element in $\operatorname{Aut}(M) \cap \Delta$ for all $i, j \in [r]$. The membership $\rho_i \rho_j^{-1} \in \operatorname{Aut}(M)$ follows from the fact that $M^{\rho_i} = M^{\rho_j}$ and the membership $\rho_i \rho_j^{-1} \in \Delta$ follows from the fact that $(\Delta \rho)^{\rho_i} = (\Delta \rho)^{\rho_j}$. (Running time.) Let $A^* \subseteq A \subseteq V_2$ be a Δ -orbit of maximal size. We claim that the maximum number of recursive calls $R(|A^*|, |A|)$ is at most $T := 2^{6|A^*|} |A|^2$. In the intransitive case, this is easy to see by induction:

$$R(|A^*|, |A|) \le 1 + \sum_{j \in [2]} R(|A^*|, |A_j|) \stackrel{\text{induction}}{\le} 1 + 2^{6|A^*|} (|A_1|^2 + |A_2|^2) \le T.$$

In the transitive case, it holds that $A^* = A$ and $s \le 2^{|A|}$ and we obtain

$$R(|A|,|A|) \le 1 + s \cdot R(\lceil |A|/2\rceil,|A|) \overset{\text{induction}}{\le} 1 + 2^{4|A|+3}|A|^2 \overset{2 \le |A|}{\le} T.$$

We consider the running time for one single call without recursive costs. All steps are polynomial time computable, except the computation of Ψ^{Can} in the transitive case. The group Ψ^{Can} can be computed in time polynomial in the index and |V|, i.e., $2^{\mathcal{O}(|A^*|)}|V|^{\mathcal{O}(1)}$. In total, we have a running time of at most $T \cdot 2^{\mathcal{O}(|A^*|)}|V|^{\mathcal{O}(1)} \subseteq 2^{\mathcal{O}(k_2)}|V|^{\mathcal{O}(1)}$ where k_2 is the size of the largest Δ -orbit of $A \subseteq V_2$.

As next step, we demonstrate how to compute canonical labelings for objects $\mathcal{X} = (\Theta \tau, \Delta \rho)$ consisting of a pair of labeling cosets.

Problem 6. Compute a function CL_{Int} with the following properties:

Input $(\Theta\tau, \Delta\rho) \in \text{Objects}(V)$ where $\Theta\tau, \Delta\rho \leq \text{Label}(V)$ and V is an unordered set.

Output A labeling coset $CL_{Int}(\Theta\tau, \Delta\rho) = \Lambda \leq Label(V)$ such that:

(CL1) $\operatorname{CL}_{\operatorname{Int}}(\Theta\tau, \Delta\rho) = \varphi \operatorname{CL}_{\operatorname{Int}}(\varphi^{-1}\Theta\tau, \varphi^{-1}\Delta\rho) \text{ for all } \varphi \in \operatorname{Iso}(V; V').$

(CL2) $\operatorname{CL}_{\operatorname{Int}}(\Theta\tau, \Delta\rho) = (\Theta \cap \Delta)\pi$ for some (and thus for all) $\pi \in \Lambda$.



Figure 1: A graph G = (V, E, P) with an ordered partition $P = (E_B, E_R)$.

In fact, Condition (CL2) given here coincides with the general Condition (CL2) stated in the preliminaries, i.e., $CL_{Int}(\Theta\tau, \Delta\rho) = Aut((\Theta\tau, \Delta\rho))\pi$ for some π . The problem can be seen as a canonization analogue to the group-intersection problem which is often used for the purpose of designing isomorphisms algorithms. The next example shows how the problem can be used for canonization purposes.

Example 7. Let G = (V, E, P) be a graph with an *ordered* partition $P = (E_B, E_R)$ of the edges $E = E_B \cup E_R$. The partition can be seen as an edge coloring which has to be preserved by automorphisms of the graph (see Figure 1). Let CL , $\operatorname{CL}_{\operatorname{Int}}$ be canonical labeling functions and define $\Delta_B \rho_B := \operatorname{CL}(E_B)$ and $\Delta_R \rho_R := \operatorname{CL}(E_R)$. Then $\operatorname{CL}_{\operatorname{Graph}}(G) := \operatorname{CL}_{\operatorname{Int}}(\Delta_B \rho_B, \Delta_R \rho_R)$ defines a canonical labeling for graphs with edges colored blue and red.

Lemma 8. A function $\operatorname{CL}_{\operatorname{Int}}$ solving Problem 6 can be computed in time $2^{\mathcal{O}(k)}|V|^{\mathcal{O}(1)}$ where k is the size of the largest Δ -orbit of V.

Proof. Let $\widetilde{V}:=\{\widetilde{v}_1,\ldots,\widetilde{v}_{|V|}\}$ be a set of size |V| disjoint from V. The set \widetilde{V} is essentially a copy of V. Define $U:=\widetilde{V} \cup V$. Let $\Delta_U \rho_U \leq \operatorname{Label}(U)$ be the labeling coset on U obtained by $\Theta \tau$ acting on \widetilde{V} and $\Delta \rho$ acting on V. More formally, we define $\Delta_U \rho_U := \{\lambda_U \in \operatorname{Label}(U) \mid \exists \gamma \in \Theta \tau, \lambda \in \Delta \rho : \text{ for all } i, j \in \{1, \ldots, |V|\} \text{ we have } \lambda_U(\widetilde{v}_i) = \gamma(v_i) + |V| \text{ and } \lambda_U(v_j) = \lambda(v_j) \}$. Define a matching $M := \{(\widetilde{v}_i, v_i) \mid i \in \{1, \ldots, |V|\} \}$ by pairing corresponding vertices. Define $\Lambda_U := \operatorname{CL}_{\operatorname{Match}}(M, \Delta_U \rho_U)$. We claim that $\Lambda := \Lambda_U \downarrow_V$ defines a canonical labeling for $(\Theta \tau, \Delta \rho)$ where " \downarrow " denotes the induced labeling coset (as defined at the beginning of Section 3).

(CL1.) Assume we have $\varphi^{-1} \Theta \tau$, $\varphi^{-1} \Delta \rho$ instead of $\Theta \tau$, $\Delta \rho$ as an input. Following the construction, we obtain M^{φ_U} instead of M and $\varphi_U^{-1} \Delta_U \rho_U$ instead of $\Delta_U \rho_U$ for some φ_U with $\varphi_U|_V = \varphi$. By (CL1) of CL_{Match}, we obtain $\varphi_U^{-1} \Lambda_U$ instead of Λ_U . Therefore, we obtain $\varphi^{-1} \Lambda$ instead of Λ .

(CL2.) We need to show that $(\operatorname{Aut}(M) \cap \Delta_U)|_V = \Theta \cap \Delta$. The inclusion $\Theta \cap \Delta \subseteq (\operatorname{Aut}(M) \cap \Delta_U)|_V$ follows from (CL1) of this reduction. We thus need to show the reversed inclusion $(\operatorname{Aut}(M) \cap \Delta_U)|_V \subseteq \Theta \cap \Delta$. So assume $\delta_U \in \operatorname{Aut}(M) \cap \Delta_U$. Let $f: \widetilde{V} \to V$ be the bijection such that $f(\widetilde{v}_i) = v_i$. Since $\delta_U \in \Delta_U$, there are some $\theta \in \Theta, \delta \in \Delta$ such that $f(\delta_U(\widetilde{v}_i)) = \theta(v_i)$ and $\delta_U(v_i) = \delta(v_i)$ for all $i \in \{1, \ldots, |V|\}$. Since $\delta_U \in \operatorname{Aut}(M)$, it holds that $f(\delta_U(\widetilde{v}_i)) = \delta_U(f(\widetilde{v}_i)) = \delta_U(v_i)$ for all $i \in \{1, \ldots, |V|\}$. Both together imply that $\theta(v_i) = f(\delta_U(\widetilde{v}_i)) = \delta_U(v_i) = \delta(v_i)$ for all $v_i \in V$. Thus $\delta_U|_V \in \Theta \cap \Delta$.

(Running time.) Observe that the exponential term in the running time of CL_{Match} just depends on the size of the largest Δ_U -orbit of $V \subseteq U$ which is simply the size of the largest Δ -orbit of V.

An algorithm similar to the one just described can be found [Mil83]. So far, we are able to canonize a pair of two atoms. This is already sufficient to canonize tuples.



Figure 2: A graph G = (V, E, P) with an (unordered) partition $P = \{E_B, E_R\}$.

Canonization of Tuples using Iterated Instances The three canonical labeling functions we have defined so far take two inputs, namely some object as first input (a point/a matching/a labeling coset) and a labeling coset as second input. We want to extend the definition to more arguments replacing the first input by a tuple of objects. This is in analogy to our definition of the stabilizer function $\operatorname{Stab}_{-}(-)$. Let CL be a canonical labeling function for pairs of objects $(\mathcal{X}, \Delta \rho)$ where $\mathcal{X} \in \operatorname{Objects}(V)$ and $\Delta \rho \leq \operatorname{Label}(V)$. For an object X_1 , we define $\operatorname{CL}(X_1; \Delta \rho)$ as $\operatorname{CL}(X_1, \Delta \rho)$. Inductively for $t \geq 2$, we define the *iterated instance* $\operatorname{CL}(X_1, \ldots, X_t; \Delta \rho)$ as $\operatorname{CL}(X_2, \ldots, X_t; \operatorname{CL}(X_1, \Delta \rho))$. To justify the definition, let X_1, \ldots, X_t be a sequence of objects and let $\Delta \rho \leq \operatorname{Label}(V)$ be a labeling coset. Then $\operatorname{CL}(X_1, \ldots, X_t; \Delta \rho)$ defines a canonical labeling for the tuple $(X_1, \ldots, X_t, \Delta \rho)$. In order to compute canonical labelings for tuples, it is therefore sufficient to canonize pairs.

5 Object Replacement

A crucial advantage of the framework we have defined is that labeling cosets are objects themselves. The next lemma shows that for a given set $\mathcal{X} = \{X_1, \dots, X_t\}$ of pairwise isomorphic objects X_i , we can replace the objects X_i by their canonical labeling cosets without losing or introducing global symmetries of the object \mathcal{X} . The benefit is that the canonical labelings of the objects X_i can be computed using a recursive approach.

Lemma 9 (Object replacement). Let $\mathcal{X} = \{X_1, \dots, X_t\}$ be an object and let CL , $\operatorname{CL}_{\operatorname{Set}}$ be canonical labeling functions and let $\Delta_i \rho_i := \operatorname{CL}(X_i)$ for each $i \in [t]$ and $\mathcal{X}^{\operatorname{Set}} := \{\Delta_1 \rho_1, \dots, \Delta_t \rho_t\}$. Assume that $X_i^{\rho_i} = X_j^{\rho_j}$ for all $i, j \in [t]$. Then $\operatorname{CL}_{\operatorname{Object}}(\mathcal{X}) := \operatorname{CL}_{\operatorname{Set}}(\mathcal{X}^{\operatorname{Set}})$ defines a canonical labeling for \mathcal{X} .

Proof. We have $X_i^{\rho_i} = X_j^{\rho_j}$ for all $i, j \in [t]$. Then, by (CL1) and (CL2) of the function CL, it holds for all $\sigma \in \text{Sym}(V)$ that $X_i^{\sigma} = X_j$, if and only if $\text{CL}(X_i^{\sigma}) = \text{CL}(X_j)$, which in turn is equivalent to $(\Delta_i \rho_i)^{\sigma} = \Delta_j \rho_j$. This implies that $\text{Aut}(\mathcal{X}) = \text{Aut}(\mathcal{X}^{\text{Set}})$.

