Permutation group algorithms based on directed graphs
(extended version)

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Abstract
We introduce a new framework for solving an important class of computational problems involving finite permutation groups, which includes calculating set stabilisers, intersections of subgroups, and isomorphisms of combinatorial structures. Our techniques generalise ‘partition backtrack’, which is the current state-of-the-art algorithm introduced by Jeffrey Leon in 1991, and which has inspired our work. Our backtrack search algorithms are organised around vertex- and arc-labelled directed graphs, which allow us to represent many problems more richly than do ordered partitions. We present the theory underpinning our framework, and we include the results of experiments showing that our techniques often result in smaller search spaces than does partition backtrack. An implementation of our algorithms is available as free software in the GRAPHBACKTRACKING package for GAP.

Note: This is an extended version of Permutation group algorithms based on directed graphs [10]. The shorter article was derived from this one, according to the comments of referees; it includes some improved exposition, and omits some proofs, examples, and other details. We recommend that the reader begins with the shorter article.

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1. Introduction

In [13], Jeffrey Leon introduced the partition backtrack algorithm for intersecting subgroups of finite symmetric groups, or their cosets, in which membership of an individual permutation can be easily decided. Many of the most important problems in computational permutation group theory can be formulated in this way, and thus can be solved with partition backtrack. These include the computation of point and set stabilisers and transporters; normalisers and centralisers of subsets and subgroups; automorphisms and isomorphisms of a wide range of combinatorial structures; element and subgroup conjugacy; and any conjunction of such problems. These problems have differing time complexities (see [15, Chapter 3], for example), but for many of them, partition backtrack currently solves the problem in the fastest known way.

Leon’s algorithm performs a backtrack search through the elements of the symmetric group, which it organises around a collection of ordered partitions. Partition backtrack builds upon the ‘individualisation-refinement’ technique of McKay, which he most recently described in [14], and which is used to compute automorphism groups and canonical labellings of finite graphs. Leon’s algorithm encodes information about the given problem into the ordered partitions, which it then uses to cleverly prune (i.e., omit superfluous parts of) the search space. Despite its excellent performance in many instances, this technique has exponential worst-case complexity, and there remain many important examples of problems that are beyond its reach. There is, therefore, still scope for improvement.

Several extensions to partition backtrack have taken further inspiration from the graph-based ideas of McKay. Theißen, for instance, used orbital graphs in [16] to significantly improve the computation of normalisers. This theme was taken up in [9], by the first three authors of the present paper, for intersections and set stabilisers. The techniques described in [9, 16] encode some information about certain orbital graphs into the ordered partitions of the search, thereby enabling better pruning of the search space. This suggests that even more powerful pruning, and ultimately better performance, could be obtained by using graphs directly, at the expense of the increased computation required at each node of the remaining search. In the present paper, we investigate precisely this idea. More specifically, we demonstrate the possibility and feasibility of placing graphs (in fact, vertex- and arc-labelled directed graphs) at the heart of backtrack search algorithms in the symmetric group, thereby generalising partition backtrack.

The purpose of this paper is to give the theoretical basis for our ideas, along with some initial experimental data. In particular, at this point, we do not concern ourselves with the time complexity or speed of our algorithms, and we do not discuss their implementation details. However, we do intend for our algorithms to be practical, and we expect that with sufficient further development into their implementations, our algorithms should perform competitively against, and even beat, partition backtrack for many classes of problems.

Note that although this paper is heavily influenced by the work of Leon [12, 13], we intend for it to be understandable without prior knowledge of his work.

This paper is organised as follows. In Section 2, we present our notation, introduce
and refer to standard concepts in graph theory and group theory, and discuss labelled
digraphs. In Section 3, we introduce stacks of labelled digraphs, which are the funda-
mental structures around which we organise our search algorithms. The remaining tools
that are crucial for our algorithms are isomorphism approximators and fixed-point ap-
proximators (Section 4), refiners (Section 5), and splitters (Section 6). We present our
algorithms and prove their correctness in Section 7, and in Section 8 we give details of
various experiments that compare our algorithms with the current state-of-the-art tech-
niques. We conclude, in Section 9, with brief comments on the results of this paper and
the directions that they suggest for further investigation.

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2. Preliminaries

Throughout this paper, \( \Omega \) denotes some finite totally-ordered set on which we define
all of our groups, digraphs, and related objects. For example, every group in this paper
is a finite permutation group on \( \Omega \), i.e. a subgroup of \( \text{Sym}(\Omega) \), the symmetric group on
\( \Omega \). We follow the standard group-theoretic notation and terminology from the literature,
such as that used in [2], and write \( \cdot \) for the composition of maps in \( \text{Sym}(\Omega) \), or we omit
a symbol for this binary operation altogether. We write \( \mathbb{N} \) for the set \( \{1, 2, 3, \ldots \} \) of all
natural numbers, and \( \mathbb{N}_0 := \mathbb{N} \cup \{0\} \). If \( n \in \mathbb{N} \), then \( S_n := \text{Sym}(\{1, \ldots, n\}) \).

For many types of objects that we define on \( \Omega \), we give a way of applying elements
of \( \text{Sym}(\Omega) \) to them (denoted by exponentiation) in a way that is structure-preserving.
For example, if we have a graph with vertex set \( \Omega \), then we can apply the same element
of \( \text{Sym}(\Omega) \) to every vertex, and obtain a new graph with the same vertex set, \( \Omega \). This
principle is used throughout this article, mainly for graphs or digraphs with vertex set
\( \Omega \), but also for sets or lists of elements in \( \Omega \), and for sets or lists of subsets of \( \Omega \) (such as
partitions of \( \Omega \)).

Let \( \mathcal{O} \) and \( \mathcal{Q} \) be digraphs with vertex set \( \Omega \) (or partitions, lists etc., as mentioned
above). Then we say that a permutation \( g \in \text{Sym}(\Omega) \) induces an isomorphism from \( \mathcal{O} \)
to \( \mathcal{Q} \) if and only if it defines a map from \( \mathcal{O} \) to \( \mathcal{Q} \), i.e. \( \mathcal{O}^g = \mathcal{Q} \), and if it is structure-
preserving. For digraphs this means that arcs are preserved, for partitions it means that
the number and sizes of cells are preserved.

We write \( \text{Iso}(\mathcal{O}, \mathcal{Q}) \) for the set of isomorphisms from \( \mathcal{O} \) to \( \mathcal{Q} \) that are induced by
elements of \( \text{Sym}(\Omega) \). If \( \text{Iso}(\mathcal{O}, \mathcal{Q}) \) is non-empty, then we call \( \mathcal{O} \) and \( \mathcal{Q} \) isomorphic,
sometimes denoted by \( \mathcal{O} \cong \mathcal{Q} \). Similarly, we consider \( \text{Aut}(\mathcal{O}) \leq \text{Sym}(\Omega) \) to be the
subgroup of \( \text{Sym}(\Omega) \) consisting of all elements that induce isomorphisms from \( \mathcal{O} \) to
itself, i.e. automorphisms. Note that, for all \( g \in \text{Iso}(\mathcal{O}, \mathcal{Q}) \), \( \text{Aut}(\mathcal{O})^g (:= \{ g^{-1}hg : h \in \text{Aut}(\mathcal{O}) \}) = \text{Aut}(\mathcal{Q}) \). In particular, if \( \mathcal{O} \cong \mathcal{Q} \), then \( \text{Iso}(\mathcal{O}, \mathcal{Q}) \) is a right coset of \( \text{Aut}(\mathcal{O}) \) and a left coset of \( \text{Aut}(\mathcal{Q}) \) in \( \text{Sym}(\Omega) \).

2.1. Ordered partitions

An ordered partition of \( \Omega \) is a list of non-empty disjoint subsets of \( \Omega \), called cells, whose union is \( \Omega \). The 'ordering' is thus defined between cells, not within a cell. For example, the list \( \{\{3, 7\}, \{1\}, \{2, 4, 5\}, \{6\}\} \) is an ordered partition of \( \{1, \ldots, 7\} \). The group \( \text{Sym}(\Omega) \) acts on the set of ordered partitions of \( \Omega \) by acting on its entries: if \( g \in \text{Sym}(\Omega) \) and \( \Pi := [C_1, \ldots, C_k] \) is an ordered partition of \( \Omega \) for some \( k \in \mathbb{N} \), then the action is defined via \( \Pi^g := [C_1^g, \ldots, C_k^g] \).

If \( k, l \in \mathbb{N} \) and \( \Pi_1 := [C_1, \ldots, C_k] \) and \( \Pi_2 := [D_1, \ldots, D_l] \) are ordered partitions of \( \Omega \), then a permutation \( g \in \text{Sym}(\Omega) \) induces an isomorphism from \( \Pi_1 \) to \( \Pi_2 \) if and only if \( C_i^g = D_i \) for all \( i \in \{1, \ldots, k\} \). Since \( \text{Sym}(\Omega) \) acts \( \Omega \)-transitively on \( \Omega \), it follows that \( \Pi_1 \) and \( \Pi_2 \) are isomorphic if and only if \( k = l \) and \( |C_i| = |D_i| \) for all \( i \in \{1, \ldots, k\} \). In addition, the automorphism group of \( \Pi_1 \) induced by \( \text{Sym}(\Omega) \) is isomorphic to \( \text{Sym}(C_1) \times \cdots \times \text{Sym}(C_k) \) in a natural way.

2.2. Labelled digraphs

A graph with vertex set \( \Omega \) is a pair \( (\Omega, E) \), where \( E \) is a set of 2-subsets of \( \Omega \). A directed graph with vertex set \( \Omega \), or digraph for short, is a pair \( (\Omega, A) \), where \( A \subseteq \Omega \times \Omega \) is a set of pairs of elements in \( \Omega \) called arcs. The elements of \( \Omega \) are called vertices in the context of graphs and digraphs. Our definition allows a digraph to have loops, which are arcs of the form \((\alpha, \alpha)\) for some vertex \( \alpha \in \Omega \).

Our techniques for searching in \( \text{Sym}(\Omega) \) are built around digraphs in which each vertex and arc is given a label from a label set \( \mathcal{L} \). We define a vertex- and arc-labelled digraph, or labelled digraph for short, to be a triple \( (\Omega, A, \text{LABEL}) \), where (\( \Omega, A \)) is a digraph and LABEL is a function from \( \Omega \cup A \) to \( \mathcal{L} \). More precisely, for any \( \delta \in \Omega \) and \((\alpha, \beta) \in A \), the label of the vertex \( \delta \) is \( \text{LABEL}(\delta) \in \mathcal{L} \), and the label of the arc \((\alpha, \beta)\) is \( \text{LABEL}(\alpha, \beta) \in \mathcal{L} \). We call such a function a labelling function.

In a theoretical sense, the properties of the labels themselves are unimportant, since we only use them to distinguish certain vertices or arcs from others, and thereby break symmetries. For convenience, therefore, we fix \( \mathcal{L} \) as some non-empty set that contains every label that we require, and which serves as the codomain of every labelling function. Thus two labelled digraphs on \( \Omega \) are equal if and only if their sets of arcs are equal, and any vertex or arc has the same label in both labelled digraphs. For the concepts in Section 4.2, we require some arbitrary but fixed total ordering to be defined on \( \mathcal{L} \).

The symmetric group on \( \Omega \) acts on the sets of graphs and digraphs with vertex set \( \Omega \), respectively, and on their labelled variants, in a natural way. We give more details about this for labelled digraphs; the forthcoming notions are defined analogously for the other kinds of graphs and digraphs that we have mentioned. Let \( \text{LABELLEDDIGRAPHS}(\Omega, \mathcal{L}) \) denote the class of all labelled digraphs on \( \Omega \) with labels in \( \mathcal{L} \), let \( \Gamma = (\Omega, A, \text{LABEL}) \in \text{LABELLEDDIGRAPHS}(\Omega, \mathcal{L}) \) and \( g \in \text{Sym}(\Omega) \). Then we define \( \Gamma^g = (\Omega, A^g, \text{LABEL}^g) \in \text{LABELLEDDIGRAPHS}(\Omega, \mathcal{L}) \), where:
(i) \(A^g := \{(\alpha^g, \beta^g) : (\alpha, \beta) \in A\}\),
(ii) \(\text{LABEL}^g(\delta) := \text{LABEL}(\delta^{g^{-1}})\) for all \(\delta \in \Omega\), and
(iii) \(\text{LABEL}^g(\alpha, \beta) := \text{LABEL}(\alpha^{g^{-1}}, \beta^{g^{-1}})\) for all \((\alpha, \beta) \in A^g\).