We extend Example 7 to (unordered) partitions by exploiting the object replacement lemma.

Example 10. Let G = (V, E, P) be a graph with an (unordered) partition $P = \{E_B, E_R\}$ of the edges $E = E_B \cup E_R$. In contrast to Example 7, the partition is not ordered. Here, there exists an automorphism that maps the set of blue edges E_B to the set of red edges E_R (see Figure 2). Let CL , $\operatorname{CL}_{\operatorname{Set}}$ be canonical labeling functions and let $\Delta_B \rho_B := \operatorname{CL}(E_B)$ and $\Delta_R \rho_R := \operatorname{CL}(E_R)$. By Lemma 9, $\operatorname{CL}_{\operatorname{Graph}}(G) := \operatorname{CL}_{\operatorname{Set}}(\{\Delta_B \rho_B, \Delta_R \rho_R\})$ defines a canonical labeling for graphs with (unordered) edge partitions.

To exploit the object replacement lemma, our upcoming algorithms in Sections 6 and 7 use the following partitioning strategy. **General Strategy** Assume we are given an object $X = \{x_1, ..., x_t\}$ that is to be canonized. Our general strategy is to construct an (unordered) partition $X = X_1 \cup ... \cup X_s$ in an isomorphism-invariant way. We call the parts X_i bundles. The isomorphism invariance of the partition into bundles in particular ensures that the set $\{X_1, ..., X_s\}$ has the same automorphism group as X. In the cases where this leads to a trivial partition (i.e., s = t or s = 1), we will use problem specific arguments to instantly make some form of progress.

The tough case will occur when the partition is non-trivial. In this case, we will recursively compute canonical labelings $\Theta_i \tau_i$ for the bundles X_i . (Since s > 1 and thus $X_i \not\subseteq X$, we are guaranteed to make progress on the recursive instance). This gives us canonical labelings for each bundle independently, but we have not taken into account any interdependencies between the bundles. This will be our next step.

First, assume that the bundles X_i are pairwise non-isomorphic. Since each bundle is canonized separately, we are now able to sort the bundles according to their canonical forms. This gives an ordered partition of the bundles $\mathcal{X} := (X_1, \dots, X_s)$ that is obtained by renaming the indices such that $X_i^{\tau_i} < X_j^{\tau_j}$, if and only if $i < j \in [s]$. Now, we can exploit the object replacement paradigm and replace the bundles by their labeling cosets without losing any information. This leads to a tuple of labeling cosets $\mathcal{X}^{\text{Int}} := (\Theta_1 \tau_1, \dots, \Theta_s \tau_s)$ for which we already have a canonization technique in Section 4.

Second, assume the bundles X_i are pairwise isomorphic. Here, we have to deal with the (unordered) partition $\mathcal{X} := \{X_1, \dots, X_s\}$. We exploit the object replacement lemma (Lemma 9) again. We replace each bundle with its labeling coset and obtain a set of labeling cosets $\mathcal{X}^{\text{Set}} := \{\Theta_1 \tau_1, \dots, \Theta_s \tau_s\}$. Doing this, we do not lose any symmetries of the object \mathcal{X} and it is now sufficient to compute a canonical labeling for the object \mathcal{X}^{Set} rather than \mathcal{X} . To canonize \mathcal{X}^{Set} , we will use a recursive approach. (Since s < t and thus $|\mathcal{X}^{\text{Set}}| < |\mathcal{X}|$, we are guaranteed to make progress on the recursive instance).

In general, we would see a mixture of the cases with some bundles being isomorphic to others but not to all. In this mixed case, we order the bundles according to their isomorphism type and perform a mixture of the other two cases.

6 Canonization of Hypergraphs

As dictated by the object replacement lemma (Lemma 9), the key problem we need to solve is to compute a canonical labeling function for objects \mathcal{X}^{Set} where the object $\mathcal{X}^{\text{Set}} = \{\Delta_1 \rho_1, \dots, \Delta_t \rho_t\}$ is a set of labeling cosets. Towards a solution of this, our next building block will be the following more specialized problem, reminiscent of hypergraph canonization.

Problem 11. Compute a function CL_{Hyper} with the following properties:

```
Input (K, \Delta \rho) \in \text{Objects}(V) where K = \{(\Delta_1 \rho_1, S_1), \dots, (\Delta_t \rho_t, S_t)\}, \ \Delta_i \rho_i \leq \text{Label}(V), \ \Delta \rho \leq \text{Label}(V), \ S_i \subseteq V \text{ for all } i \in [t], \ S_i \neq S_j \text{ for } i \neq j \text{ and } V \text{ is an unordered set.}
```

Output A labeling coset $CL_{Hyper}(K, \Delta \rho) = \Lambda \leq Label(V)$ such that:

(CL1) $\operatorname{CL}_{\operatorname{Hyper}}(K, \Delta \rho) = \varphi \operatorname{CL}_{\operatorname{Hyper}}(K^{\varphi}, \varphi^{-1} \Delta \rho) \text{ for all } \varphi \in \operatorname{Iso}(V; V').$

(CL2) $\operatorname{CL}_{\operatorname{Hyper}}(K, \Delta \rho) = \{ \delta \in \Delta \mid \exists \psi \in \operatorname{Sym}(t) \forall i \in [t] : (\Delta_i \rho_i, S_i)^{\delta} = (\Delta_{\psi(i)} \rho_{\psi(i)}, S_{\psi(i)}) \} \pi$ for some (and thus for all) $\pi \in \Lambda$.

As usual, Conditions (CL1) and (CL2) given here coincide with the general Condition (CL1) and (CL2). In particular, $CL_{Hyper}(K, \Delta \rho) = Aut((K, \Delta \rho))\pi$ for some π .

Lemma 12. A function $\operatorname{CL}_{\operatorname{Hyper}}$ solving Problem 11 can be computed in time $2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest Δ -orbit of V.

In an instance of Problem 11, each labeling coset $\Delta_i \rho_i$ comes with a subset S_i of V and these subsets are pairwise distinct. In the special case where $\Delta_i \rho_i = \text{Label}(V)$ for all $i \in [t]$, the problem is equivalent to hypergraph canonization. However, we need the more general version for a recursive approach. Nevertheless, we think of the sets S_i as hyperedges. Before giving a detailed proof we describe the general strategy.

Intuition for the Hypergraph Algorithm To solve Problem 11, we will maintain at any point in time a Δ -invariant set $A \subseteq V$ for which the following condition (Condition (A)) holds: $S_i \cap A \neq S_j \cap A$ for all $i \neq j$. This set A measures our progress in the sense that the number of hyperedges t is bounded by $2^{|A|}$. In the base case, if |A| is smaller than an absolute constant, we have a constant number of hyperedges and can apply a brute force algorithm.

If Δ acts transitively on A (the transitive case), we branch on all possible splits of A into two equally sized sets A_1, A_2 , shrinking Δ in the process, and achieving that Δ is not transitive anymore.

The trickiest case is when Δ does not act transitively on A. This gives us a canonical Δ invariant partition $A = A_1 \cup A_2$ (the intransitive case). Here, we need to apply recursion. A primitive approach by recursing on A_1 and subsequently on A_2 does not work, since it would not maintain the Condition (A) which ensures that we can handle the base case. Instead, we define a partition into bundles $K = K_1 \cup ... \cup K_s$ of the set K as proposed by our general strategy. In the concrete situation for hypergraphs, we can define bundles as follows. We say that two hyperedges S_i and S_j are in the same bundle, if and only if the hyperedges agree in the first part A_1 (i.e., $S_i \cap A_1 = S_j \cap A_1$) (see Figure 3). This gives an (unordered) partition of the set of hyperedges $K = K_1 \cup ... \cup K_s$, where each subset of hyperedges K_i corresponds to a bundle. In the extreme case where each hyperedge forms its own bundle, and hence s = t, we can restrict our focus A to the set A_1 and we still maintain Condition (A), making progress. In the other extreme, if all hyperedges correspond to the same bundle, and hence s = 1, we can restrict our set A to the A_2 . It remains to explain the case in which we have a proper bundling. For this observe that the bundles themselves form instances of our original problem so we can compute a canonical labeling $\Theta_i \tau_i := \mathrm{CL}_{\mathrm{Hyper}}(K_i)$ for each of the bundles recursively. Following our general strategy, we next compute a canonical labeling for the set of bundles taking the relation between the bundles into account.

For the case that the bundles K_{ℓ} are pairwise non-isomorphic, we directly follow our general strategy. We order the bundles according to their isomorphism type and canonize them sequentially using iterated instances from Section 4.

Assume now that the bundles K_i are pairwise isomorphic. In this case, we have an (unordered) partition $\mathcal{K} := \{K_1, \dots, K_s\}$ consisting of the pairwise isomorphic bundles. Here, we exploit the object replacement paradigm (Lemma 9). We replace each bundle with its labeling coset and obtain a set of labeling cosets $\mathcal{K}^{\text{Set}} := \{\Theta_1 \tau_1, \dots, \Theta_s \tau_s\}$. Doing this, we do not lose any symmetries of the hypergraph \mathcal{K} and it is now sufficient to compute a canonical labeling of the object \mathcal{K}^{Set} rather than \mathcal{K} . To canonize \mathcal{K}^{Set} using recursion, we have to interpret this set of labeling cosets as an instance of our hypergraph problem. For this, observe that restricted to the set $A_1 \subseteq A \subseteq V$ the set \mathcal{K}^{Set} must induce a hypergraph structure since the bundles pairwise disagree on A_1 (see the left side of Figure 3). This allows us to compute the canonical labeling for \mathcal{K}^{Set} recursively using our hypergraph algorithm.

In the general case, in which some bundles being isomorphic to others but not to all, we perform a mixture of the two cases just described.

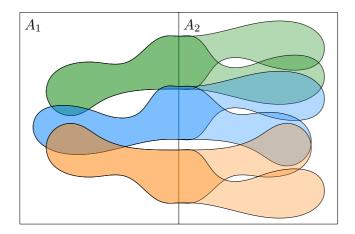


Figure 3: Bundling the hyperedges: six hyperedges are bundled into 3 bundles (shown in distinct colors) each consisting of two hyperedges.

Comparison to Previous Algorithms The first $2^{\mathcal{O}(|V|)}$ -time hypergraph-isomorphism algorithm is due to Luks [Luk99]. In a dynamic programming fashion, he computed the isomorphisms by intersecting cosets of isomorphisms between already computed subhypergraphs. This approach makes use of the coset-intersection problem for permutation groups.

Using Luks's approach as a starting point, in [ADKT15] an algorithm is developed for the setting of bounded color classes. Indeed, the authors found a way to exploit ordered partitions by using the bundling technique described here. However, within the color classes they used essentially Luks's dynamic programming algorithm to compute the isomorphisms.

The crucial novelty in our algorithm is the more general definition of the problem in which labeling cosets occur as part of the input structure. This allows us to completely give up dynamic programming, and instead use the bundling technique in a recursive way. Treating cosets (which are the results of recursive canonization calls) as objects themselves allows us to recurse on substructures.

This in turn allows us to compute canonical labelings for hypergraphs resolving the open question of both papers.

Another advantage of our approach is that it allows for a polynomial-time algorithm if the group Δ is of a certain restricted structure (such as having bounded size composition factors, see Corollary 25).

Detailed Description of the Hypergraph Algorithm We proceed to prove Lemma 12 by giving a detailed description and analysis of our hypergraph canonization algorithm.

Proof of Lemma 12. For the purpose of recursion, we need an additional input parameter. Specifically, we use a subset $A \subseteq V$ such that $\Delta \subseteq \operatorname{Stab}(A)$. Initially, we set A = V. For this parameter, we always require that

(A)
$$S_i \cap A \neq S_j \cap A$$
 for all $i \neq j$.

An algorithm for $\mathrm{CL}_{\mathrm{Hyper}}(K, A, \Delta \rho)$:

If $|A| \le 1$: (Because of Property (A), it holds that $|K| \le 2$.)

```
If |K| = 1: Return \operatorname{CL}_{\operatorname{Int}}(\Delta_1 \rho_1, \operatorname{Label}(S_1) \uparrow^V; \Delta \rho).
                  (This is an iterated instance as defined in Section 4.)
         If |K| = 2:
                  Rename the indices of elements in K such that S_1 \cap A = \emptyset and S_2 \cap A = A.
                  Return \operatorname{CL}_{\operatorname{Int}}(\Delta_1 \rho_1, \operatorname{Label}(S_1) \uparrow^V, \Delta_2 \rho_2, \operatorname{Label}(S_2) \uparrow^V; \Delta \rho).
                  (This is an iterated instance as defined in Section 4.)
If \Delta is intransitive on A:
         Partition A = A_1 \cup A_2 where A_1 is a \Delta-orbit such that A_1^{\rho} is minimal.
         (Minimal w.r.t. the order "<" defined in Section 3.)
         Define S_{i,1} := S_i \cap A_1 for each i \in [t].
         Define an (unordered) partition K := K_1 \cup ... \cup K_s with \mathcal{K} := \{K_1, ..., K_s\} such that:
         S_{i,1} = S_{j,1}, if and only if (\Delta_i \rho_i, S_i), (\Delta_j \rho_j, S_j) \in K_\ell for some \ell \in [s].
         If s = t: (Thus S_{i,1} \neq S_{j,1} for all i \neq j.)
                  Recurse and return \Lambda := CL_{Hyper}(K, A_1, \Delta \rho).
         If s = 1: (Thus S_{i,1} = S_{j,1} for all i, j \in [t] and thus S_i \cap A_2 \neq S_j \cap A_2 for all i \neq j.)
                  Recurse and return \Lambda := CL_{Hyper}(K, A_2, \Delta \rho).
         If 1 < s < t: (Thus S_{i,1} = S_{j,1} for some i \neq j, but not for all i \neq j.)
                  (We compute a canonical labeling for K.)
                  Compute \Theta_i \tau_i := \mathrm{CL}_{\mathrm{Hyper}}(K_i, A_2, \Delta \rho) for each i \in [s] recursively.
                  For each K_i pick a (\Delta_i \rho_i, S_i) \in K_i and set R_i := S_{i,1}.
                  (Here R_i does not depend on the choice of j.)
                  Let \mathcal{K}^{\text{Hyper}} := \{(\Theta_1 \tau_1, R_1), \dots, (\Theta_s \tau_s, R_s)\}.
Define an ordered partition \mathcal{K}^{\text{Hyper}} = \mathcal{K}_1^{\text{Hyper}} \cup \dots \cup \mathcal{K}_r^{\text{Hyper}} such that
                  (K_i, \Delta \rho)^{\tau_i} \prec (K_j, \Delta \rho)^{\tau_j}, if and only if (\Theta_i \tau_i, R_i) \in \mathcal{K}_p^{\text{Hyper}} and (\Theta_j \tau_j, R_j) \in \mathcal{K}_q^{\text{Hyper}} for
                  some p, q \in [r] with p < q.
                  Recurse and return \Lambda := \mathrm{CL}_{\mathrm{Hyper}}((\mathcal{K}_1^{\mathrm{Hyper}}, A_1), \dots, (\mathcal{K}_r^{\mathrm{Hyper}}, A_1); \Delta \rho).
                  (This is an iterated instance as defined in Section 4.)
If \Delta is transitive on A:
         Let A^{\operatorname{Can}} := A^{\rho} and \Delta^{\operatorname{Can}} := (\Delta \rho)^{\rho}.
         Partition A^{\operatorname{Can}} = A_1^{\operatorname{Can}} \cup A_2^{\operatorname{Can}} such that |A_1^{\operatorname{Can}}| = \lfloor |A^{\operatorname{Can}}|/2 \rfloor and A_1^{\operatorname{Can}} is minimal.
         (Minimal w.r.t. the order "<" defined in Section 3.)
         Compute \Psi^{\operatorname{Can}} := \operatorname{Stab}_{\Delta^{\operatorname{Can}}}(A_1^{\operatorname{Can}}, A_2^{\operatorname{Can}}).
          (The group can be computed using a membership test as stated in the preliminaries.)
         Decompose \Delta^{\operatorname{Can}} into left cosets of \Psi^{\operatorname{Can}} and write \Delta^{\operatorname{Can}} = \bigcup_{i \in [s]} \delta_i^{\operatorname{Can}} \Psi^{\operatorname{Can}}.
         Compute \Delta_i \rho_i := \mathrm{CL}_{\mathrm{Hyper}}(K, A, \rho \delta_i^{\mathrm{Can}} \Psi^{\mathrm{Can}}) for each i \in [s] recursively.
         Rename the indices in [s] such that:
         (K,\Delta\rho)^{\rho_1} = \ldots = (K,\Delta\rho)^{\rho_r} \prec (K,\Delta\rho)^{\rho_{r+1}} \leq \ldots \leq (K,\Delta\rho)^{\rho_s}.
         Return \Lambda := \langle \Delta_1 \rho_1, \dots, \Delta_r \rho_r \rangle.
          (This is the smallest coset containing these cosets as defined in the preliminaries.)
```

- (A.) Towards showing correctness of the algorithm, we first argue that Condition (A) remains satisfied in recursive calls. In the intransitive case, Condition (A) remains satisfied for the recursive calls by construction of the partition of K. In the transitive case, K and K remain unchanged, and therefore Condition (A) also remains satisfied.
- (CL1.) As usual, Property (CL1) follows since all ordered sequences and all partitions are defined in an isomorphism-invariant way.

(CL2.) Consider the Case $|A| \leq 1$. If |K| = 1, then $\operatorname{Aut}((K, \Delta \rho))$ is equal to the intersection $\Delta_1 \cap \operatorname{Stab}(S_1) \cap \Delta$. Analogously, if |K| = 2, then $\operatorname{Aut}((K, \Delta \rho))$ is equal to $\Delta_1 \cap \operatorname{Stab}(S_1) \cap \Delta_2 \cap \operatorname{Stab}(S_2) \cap \Delta$.

We consider the intransitive case. In the Cases s=t and s=1, (CL2) holds by induction. We consider the Case 1 < s < t. By induction, it holds that Λ defines a canonical labeling for $(\mathcal{K}_1^{\text{Hyper}}, \dots, \mathcal{K}_r^{\text{Hyper}}, \Delta \rho)$. Since R_i was chosen in an isomorphism-invariant way, Λ defines a canonical labeling for $(\mathcal{J}_1^{\text{Hyper}}, \dots, \mathcal{J}_r^{\text{Hyper}}, \Delta \rho)$ where $\mathcal{J}_i^{\text{Hyper}} = \{\Lambda \mid (\Lambda, R) \in \mathcal{R}_i^{\text{Hyper}}\}$ for $i \in [r]$. Because of the object replacement lemma (Lemma 9), it holds that Λ defines a canonical labeling for $(\mathcal{J}_1, \dots, \mathcal{J}_r, \Delta \rho)$ where $\mathcal{J} = \mathcal{J}_1 \cup \dots \cup \mathcal{J}_r$ such that $K_i \in \mathcal{J}_\ell$, if and only if $\Theta_i \tau_i \in \mathcal{J}_\ell^{\text{Hyper}}$. Since $(\mathcal{J}_1, \dots, \mathcal{J}_r)$ is an isomorphism-invariant ordered partition of $\mathcal{J} = \mathcal{K}$, it holds that Λ defines a canonical labeling for $(\mathcal{K}, \Delta \rho)$. Again, $\mathcal{K} = \{K_1, \dots, K_s\}$ is an isomorphism-invariant (unordered) partition of $K = K_1 \cup \dots \cup K_s$ and therefore Λ defines a canonical labeling for $(K, \Delta \rho)$.

The transitive case is similar to the analysis in Lemma 5.

(Running time.) Let $A^* \subseteq A$ be a Δ -orbit of maximal size. We claim that the maximum number of recursive calls given these parameters $R(|A^*|, |A|, |K|)$ is at most $T := 2^{6|A^*|}|A||K|^3$.

In the Case $|A| \le 1$, we do not have further recursive calls. The transitive case is similar to the analysis in Lemma 5. In the intransitive cases if s = t or s = 1, there is only one recursive call and the size of A decreases.

We consider the intransitive case when 1 < s < t. Here, we have recursive calls on K_1, \ldots, K_s and $\mathcal{K}_1^{\mathrm{Hyper}}, \ldots \mathcal{K}_r^{\mathrm{Hyper}}$. The cardinalities of $|A^*|$ and |A| never increase for recursive calls.

$$R(|A^*|, |A|, |K|) \leq 1 + \sum_{i=1}^{r} R(|A_i^*|, |A_1|, |\mathcal{K}_i^{\text{Hyper}}|) + \sum_{i=1}^{s} R(|A^*|, |A_2|, |K_i|)$$

$$\stackrel{\text{induction}}{\leq 1 + \sum_{i=1}^{r} T(|A_i^*|, |A_1|, |\mathcal{K}_i^{\text{Hyper}}|) + \sum_{i=1}^{s} T(|A^*|, |A_2|, |K_i|)}$$

$$\leq 1 + T(|A^*|, |A|, \sum_{i=1}^{r} |\mathcal{K}_i^{\text{Hyper}}|) + \sum_{i=1}^{s} T(|A^*|, |A|, |K_i|)$$

$$= 1 + 2^{6|A^*|} |A| (s^3 + \sum_{i=1}^{s} |K_i|^3) \leq T,$$

where for the last inequality we argue as follows: we use that $s \neq t$ and thus there is an $i \in [s]$ such that $|K_i| \geq 2$. Without loss of generality, we assume $|K_1| \geq 2$. For $i \neq 1$, we use $|K_i| \geq 1$.

$$|K|^{3} = \left(\sum_{i=1}^{s} |K_{i}|\right)^{3} = \sum_{i=1}^{s} |K_{i}|^{3} + \sum_{\substack{2 \le i, j, \ell \le s \\ |\{i, j, \ell\}| \ge 2}} |K_{i}||K_{j}||K_{\ell}| + \sum_{2 \le i, j \le s} 3|K_{1}||K_{i}||K_{j}| + \sum_{2 \le i \le s} 3|K_{1}|^{2}|K_{i}|$$

$$\geq \sum_{i=1}^{s} |K_{i}|^{3} + \left((s-1)^{3} - (s-1)\right) + 6(s-1)^{2} + 12(s-1)$$

$$= \sum_{i=1}^{s} |K_{i}|^{3} + s^{3} + 3s^{2} + 2s - 6 \stackrel{s>1}{>} \sum_{i=1}^{s} |K_{i}|^{3} + s^{3}$$

We consider the running time for one single call without recursive costs. Such a call can be computed in time $2^{\mathcal{O}(k)}|V|^{\mathcal{O}(1)}$ where k is the largest Δ -orbit of V. In total, we have a running time of at most $T \cdot 2^{\mathcal{O}(k)}|V|^{\mathcal{O}(1)} \subseteq 2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest Δ -orbit of V.