In other words, the arcs are mapped according to \(g\), and the label of a vertex or arc in \(\Gamma^g\) is the label of its preimage in \(\Gamma\). This implies that the labels that appear in \(\Gamma^g\) are exactly those that appear in \(\Gamma\). This gives rise to a group action of \(\text{Sym}(\Omega)\) on \(\text{LABELLEDDIGRAPHS}(\Omega, \mathcal{L})\), since the identity permutation \(\text{id}_\Omega\) fixes any labelled digraph \(\Gamma\), and \(\Gamma^{gh} = (\Gamma^g)^h\) for all \(g, h \in \text{Sym}(\Omega)\).

Let \(\Gamma, \Delta \in \text{LABELLEDDIGRAPHS}(\Omega, \mathcal{L})\). A permutation \(g \in \text{Sym}(\Omega)\) induces an isomorphism from \(\Gamma\) to \(\Delta\) if and only if \(\Gamma^g = \Delta\). This means that \(g\) maps each vertex to a vertex with the same label, maps each arc to an arc with the same label, and maps pairs of vertices in \(\Omega\) that do not form arcs to pairs that do not form arcs.

The action of a permutation on a labelled digraph is illustrated in Example 2.1.

**Example 2.1.** Let \(\Omega = \{1, \ldots, 5\}\), \(A = \{(2, 2), (2, 3), (3, 2), (3, 5), (5, 1), (5, 4)\} \subseteq \Omega \times \Omega\), and \(\mathcal{L} = \{\text{black, white, solid, dashed}\}\). We define a labelling function \(\text{LABEL} : \Omega \cup A \rightarrow \mathcal{L}\) as follows: for all \(\delta \in \Omega\) and all \((\alpha, \beta) \in A\), let

\[
\text{LABEL}(\delta) = \begin{cases} 
  \text{black} & \text{if } \delta \text{ is prime,} \\
  \text{white} & \text{otherwise},
\end{cases}
\]

and

\[
\text{LABEL}(\alpha, \beta) = \begin{cases} 
  \text{solid} & \text{if } \alpha \leq \beta, \\
  \text{dashed} & \text{if } \alpha > \beta.
\end{cases}
\]

![Figure 2.2](image-url)  
*Figure 2.2:* The labelled digraphs \(\Gamma\) and \(\Gamma^{(1\ 5)(2\ 3)}\) from Example 2.1.

The diagram on the left of Figure 2.2 depicts the labelled digraph \(\Gamma := (\Omega, A, \text{LABEL})\), and the diagram on the right of Figure 2.2 depicts \(\Gamma^{(1\ 5)(2\ 3)}\), where each vertex and arc has a style corresponding to its label. Note that the diagrams look identical, except that the vertices are numbered differently, according to \((1\ 5)(2\ 3)\). This permutation induces an isomorphism from \(\Gamma\) to \(\Gamma^{(1\ 5)(2\ 3)}\), by definition, but it does not induce an automorphism of \(\Gamma\), since \(\Gamma \neq \Gamma^{(1\ 5)(2\ 3)}\). This can be seen, for instance, by noting that there is a loop at 2 in \(\Gamma\), but not in \(\Gamma^{(1\ 5)(2\ 3)}\), or by noting that the vertex 1 has the label \text{white} in \(\Gamma\), while it has the label \text{black} in \(\Gamma^{(1\ 5)(2\ 3)}\).

The unique non-trivial automorphism of \(\Gamma\) induced by \(\text{Sym}(\Omega)\) is the transposition \((1\ 4)\). Since the set \(\text{Iso}(\Gamma, \Gamma^{(1\ 5)(2\ 3)})\) of induced isomorphisms from \(\Gamma\) to \(\Gamma^{(1\ 5)(2\ 3)}\) is
the right coset of $\text{Aut}(\Gamma)$ that contains $(1\ 5)(2\ 3)$, it follows that the second and final isomorphism from $\Gamma$ to $\Gamma^{(1\ 5)(2\ 3)}$ is the permutation $(1\ 4\ 5)(2\ 3) = (1\ 4) \cdot (1\ 5)(2\ 3)$. Indeed,

$$\Gamma^{(1\ 4) \cdot (1\ 5)(2\ 3)} = \left( \Gamma^{(1\ 4)} \right)^{(1\ 5)(2\ 3)} = \Gamma^{(1\ 5)(2\ 3)}.$$

We have chosen to build our techniques around labelled digraphs because then they can be straightforwardly applied to a wide range of the graphs and digraphs that occur in practice. This is because graphs, digraphs, and so-called multigraphs and multidigraphs can be converted into labelled digraphs in such a way that the sets of isomorphisms that we are interested in do not change.

2.3. Orbital graphs

Some previous work, such as that of Theißen [16] and an article [9] by the first three authors of this paper, shows that orbital graphs can be useful for representing properties of groups and cosets when performing a partition backtrack search in $\text{Sym}(\Omega)$.

**Definition 2.3 (Orbital graph).** Let $G \leq \text{Sym}(\Omega)$, and let $\alpha, \beta \in \Omega$ be such that $\alpha \neq \beta$. Then the orbital graph of $G$ with base-pair $(\alpha, \beta)$ is the digraph $(\Omega, \{(\alpha^g, \beta^g) : g \in G\})$, which is denoted by $\Gamma(G, \Omega, (\alpha, \beta))$.

Although an orbital graph is a digraph rather than a graph, we retain the original name because it has become standard in the literature. The next lemma is a well-known result about orbital graphs (see for example [2, Section 3.2] or [9, Lemma 17]).

**Lemma 2.4.** Let $G \leq \text{Sym}(\Omega)$. Then $G$ acts on each of its orbital graphs as an arc-transitive group of digraph automorphisms. (This means that, given any two arcs, there exists some $g \in G$ mapping one to the other.)

\[\Gamma(C_6, \{1, \ldots, 6\}, (1, 2)) \quad \Gamma(C_6, \{1, \ldots, 6\}, (1, 3)) \quad \Gamma(C_6, \{1, \ldots, 6\}, (1, 4))\]

**Figure 2.5:** Diagrams of three orbital graphs of the group $C_6 := \langle(1\ 2\ 3\ 4\ 5\ 6)\rangle \leq S_6$ with, from left to right, base-pairs $(1, 2)$, $(1, 3)$, and $(1, 4)$. The automorphism group of $\Gamma(C_6, \{1, \ldots, 6\}, (1, 2))$ induced by $S_6$ is $C_6$, whereas the automorphism groups of the other two orbital graphs properly contain $C_6$.

Lemma 2.4 implies that the group of digraph automorphisms (induced by $\text{Sym}(\Omega)$) of an orbital graph of a group $G$ is an overestimate for $G$. Approximations obtained in this way can differ greatly in their precision. At one extreme, a group is **absolutely orbital graph recognisable**, in the terminology of [4], if it is equal to the induced automorphism
group of each of its orbital graphs. The dihedral group \( \langle (1\ 2\ 3\ 4), (1\ 3) \rangle \) of order 8 in \( S_4 \) has this property, for example. At the other extreme, a group that acts 2-transitively on \( \Omega \) has a unique orbital graph, which contains every possible non-loop arc, and thus has automorphism group \( \text{Sym}(\Omega) \). It follows that 2-transitive groups cannot be differentiated by the automorphism groups of their orbital graphs.

There are many further kinds of behaviours between these extremes: a group is called 2-closed if it is equal to the intersection of the automorphism groups of its orbital graphs. We can consider a 2-closed group to be one where the collection of its orbital graphs represents the group exactly. These groups are particularly well-suited to the techniques of our paper, because they can be encoded in a stack of labelled digraphs capturing all relevant information. We will introduce this idea in Section 3. Groups that are absolutely orbital graph recognisable are 2-closed, but there are many 2-closed groups that are not absolutely orbital graph recognisable. The Klein four-group \( V := \langle (1\ 2)(3\ 4), (1\ 3)(2\ 4) \rangle \) is 2-closed, for instance, even though none of its orbital graphs has automorphism group equal to \( V \).

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**Example 2.7.** The automorphism groups of the Klein four-group \( V := \langle (1\ 2)(3\ 4), (1\ 3)(2\ 4) \rangle \) are dihedral groups with 8 elements. (See Figure 2.6.) However, the intersection of any two such automorphism groups is \( V \). Therefore \( V \) is 2-closed, but not absolutely orbital graph recognisable.

Any subgroup \( G \leq \text{Sym}(\Omega) \) leaves each of its orbits on \( \Omega \) invariant. In other words, if \( O_1, \ldots, O_k \subseteq \Omega \) are the distinct orbits of \( G \) on \( \Omega \), then \( G \) is contained in the stabiliser \( \{ g \in \text{Sym}(\Omega) : [O_1^g, \ldots, O_k^g] = [O_1, \ldots, O_k] \} \) of \( [O_1, \ldots, O_k] \) in \( \text{Sym}(\Omega) \), which is isomorphic to the direct product \( \text{Sym}(O_1) \times \cdots \times \text{Sym}(O_k) \). As discussed later in Example 5.18, stabilisers of this kind can be perfectly represented by labelled digraphs. This means that, for any non-transitive group \( G \), we can use its orbits to produce a labelled digraph whose automorphism group both contains \( G \), and is properly contained in \( \text{Sym}(\Omega) \). In particular, this labelled digraph represents \( G \) better than does any labelled digraph whose automorphism group is \( \text{Sym}(\Omega) \), which is the worst possible case.

In [9], the authors say that an orbital graph \( \Gamma \) of a group \( G \) is futile if and only if \( \text{Aut}(\Gamma) \) is the stabiliser of a list of the orbits of \( G \). In essence, this means that the orbital graph is no better at representing \( G \) than the set of orbits of \( G \). Such an orbital graph has little computational value, since the orbits of a group can be represented by an ordered partition, which can be constructed, computed with, and stored much more cheaply than can an orbital graph.

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![Figure 2.6: The orbital graphs of the Klein four-group \( V := \langle (1\ 2)(3\ 4), (1\ 3)(2\ 4) \rangle \).](image-url)
3. Stacks of labelled digraphs

In this section we introduce labelled digraph stacks. We organise our search algorithms around these stacks, much like how partition backtrack is organised around stacks of ordered partitions. The essential idea is to represent the subsets of Sym(Ω), for whose intersection we are searching, as the set of isomorphisms from a suitable labelled digraph stack to another. We explain this in Section 7.

A labelled digraph stack on Ω is a finite (possibly empty) list of labelled digraphs on Ω. We denote the collection of all labelled digraph stacks on Ω by DigraphStacks(Ω). The length of a labelled digraph stack S, written |S|, is the number of entries that it contains. A labelled digraph stack of length 0 is called empty, and we denote the empty labelled digraph stack on Ω by EmptyStack(Ω). We use a notation typical for lists, whereby if i ∈ {1, . . . , |S|}, then S[i] denotes the i-th labelled digraph in the stack S.

We allow any labelled digraph stack on Ω to be appended onto the end of another. If S, T ∈ DigraphStacks(Ω) have lengths k and l, respectively, then we define S∥T to be the labelled digraph stack [S[1], . . . , S[k], T[1], . . . , T[l]] of length k + l formed by appending T to S.