Corollary 13. Canonical labelings for hypergraphs can be computed in time $2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest color class of V.

Proof. Given a hypergraph with hyperedges $\{S_1, \ldots, S_t\}$ and a coloring (C_1, \ldots, C_t) of $V = C_1 \cup \ldots \cup C_t$, we use the previous algorithm to compute a canonical labeling for $(K, \Delta \rho)$ where $K = \{(\text{Label}(V), S_1), \ldots, (\text{Label}(V), S_t)\}$ and $\Delta \rho = \{\lambda \in \text{Label}(V) \mid \forall i, j \in [t], i < j \forall v_i \in C_i, v_j \in C_j : \lambda(v_i) < \lambda(v_j)\}.$

7 Canonization of Sets

In this section, we are looking for a canonical labeling function for objects \mathcal{X} in the case where $\mathcal{X} = (\{\Delta_1 \rho_1, \dots, \Delta_t \rho_t\}, \Delta \rho)$. As we will see in Section 8, canonical labelings for objects in general can be reduced to this case in polynomial time.

Problem 14. Compute a function CL_{Set} with the following properties:

Input $(J, \Delta \rho) \in \text{Objects}(V)$ where $J = \{\Delta_1 \rho_1, \dots, \Delta_t \rho_t\}, \ \Delta_i \rho_i \leq \text{Label}(V)$ for all $i \in [t]$, $\Delta \rho \leq \text{Label}(V)$ and V is an unordered set.

Output A labeling coset $CL_{Set}(J, \Delta \rho) = \Lambda \leq Label(V)$ such that:

(CL1) $\operatorname{CL}_{\operatorname{Set}}(J,\Delta\rho) = \varphi \operatorname{CL}_{\operatorname{Set}}(J^{\varphi}, \varphi^{-1}\Delta\rho) \text{ for all } \varphi \in \operatorname{Iso}(V;V').$

(CL2) $\operatorname{CL}_{\operatorname{Set}}(J, \Delta \rho) = \{ \delta \in \Delta \mid \exists \psi \in \operatorname{Sym}(t) \forall i \in [t] : \delta^{-1} \Delta_i \rho_i = \Delta_{\psi(i)} \rho_{\psi(i)} \} \pi \text{ for some (and thus for all) } \pi \in \Lambda.$

As usual, Conditions (CL1) and (CL2) coincide with the general the conditions. In particular, $\text{CL}_{\text{Set}}(J,\Delta\rho) = \text{Aut}((J,\Delta\rho))\pi$ for some π .

Lemma 15. A function $\operatorname{CL}_{\operatorname{Set}}$ solving Problem 14 can be computed in time $2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest Δ -orbit of V.

Intuition for the Sets of Labeling Cosets Algorithm As it was the case for hypergraph algorithm, we need a generalization of our problem for a recursive approach. We extend the instances to sets of the form $L = \{(\Delta_1 \rho_1, \Theta_1 \tau_1), \dots, (\Delta_t \rho_t, \Theta_t \tau_t)\}$. For the initial instance, $\Theta_i \tau_i$ is simply set to equal $\Delta_i \rho_i$. The labeling cosets $\Theta_i \tau_i$ can be seen as an analogue to the hyperedges S_i in Problem 11 and are used to define a bundling of the instance L. Compared to hyperedges S_i the labeling cosets $\Theta_i \tau_i$ can describe global interdependencies. While Condition (A) for hypergraphs describes a local distinctness, for our new problem, we define adequate Conditions (C) and (AC) describing a more refined distinctness of the cosets. But again, the size of a set $A \subseteq V$ is used to measure our progress in the sense that the size |L| is bounded in terms of |A|. Additionally, we will ensure a uniformity condition (Condition (D)) which helps us in various situations. In the algorithm, following our general strategy, we heavily use the partitioning techniques.

First, we consider the case in which at least one group Θ_i is intransitive on the set A. The uniformity (D) implies that all groups Θ_i must be intransitive. In particular, each Θ_i can be associated with the orbit $A_{i,1} \subseteq A$ that has minimal image under τ_i .

If all orbits $A_{i,1}$ and $A_{j,1}$ are distinct for $i \neq j$, the sets $A_{i,1} \subseteq A$ form a hypergraph and we apply our hypergraph algorithm. If the orbits $A_{i,1}$ and $A_{j,1}$ are equal for all $i, j \in [t]$, we can define a set $A_1 := A_{i,1}$ which does not depend on the choice of $i \in [t]$. This gives us a canonical partition $A = A_1 \cup A \setminus A_1$ of the set A we are focusing on. With a similar idea as for hypergraphs, we are able to use the partition of A to define a partition $L = L_1 \cup \ldots \cup L_s$ of L into bundles. In the extreme cases (s = t or s = 1), we use the concrete definition of the partition to reduce the

size of the set A, making progress. The case of a proper partition can be handled by bundling and recursion as usual (one has to be careful that (C) and (AC) are maintained for the recursive call). Also in the remaining subcase where some of the orbits $A_{i,1} \subseteq A$ being equal to others but not to all, we can define a partition into bundles and recurse on that.

Second, we consider the case in which all groups Θ_i are transitive on the focus set A. A crucial difference here is that instead of splitting the underlying vertex A by decomposing only one single group, we split all the labeling cosets $\Theta_i \tau_i$ by decomposing them into left cosets. This leads to the case of intransitive groups Θ_i which we already handled.

Detailed Description of the Sets of Labeling Cosets Algorithm Proving Lemma 15, we give a detailed description and analysis of the algorithm for sets of labeling cosets.

Proof of Lemma 15. We generalize the problem and instead of J we take as an input a set of pairs of labeling cosets $L = \{(\Delta_1 \rho_1, \Theta_1 \tau_1), \dots, (\Delta_t \rho_t, \Theta_t \tau_t)\}$. For the purpose of recursion, we need some additional input parameters. Specifically, we use subsets $A, C \subseteq V$ such that $\Theta_i \leq \operatorname{Stab}(A, C)$ for all $i \in [t]$. Initially, we set A = V and $C = \emptyset$ and $\Theta_i \tau_i = \Delta_i \rho_i$ for all $i \in [t]$. Furthermore, we require that

```
(C) \Theta_i \tau_i |_C = \Theta_i \tau_i |_C for all i, j \in [t], and
(AC) \Theta_i \tau_i |_{A \cup C} \neq \Theta_j \tau_j |_{A \cup C} for all i \neq j.
An algorithm for \mathrm{CL}_{\mathrm{Set}}(L,A,C,\Delta\rho):
If |L| = 0: Return \operatorname{CL}_{\operatorname{Int}}(\operatorname{Label}(A)\uparrow^V, \operatorname{Label}(C)\uparrow^V; \Delta\rho).
           (This is an iterated instance as defined in Section 4.)
If |A| \leq 1:
           Rename the indices in [t] such that A^{\tau_1} < \ldots < A^{\tau_t}.
            (The ordering is strict, for a proof see (Correctness.) below the algorithm.)
           Return \Lambda := \operatorname{CL}_{\operatorname{Int}}(\Delta_1 \rho_1, \dots, \Delta_t \rho_t, \Theta_1 \tau_1, \dots, \Theta_t \tau_t; \Delta \rho).
            (This is an iterated instance as defined in Section 4.)
Let A_i^{\operatorname{Can}} \coloneqq A^{\tau_i}, C_i^{\operatorname{Can}} \coloneqq C^{\tau_i} and \Theta_i^{\operatorname{Can}} \coloneqq (\Theta_i \tau_i)^{\tau_i} for each i \in [t].
\begin{split} &\textit{If } (A_i^{\operatorname{Can}}, C_i^{\operatorname{Can}}, \Theta_i^{\operatorname{Can}}) \neq (A_j^{\operatorname{Can}}, C_j^{\operatorname{Can}}, \Theta_j^{\operatorname{Can}}) \textit{ for some } i, j \in [t]: \\ &\operatorname{Define an } \textit{ ordered } \operatorname{partition } L = L_1 \cup \ldots \cup L_s \text{ such that: } \\ &(A_i^{\operatorname{Can}}, C_i^{\operatorname{Can}}, \Theta_i^{\operatorname{Can}}) \prec (A_j^{\operatorname{Can}}, C_j^{\operatorname{Can}}, \Theta_j^{\operatorname{Can}}), \textit{ if and only if } \end{split}
            (\Delta_i \rho_i, \Theta_i \tau_i) \in L_p and (\Delta_j \rho_j, \Theta_j \tau_j) \in L_q for some p, q \in [s] with p < q.
           Recurse and return \Lambda := \mathrm{CL}_{\mathrm{Set}}((L_1, A, C), \dots, (L_s, A, C); \Delta \rho).
            (This is an iterated instance as defined in Section 4.)
Now, we have the following property (D): (A_i^{\text{Can}}, C_i^{\text{Can}}, \Theta_i^{\text{Can}}) = (A_i^{\text{Can}}, C_i^{\text{Can}}, \Theta_i^{\text{Can}}) for all i, j \in
[t].
If \Theta_i is intransitive on A for some (and because of (D) for all) i \in [t]:
           For each i \in [t] write A = A_{i,1} \cup A_{i,2} where A_{i,1} is a \Theta_i-orbit and such that A_{i,1}^{\tau_i} is minimal.
           (Minimal w.r.t. the order "<" defined in Section 3.)
           If A_{i,1} = A_{j,1} for all i, j \in [t]:
                      Let A_1 := A_{i,1} for some (and thus all) i \in [t].
                      Let \Lambda_i := \Theta_i \tau_i|_{A_1 \cup C} for each i \in [t].
                      Define an (unordered) partition L = L_1 \cup ... \cup L_s with \mathcal{L} := \{L_1, ..., L_s\} such that:
```

 $\Lambda_i = \Lambda_j$, if and only if $(\Delta_i \rho_i, \Theta_i \tau_i), (\Delta_j \rho_j, \Theta_j \tau_j) \in L_\ell$ for some $\ell \in [s]$.

```
If s = t: (Thus \Lambda_i \neq \Lambda_j for all i \neq j.)
                              Recurse and return \Lambda := \mathrm{CL}_{\mathrm{Set}}(L, A_1, C, \Delta \rho)
                      If s = 1: (Thus \Lambda_i = \Lambda_j for all i, j \in [t].)
                              Recurse and return \Lambda := \mathrm{CL}_{\mathrm{Set}}(L, A_2, A_1 \cup C, \Delta \rho)
                      If 1 < s < t: (Thus \Lambda_i = \Lambda_j for some i \neq j, but not for all i \neq j.)
                               (We compute a canonical labeling for \mathcal{L}.)
                              Compute \Pi_i \eta_i := \operatorname{CL}_{\operatorname{Set}}(L_i, A_2, A_1 \cup C, \Delta \rho) for each i \in [s] recursively.
                              For each L_i pick a (\Delta_j \rho_j, \Theta_j \tau_j) \in L_i and set \widehat{\Gamma}_i := \Lambda_j.
                              (The set \widehat{\Gamma}_i does not depend on the choice of j, but \widehat{\Gamma}_i is not a labeling coset.)
                              Let \Gamma_i := \{ \gamma \in \text{Label}(V) \mid \gamma |_{A_1 \cup C} \in \widehat{\Gamma}_i \} \leq \text{Label}(V).
                              (The definition of \Gamma_i rectifies that \widehat{\Gamma}_i is not a labeling coset.)
                              Set \mathcal{L}^{\operatorname{Set}} := \{(\Pi_1 \eta_1, \Gamma_1), \dots, (\Pi_s \eta_s, \Gamma_s)\}.
                             Define an ordered partition \mathcal{L}^{\operatorname{Set}} = \mathcal{L}_{1}^{\operatorname{Set}} \cup \ldots \cup \mathcal{L}_{r}^{\operatorname{Set}} such that: (L_{i}, \Delta \rho)^{\eta_{i}} < (L_{j}, \Delta \rho)^{\eta_{j}}, if and only if (\Pi_{i}\eta_{i}, \Gamma_{i}) \in \mathcal{L}_{p}^{\operatorname{Set}} and (\Pi_{j}\eta_{j}, \Gamma_{j}) \in \mathcal{L}_{q}^{\operatorname{Set}} for
                              some p, q \in [r] with p < q.
                              Recurse and return \Lambda := \mathrm{CL}_{\mathrm{Set}}((\mathcal{L}_1^{\mathrm{Set}}, A_1, C), \dots, (\mathcal{L}_r^{\mathrm{Set}}, A_1, C); \Delta \rho).
                              (This is an iterated instance as defined in Section 4.)
           If A_{i,1} \neq A_{j,1} for some i, j \in [t]:
                      Define an (unordered) partition L = L_1 \cup ... \cup L_s with \mathcal{L} := \{L_1, ..., L_s\} such that:
                      A_{i,1} = A_{j,1}, if and only if (\Delta_i \rho_i, \Theta_i \tau_i), (\Delta_j \rho_j, \Theta_j \tau_j) \in L_\ell for some \ell \in [s].
                      (Observe that 1 < s \le t.)
                      (We compute a canonical labeling for \mathcal{L}.)
                      Compute \Pi_i \eta_i := \operatorname{CL}_{\operatorname{Set}}(L_i, A, C, \Delta \rho) for each i \in [s] recursively.
                      For each L_i pick a (\Delta_i \rho_i, \Theta_i \tau_i) \in L_i and set S_i := A_{i,1}.
                      (The set S_i does not depend on the choice of j.)
                     Set \mathcal{L}^{\text{Hyper}} := \{(\Pi_1 \eta_1, S_1), \dots, (\Pi_s \eta_s, S_s)\}.
Define an ordered partition \mathcal{L}^{\text{Hyper}} = \mathcal{L}_1^{\text{Hyper}} \cup \dots \cup \mathcal{L}_r^{\text{Hyper}} such that:
                     (L_i, \Delta \rho)^{\eta_i} \prec (L_j, \Delta \rho)^{\eta_j}, if and only if (\Pi_i \eta_i, S_i) \in \mathcal{L}_p^{\text{Hyper}} and (\Pi_j \eta_j, S_j) \in \mathcal{L}_q^{\text{Hyper}} and
                      p < q \in [r].
                     Return \Lambda := \mathrm{CL}_{\mathrm{Hyper}}((\mathcal{L}_1^{\mathrm{Hyper}}, V), \dots, (\mathcal{L}_r^{\mathrm{Hyper}}, V); \Delta \rho) using Lemma 12.
                      (This is an iterated instance as defined in Section 4.)
If \Theta_i is transitive on A for some (and because of (D) for all) i \in [t]:
           Let A^{\operatorname{Can}} \coloneqq A_i^{\operatorname{Can}}, C^{\operatorname{Can}} \coloneqq C_i^{\operatorname{Can}} and \Theta^{\operatorname{Can}} \coloneqq \Theta_i^{\operatorname{Can}} for some i \in [t].
           (Because of (D), the definitions do not depend on the choice of i \in [t].)
           Partition A^{\operatorname{Can}} = A_1^{\operatorname{Can}} \cup A_2^{\operatorname{Can}} such that |A_1^{\operatorname{Can}}| = \lfloor |A^{\operatorname{Can}}|/2 \rfloor and A_1^{\operatorname{Can}} is minimal.
           (Minimal w.r.t. the order "<" defined in Section 3.)
           Define \Psi^{\operatorname{Can}} := \operatorname{Stab}_{\Theta^{\operatorname{Can}}}(A_1^{\operatorname{Can}}, A_2^{\operatorname{Can}}).
            (The group can be computed using a membership test as stated in the preliminaries.)
           Decompose \Theta^{\text{Can}} into left cosets of \Psi^{\text{Can}} and write \Theta^{\text{Can}} = \bigcup_{i \in [s]} \theta_i^{\text{Can}} \Psi^{\text{Can}}.
           Let \Theta_C^{\operatorname{Can}} \coloneqq \Theta^{\operatorname{Can}}|_{C^{\operatorname{Can}}} and \Psi_C^{\operatorname{Can}} \coloneqq \Psi^{\operatorname{Can}}|_{C^{\operatorname{Can}}}.

Decompose \Theta_C^{\operatorname{Can}} into left cosets of \Psi_C^{\operatorname{Can}} and write \Theta_C^{\operatorname{Can}} = \bigcup_{i \in [r]} \theta_{C,i}^{\operatorname{Can}} \Psi_C^{\operatorname{Can}}.
            (Observe that r \leq s.)
           For some j \in [t], define a set of cosets N := \{\Gamma_1, \ldots, \Gamma_r\} where \Gamma_i := \tau_j|_C \theta_{C,i}^{\operatorname{Can}} \Psi_C^{\operatorname{Can}}.
            (Because of (C), the set N does not depend on the choice of j \in [t].)
           Define L_i := \{(\Delta_j \rho_j, \tau_j \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}}) \mid j \in [t], \ell \in [s], (\tau_j \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}}) \mid_C = \Gamma_i \} for each i \in [r].
           Compute \Pi_i \eta_i := \mathrm{CL}_{\mathrm{Set}}(L_i, A, C, \Delta \rho) for each i \in [r] recursively.
```

```
Rename the indices of elements in N = \{\Gamma_1, \dots, \Gamma_r\} such that:
(L,\Delta\rho)^{\eta_1} = \ldots = (L,\Delta\rho)^{\eta_q} < (L,\Delta\rho)^{\eta_{q+1}} \leq \ldots \leq (L,\Delta\rho)^{\eta_r}.
(The ordering does not depend on the choice of the \eta_i, for a proof see (CL1.).)
Return \Lambda := \langle \Pi_1 \eta_1, \dots, \Pi_q \eta_q \rangle.
(This is the smallest coset containing these cosets as defined in the preliminaries.)
```

(Correctness.) We consider the case $|A| \leq 1$. We show that we obtain a strict ordering indeed. If $A = \emptyset$, then because of (C) and (AC), it holds that |L| = 1, so the ordering is strict. Let us assume that |A| = 1. Since A is Θ_i -invariant and consists of one element, it holds that $\Theta_i|_{A\cup C}$ is a direct product of $\Theta_i|_A$ and $\Theta_i|_C$ for all $i\in[t]$. But because of (C), it holds that $(\Theta_i \tau_i)|_A \neq (\Theta_i \tau_i)|_A$ for all $i \neq j$ and therefore the ordering is strict.

(C and AC.) We show that (C) and (AC) remain satisfied for the recursive calls. Consider the case $(A_i^{\text{Can}}, C_i^{\text{Can}}, \Theta_i^{\text{Can}}) \neq (A_j^{\text{Can}}, C_j^{\text{Can}}, \Theta_j^{\text{Can}})$. Observe that if (C) and (AC) hold for the set L, then they also hold for each subset of $L_i \subseteq L$. Therefore, in this case (C) and (AC) remain satisfied.

Consider the intransitive case, when $A_{i,1} = A_{j,1}$. In the cases s = t and s = 1, the conditions (C) and (AC) hold for chosen subsets of A by construction. In the Case 1 < s < t, the labeling cosets Γ_i satisfy (C) and (AC) by construction of the partition.

Consider the intransitive case, when $A_{i,1} \neq A_{j,1}$. Here, we only have recursive calls for subsets $L_i \subseteq L$ with A and C unchanged.

Consider the transitive case. Condition (C) holds by construction. Next, we show that also (AC) remains satisfied. Condition (D) implies $\Theta_i^{\text{Can}}|_{A_i^{\text{Can}} \cup C_i^{\text{Can}}} = \Theta_j^{\text{Can}}|_{A_j^{\text{Can}} \cup C_j^{\text{Can}}}$ which means that $\Theta_i \tau_i|_{A \cup C}$ and $\Theta_j \tau_i|_{A \cup C}$ are cosets of the same group. Together with (AC), this implies that $\Theta_i \tau_i|_{A \cup C} \cap \Theta_j \tau_j|_{A \cup C} = \emptyset$. For this reason, also subsets of these cosets are disjoint, i.e., $\tau_i \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}}|_{A \cup C} \cap \tau_j \theta_{\ell'}^{\operatorname{Can}} \Psi^{\operatorname{Can}}|_{A \cup C} = \emptyset$ for $i \neq j$ and $\ell, \ell' \in [s]$. The same disjointness holds for i = j and $\ell \neq \ell'$ since $(\theta_\ell^{\operatorname{Can}}|_{A^{\operatorname{Can}} \cup C^{\operatorname{Can}}})^{-1} \theta_{\ell'}^{\operatorname{Can}}|_{A^{\operatorname{Can}} \cup C^{\operatorname{Can}}} \in \Psi^{\operatorname{Can}}|_{A^{\operatorname{Can}} \cup C^{\operatorname{Can}}}$ implies $\ell = \ell'$. In particular, the cosets $\tau_i \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}}|_{A \cup C}$ and $\tau_j \theta_{\ell'}^{\operatorname{Can}} \Psi^{\operatorname{Can}}|_{A \cup C}$ are distinct for $(i, \ell) \neq (j, \ell')$.

(CL1.) This is not hard to see as almost all ordered sequences and all partitions are defined in an isomorphism-invariant way. There is only one case that needs attention. In the transitive case, we define an ordering that might a priori depend on the choice of η_i for $i \in [r]$. To prove that this is indeed not the case, we claim that $\operatorname{Aut}(L_i) \subseteq \operatorname{Aut}(L)$. Let $\sigma \in \operatorname{Aut}(L_i)$ for $i \in [r]$. Let $j \in [t]$. There is at least one $\ell \in [s]$ such that $(\Delta_j \rho_j, \tau_j \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}}) \in L_i$ since $\{(\tau_j \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}})|_C \mid \ell \in [s]\} = \{\tau_j|_C \theta_{C,i}^{\operatorname{Can}} \Psi_C^{\operatorname{Can}} \mid i \in [r]\} = \{\Gamma_1, \dots, \Gamma_r\}$. By definition of $\operatorname{Aut}(L_i)$, there are $j' \in [t]$ and $\ell' \in [s]$ such that $(\Delta_j \rho_j, \tau_j \theta_\ell^{\operatorname{Can}} \Psi^{\operatorname{Can}})^{\sigma} = (\Delta_{j'} \rho_{j'}, \tau_{j'} \theta_{\ell'}^{\operatorname{Can}} \Psi^{\operatorname{Can}})$. This implies $(\Delta_j \rho_j, \Theta_j \tau_j)^{\sigma} = (\Delta_{j'} \rho_{j'}, \Theta_{j'} \tau_{j'})$. Since for all $j \in [t]$, there is such a $j' \in [t]$, this implies $\sigma \in \operatorname{Aut}(L)$.