We define an action of Sym(Ω) on DigraphStacks(Ω) via the action of Sym(Ω) on the set of all labelled digraphs on Ω. More specifically, for all S ∈ DigraphStacks(Ω) and g ∈ Sym(Ω), we define Sg to be the labelled digraph stack of length |S| with Sg[i] = S[i]g for all i ∈ {1, . . . , |S|}. In other words, Sg is the labelled digraph stack obtained from S by applying g to each of its entries. An isomorphism from S to another labelled digraph stack T (induced by Sym(Ω)) is therefore a permutation g ∈ Sym(Ω) such that Sg = T. In particular, only digraph stacks of equal lengths can be isomorphic, which means that results concerning isomorphisms of labelled digraph stacks only need to consider those with equal lengths. Note that every permutation in Sym(Ω) induces an automorphism of EmptyStack(Ω).

Remark 3.1. Let S, T, U, V ∈ DigraphStacks(Ω). It follows from the definitions that

\[
\text{Iso}(S, T) = \begin{cases} 
\emptyset & \text{if } |S| \neq |T|, \\
\bigcap_{i=1}^{|S|} \text{Iso}(S[i], T[i]) & \text{if } |S| = |T|,
\end{cases}
\text{and that } \text{Aut}(S) = \bigcap_{i=1}^{|S|} \text{Aut}(S[i]).
\]

In addition Aut(S∥U) ≤ Aut(S), and if |S| = |T|, then Iso(S∥U,T∥V) ⊆ Iso(S, T). Roughly speaking, the automorphism group of a labelled digraph stack, and the set of isomorphisms from one labelled digraph stack to another one of equal length, potentially become smaller as new entries are added to the stacks.

We illustrate some of the foregoing concepts in Example 3.2.

Example 3.2. Let Ω = {1, . . . , 6} and ℳ = {black, white, solid, dashed}. Here we define a labelled digraph stack S on Ω that has length 3, by describing each of its members.

We define the first entry of S via the orbital graph of \(K := \langle (12)(34)(56), (246) \rangle\) with base-pair (1, 3). The automorphism group of this orbital graph (as always, induced by Sym(Ω)) is K itself; in other words, this orbital graph perfectly represents K by its
automorphism group. In order to define $S[1]$, we convert this orbital graph into a labelled digraph by assigning the label white to each vertex and assigning the label solid to each arc. This does not change the automorphism group of the digraph.

We define the second entry of $S$ to be the labelled digraph on $\Omega$ without arcs, whose vertices 1 and 2 are labelled black, and whose remaining vertices are labelled white. The automorphism group of this labelled digraph is the setwise stabiliser of $\{1, 2\}$ in $\text{Sym}(\Omega)$.

We define the third entry of $S$ to be the labelled digraph $S[3]$ shown in Figure 3.3, with arcs and labels as depicted there; its automorphism group is $\langle (1\ 2), (3\ 4)(5\ 6) \rangle$.

Given the automorphism groups of the individual entries of $S$, as described above, it follows that the automorphism group of $S$ consists of precisely those elements of $K$ that stabilise the set $\{1, 2\}$, and that are automorphisms of the labelled digraph $S[3]$. Hence this group is $\langle (1\ 2)(3\ 4)(5\ 6) \rangle$. Since $(1\ 2)$ is an automorphism of $S[2]$ and $S[3]$, but not of $S[1]$, it follows that $S^{(1\ 2)} = [S[1]^{(1\ 2)}, S[2], S[3]] \neq S$. We also note that $\text{Iso}(S, S^{(1\ 2)})$ is the right coset $\text{Aut}(S) \cdot (1\ 2) = \{(1\ 2), (3\ 4)(5\ 6)\}$ of $\text{Aut}(S)$ in $\text{Sym}(\Omega)$.

![Diagrams of the labelled digraphs in the labelled digraph stack S from Example 3.2. The vertices and arcs of these labelled digraphs are styled according to their labels, which are chosen from the set \{black, white, solid, dashed\}.](image)

Figure 3.3: Diagrams of the labelled digraphs in the labelled digraph stack $S$ from Example 3.2. The vertices and arcs of these labelled digraphs are styled according to their labels, which are chosen from the set {black, white, solid, dashed}.

As well as the obvious difference of being defined in terms of labelled digraphs rather than ordered partitions, there are further conceptual differences between labelled digraph stacks and the ordered partitions stacks that Leon uses in [12, 13] for his search algorithms. For example, the entries of a labelled digraph stack on $\Omega$ can be any labelled digraphs on $\Omega$, whereas each subsequent ordered partition in one of Leon’s ordered partition stacks is required to be finer than the previous entry (for some definition of ‘finer’). We explore this further in Section 3.1. Furthermore, one can simply write down the automorphisms and isomorphisms of ordered partition stacks induced by $\text{Sym}(\Omega)$ with trivial calculation, but this is computationally expensive for labelled digraph stacks, in general. This reflects the fact that a far greater range of sets of permutations can be represented by labelled digraph stacks than can be represented by ordered partition stacks.

### 3.1. The squashed labelled digraph of a stack

As mentioned previously, in the definition of a labelled digraph stack, we have not included any requirement of entries of a stack becoming ‘finer’. This is because it can
be computationally expensive to find out the automorphism groups of labelled digraphs and their stacks, and we therefore do not wish to require that the automorphism groups of a labelled digraph stack and its entries are always known.

Moreover, without a requirement of entries becoming ‘finer’, it is much easier to append new labelled digraphs to a stack, which is the primary topic of Section 5. The computational purpose of extending a stack is simply to add new information about the current part of the search space; there is no need to duplicate old information. The automorphism groups of the pre-existing entries of a stack can always be obtained from the entries themselves, and so from this perspective, it is not necessary for each new entry to contain old information about the previous entries.

On the other hand, having a labelled digraph whose automorphism group is equal to that of a given labelled digraph stack (analogous to the final entry of an ordered partition stack) proves to be convenient for our exposition, especially for Section 4, even though it is not fundamentally required for the correctness of our algorithms. However, we define this special labelled digraph to be a new object that is defined from the stack, rather than being part of the stack itself. More specifically, in the remainder of Section 3.1, we introduce a way of converting labelled digraph stacks into labelled digraphs in a way that preserves isomorphisms. This is a short way of saying that the sets of isomorphisms that we are interested in do not change in the process.

In order to make the following definition, we first fix a special symbol $\# \notin \mathcal{L}$ that is never to be used as the label of a vertex or an arc in any labelled digraph.

**Definition 3.4.** Let $S$ be a labelled digraph stack on $\Omega$, with $S[i] := (\Omega, A_i, \text{LABEL}_i)$ being some labelled digraph on $\Omega$ for each $i \in \{1, \ldots, |S|\}$. Then the **squashed labelled digraph** of $S$, denoted by $\text{Squash}(S)$, is the labelled digraph $(\Omega, A, \text{LABEL})$, where

- $A = \bigcup_{i=1}^{|S|} A_i$,
- $\text{LABEL}(\delta) = [\text{LABEL}_1(\delta), \ldots, \text{LABEL}_{|S|}(\delta)]$ for all $\delta \in \Omega$, and
- $\text{LABEL}(\alpha, \beta)$ is the list of length $|S|$ for all $(\alpha, \beta) \in \bigcup_{i=1}^{|S|} A_i$, where

$$\text{LABEL}(\alpha, \beta)[i] = \begin{cases} \text{LABEL}_i(\alpha, \beta) & \text{if } (\alpha, \beta) \in A_i, \\ \# & \text{if } (\alpha, \beta) \notin A_i, \end{cases} \quad \text{for all } i \in \{1, \ldots, |S|\}.$$

Note that the labelling function of the squashed labelled digraph of a stack can be used to reconstruct all information about the stack from which it was created. We also point out that $\text{Squash}(S)^g = \text{Squash}(S^g)$ for all $S \in \text{DIGRAPHSTACKS}(\Omega)$ and $g \in \text{Sym}(\Omega)$.

In the following lemma, we prove that the set of isomorphisms induced by $\text{Sym}(\Omega)$ from one labelled digraph stack $S$ to another $T$ consists of exactly those elements of $\text{Sym}(\Omega)$ that induce isomorphisms from $\text{Squash}(S)$ to $\text{Squash}(T)$.

**Lemma 3.5.** Let $S, T \in \text{DIGRAPHSTACKS}(\Omega)$. Then

$$\text{Iso}(S, T) = \text{Iso}(\text{Squash}(S), \text{Squash}(T)).$$
Proof. If $S$ and $T$ have different lengths, then they are non-isomorphic by definition, and $\text{SQUASH}(S)$ and $\text{SQUASH}(T)$ are non-isomorphic because their labels have different lengths.

For the remainder of the proof, we suppose that $S$ and $T$ have some common length $k \in \mathbb{N}_0$. Let $\mu$ and $\nu$ denote the labelling functions of $\text{SQUASH}(S)$ and $\text{SQUASH}(T)$, respectively, and for each $i \in \{1, \ldots, k\}$, let $S[i] = (\Omega, A_i, \sigma_i)$ and $T[i] = (\Omega, B_i, \tau_i)$.

The sets whose equality we wish to prove are subsets of $\text{Sym}(\Omega)$, so let $g \in \text{Sym}(\Omega)$ be arbitrary. We prove that $g \in \text{Iso}(S, T)$ if and only if $g \in \text{Iso}(\text{SQUASH}(S), \text{SQUASH}(T))$ by just following the relevant definitions closely.

$$g \in \text{Iso}(S, T) \iff S[i]^g = T[i] \text{ for all } i \in \{1, \ldots, |S|\}$$

$$\iff A_i^g = B_i \text{ and } \sigma_i^g = \tau_i \text{ for each } i \in \{1, \ldots, k\}$$

$$\iff A_i^g = B_i \text{, } \sigma_i(\delta) = \tau_i(\delta^g), \text{ and } \sigma_i(\alpha, \beta) = \tau_i(\alpha^g, \beta^g)$$

for each $i \in \{1, \ldots, k\}$, $\delta \in \Omega$, and $(\alpha, \beta) \in A_i$

$$\iff A_i^g = B_i \text{, } \mu(\delta) = \nu(\delta^g), \text{ and } \mu(\alpha, \beta) = \nu(\alpha^g, \beta^g)$$

for each $i \in \{1, \ldots, k\}$, $\delta \in \Omega$, and $(\alpha, \beta) \in A_1 \cup \cdots \cup A_k$

$$\iff (A_1 \cup \cdots \cup A_k)^g = B_1 \cup \cdots \cup B_k, \mu(\delta) = \nu(\delta^g), \text{ and }$$

$$\mu(\alpha, \beta) = \nu(\alpha^g, \beta^g) \text{ for each } \delta \in \Omega \text{ and } (\alpha, \beta) \in A_1 \cup \cdots \cup A_k$$

$$\iff (A_1 \cup \cdots \cup A_k)^g = B_1 \cup \cdots \cup B_k \text{ and } \mu^g = \nu$$

$$\iff g \in \text{Iso}(\text{SQUASH}(S), \text{SQUASH}(T)).$$

Example 3.6. Let $S$ be the labelled digraph stack from Example 3.2. Since $|S| = 3$, the labels of vertices and arcs in $\text{SQUASH}(S)$ are lists of length 3. The vertex labels of $\text{SQUASH}(S)$ are:

- $\text{LABEL}(1) = \text{LABEL}(2) = [\text{white, black, white}]$, shown as black in Figure 3.7,
- $\text{LABEL}(3) = \text{LABEL}(4) = [\text{white, white, white}]$, shown as white in Figure 3.7, and
- $\text{LABEL}(5) = \text{LABEL}(6) = [\text{white, white, black}]$, shown as grey in Figure 3.7.

There are ten arcs in $\text{SQUASH}(S)$, which in total have five different labels:

- $\text{LABEL}(1, 3) = \text{LABEL}(2, 4) = [\text{solid, #, #}]$, shown as thin in Figure 3.7,
- $\text{LABEL}(3, 4) = \text{LABEL}(4, 3) = [\#, #, \text{solid}]$, shown as dotted in Figure 3.7,
- $\text{LABEL}(5, 2) = \text{LABEL}(6, 1) = [\#, #, \text{dashed}]$, shown as dashed in Figure 3.7,
- $\text{LABEL}(3, 5) = \text{LABEL}(4, 6) = [\text{solid, #, solid}]$, shown as thick in Figure 3.7, and
- $\text{LABEL}(5, 1) = \text{LABEL}(6, 2) = [\text{solid, #, dashed}]$, shown as wavy in Figure 3.7.