(CL2.) In the Case $|A| \leq 1$, the strict ordering of the sequence implies that $\sigma^{-1}\Theta_i\tau_i \neq \Theta_j\tau_j$ for all $\sigma \in \operatorname{Aut}(A)$ and all $i \neq j$. Therefore, $\operatorname{Aut}((L, A, C, \Delta \rho)) = \Delta_1 \cap \ldots \cap \Delta_t \cap \Theta_1 \cap \ldots \cap \Theta_t \cap A_t \cap A$ Stab $(A, C) \cap \Delta$ where Stab(A, C) can be omitted since $\Theta_1 \leq \operatorname{Stab}(A, C)$. We consider the Case $(A_i^{\operatorname{Can}}, C_i^{\operatorname{Can}}, \Theta_i^{\operatorname{Can}}) \neq (A_j^{\operatorname{Can}}, C_j^{\operatorname{Can}}, \Theta_j^{\operatorname{Can}})$. Here, $\mathcal{L} = (L_1, \ldots, L_s)$ is an

isomorphism-invariant ordered partition of $L = L_1 \cup ... \cup L_s$ and therefore $Aut(\mathcal{L}) = Aut(L)$.

Consider the intransitive case, when $A_{i,1} = A_{j,1}$ and s = t or s = 1. Condition (D) and $L \neq \emptyset$ also ensure $Aut(L) \leq Stab(A, C)$. Therefore, changing these parameters in an isomorphisminvariant way does not affect the automorphism group. In the Case 1 < s < t, the labeling coset Λ defines a canonical labeling for $(\mathcal{L}_1^{\operatorname{Set}}, \dots, \mathcal{L}_r^{\operatorname{Set}}, \Delta \rho)$ by induction. Since Γ_i was chosen in an isomorphism-invariant way, Λ defines a canonical labeling for $(\mathcal{J}_1^{\text{Set}}, \dots, \mathcal{J}_r^{\text{Set}}, \Delta \rho)$ where $\mathcal{J}_{i}^{\mathrm{Set}} = \{ \Lambda \mid (\Lambda, \Gamma) \in \mathcal{L}_{i}^{\mathrm{Set}} \}$ for $i \in [r]$. Because of the object replacement lemma (Lemma 9), it holds that Λ defines a canonical labeling for $(\mathcal{J}_1, \ldots, \mathcal{J}_r, \Delta \rho)$ where $\mathcal{J} = \mathcal{J}_1 \cup \ldots \cup \mathcal{J}_r$ such that $L_i \in \mathcal{J}_\ell$, if and only if $\Pi_i \eta_i \in \mathcal{J}_\ell^{\operatorname{Set}}$. Since $(\mathcal{J}_1, \ldots, \mathcal{J}_r)$ is an isomorphism-invariant ordered partition of $\mathcal{J} = \mathcal{L}$, it holds that Λ defines a canonical labeling for $(\mathcal{L}, \Delta \rho)$. Again, $\mathcal{L} = \{L_1, \ldots, L_s\}$ is an isomorphism-invariant (unordered) partition of $L = L_1 \cup \ldots \cup L_s$ and therefore Λ defines a canonical labeling for $(L, \Delta \rho)$.

Consider the intransitive case, when $A_{i,1} \neq A_{j,1}$. Here, the proof is analogous to the previous Case 1 < s < t. Also here, Λ defines a canonical labeling of $(\mathcal{L}_1^{\text{Hyper}}, \dots, \mathcal{L}_r^{\text{Hyper}}, \Delta \rho)$. Since S_i was chosen in an isomorphism-invariant way, the labeling coset Λ defines a canonical labeling for $(\mathcal{J}_1^{\text{Hyper}}, \dots, \mathcal{J}_r^{\text{Hyper}}, \Delta \rho)$ where $\mathcal{J}_i^{\text{Hyper}} = \{\Lambda \mid (\Lambda, S) \in \mathcal{L}_i^{\text{Hyper}}\}$ for $i \in [r]$. Because of the object replacement lemma (Lemma 9), it holds that Λ defines a canonical labeling for $(\mathcal{J}_1, \dots, \mathcal{J}_r, \Delta \rho)$ where $\mathcal{J} = \mathcal{J}_1 \cup \dots \cup \mathcal{J}_r$ such that $L_i \in \mathcal{J}_\ell$, if and only if $\Pi_i \eta_i \in \mathcal{J}_\ell^{\text{Hyper}}$. Since $(\mathcal{J}_1, \dots, \mathcal{J}_r)$ is an isomorphism-invariant ordered partition of $\mathcal{J} = \mathcal{L}$, it holds that Λ defines a canonical labeling for $(\mathcal{L}, \Delta \rho)$. Again, $\mathcal{L} = \{L_1, \dots, L_s\}$ is an isomorphism-invariant (unordered) partition of $L = L_1 \cup \dots \cup L_s$ and therefore Λ defines a canonical labeling for $(L, \Delta \rho)$.

Consider the transitive case. We claim that $\Lambda = \operatorname{Aut}((L, \Delta \rho))\pi$ for some (and thus for all) $\pi \in \Lambda$. The inclusion $\operatorname{Aut}((L, \Delta \rho))\pi \subseteq \Lambda$ follows from (CL1) of this algorithm. It remains to show $\Lambda \subseteq \operatorname{Aut}((L, \Delta \rho))\pi$. We need to show that $\eta_i \eta_j^{-1}$ is an element in $\operatorname{Aut}((L, \Delta \rho))$ for all $i, j \in [q]$. The membership follows from the fact that $(L, \Delta \rho)^{\eta_i} = (L, \Delta \rho)^{\eta_j}$.

(Running time.) Let $A^* \subseteq A$ be a Θ_i -orbit of maximal size over all $i \in [t]$. We claim that the maximum number of recursive calls given these parameters $R(|A^*|, |A|, |L|)$ is at most $T := 2^{14|A^*|}|A||L|^3$.

In the Case $(A_i^{\text{Can}}, C_i^{\text{Can}}, \Theta_i^{\text{Can}}) \neq (A_j^{\text{Can}}, C_j^{\text{Can}}, \Theta_j^{\text{Can}})$ and in the intransitive cases, we make progress on |A| or |L| similar to the analysis of Lemma 12.

We consider the transitive case. Here, we have recursive calls on L_1, \ldots, L_r . Observe that $\sum_{i=1}^r |L_i| = s|L| \le 2^{|A|}|L|$. For the recursive calls, we make progress on $|A^*| = |A|$.

$$R(|A|, |A|, |L|) \leq 1 + \sum_{i=1}^{r} R(\lceil |A|/2 \rceil, |A|, |L_{i}|)$$
induction
$$\leq 1 + \sum_{i=1}^{r} T(\lceil |A|/2 \rceil, |A|, |L_{i}|)$$

$$\leq 1 + T(|A|/2 + 1/2, |A|, \sum_{i=1}^{r} |L_{i}|) \leq 1 + 2^{10|A|+7} |A||L|^{3} \stackrel{2 \leq |A|}{\leq} T.$$

This gives at most T recursive calls for the instance $(L, A, C, \Delta \rho)$.

Summing up, our argument so far shows a bound of $2^{14|A^*|}|A||L|^3$ on the number of recursive calls, where A^* is the maximum size Θ_i -orbit within A. Applying the algorithm on an instance $(J, \Delta \rho)$ gives us a bound of $2^{\mathcal{O}(k)}|V||J|^3$ on the number of recursive calls, where k is the size of the largest Δ_i -orbit of V over all $i \in [t]$. However, the running time claimed by the theorem is in terms of the largest Δ -orbit rather than the Δ_i -orbits. To achieve this, we add a preprocessing step before the algorithm that ensures that the Δ_i -orbits are no larger than the Δ -orbits.

Given the instance $(J, \Delta \rho)$, this can be done as follows. Compute $\Delta'_i \rho'_i := \operatorname{CL}_{\operatorname{Int}}(\Delta_i \rho_i, \Delta \rho)$ for each $\Delta_i \rho_i \in J$. Set $J' := \{\Delta'_1 \rho'_1, \ldots, \Delta'_t \rho'_t\}$. Then define an ordered partition $J' = J'_1 \cup \ldots \cup J'_s$ such that: $(\Delta_i \rho_i, \Delta \rho)^{\rho'_i} < (\Delta_j \rho_j, \Delta \rho)^{\rho'_j}$, if and only if $\Delta'_i \rho'_i \in J'_p$ and $\Delta'_j \rho'_j \in J'_q$ and $p < q \in [s]$. This gives a new (iterated) instance $(J'_1, \ldots, J'_s, \Delta \rho)$ which can be processed by our algorithm that we just presented. A canonical labeling for the new instance defines a canonical labeling also for $(J, \Delta \rho)$ by the object replacement lemma. Furthermore, the new instance has the property that for all $\Delta'_i \rho'_i \in J'_i$ and all $j \in [s]$ the Δ'_i -orbits are not larger than the Δ -orbits.

8 Canonization of Objects

As argued in Lemma 9, for the purpose of a canonical labeling, objects can be replaced with their canonical labelings. With Lemma 15, we are able to compute canonical labelings for a set of labeling cosets. In this section, we will combine both techniques to compute a canonical labeling function for objects in general.

Problem 16. Compute a function CL_{Object} with the following properties:

```
Input (\mathcal{X}, \Delta \rho) \in \text{Objects}(V) where \Delta \rho \leq \text{Label}(V) and V is an unordered set.
```

Output A labeling coset $\mathrm{CL}_{\mathrm{Object}}(\mathcal{X}, \Delta \rho) = \Lambda \leq \mathrm{Label}(V)$ such that:

(CL1) $\operatorname{CL}_{\operatorname{Object}}(\mathcal{X}, \Delta \rho) = \varphi \operatorname{CL}_{\operatorname{Object}}(\mathcal{X}^{\varphi}, \varphi^{-1} \Delta \rho) \text{ for all } \varphi \in \operatorname{Iso}(V; V').$

(CL2) $CL_{Object}(\mathcal{X}, \Delta \rho) = Aut((\mathcal{X}, \Delta \rho))\pi$ for some (and thus for all) $\pi \in \Lambda$.

Theorem 17. A function $\mathrm{CL}_{\mathrm{Object}}$ solving Problem 16 can be computed in time $2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest Δ -orbit of V.

```
Proof. An algorithm for CL_{Object}(\mathcal{X}, \Delta \rho):
```

If $\mathcal{X} = v \in V$: Return $\mathrm{CL}_{\mathrm{Point}}(v, \Delta \rho)$.

If $\mathcal{X} = \Theta \tau \leq \text{Label}(V)$: Return $\text{CL}_{\text{Int}}(\Theta \tau, \Delta \rho)$.

If
$$\mathcal{X} = (X_1, \dots, X_t)$$
:

Compute $\Delta_i \rho_i := \mathrm{CL}_{\mathrm{Object}}(X_i, \Delta \rho)$ for each $i \in [t]$ recursively.