Since automorphisms of labelled digraphs preserve the sets of vertices with any particular label, it is clear that $\text{Aut}(\text{SQUASH}(S)) \leq \langle (1 \ 2), (3 \ 4), (5 \ 6) \rangle$. This containment is proper, since $\text{Aut}(\text{SQUASH}(S)) = \text{Aut}(S)$ by Lemma 3.5, and $\text{Aut}(S) = \langle (1 \ 2)(3 \ 4)(5 \ 6) \rangle$, as
Figure 3.7: A depiction of the squashed labelled digraph \text{SQUASH}(S) from Example 3.6, which is constructed from the labelled digraph stack \text{S} from Example 3.2.

discussed in Example 3.2. Indeed, inspection of the arc labels in \text{SQUASH}(S) shows that any automorphism that interchanges the pair of points in any of \{1, 2\}, \{3, 4\}, or \{5, 6\} also interchanges the other pairs.

4. Approximating isomorphisms and fixed points of stacks

One might assume that organising a search around some kind of object (where the set of elements we are searching for is overestimated by the set of isomorphisms from one such object to another) requires knowing exactly what these isomorphisms are. When searching with labelled digraphs stacks, for instance, this would entail performing many potentially-expensive labelled digraph isomorphism computations. However, as we show in this paper, this is not necessary. One may instead overestimate the set of isomorphisms rather than compute them exactly. Unsurprisingly, worse approximations typically lead to larger searches, but since an overestimate of an overestimate is again just an overestimate, doing this does not significantly change the search technique.

There is therefore a trade-off between the accuracy of such overestimates, and the amount of effort spent in computing them. In Definition 4.1, we introduce the concept of an isomorphism approximator for pairs of labelled digraphs stacks, which is a vital component of the algorithms described in Section 7. Later we give several examples of such functions.

Definition 4.1. An isomorphism approximator for labelled digraph stacks is a function \text{APPROX} that maps a pair of labelled digraph stacks on \Omega to either the empty set \emptyset, or a right coset of a subgroup of \text{Sym}(\Omega), such that the following statements hold for all \text{S}, \text{T} \in \text{DIGRAPHSTACKS}(\Omega) (we write \text{APPROX}(S) as an abbreviation for \text{APPROX}(S, S)):

(i) Iso(S, T) \subseteq \text{APPROX}(S, T).

(ii) If |S| \neq |T|, then \text{APPROX}(S, T) = \emptyset.

(iii) If \text{APPROX}(S, T) \neq \emptyset, then \text{APPROX}(S, T) = \text{APPROX}(S) \cdot h for some \ h \in \text{Sym}(\Omega).

Let \text{APPROX} be an isomorphism approximator and let \text{S}, \text{T} \in \text{DIGRAPHSTACKS}(\Omega). As discussed previously, the set Iso(S, T) of isomorphisms induced by \text{Sym}(\Omega) from \text{S}
to $T$ is either empty, or it is a right coset of $\text{Aut}(S)$. Since $\text{id}_\Omega \in \text{Iso}(S,S) = \text{Aut}(S)$, it follows by definition that $\text{Approx}(S)$ is a subgroup of $\text{Sym}(\Omega)$ that contains $\text{Aut}(S)$, the automorphism group of $S$ induced by $\text{Sym}(\Omega)$. In other words, $\text{Approx}(S)$ is an overestimate for $\text{Aut}(S)$. The value of $\text{Approx}(S,T)$ should be interpreted as follows.

By Definition 4.1(i), $\text{Approx}(S,T)$ gives a true overestimate for $\text{Iso}(S,T)$. Therefore, if $\text{Approx}(S,T) = \emptyset$, then the approximator has correctly determined that $S$ and $T$ are non-isomorphic. In particular, by Definition 4.1(ii), an isomorphism approximator correctly determines that stacks of different lengths are non-isomorphic. Otherwise, the approximator returns a right coset in $\text{Sym}(\Omega)$ of its overestimate for $\text{Aut}(S)$.

For practical purposes, it is most convenient for a computer implementation of an isomorphism approximator to return a coset of the form $\text{Approx}(S) \cdot h$ by explicitly giving the group $\text{Approx}(S)$, typically by a list of generators, along with a coset representative.

Any sensible isomorphism approximator returns $\emptyset$ for labelled digraph stacks where the $i^{\text{th}}$ entries contain different numbers of arcs or vertices with any label. However, for simplicity, the definition only contains conditions that our techniques require.

In Section 5.2, we require the ability to approximate a set of fixed points of the automorphism group of any labelled digraph stack. A point $\omega \in \Omega$ is a fixed point of a subgroup $G \leq \text{Sym}(\Omega)$ if and only if $\omega^g = \omega$ for all $g \in G$. This is particularly useful when it comes to using orbits and orbital graphs in our search techniques. For stacks of ordered partitions, it is possible to simply read off the fixed points, but once again, this is something that can be much more computationally expensive for stacks of labelled digraphs. Therefore we introduce the following definition.

**Definition 4.2.** A fixed-point approximator for labelled digraph stacks is a function $\text{Fixed}$ that maps each labelled digraph stack on $\Omega$ to a finite list in $\Omega$, such that for each $S \in \text{DigraphStacks}(\Omega)$:

(i) Each entry in $\text{Fixed}(S)$ is a fixed point of $\text{Aut}(S)$, and

(ii) $\text{Fixed}(S)^g = \text{Fixed}(S^g)$ for all $g \in \text{Sym}(\Omega)$.

Definition 4.2(ii) ensures that a fixed-point approximator is compatible with the techniques that we describe in Section 5.2. A fixed-point approximator is permitted to return lists with duplicate entries, although duplicate entries would seem to have no practical benefit.

**4.1. Computing automorphisms and isomorphisms exactly**

For Definition 4.4, we require the concept of a canoniser of labelled digraphs.

**Definition 4.3.** A canoniser of labelled digraphs is a function $\text{Canon}$ from the set of labelled digraphs on $\Omega$ to $\text{Sym}(\Omega)$ such that, for all labelled digraphs $\Gamma$ and $\Delta$, $\Gamma^\text{Canon}(\Gamma) = \Delta^\text{Canon}(\Delta)$ if and only if $\Gamma$ and $\Delta$ are isomorphic.

In essence, a canoniser assigns each object to a permutation that maps the object to some canonically chosen member of its isomorphism class. Canonisers are defined analogously for vertex-labelled digraphs (i.e. digraphs where the labelling function is
defined on the set of vertices only). There are several widely-used computational tools for canonising vertex-labelled digraphs, such as bliss [11] and nauty [14]. These tools compute the automorphism group of a vertex-labelled digraph at the same time as they canonise it. Since it is relatively easy to convert labelled digraphs into vertex-labelled digraphs in a way that preserves isomorphisms, it is possible to use such tools to canonise and compute automorphism groups of labelled digraphs.

**Definition 4.4** (Canonising and computing automorphisms exactly). Let CANON be a canoniser of labelled digraphs. We define functions FIXED and APPROX as follows: for all $S, T ∈ \text{DIGRAPHSTACKS}(Ω)$, let $g = \text{CANON}(\text{SQUASH}(S))$ and $h = \text{CANON}(\text{SQUASH}(T))$, let $L$ be the list $[i ∈ Ω : i$ is fixed by $\text{AUT}(\text{SQUASH}(S)^g)]$, ordered as usual in $Ω$, and define

$$\text{FIXED}(S) = L^{g^{-1}}, \quad \text{and}$$

$$\text{APPROX}(S, T) = \begin{cases} \text{AUT}(\text{SQUASH}(S)) · gh^{-1} & \text{if } \text{SQUASH}(S)^g = \text{SQUASH}(T)^h, \\ \emptyset & \text{otherwise}. \end{cases}$$

**Lemma 4.5.** Let the functions APPROX and FIXED be given as in Definition 4.4. Then APPROX is an isomorphism approximator, and FIXED is a fixed-point approximator. Moreover, for all $S, T ∈ \text{DIGRAPHSTACKS}(Ω)$, $\text{APPROX}(S, T) = \text{ISO}(S, T)$.

**Proof.** Throughout the proof, we repeatedly use Lemma 3.5 and Definition 4.3. As in Definition 4.3, let $g = \text{CANON}(\text{SQUASH}(S))$ and $h = \text{CANON}(\text{SQUASH}(T))$.

First, we show that $\text{APPROX}(S, T) = \text{ISO}(S, T)$, which implies that Definition 4.1(i) and (ii) hold. If $S \not\cong T$, then $\text{SQUASH}(S)^g \not\cong \text{SQUASH}(T)^h$, and so $\text{APPROX}(S, T) = \text{ISO}(S, T) = \emptyset$. Otherwise $S \cong T$, in which case $gh^{-1} ∈ \text{ISO}(\text{SQUASH}(S), \text{SQUASH}(T)) = \text{ISO}(S, T)$. Therefore

$$\text{APPROX}(S, T) = \text{AUT}(\text{SQUASH}(S)) · gh^{-1} = \text{AUT}(S) · gh^{-1} = \text{ISO}(S, T).$$

Definition 4.1(iii) clearly holds. Therefore APPROX is an isomorphism approximator.

Define $L = [i ∈ Ω : i$ is fixed by $\text{AUT}(\text{SQUASH}(S)^g)]$, ordered as usual in $Ω$. Since $\text{AUT}(S)^g = \text{AUT}(\text{SQUASH}(S)^g) = \text{AUT}(\text{SQUASH}(S)^g)$, it follows that $L$ consists of fixed points of $\text{AUT}(S)^g$, and so $\text{FIXED}(S)$ (which equals $L^{g^{-1}}$) consists of fixed points of $\text{AUT}(S)$. Therefore Definition 4.2(i) holds. To show that Definition 4.2(ii) holds, let $x ∈ \text{SYM}(Ω)$ be arbitrary and define $r = \text{CANON}(\text{SQUASH}(S^x))$. Since $\text{SQUASH}(S)$ and $\text{SQUASH}(S^x)$ are isomorphic, it follows that $\text{SQUASH}(S)^g = \text{SQUASH}(S^x)^r$. In particular, $L = [i ∈ Ω : i$ is fixed by $\text{AUT}(\text{SQUASH}(S^x)^g)]$, and $g^{-1}xr$ is an automorphism of $\text{SQUASH}(S)^g$, which means that $g^{-1}xr$ fixes every entry of $L$. Thus

$$\text{FIXED}(S)^x = L^{g^{-1}x} = L^{(g^{-1}xr)r^{-1}} = L^{r^{-1}} = \text{FIXED}(S^x). \quad □$$

### 4.2. Approximations via equitable vertex labellings

In order to present the approximator functions of this section, we require the notion of an equitable vertex labelling for a labelled digraph. Here we use the term *vertex labelling* as an abbreviation for the restriction of a digraph labelling function to the set of vertices, $Ω$. 


4.2.1. Equitable vertex labellings

Definition 4.6. The vertex labelling of a labelled digraph \((\Omega, A, \text{LABEL})\) is equitable if and only if, for all vertices \(\alpha, \beta \in \Omega\) with the same label, and for all vertex labels \(y\) and arc labels \(z\):

\[
|\{(\alpha, \delta) \in A : \text{LABEL}(\delta) = y \text{ and } \text{LABEL}(\alpha, \delta) = z\}| = |\{(\beta, \delta) \in A : \text{LABEL}(\delta) = y \text{ and } \text{LABEL}(\beta, \delta) = z\}|, \text{ and }
\]

\[
|\{(\delta, \alpha) \in A : \text{LABEL}(\delta) = y \text{ and } \text{LABEL}(\delta, \alpha) = z\}| = |\{(\delta, \beta) \in A : \text{LABEL}(\delta) = y \text{ and } \text{LABEL}(\delta, \beta) = z\}|.
\]

In other words, the vertex labelling is equitable if and only if, for all vertex labels \(x\) and \(y\) and arc labels \(z\), every vertex with label \(x\) has some common number of out-neighbours with label \(y\) via arcs with label \(z\), and similarly, every vertex with label \(x\) has some common number of in-neighbours with label \(y\) via arcs with label \(z\).