Return $\Lambda := \operatorname{CL}_{\operatorname{Int}}(\Delta_1 \rho_1, \dots, \Delta_t \rho_t; \Delta \rho)$ using the algorithm from Lemma 8.

(This is an iterated instance as defined in Section 4.)

If
$$X = \{X_1, ..., X_t\}$$
:

Compute $\Delta_i \rho_i := \mathrm{CL}_{\mathrm{Object}}(X_i, \Delta \rho)$ for each $i \in [t]$ recursively.

Set $\mathcal{X}^{\text{Set}} := \{\Delta_1 \rho_1, \dots, \Delta_t \rho_t\}.$

Define an ordered partition $\mathcal{X}^{\text{Set}} = \mathcal{X}_1^{\text{Set}} \cup \ldots \cup \mathcal{X}_s^{\text{Set}}$ such that:

 $X_i^{\rho_i} < X_j^{\rho_j}$, if and only if $\Delta_i \rho_i \in \mathcal{X}_p^{\text{Set}}$ and $\Delta_j \rho_j \in \mathcal{X}_q^{\text{Set}}$ for some $p, q \in [s]$ with p < q.

Return $\Lambda := \mathrm{CL}_{\mathrm{Set}}(\mathcal{X}_1^{\mathrm{Set}}, \dots, \mathcal{X}_s^{\mathrm{Set}}; \Delta \rho)$ using the algorithm from Lemma 15.

(This is an iterated instance as defined in Section 4.)

- (CL1.) This is easy to see as the partition of \mathcal{X}^{Set} is defined in an isomorphism-invariant way.
- (CL2.) The Case $\mathcal{X} = \{X_1, \dots, X_t\}$ follows from the object replacement lemma (Lemma 9). The other cases use canonical labeling functions we described in previous sections.

(Running time.) With a dynamic programming approach, we build up a table in which we store a canonical labeling for each $(\mathcal{Y}, \Delta \rho)$ with $\mathcal{Y} \in \mathrm{TClosure}(\mathcal{X})$. Note that in each recursive call to $\mathrm{CL}_{\mathrm{Object}}$ the coset $\Delta \rho$ remains unchanged and thus each recursive call is indeed of the form $(\mathcal{Y}, \Delta \rho)$ with $\mathcal{Y} \in \mathrm{TClosure}(\mathcal{X})$. We thus get at most $|\mathrm{TClosure}(\mathcal{X})| \in \mathcal{O}(n)$ recursive calls. For the (non-recursive) calls to $\mathrm{CL}_{\mathrm{Int}}$ and $\mathrm{CL}_{\mathrm{Set}}$, we use the respective algorithms from the previous sections to compute the solutions within the desired running time.

Corollary 18. Canonical labelings for combinatorial objects can be computed in time $2^{\mathcal{O}(k)}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest color class of V.

Proof. Given an object $\mathcal{X} \in \text{Objects}(V)$ and a coloring (C_1, \ldots, C_t) of $V = C_1 \cup \ldots \cup C_t$, we use the previous algorithm to compute a canonical labeling for $(\mathcal{X}, \Delta \rho)$ where $\Delta \rho = \{\lambda \in \text{Label}(V) \mid \forall i, j \in [t], i < j \forall v_i \in C_i, v_j \in C_j : \lambda(v_i) < \lambda(v_j)\}.$

Canonization of Strings and Codes A string or code word with positions V over a finite alphabet Σ is a function $\mathfrak{x}:V\to\Sigma$. A code is a set of code words.

Isomorphism of codes, also known as code equivalence, was considered in [BCGQ11] and in [BCQ12]. With our general result for objects, we achieve the same time bound even for canonization.

Corollary 19. Canonical labelings for codes can be computed in time $2^{\mathcal{O}(|V|)}|\mathcal{A}|^{\mathcal{O}(1)}$ where |V| is the length of the code words and $|\mathcal{A}|$ is the size of the code (i.e., the number of code words).

Proof. We need to explain how to encode a string with our formalism. Observe that Σ is an alphabet which has to be fixed pointwise by automorphisms. For this reason, we can encode the elements in Σ as \emptyset , $\{\emptyset\}$, ... and so on. A string \mathfrak{x} can be encoded as a function and thus as a set of pairs $\{(v,\mathfrak{x}(v)) \mid v \in V\}$.

We can also draw conclusions for canonization of permutation groups up to permutational isomorphism.

Corollary 20. Canonical labelings for permutation groups (up to permutational isomorphism) can be computed in time $2^{\mathcal{O}(|V|)}|\Delta|^{\mathcal{O}(1)}$ where V is the permutation domain and $|\Delta|$ is the order of the group.

Proof. We encode an element $\delta \in \Delta \leq \operatorname{Sym}(V)$ explicitly as permutation over V by using the set $M(\delta) := \{(v, v^{\delta}) \mid v \in V\}$. Canonizing $\{M(\delta) \mid \delta \in \Delta\}$ is the same as canonizing the group Δ up to permutational isomorphism.

9 Canonical Generating Sets

The algorithms we have described throughout the paper canonize combinatorial objects. When given an unordered object as an input, they produce a canonical ordered object as an output. However, this does not immediately give us a canonical encoding of the output (i.e., is does not provide a canonical output string) as there may be multiple ways to represent the same ordered object. Indeed, in Section 3, we described how we represent objects using generating sets and colored directed graphs. Usually it is not very crucial which encoding we use to translate the generating sets and colored directed graphs into a binary string which can be processed by an algorithm or a Turing machine. However, especially in the context of canonization, it would be desirable to ensure that if two implicitly given ordered objects $\mathcal{X}, \mathcal{Y} \in \text{Objects}(\{1, \dots, |V|\})$ are equal, then they also have the same string encoding $\text{enc}(\mathcal{X}) = \text{enc}(\mathcal{Y})$. For explicitly given objects \mathcal{X} over $\{1, \dots, |V|\}$, this can be achieved since all elements in TClosure(\mathcal{X}) are linearly ordered by "<". Therefore, the crucial question is how to uniquely encode the implicitly given labeling cosets $\Delta \rho \leq \text{Label}(\{1, \dots, |V|\})$. To answer this question, we make use of canonical generating sets.

Lemma 21 ([AGvM⁺18], Lemma 6.2, [GNSW18], Lemma 21). There is a polynomial-time algorithm that, given a labeling coset $\Delta \rho \leq \text{Label}(\{1,..,|V|\})$ via a generating set, computes a generating set for $\Delta \rho$. The output only depends on $\Delta \rho$ (and not on the given generating set).

With this lemma, we can find a canonical generating set for labeling cosets over natural numbers. Using the order "<", we can thus compute for every ordered object a string that uniquely encodes the object.

Lemma 22. There is an injective encoding enc: Objects $(\{1, ... |V|\}) \rightarrow \{0, 1\}^*$ that maps ordered objects to (0-1)-strings. The encoding enc and its inverse are polynomial-time computable (for objects given via generating sets and colored directed graphs).

There is a second application of canonical generating sets in our context. For this, let us consider the bottleneck of our canonization algorithms. The recursions perform efficiently, except for the transitive cases. The concrete situation is that we have some group $\Delta^{\text{Can}} \leq \text{Sym}(\{1,\ldots,|V|\})$ acting transitively on a set $A^{\text{Can}} \subseteq \{1,\ldots,|V|\}$. In this case, the algorithm computes a subgroup $\Psi^{\text{Can}} \leq \Delta^{\text{Can}}$, decomposes Δ^{Can} into cosets of Ψ^{Can} and recurses. Here, the branching degree of the algorithm is the index of the subgroup Ψ^{Can} in Δ^{Can} . However, progress is made since the Ψ^{Can} -orbits on A^{Can} are smaller than the Δ^{Can} -orbits on A^{Can} . Luks's group theoretic framework [Luk82], which solves isomorphism for bounded degree graphs in polynomial time, attacks this bottleneck. He used group theoretic insights to argue that if Δ^{Can} is of a group of a certain type (a so called Γ_d -group), then there is a subgroup of relatively small index and small orbit size. Babai's algorithm in turn, attacks the bottleneck of Luks's approach which is characterized by giant homomorphisms from Δ^{Can} to some symmetric group. In the rest of this section, we discuss how these approaches can be employed within our canonization framework by the use of canonical generating sets.

A block system $\mathcal{B} = \{B_1, \dots, B_t\}$ for a group $\Delta \leq \operatorname{Sym}(V)$ is a Δ -invariant partition \mathcal{B} of $V = B_1 \cup \dots \cup B_t$. For a group $\Delta \leq \operatorname{Sym}(V)$, the composition width of Δ , denoted as $\operatorname{cw}(\Delta)$, is the smallest integer k such that all composition factors of Δ are isomorphic to a subgroup of $\operatorname{Sym}(k)$. Luks's approach exploits that one can efficiently compute a minimal block system for a given group. One then computes the subgroup Ψ that stabilizes all the blocks setwise. Babai, Cameron and Pálfy [BCP82] showed that for groups of bounded composition width such a Ψ is of relatively small index. Therefore, going down to the subgroup Ψ is not too costly, but still reduces the size of the orbits in the recursive calls significantly. Together these results prove the following.

Theorem 23 ([Luk82] and [BCP82],[BKL83]). Let $\Delta \leq \operatorname{Sym}(V)$ be a group that is transitive on a set $A \subseteq V$. There is a subgroup $\Psi \leq \Delta$ and $b \in \mathbb{N}$ such that:

- (1) The size of the Ψ -orbits on A is bounded by b.
- (2) The index $[\Delta : \Psi]$ is bounded by $(|A|/b)^{\mathcal{O}(cw(\Delta))}$.

Furthermore, there is an algorithm A that given $A \subseteq V$ and a generating set for Δ , computes a generating set for a subgroup $\Psi \leq \Delta$. The algorithm runs in time $|V|^{\mathcal{O}(\mathrm{cw}(\Delta))}$.

Proof sketch. Let $\mathcal{B} = \{B_1, \ldots, B_t\}$ be a minimal block system for $A \subseteq V$ and let $b := |A|/t = |B_1|$. Define $\Psi := \operatorname{Stab}_{\Delta}(B_1, \ldots, B_t)$. The bound on the index follows from a bound of the size of primitive permutation groups of degree t. While Babai, Cameron, Pálfy [BCP82] implicitly proved a bound of $t^{\omega(\operatorname{cw}(\Delta))}$ where $\omega \in \mathcal{O}(n \log n)$, it was later observed that ω can be chosen linear as stated in [BKL83], see [LS99].

For us, a crucial detail here is that the minimal block system and thus Ψ is not unique. For an isomorphism algorithm, it is usually sufficient to compute an arbitrary subgroup $\Psi \leq \Delta$ with Properties (1) and (2). However, for the purpose of canonization, we will need that for each group Δ one particular subgroup $\Psi \leq \Delta$ will be computed and the choice of Ψ has to be consistent across different calls of algorithm A. More precisely, we need that for two inputs I and I' which are both encodings for the pair (A, Δ) , the algorithm A with input I has the same output as A with input I'. For canonization algorithms as in [BL83] this consistency was

achieved by computing one particular, so called *smallest*, minimal block system \mathcal{B}^* . However, such an approach needs some insight into the proof of Theorem 23 and one has to argue that the proof can be extended rather than using the theorem as a black box only.