By including arc labels, Definition 4.6 extends the well-known concepts of equitable colourings [14, Section 3.1] and partitions [9, Definition 29] of vertex-labelled graphs and digraphs, and enables us to estimate automorphism groups and sets of isomorphisms.

It is possible to define a procedure that takes a labelled digraph \(\Gamma\), and returns a new equitable vertex labelling for \(\Gamma\), where vertices with the same equitable label have the same original label in \(\Gamma\). The approximation for \(\text{Aut}(\Gamma)\) that can be obtained from such an equitable vertex labelling procedure turns out to be a potentially better approximation for \(\text{Aut}(\Gamma)\) than the one derived from the original vertex labelling. We present an example of such a procedure in Algorithm 4.8, which is an adaptation of existing algorithms for computing equitable partitions of vertex-labelled digraphs, such as those in [14, Algorithm 1] and [9, Algorithm 2].

In the following lemma, we present several properties of the function defined by Algorithm 4.8, and then we present and discuss the algorithm. Note that (iii) and (iv) follow from (ii), which itself follows from the careful ordering of the lists in Algorithm 4.8. The proof is otherwise omitted, because it is mathematically straightforward.

Lemma 4.7. Let \(\text{EQUITABLE}\) be the function defined by Algorithm 4.8, and let \(\Gamma\) and \(\Delta\) be labelled digraphs on \(\Omega\). Then there exist \(k, l \in \mathbb{N}_0\), labels \(x_1, \ldots, x_k, y_1, \ldots, y_l\), and subsets \(U_1, \ldots, U_k, V_1, \ldots, V_l \subseteq \Omega\) such that

\[
\text{EQUITABLE}(\Gamma) = [(x_1, U_1), \ldots, (x_k, U_k)] \text{ and } \text{EQUITABLE}(\Delta) = [(y_1, V_1), \ldots, (y_l, V_l)].
\]

Then the following hold:

(i) \(\text{EQUITABLE}(\Gamma)\) defines an equitable vertex-labelling for \(\Gamma\).

(ii) \(\text{EQUITABLE}(\Gamma^g) = [(x_1, U_1^g), \ldots, (x_k, U_k^g)]\) for all \(g \in \text{Sym}(\Omega)\).

(iii) \(\text{Aut}(\Gamma) \leq \{g \in \text{Sym}(\Omega) : [O_1^g, \ldots, O_k^g] = [O_1, \ldots, O_k]\}\).

(iv) \(\text{Iso}(\Gamma, \Delta)\)

\[
\begin{cases} 
\emptyset, & \text{if } k \neq l \text{ or } x_i \neq y_i \text{ for any } i, \\
\{g \in \text{Sym}(\Omega) : [U_1^g, \ldots, U_k^g] = [V_1, \ldots, V_k]\}, & \text{otherwise.}
\end{cases}
\]
Algorithm 4.8 Equitable: Equitable vertex labelling for a labelled digraph.

**Input:** A labelled digraph $\Gamma := (\Omega, A, \text{Label})$, with labels from a totally-ordered set.

**Output:** A list that defines an equitable vertex labelling for $\Gamma$, such that:

- vertices with the same equitable label have the same original label, and
- vertices in the same orbit of $\text{Aut}(\Gamma)$ have the same equitable label.

1. \(\text{NewLabels} := \{(x, \{\alpha \in \Omega : \text{Label}(\alpha) = x\}) : x \in \text{Label}(\Omega)\}\), a set of pairs.
2. Convert \(\text{NewLabels}\) into a list, ordered by first component.
3. \(\text{ToProcess} := \text{NewLabels}\).
4. while \(\text{ToProcess}\) is non-empty and \(|\text{NewLabels}| < |\Omega|\) do
   5. Remove the first entry \((x, U)\) of \(\text{ToProcess}\).
   6. \(L := \{\text{Label}(\alpha, \beta) : (\alpha, \beta) \in A, \text{ and } \alpha \in U \text{ or } \beta \in U\}\).
   7. Convert \(L\) into a list, ordered by the ordering of labels.
   8. for \((y, V) \in \text{NewLabels}\) do
      9. for \(\alpha \in V\) and \(i \in \{1, \ldots, |L|\}\) do
         10. \(f(\alpha)[i] := (|\{\beta \in U : \text{Label}(\alpha, \beta) = L[i]\}|, |\{\beta \in U : \text{Label}(\beta, \alpha) = L[i]\}|)\).
            \(\triangleright f\) is a function, and \(f(\alpha)\) is a list of \(|L|\) elements of \(\mathbb{N}_0 \times \mathbb{N}_0\).
      11. Partition \(V\) into \(V_1, \ldots, V_k\) according to, and ordered lexicographically by, \(f\).
          \(\triangleright\) for all \(\alpha, \beta \in V\), there exist unique \(i, j \in \{1, \ldots, k\}\) with \(\alpha \in V_i\) and \(\beta \in V_j\); \(i < j\) if and only if \(f(\alpha) < f(\beta)\). Note that \(f\)-values are totally ordered.
      12. for \(i \in \{1, \ldots, k\}\) do
          13. \(y_i := [y, x, L, f(\min(V_i))]\) \(\triangleright y_i\) is the new label for the vertices in \(V_i\).
      14. Replace \((y, V)\) in \(\text{NewLabels}\) by \((y_1, V_1), \ldots, (y_k, V_k)\), in this order.
      15. if \(k > 1\) then
          16. Remove \((y, V)\) from \(\text{ToProcess}\), if present.
          17. Add \((y_1, V_1), \ldots, (y_k, V_k)\) to the end of \(\text{ToProcess}\), in this order.
   18. return \(\text{NewLabels}\).

To summarise, given a labelled digraph, Algorithm 4.8 repeatedly tests whether each set of vertices with the same label satisfies the condition in Definition 4.6. For each such set and label, either the condition is satisfied, and a new label for this set is devised that encodes the old label and information about how the condition was satisfied, or the condition is not satisfied, and the vertices are given new labels that encode the old label and information about why the new labels were created.

By choosing meaningful vertex labels this way, rather than retaining the existing labels and defining new labels arbitrarily, we can distinguish more pairs of labelled digraphs as non-isomorphic via Lemma 4.7(iv). The next example illustrates this principle.

**Example 4.9.** Let \(\Gamma\) be the labelled digraph on \(\Omega\) with all possible arcs, and let \(\Delta\) be the labelled digraph on \(\Omega\) without arcs, where every vertex and arc in \(\Gamma\) and \(\Delta\) has the label \(x\), for some arbitrary but fixed \(x \in \Omega\). Then Lemma 4.7(iv) allows us to algorithmically deduce that \(\Gamma\) and \(\Delta\) are non-isomorphic, even though both are regular (i.e. every vertex has a common number of in-neighbours, and a common number of
out-neighbours), and they even have the same induced automorphism group, namely \( \text{Sym}(\Omega) \). The \textsc{Equitable} procedure from Algorithm 4.8 assigns the vertices in \( \Gamma \) a label that encodes that each vertex has \( |\Omega| \) in- and out-neighbours, and it assigns the vertices in \( \Delta \) a label that encodes that each vertex has no in- or out-neighbours. Therefore, the labels given by \textsc{Equitable}(\( \Gamma \)) and \textsc{Equitable}(\( \Delta \)) are different, and so \( \Gamma \) and \( \Delta \) are non-isomorphic by Lemma 4.7(iv). A note of warning: the choice of new labels plays a role! If new labels were instead, say, chosen to be incrementally increasing integers starting at 1, then we would have \textsc{Equitable}(\( \Gamma \)) = \textsc{Equitable}(\( \Delta \)), and the deduction that we explained above would not be possible.

In the previous example it is obvious to us the digraphs are non-isomorphic, but for many more complicated examples, Lemma 4.7(iv) can still be used to detect less obvious non-isomorphism.

4.2.2. Strong and weak approximations via equitable vertex labelling

**Definition 4.10** (Strong equitable labelling). Let \textsc{Equitable} be the function defined by Algorithm 4.8, and let \( S, T \in \text{DigraphStacks}(\Omega) \). Then there exist \( k, l \in \mathbb{N}_0 \), labels \( x_1, \ldots, x_k \), and \( y_1, \ldots, y_l \), and subsets \( U_1, \ldots, U_k, V_1, \ldots, V_l \subseteq \Omega \) such that

\[
\text{Equitable}(\text{Squash}(S)) = [(x_1, U_1), \ldots, (x_k, U_k)], \quad \text{and} \quad \text{Equitable}(\text{Squash}(T)) = [(y_1, V_1), \ldots, (y_l, V_l)].
\]

Let \( G \) denote the stabiliser of the list \( [U_1, \ldots, U_k] \) in \( \text{Sym}(\Omega) \), and define

\[
\text{Approx}(S, T) = \begin{cases} 
G \cdot h & \text{if } |S| = |T|, \ k = l, \ \text{and for all } i, x_i = y_i \ \text{and } |U_i| = |V_i|; \\
\varnothing & \text{otherwise},
\end{cases}
\]

where \( h \in \text{Sym}(\Omega) \) is any permutation with the property that \( U_i^h = V_i \) for each \( i \in \{1, \ldots, k\} \). Note that for all \( g, h \in \text{Sym}(\Omega) \), \( U_i^g = U_i^h \) for all \( i \) if and only if \( g \) and \( h \) represent the same right coset of \( G \) in \( \text{Sym}(\Omega) \). Finally, we define

\[
\text{Fixed}(S) = [u_{i_1}, \ldots, u_{i_m}],
\]

where \( i_1 < \cdots < i_m \) and the sets \( U_{ij} = \{u_{ij}\} \) for each \( j \in \{1, \ldots, m\} \) are exactly the singletons amongst \( U_1, \ldots, U_k \).

**Definition 4.11** (Weak equitable labelling). Let \textsc{Equitable} be the function defined by Algorithm 4.8, and let \( S, T \in \text{DigraphStacks}(\Omega) \). For each \( i \in \{1, \ldots, |S|\} \), \( j \in \{1, \ldots, |T|\} \), there exist \( k_i, l_j \in \mathbb{N}_0 \), labels \( x_{i,1}, \ldots, x_{i,k_i}, y_{j,1}, \ldots, y_{j,l_j} \), and subsets \( U_{i,1}, \ldots, U_{i,k_i}, V_{j,1}, \ldots, V_{j,l_j} \subseteq \Omega \) such that

\[
\text{Equitable}(S[i]) = [(x_{i,1}, U_{i,1}), \ldots, (x_{i,k_i}, U_{i,k_i})], \quad \text{and} \quad \text{Equitable}(T[j]) = [(y_{j,1}, V_{j,1}), \ldots, (y_{j,l_j}, V_{j,l_j})].
\]

If either \( |S| \neq |T| \), or else if \( k_i \neq l_j \) for some \( i \in \{1, \ldots, |S|\} \), or else if \( x_{i,j} \neq y_{i,j} \) for some \( i \in \{1, \ldots, |S|\} \) and \( j \in \{1, \ldots, k_i\} \), then we define \( \text{Approx}(S, T) = \varnothing \). Otherwise,
we proceed by ‘intersecting’ the equitable vertex labellings for \( S \), and we do the same with those for \( T \).

More specifically, we define functions \( f \) and \( g \) that map vertices to lists of finite length with entries in \( \mathbb{N} \). For each \( \alpha \in \Omega \), we define \( f(\alpha) \) to be a list of length \( |S| \) where, for each \( i \in \{1, \ldots, |S|\} \), \( f(\alpha)[i] \) is the unique \( j \in \{1, \ldots, k_i\} \) such that \( \alpha \in U_{i,j} \). Similarly, for each \( \alpha \in \Omega \), we define \( g(\alpha) \) to be a list of length \( |T| \) where, for each \( i \in \{1, \ldots, |T|\} \), \( g(\alpha)[i] \) is the unique \( j \in \{1, \ldots, k_i\} \) such that \( \alpha \in V_{i,j} \). Therefore \( f \) and \( g \), respectively, encode the equitable label of a vertex at each level of \( S \) and \( T \). Then we define subsets \( W_1, \ldots, W_m \) of \( \Omega \) according to, and ordered lexicographically by, \( f \)-value, and similarly we define subsets \( T_1, \ldots, T_n \) of \( \Omega \) via \( g \).

Given all of this, we let \( G \) denote the stabiliser of \( W_1, \ldots, W_m \) in \( \text{Sym}(\Omega) \) and define

\[
\text{APPROX}(S, T) = \begin{cases} 
G \cdot h & \text{if } |S| = |T|, \ m = n, \ \text{and for all } i, \\
|W_i| = |T_i| \text{ and } f(\min(W_i)) = g(\min(T_i)), \\
\emptyset & \text{otherwise,}
\end{cases}
\]

where \( h \in \text{Sym}(\Omega) \) is any permutation with the property that \( W_i^h = T_i \) and \( \min(W_i) \) is the minimum with respect to the ordering of \( \Omega \). Finally, we define

\[
\text{FIXED}(S) = [w_{i_1}, \ldots, w_{i_t}],
\]

where \( i_1 < \cdots < i_t \) and the sets \( W_{i_j} = \{w_{i_j}\} \) for each \( j \in \{1, \ldots, t\} \) are exactly the singletons amongst \( W_1, \ldots, W_m \).

The following lemma holds by Lemma 4.7.

**Lemma 4.12.** The functions \( \text{APPROX} \) from Definitions 4.10 and 4.11 are isomorphism approximators, and the functions \( \text{FIXED} \) are fixed-point approximators.

### 4.3. Comparing approximators

In this section, we give an example that compares the isomorphism approximators from Sections 4.1 and 4.2. In principle, approximations via weak equitable labellings should be the cheapest to compute, and those via canonising should be the most expensive. On the other hand, those via weak equitable labelling should be the least accurate, and those via canonising the most accurate. The reason that strong equitable labelling sometimes provides better approximations than weak equitable labelling is that it considers all of the entries of the stack simultaneously, whereas the weak version only considers each entry of the stack individually.

**Example 4.13.** Let the labelled digraphs \( \Gamma_1, \Gamma_2, \Delta_1, \) and \( \Delta_2 \) be defined as in Figure 4.14. The label of every vertex in \( \Gamma_1, \Gamma_2, \Delta_1, \) and \( \Delta_2 \) is \textit{white}, and each arc has the label \textit{solid} or \textit{dashed}, according to its depiction. Every vertex in \textsc{Squash}([\( \Gamma_1, \Gamma_2 \)]) and \textsc{Squash}([\( \Delta_1, \Delta_2 \)]) has the same label \textit{[white, white]}; arcs with label \textit{[#]} are shown as \textit{solid}, arcs with label \textit{[#]} are shown as \textit{dashed}, and arcs with label \textit{[solid, dashed]} are shown as \textit{dotted}. We order labels via:

\[
dashed < \text{solid} < \text{white} < \text{[white, white]} < \text{[#]} < \text{[dashed]} < \text{[solid, dashed]}.\]
Weak equitable labelling: Since $\Gamma_1$, $\Gamma_2$, $\Delta_1$, and $\Delta_2$ are regular (i.e. in each of them, all vertices have a common number of in-neighbours and a common number of out-neighbours), the equitable vertex labelling algorithm cannot make progress, as it only considers each labelled digraph individually.

More specifically, Algorithm 4.8 gives the label $[\text{white}, \text{white}, [\text{solid}], (2, 2)]$ to every vertex in $\Gamma_1$ and $\Delta_1$ (encoding that every white vertex has two white in-neighbours and two white out-neighbours via solid arcs), and it labels every vertex in $\Gamma_2$ and $\Delta_2$ with $[\text{white}, \text{white}, [\text{dashed}], (1, 1)]$ (since every white vertex has one white out-neighbour and one white in-neighbour via dashed arcs).

Therefore, weak equitable labelling gives the worst possible overestimation

$$\text{APPROX}([\Gamma_1, \Gamma_2], [\Delta_1, \Delta_2]) = S_6.$$  

Strong equitable labelling: Algorithm 4.8 assigns the new label

$$[[\text{white}, \text{white}], [\text{white}, \text{white}], [[\#], [\text{dashed}], [\text{solid}, \#]], [(1, 1), (2, 2)],$$

to the vertices 3 and 6 of SQUASH($[\Gamma_1, \Gamma_2]$) and the vertices 1 and 5 of SQUASH($[\Delta_1, \Delta_2]$).

This encodes that these vertices (which previously had label $[\text{white}, \text{white}]$) each have one in- and one out-neighbour with label $[\text{white}, \text{white}]$ via $[\#], [\text{dashed}]$ arcs, and two such in-neighbours and two such out-neighbours via $[\text{solid}, \#]$ arcs. In addition, the algorithm then labels the remaining vertices, namely 1, 2, 4, and 5 in SQUASH($[\Gamma_1, \Gamma_2]$), and 2, 3, 4, and 6 in SQUASH($[\Delta_1, \Delta_2]$), as

$$[[\text{white}, \text{white}], [\text{white}, \text{white}], [[\text{solid}, \#], [\text{solid}, \text{dashed}]], [(1, 1), (1, 1)]].$$
For each squashed labelled digraph, the algorithm updates these new labels with information about why these sets of vertices cannot be further subdivided. Ultimately, strong equitable labelling gives
\[ \text{APPROX}([\Gamma_1, \Gamma_2], [\Delta_1, \Delta_2]) = \langle (3 6), (1 2), (1 2 4 5) \rangle \cdot (1 2 3)(5 6). \]

Note that \(|\text{APPROX}([\Gamma_1, \Gamma_2], [\Delta_1, \Delta_2])| = 4! \cdot 2! = 48\), and so this is a much smaller overestimate.

The coset representative \(g := (1 2 3)(5 6)\) was chosen arbitrarily from \(S_6\), subject to satisfying the property that \(\{1, 2, 4, 5\}^g = \{2, 3, 4, 6\}\) and \(\{3, 6\}^g = \{1, 5\}\). Note that \(g\) happens not to be an isomorphism from \([\Gamma_1, \Gamma_2]\) to \([\Delta_1, \Delta_2]\).

**Canonising and computing exactly:** We compute (using BLISS [11] via the GAP [3] package DIGRAPHS [1]) that \(\text{Aut}(\text{SQUASH}([\Gamma_1, \Gamma_2])) = \langle (1 2)(3 6)(4 5), (1 4)(2 5)(3 6) \rangle\) and \((1 2 3 5 6)\) induces an isomorphism from \(\text{SQUASH}([\Gamma_1, \Gamma_2])\) to \(\text{SQUASH}([\Delta_1, \Delta_2])\). Thus
\[ \text{Iso}([\Gamma_1, \Gamma_2], [\Delta_1, \Delta_2]) = \langle (1 2)(3 6)(4 5), (1 4)(2 5)(3 6) \rangle \cdot (1 2 3 5 6). \]

In particular, \(|\text{Iso}([\Gamma_1, \Gamma_2], [\Delta_1, \Delta_2])| = 4\), which shows us how far away we still were from a perfect estimate with the other approximators.

**5. Adding information to stacks with refiners**

In this section we introduce and discuss refiners for labelled digraph stacks. We use refiners to encode information about a search problem into the stacks around which the search is organised, in order to prune the search space.

**Definition 5.1.** A refiner for a set of permutations \(U \subseteq \text{Sym}(\Omega)\) is a pair of functions \((f_L, f_R)\) from \(\text{DIGRAPHSTACKS}(\Omega)\) to itself, such that, for all \(S, T \in \text{DIGRAPHSTACKS}(\Omega)\) with \(S \cong T\):
\[ U \cap \text{Iso}(S, T) \subseteq U \cap \text{Iso}(f_L(S), f_R(T)). \]

While refiners depend on a subset of \(\text{Sym}(\Omega)\), we do not include this in our notation in order to make it less complicated. Note that the condition in Definition 5.1 is satisfied for all non-isomorphic labelled digraph stacks \(S\) and \(T\), and so the condition that \(S \cong T\) in Definition 5.1 could be removed without altering the notion of a refiner.

As a trivial example, every pair of functions from \(\text{DIGRAPHSTACKS}(\Omega)\) to itself is a refiner for the empty set. It is valid, and indeed common, to search for the empty set: for instance, one might wish to use the techniques in this paper to search for the set of isomorphisms from one labelled digraph to another that, in the end, prove to be non-isomorphic. Thus it is important that Definition 5.1 accommodates the empty set.

The functions \(f_L\) and \(f_R\) of a refiner \((f_L, f_R)\) are also permitted to produce empty labelled digraph stacks. If, for example, we set \(f\) to be the constant function that maps every labelled digraph stack on \(\Omega\) to \(\text{EMPTYSTACK}(\Omega)\), then \((f, f)\) is a refiner for any set \(U \subseteq \text{Sym}(\Omega)\). This is because every permutation in \(\text{Sym}(\Omega)\), by definition, induces an
autormorphism of $\text{EMPTY\_STACK}(\Omega)$. It follows that $U \cap \text{Iso}(f(S), f(T)) = U \cap \text{Sym}(\Omega) = U$ for all $S, T \in \text{DIGRAPH\_STACKS}(\Omega)$ in this case.

In the following lemma, we formulate additional equivalent definitions of refiners.

**Lemma 5.2.** Let $(f_L, f_R)$ be a pair of functions from $\text{DIGRAPH\_STACKS}(\Omega)$ to itself and let $U \subseteq \text{Sym}(\Omega)$. Then the following are equivalent:

(i) $(f_L, f_R)$ is a refiner for $U$.

(ii) For all isomorphic $S, T \in \text{DIGRAPH\_STACKS}(\Omega)$:

$$U \cap \text{Iso}(S, T) = U \cap \text{Iso}(S\|f_L(S), T\|f_R(T)),$$

(iii) For all isomorphic $S, T \in \text{DIGRAPH\_STACKS}(\Omega)$ and $g \in U$:

if $S^g = T$, then $f_L(S)^g = f_R(T)$.

**Proof.** (i) $\Rightarrow$ (ii). Let $S, T \in \text{DIGRAPH\_STACKS}(\Omega)$, and suppose that $S$ and $T$ are isomorphic. Then $U \cap \text{Iso}(S, T) \subseteq U \cap \text{Iso}(f_L(S), f_R(T))$ by assumption, and since $S$ and $T$ have equal lengths, it follows that

$$\text{Iso}(S, T) \cap \text{Iso}(f_L(S), f_R(T)) = \text{Iso}(S\|f_L(S), T\|f_R(T))$$

by Remark 3.1. Hence

$$U \cap \text{Iso}(S, T) = U \cap \text{Iso}(S, T) \cap (U \cap \text{Iso}(f_L(S), f_R(T))) = U \cap (\text{Iso}(S, T) \cap \text{Iso}(f_L(S), f_R(T))) = U \cap \text{Iso}(S\|f_L(S), T\|f_R(T)).$$

(ii) $\Rightarrow$ (iii). Let $S, T \in \text{DIGRAPH\_STACKS}(\Omega)$ be isomorphic, and let $u \in U$. If $S^u = T$, then $u \in \text{Iso}(S, T)$ by definition, and so $u \in \text{Iso}(S\|f_L(S), T\|f_R(T))$ by assumption. Since $S$ and $T$ have equal lengths, and $S\|f_L(S)$ and $T\|f_R(T)$ have equal lengths, it follows that so too do $f_L(S)$ and $f_R(T)$. Then $f_L(S)^u = f_R(T)$, since for each $i \in \{1, \ldots, |f_L(S)|\}$,

$$f_L(S)[i]^u = (S\|f_L(S))[i]\| + i]^u = (T\|f_R(T))[i] + i = f_R(T)[i].$$

(iii) $\Rightarrow$ (i). This implication is immediate. \hfill $\square$

Perhaps Lemma 5.2(ii) most clearly indicates the relevance of refiners to search.