Using canonical generating sets for objects over natural numbers, we can reformulate the theorem. The difference is that in the reformulation the subgroup can be chosen in a unique way. This method is quite general as it indeed uses Theorem 23 as a black box only.

Theorem 24 ([BL83] and [BCP82],[BKL83]). Let $\Delta^{\operatorname{Can}} \leq \operatorname{Sym}(\{1,\ldots,|V|\})$ be a group that is transitive on a set $A^{\operatorname{Can}} \subseteq \{1,\ldots,|V|\}$. There is a subgroup $\Psi^{\operatorname{Can}} \leq \Delta^{\operatorname{Can}}$ and $b \in \mathbb{N}$ such that:

- (1) The size of the Ψ^{Can} -orbits on A^{Can} are bounded by b.
- (2) The index $[\Delta^{\operatorname{Can}} : \Psi^{\operatorname{Can}}]$ is bounded by $(|A^{\operatorname{Can}}|/b)^{\mathcal{O}(\operatorname{cw}(\Delta^{\operatorname{Can}}))}$.

Furthermore, there is an algorithm B that given $A^{\operatorname{Can}} \subseteq \{1,\ldots,|V|\}$ and a generating set for $\Delta^{\operatorname{Can}}$, computes a generating set for the subgroup $\Psi^{\operatorname{Can}} \leq \Delta^{\operatorname{Can}}$. The group $\Psi^{\operatorname{Can}}$ only depends on A^{Can} and $\Delta^{\operatorname{Can}}$ (and not on the given generating set for $\Delta^{\operatorname{Can}}$). The algorithm runs in time $|V|^{\mathcal{O}(\operatorname{cw}(\Delta^{\operatorname{Can}}))}$.

Proof. Let $(\delta_1^{\operatorname{Can}}, \dots, \delta_t^{\operatorname{Can}})$ be a canonical generating set of $\Delta^{\operatorname{Can}}$ ordered according to " \prec ". We execute the algorithm A from Theorem 23 with input $(A^{\operatorname{Can}}, (\delta_1^{\operatorname{Can}}, \dots, \delta_t^{\operatorname{Can}}))$ and return its output.

Using the result of the previous theorem, we can achieve a running time for canonization expressible in terms of the composition width of Δ .

Corollary 25. A function CL_{Object} solving Problem 16 can be computed in time $k^{\mathcal{O}(cw(\Delta))}n^{\mathcal{O}(1)}$ where n is the input size and k is the size of the largest Δ -orbit of V.

Proof. In the transitive case of the algorithms for CL_{Match} , CL_{Hyper} and CL_{Set} , we are in the situation of a group Δ^{Can} (or Θ^{Can} respectively) that is transitive on a set A^{Can} . To achieve the running time, we replace the line "Define $\Psi^{Can} := \operatorname{Stab}_{\Delta^{Can}}(A_1^{Can}, A_2^{Can})$ " with "Define Ψ^{Can} as the output of algorithm B from Theorem 24 with input A^{Can} and Δ^{Can} ".

(Running time.) The critical point for the running time analysis is that a recursion of the type $R(|A^*|) \le (|A^*|/b)^{\mathcal{O}(\mathrm{cw}(\Delta))} R(b)$ leads to some function $R(|A^*|) \in |A^*|^{\mathcal{O}(\mathrm{cw}(\Delta))}$.

We remark that there is a particular technique [BKL83] to improve the running time for isomorphism algorithms from $k^{\mathcal{O}(\mathrm{cw}(\Delta))}n^{\mathcal{O}(1)}$ to $k^{\mathcal{O}(\mathrm{cw}(\Delta)/\log\mathrm{cw}(\Delta))}n^{\mathcal{O}(1)}$. As this technique exploits the precise structure of large primitive groups and needs some detailed background, we will not describe it here.

10 Outlook and Open Questions

We presented a general framework to devise canonization algorithms for combinatorial objects. It allows for the use of various other algorithms developed in the context of isomorphism problems, without having to worry about isomorphism invariance. We believe that it not only should be possible to use the framework to design further canonization algorithms, but that the framework will simplify the task. Especially the use of canonical generating sets simplifies the task to adapt theorems used for isomorphism to adequate canonization variants. Naturally, the bounded degree isomorphism algorithm of [GNS18] should then be amenable to canonization. However, this remains as future work.

We ask whether canonization of combinatorial objects can be performed in time $n^{\text{polylog}(|V|)}$ where n is the size of the object. Such a running time is of deep interest for a canonization algorithm for graphs of tree width at most k running in time $|V|^{\text{polylog}(k)}$ which in turn would generalize Babai's quasipolynomial time bound. However, even for the isomorphism-version of this problem we have no such algorithm yet.

A different question to this end is whether the time bound that we presented in this paper (of $2^{\mathcal{O}(|V|)}n^{\mathcal{O}(1)}$ for objects of size n) can be improved to moderately exponential $2^{\mathcal{O}(|V|^{1-\varepsilon})}n^{\mathcal{O}(1)}$ for some $\varepsilon > 0$

It remains an open problem whether isomorphism of permutation groups over a permutation domain V (that however are implicitly given via a generating set) can be decided in time $2^{\mathcal{O}(|V|)}$ regardless of the order of the groups [BCGQ11, Cod11]. Our framework might help to design such an isomorphism algorithm. Indeed, in Section 8, we showed how codes and permutation groups can be encoded as combinatorial objects. However, we did so by explicitly listing all elements. To encode implicitly given permutation groups, our framework can readily be extended to allowing implicitly represented cosets of V to the set V itself as a new third form of atom, but at this point we do not see how to handle the arising objects efficiently.

References

- [ADKT15] Vikraman Arvind, Bireswar Das, Johannes Köbler, and Seinosuke Toda. Colored hypergraph isomorphism is fixed parameter tractable. *Algorithmica*, 71(1):120–138, 2015.
- [AGvM⁺18] Eric Allender, Joshua A Grochow, Dieter van Melkebeek, Cristopher Moore, and Andrew Morgan. Minimum circuit size, graph isomorphism, and related problems. SIAM Journal on Computing, 47(4):1339–1372, 2018.
- [Bab16] László Babai. Graph isomorphism in quasipolynomial time [extended abstract]. In Daniel Wichs and Yishay Mansour, editors, Proceedings of the 48th Annual ACM SIGACT Symposium on Theory of Computing, STOC 2016, Cambridge, MA, USA, June 18-21, 2016, pages 684–697. ACM, 2016.
- [Bab19] László Babai. Canonical form for graphs in quasipolynomial time. In *Proceedings* of the 51th Annual ACM SIGACT Symposium on Theory of Computing, STOC 2019, Phoenix, AZ, USA, June 23-26, 2019. ACM, 2019. To appear.
- [BC08] László Babai and Paolo Codenotti. Isomorhism of hypergraphs of low rank in moderately exponential time. In 49th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2008, October 25-28, 2008, Philadelphia, PA, USA, pages 667–676. IEEE Computer Society, 2008.
- [BCGQ11] László Babai, Paolo Codenotti, Joshua A. Grochow, and Youming Qiao. Code equivalence and group isomorphism. In Dana Randall, editor, *Proceedings of the Twenty-Second Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2011, San Francisco, California, USA, January 23-25, 2011*, pages 1395–1408. SIAM, 2011.
- [BCP82] László Babai, Peter J. Cameron, and Péter P. Pálfy. On the orders of primitive groups with restricted nonabelian composition factors. *J. Algebra*, 79(1):161–168, 1982.

- [BCQ12] László Babai, Paolo Codenotti, and Youming Qiao. Polynomial-time isomorphism test for groups with no abelian normal subgroups (extended abstract). In *ICALP* (1), volume 7391 of *Lecture Notes in Computer Science*, pages 51–62. Springer, 2012.
- [BKL83] László Babai, William M. Kantor, and Eugene M. Luks. Computational complexity and the classification of finite simple groups. In 24th Annual Symposium on Foundations of Computer Science, Tucson, Arizona, USA, 7-9 November 1983, pages 162–171. IEEE Computer Society, 1983.
- [BL83] László Babai and Eugene M Luks. Canonical labeling of graphs. In *Proceedings* of the fifteenth annual ACM symposium on Theory of computing, pages 171–183. ACM, 1983.
- [BMW17] Peter A. Brooksbank, Joshua Maglione, and James B. Wilson. A fast isomorphism test for groups whose lie algebra has genus 2. *Journal of Algebra*, 473:545 590, 2017.
- [Cod11] Paolo Codenotti. Testing isomorphism of combinatorial and algebraic structures. The University of Chicago, 2011.
- [GNS18] Martin Grohe, Daniel Neuen, and Pascal Schweitzer. A faster isomorphism test for graphs of small degree. CoRR, abs/1802.04659, 2018.
- [GNSW18] Martin Grohe, Daniel Neuen, Pascal Schweitzer, and Daniel Wiebking. An improved isomorphism test for bounded-tree-width graphs. CoRR, abs/1803.06858, 03 2018.
- [GQ15] Joshua A. Grochow and Youming Qiao. Polynomial-time isomorphism test of groups that are tame extensions (extended abstract). In Khaled M. Elbassioni and Kazuhisa Makino, editors, Algorithms and Computation 26th International Symposium, ISAAC 2015, Nagoya, Japan, December 9-11, 2015, Proceedings, volume 9472 of Lecture Notes in Computer Science, pages 578–589. Springer, 2015.
- [GQ17] Joshua A. Grochow and Youming Qiao. Algorithms for group isomorphism via group extensions and cohomology. SIAM J. Comput., 46(4):1153–1216, 2017.
- [GS15] Martin Grohe and Pascal Schweitzer. Isomorphism testing for graphs of bounded rank width. *CoRR*, abs/1505.03737, 2015.
- [LS99] Martin Liebeck and Aner Shalev. Simple groups, permutation groups, and probability. *Journal of the American Mathematical Society*, 12(2):497–520, 1999.
- [Luk82] Eugene M. Luks. Isomorphism of graphs of bounded valence can be tested in polynomial time. *J. Comput. Syst. Sci.*, 25(1):42–65, 1982.
- [Luk99] Eugene M. Luks. Hypergraph isomorphism and structural equivalence of boolean functions. In Jeffrey Scott Vitter, Lawrence L. Larmore, and Frank Thomson Leighton, editors, *Proceedings of the Thirty-First Annual ACM Symposium on Theory of Computing, May 1-4, 1999, Atlanta, Georgia, USA*, pages 652–658. ACM, 1999.

- [LW12] Mark L. Lewis and James B. Wilson. Isomorphism in expanding families of indistinguishable groups. *Groups Complexity Cryptology*, 4(1):73–110, 2012.
- [Mat79] Rudolf Mathon. A note on the graph isomorphism counting problem. *Inf. Process. Lett.*, 8(3):131–132, 1979.
- [Mil83] Gary Miller. Isomorphism testing and canonical forms for k-contractable graphs (a generalization of bounded valence and bounded genus). In *Foundations of Computation Theory*, pages 310–327. Springer, 1983.
- [RW15] David J. Rosenbaum and Fabian Wagner. Beating the generator-enumeration bound for p-group isomorphism. *Theor. Comput. Sci.*, 593:16–25, 2015.
- [Ser03] Ákos Seress. Permutation group algorithms, volume 152 of Cambridge Tracts in Mathematics. Cambridge University Press, Cambridge, 2003.