Suppose that we wish to search for the intersection $U_1 \cap \cdots \cap U_n$ of some subsets of $\text{Sym}(\Omega)$. Let $i \in \{1, \ldots, n\}$, let $(f_L, f_R)$ be a refiner for $U_i$, and let $S$ and $T$ be isomorphic labelled digraph stacks on $\Omega$, such that $\text{Iso}(S, T)$ overestimates (i.e. contains) $U_1 \cap \cdots \cap U_n$.

We may use the refiner $(f_L, f_R)$ to refine the pair of stacks $(S, T)$: we apply the functions $f_L$ and $f_R$, respectively, to the stacks $S$ and $T$ and obtain an extended pair of stacks $(S\|f_L(S), T\|f_R(T))$. We call this process refinement. Note that the refiner for $U_i$ need not consider the other sets in the intersection.
By Lemma 5.2(ii), the set of induced isomorphisms Iso(S∥f_L(S), T∥f_R(T)) contains the elements of U_i that belonged to Iso(S, T). Since U_i contains U_1 ∩ ... ∩ U_n, it follows that Iso(S∥f_L(S), T∥f_R(T)) is again an overestimate for U_1 ∩ ... ∩ U_n; it is contained in the previous overestimate by Remark 3.1. Moreover, Iso(S∥f_L(S), T∥f_R(T)) may lack some elements of Iso(S, T) \ (U_1 ∩ ... ∩ U_n), in which case we have produced a smaller overestimate for the result, and thereby reduced the size of the remaining search space. We may then repeat this process, perhaps with a different refiner, in the hope of reducing the search space further still.

The condition in Lemma 5.2(iii) is often most convenient for verifying that a pair of functions is a refiner for some set, as is done in Example 5.3.

**Example 5.3** (Refiner for set stabiliser and transporter in Sym(Ω)). Let A, B ⊆ Ω and let
\[
S_{A,B} = \{ g \in \text{Sym}(Ω) : A^g = B \}
\]
denote the set of permutations of Ω that map A to B. Note that S_{A,A} is the set stabiliser Sym(Ω)_A of A in Sym(Ω), and that in general, either S_{A,B} is empty, or it is a right coset of Sym(Ω)_A and a left coset of Sym(Ω)_B in Sym(Ω).

Define a labelled digraph Γ_A without arcs, where the vertices in A have the label in, and the remaining vertices have the label out. Furthermore, let \text{STAB}_A be the function that maps every labelled digraph stack on Ω to the stack [Γ_A]. Define Γ_B and \text{STAB}_B analogously. Then (\text{STAB}_A, \text{STAB}_B) is a refiner for the set S_{A,B} by Lemma 5.2(iii), since
\[
\text{STAB}_A(S)^g = [Γ_A]^g = [Γ_A^g] = [Γ_B] = \text{STAB}_B(T)
\]
for all S, T ∈ \text{DIGRAPHSTACKS}(Ω) and for all g ∈ S_{A,B}.

The refiner in Example 5.3 is particularly straightforward: the functions \text{STAB}_A and \text{STAB}_B are constant, and they return stacks of length one containing labelled digraphs without arcs and only two different vertex labels. Moreover, the isomorphisms between these stacks are precisely the permutations in Sym(Ω) that map A to B as sets.

Note that when Example 5.3 gives a refiner (f_L, f_R) for a subgroup of Sym(Ω) rather than just a subset, for example when A = B and the subgroup is the setwise stabiliser of A in Sym(Ω), then f_L = f_R. Lemma 5.4 shows that this property is shared by every refiner for a set that contains the identity map on Ω.

**Lemma 5.4** (cf. [12, Prop 2], [13, Lemma 6]). Let (f_L, f_R) be a refiner for a subset U ⊆ Sym(Ω) that contains the identity map, idΩ. Then f_L = f_R.

*Proof.* Let S ∈ \text{DIGRAPHSTACKS}(Ω) be arbitrary. Since id_Ω ∈ U and (f_L, f_R) is a refiner for U, it follows by Lemma 5.2(iii) that f_L(S) = f_L(S)^{id_Ω} = f_R(S). \qed

Lemma 5.2(iii) implies the following lemma.

**Lemma 5.5.** Let f be a function from \text{DIGRAPHSTACKS}(Ω) to itself, and let U be a subset of Sym(Ω) containing id_Ω. Then (f, f) is a refiner for U if and only if f(S^g) = f(S)^g for all g ∈ U and S ∈ \text{DIGRAPHSTACKS}(Ω).
Next, we see that any refiner for a non-empty set can be derived from a function \( f \) that satisfies the condition in Lemma 5.5.

**Lemma 5.6.** Let \( U \) be a non-empty subset of \( \text{Sym}(\Omega) \), fix \( h \in U \) arbitrarily, and let \( f \) and \( g \) be functions from \( \text{DigraphStacks}(\Omega) \) to itself. Then the following are equivalent:

(i) \((f, g)\) is a refiner for \( U \).

(ii) \((f, f)\) is a refiner for \( Uh^{-1} \), and \( g(S) = f(S^{h^{-1}})^{h} \) for all \( S \in \text{DigraphStacks}(\Omega) \).

In particular, if \( U \) is a right coset of a subgroup \( G \leq \text{Sym}(\Omega) \), then \((f, g)\) is a refiner for \( U \) if and only if \((f, f)\) is a refiner for the group \( G \), and \( g(S) = f(S^{h^{-1}})^{h} \) for all \( S \in \text{DigraphStacks}(\Omega) \).

**Proof.** (i) \(\Rightarrow\) (ii). Let \( S \in \text{DigraphStacks}(\Omega) \). Since \((f, g)\) is a refiner for \( U \), it follows by Lemma 5.2(iii) that \( g(S^{h}) = f(S^{h}) \).

Moreover, \( S \) was chosen arbitrarily, and so \( g(S) = g((S^{h^{-1}})^{h}) = f(S^{h^{-1}})^{h} \). Furthermore, if \( y \in Uh^{-1} \) is arbitrary, then

\[
(f(S))^{y} = (f(S)^{y})^{h^{-1}} = g((S^{y}h^{-1})^{h}) = f(S^{yh^{-1}})^{h} = f(S^{y}).
\]

Therefore \((f, g)\) is a refiner for \( Uh^{-1} \) by Lemma 5.2(iii).

(ii) \(\Rightarrow\) (i). Let \( S, T \in \text{DigraphStacks}(\Omega) \), suppose that \( S \) and \( T \) are isomorphic, and let \( x \in U \). Since \((f, f)\) is a refiner for \( Uh^{-1} \) and \( xh^{-1} \in Uh^{-1} \), it follows by Lemma 5.5 that \( f(S)^{xh^{-1}} = f(S^{xh^{-1}}) \).

Thus, if \( S^{x} = T \), then

\[
(f(S)^{x} = f(S)^{xh^{-1}}h = f(S^{xh^{-1}})^{h} = f(T^{h^{-1}})^{h} = g(T),
\]

and so \((f, g)\) is a refiner for \( U \) by Lemma 5.2(iii).

For some pairs of functions, such as those in Example 5.3 and the upcoming Example 5.9, one may use the following results to show that the pair gives a refiner.

**Lemma 5.7.** Let \( U \subseteq \text{Sym}(\Omega) \), and let \( f_{L}, f_{R} \) be functions from \( \text{DigraphStacks}(\Omega) \) to itself such that \( U \subseteq \text{Iso}(f_{L}(S), f_{R}(T)) \) for all isomorphic \( S, T \in \text{DigraphStacks}(\Omega) \). Then \((f_{L}, f_{R})\) is a refiner for \( U \).

**Proof.** Let \( S, T \in \text{DigraphStacks}(\Omega) \) be isomorphic. By Remark 3.1 and the assumption on \((f_{L}, f_{R})\) we have that

\[
U \cap \text{Iso}(S, T) = (U \cap \text{Iso}(f_{L}(S), f_{R}(T))) \cap \text{Iso}(S, T)
= U \cap (\text{Iso}(S, T) \cap \text{Iso}(f_{L}(S), f_{R}(T)))
= U \cap \text{Iso}(S\|f_{L}(S), T\|f_{R}(T)).
\]

Therefore, by Lemma 5.2(ii), \((f_{L}, f_{R})\) is a refiner for \( U \).

**Corollary 5.8.** Let \( G \leq \text{Sym}(\Omega) \), and let \( f \) be a function from \( \text{DigraphStacks}(\Omega) \) to itself with constant value \( S \in \text{DigraphStacks}(\Omega) \), such that \( G \leq \text{Aut}(S) \). Then \((f, f)\) is a refiner for \( G \).
Example 5.9 (Refiner for set of subsets stabiliser and transporter). Let $k \in \mathbb{N}_0$ and $U_i \subseteq \Omega$ for all $i \in \{1, \ldots, k\}$, let $\mathcal{U} = \{U_1, \ldots, U_k\}$, and let $\Gamma_\mathcal{U}$ be the labelled digraph on $\Omega$ whose set of arcs is

$$\{(\alpha, \beta) \in \Omega \times \Omega : \alpha \neq \beta \text{ and } \{\alpha, \beta\} \subseteq U_i \text{ for some } i\};$$

where the label of each vertex $\alpha \in \Omega$ is a list of length $\max\{|U_i| : i \in \{1, \ldots, k\}\}$, with $i$th entry

$$|\{j \in \{1, \ldots, k\} : \alpha \in U_j \text{ and } |U_j| = i\}|, k,$$

and the label of each arc $(\alpha, \beta)$ in the digraph is a list of the same length, with $i$th entry

$$|\{j \in \{1, \ldots, k\} : \alpha, \beta \in U_j \text{ and } |U_j| = i\}|, k).$$

The label of a vertex (or arc) encodes, for each size of subset, the number of all subsets that have that size and contain that vertex (or arc). For every $S \in \text{DIGRAPHSTACKS}(\Omega)$, we define $f_\mathcal{U}(S) = \Gamma_\mathcal{U}$. In addition, for all $g \in \text{Sym}(\Omega)$, we define $\mathcal{U}^g = \{U_1^g, \ldots, U_k^g\}$.

Let $\mathcal{U}$ and $\mathcal{V}$ be arbitrary sets of subsets of $\Omega$. Since the labelled digraphs $\Gamma_\mathcal{U}$ and $\Gamma_\mathcal{V}$ were defined so that $\{g \in \text{Sym}(\Omega) : \mathcal{U}^g = \mathcal{V}\} \subseteq \text{Iso}(\Gamma_\mathcal{U}, \Gamma_\mathcal{V})$, it follows by Lemma 5.7 that $(f_\mathcal{U}, f_\mathcal{V})$ is a refiner for the set $\{g \in \text{Sym}(\Omega) : \mathcal{U}^g = \mathcal{V}\}$, and Corollary 5.8 yields that $(f_\mathcal{U}, f_\mathcal{V})$ is a refiner for the group $\{g \in \text{Sym}(\Omega) : \mathcal{U}^g = \mathcal{U}\}$.

For a specific example, we consider the sets of subsets $U = \{\{1\}, \{1, 2, 3\}, \{2, 4\}\}$, and $\mathcal{V} := \{\{5\}, \{2, 3, 4\}, \{3, 4\}\}$. Both $\mathcal{U}$ and $\mathcal{V}$ contain three subsets, which have sizes 1, 2 and 3, and so, at least superficially, it seems plausible there may exist elements of $\mathcal{S}_3$ that map $\mathcal{U}$ to $\mathcal{V}$. In order to search for the transporter set $\{g \in \mathcal{S}_3 : \mathcal{U}^g = \mathcal{V}\}$, then (with all the following notation as defined above) we can use the refiner $(f_\mathcal{U}, f_\mathcal{V})$ to produce labelled digraphs $\Gamma_\mathcal{U}$ and $\Gamma_\mathcal{V}$, such that $\text{Iso}(\Gamma_\mathcal{U}, \Gamma_\mathcal{V})$ contains the transporter set. These labelled digraphs are depicted in Figure 5.10; although we do not give the correspondence explicitly, a pair of vertices or a pair of arcs have the same visual style if and only if they have the same label.

![Figure 5.10](image-url)

**Figure 5.10:** Demonstration of the labelled digraphs $\Gamma_\mathcal{U}$ and $\Gamma_\mathcal{V}$ from Example 5.9, for the sets of subsets $\mathcal{U} = \{\{1\}, \{1, 2, 3\}, \{2, 4\}\}$ and $\mathcal{V} = \{\{5\}, \{2, 3, 4\}, \{3, 4\}\}$ of $\{1, \ldots, 5\}$.

There are many ways to show that $\Gamma_\mathcal{U}$ and $\Gamma_\mathcal{V}$ are non-isomorphic: for example, they have different numbers of arcs. Hence no permutation in $\mathcal{S}_5$ maps $\mathcal{U}$ to $\mathcal{V}$.
5.1. Perfect refiners

Refiners differ in their ability to encode information into a pair of labelled digraph stacks. For some sets, there are refiners that capture all of the information about the set. Such refiners are the focus of this section.

**Lemma 5.11.** Let $U \subseteq \text{Sym}(\Omega)$, and let $f_L, f_R$ be functions from $\text{DIGRAPHSTACKS}(\Omega)$ to itself such that

$$U \cap \text{Iso}(S, T) = \text{Iso}(S \parallel f_L(S), T \parallel f_R(T))$$

for all $S, T \in \text{DIGRAPHSTACKS}(\Omega)$. Then $(f_L, f_R)$ is a refiner for $U$.

**Proof.** Let $S, T \in \text{DIGRAPHSTACKS}(\Omega)$ be isomorphic. The hypothesis implies that $\text{Iso}(S \parallel f_L(S), T \parallel f_R(T)) \subseteq U$, and hence that

$$U \cap \text{Iso}(S, T) = U \cap \text{Iso}(S \parallel f_L(S), T \parallel f_R(T)).$$

Thus $(f_L, f_R)$ is a refiner for $U$ by Lemma 5.2(ii).

Refiners with the property from Lemma 5.11 are called **perfect refiners**. Roughly speaking, a perfect refiner $(f_L, f_R)$ for a subset $U \subseteq \text{Sym}(\Omega)$ is used during a search algorithm to take a pair of isomorphic labelled digraph stacks $S$ and $T$, and refine the stacks in such a way as to leave exactly those isomorphisms from $S$ to $T$ that are contained in $U$. In particular, a perfect refiner never needs to be applied more than once in any branch of a search, because all information about $U$ is already encoded into the stacks after its first application.

Next we give alternative ways of proving that a pair of functions forms a perfect refiner for a particular set.

**Lemma 5.12.** Let $U \subseteq \text{Sym}(\Omega)$, and let $f_L, f_R$ be functions from $\text{DIGRAPHSTACKS}(\Omega)$ to itself such that $U = \text{Iso}(f_L(S), f_R(T))$ for all $S, T \in \text{DIGRAPHSTACKS}(\Omega)$. Then $(f_L, f_R)$ is a perfect refiner for $U$.

**Proof.** Let $S, T \in \text{DIGRAPHSTACKS}(\Omega)$ be isomorphic. Using Remark 3.1 and the assumption on $(f_L, f_R)$, it follows that

$$U \cap \text{Iso}(S, T) = \text{Iso}(f_L(S), f_R(T)) \cap \text{Iso}(S, T) = \text{Iso}(S \parallel f_L(S), T \parallel f_R(T)).$$

**Corollary 5.13.** Let $G \leq \text{Sym}(\Omega)$, and let $f$ be a function from $\text{DIGRAPHSTACKS}(\Omega)$ to itself with constant value $S \in \text{DIGRAPHSTACKS}(\Omega)$, such that $G = \text{Aut}(S)$. Then $(f, f)$ is a perfect refiner for $G$.

We have already seen a perfect refiner in Example 5.3; this is particularly straightforward to verify with Lemma 5.12. We give several further examples of perfect refiners in Section 5.1.1. Not every subset of $\text{Sym}(\Omega)$ has a perfect refiner, however.

**Lemma 5.14.** Let $U \subseteq \text{Sym}(\Omega)$. Then there exists a perfect refiner for $U$ if and only if $U = \text{Iso}(S, T)$ for some $S, T \in \text{DIGRAPHSTACKS}(\Omega)$.
Proof. \((\Rightarrow)\) Let \((f_L, f_R)\) be a perfect refiner for \(U\). The result follows by applying the condition in Lemma 5.11 with \(S = T = \text{EmptyStack}(\Omega)\).

\((\Leftarrow)\) Let \(S, T \in \text{DigraphStacks}(\Omega)\) be such that \(U = \text{Iso}(S, T)\). Define \(f_L\) and \(f_R\) to be functions from \(\text{DigraphStacks}(\Omega)\) to itself with constant values \(S\) and \(T\), respectively. Then \((f_L, f_R)\) is a perfect refiner for \(U\) by Lemma 5.12.

Lemma 5.14 implies that a non-empty subset has a perfect refiner if and only if it is a coset of the \(\text{Sym}(\Omega)\)-induced automorphism group of a labelled digraph. Note that not every subgroup of \(\text{Sym}(\Omega)\) is the automorphism group of a labelled digraph.

5.1.1. Examples of perfect refiners

In this section, we give examples of perfect refiners for subgroups and their cosets, in order to thoroughly explain, especially in the first example, the idea of a perfect refiner. As we saw in Lemmas 5.5 and 5.6, the crucial step when creating a refiner for a subgroup \(G \leq \text{Sym}(\Omega)\), or for one of its cosets, is to define a function \(f\) from \(\text{DigraphStacks}(\Omega)\) to itself such that \(f(Sg) = f(S)g\) for all \(S \in \text{DigraphStacks}(\Omega)\) and \(g \in G\).

**Example 5.15** (Perfect refiner for permutation centraliser and conjugacy). For every \(g \in \text{Sym}(\Omega)\), let \(\Gamma_g\) be the labelled digraph on \(\Omega\) whose set of arcs is \(\{(\alpha, \beta) \in \Omega \times \Omega : \alpha^g = \beta\}\), and in which all labels are defined to be 0. For every \(S \in \text{DigraphStacks}(\Omega)\), define \(f_g(S) = [\Gamma_g]\). Let \(g, h \in \text{Sym}(\Omega)\) be arbitrary. Then \((f_g, f_g)\) is a perfect refiner for the centraliser of \(g\) in \(\text{Sym}(\Omega)\) by Corollary 5.13, and by Lemma 5.12, \((f_g, f_h)\) is a perfect refiner for the set \(\{x \in \text{Sym}(\Omega) : g^x = h\}\).

We illustrate one such instance of this perfect refiner. Let \(g = (12)(365) \in S_6\), let \(U\) denote the centraliser of \(g\) in \(S_6\), and define the labelled digraph \(\Gamma_g\) and function \(f_g\) as above. A diagram of \(\Gamma_g\) is shown in Figure 5.16. Note that there is a loop at vertex 4, and only at vertex 4, because 4 is the unique fixed point of \(g\) on \(\{1, \ldots, 6\}\).

![Figure 5.16](image-url)

**Figure 5.16:** The labelled digraph \(\Gamma_g\) for \(g = (12)(365)\), from Example 5.15.

In order to use Corollary 5.13 to verify that \((f_g, f_g)\) is a perfect refiner for \(U\), we must prove that \(\text{Aut}([\Gamma_g]) = U\). Note that \(\text{Aut}([\Gamma_g]) = \text{Aut}(\Gamma_g)\). Every automorphism of \(\Gamma_g\) fixes the unique vertex with a loop, and it also stabilises the connected components (because they have different sizes), and induces automorphisms on them. Therefore \(\text{Aut}(\Gamma_g)\) is contained in the subgroup \(\langle (12), (35), (36) \rangle\) of \(S_6\). But none of the transpositions in \(\langle (35), (36) \rangle\) is an automorphism of \(\Gamma_g\), because the arcs between 3, 5, and 6 only go in one direction. Hence \(\text{Aut}(\Gamma_g) = \langle (12), (365) \rangle = U\), as required.
Example 5.17 (Perfect refiner for labelled digraph automorphism and isomorphism). For every labelled digraph $\Gamma$ on $\Omega$ and every $S \in \text{DIGRAPHSTACKS}(\Omega)$, let $f_\Gamma(S) = [\Gamma]$. Note that $f_\Gamma(S)^g = [\Gamma^g] = [\Gamma] = f_\Gamma(S)$ for all $g \in \text{Aut}(\Gamma)$.

Let $\Gamma$ and $\Delta$ be arbitrary labelled digraphs on $\Omega$. Then $(f_\Gamma, f_\Delta)$ is a perfect refiner for $\text{Iso}(\Gamma, \Delta)$ by Lemma 5.12, and $(f_\Gamma, f_\Gamma)$ is a perfect refiner for $\text{Aut}(\Gamma)$ by Corollary 5.13.

Example 5.18 (Perfect refiner for list of subsets stabiliser and transporter). Whenever $k \in \mathbb{N}_0$ and $U_i \subseteq \Omega$ for each $i \in \{1, \ldots, k\}$ and $U := [U_1, \ldots, U_k]$, we let $\Gamma_U$ be the labelled digraph on $\Omega$ without arcs, where the label of each vertex $\alpha \in \Omega$ is $\{i \in \{1, \ldots, k\} : \alpha \in U_i\}$. For every $S \in \text{DIGRAPHSTACKS}(\Omega)$, define $f_U(S) = [\Gamma_U]$. If $g \in \text{Sym}(\Omega)$, then $U^g := [U_1^g, \ldots, U_k^g]$.

Let $U$ and $V$ be arbitrary lists of subsets of $\Omega$ with all the notation as explained above. Then $(f_U, f_V)$ is a perfect refiner for the set $\{g \in \text{Sym}(\Omega) : U^g = V\}$ by Lemma 5.12, and $(f_U, f_U)$ is a perfect refiner for the group $\{g \in \text{Sym}(\Omega) : U^g = U\}$ by Corollary 5.13.

To illustrate this, let $\Omega = \{1, \ldots, 6\}$ and $U = \{(1,3,6), (3,5), (2,4), (2,3,4)\}$. It follows that

$$\{g \in S_6 : [\{1,3,6\}, \{3,5\}, \{2,4\}, \{2,3,4\}]^g = U\} = \text{Aut}(\Gamma_U) = \langle (16), (24) \rangle.$$

$$\begin{array}{c}
\{1\} & \{1\} \\
6 & 1 \\
\hline
\{2\} & \{2\} & \{3,4\} \\
5 & \{3\} & \{1,2,4\} \\
\{4\} & \{3,4\} \\
\end{array}$$

Figure 5.19: The labelled digraph $\Gamma_{\{(1,3,6),(3,5),(2,4),(2,3,4)\}}$ from Example 5.18.

If $n, m \in \mathbb{N}$ and we encode a list $[x_1, \ldots, x_m]$ in $\Omega$ as the list of singleton subsets $[[x_1], \ldots, [x_m]]$, and we encode a subset $\{y_1, \ldots, y_n\} \subseteq \Omega$ as the list $[[y_1], \ldots, [y_n]]$, then we see that Example 5.18 can be used to create perfect refiners for the sets of permutations that stabilise or transport lists in $\Omega$ or subsets of $\Omega$.

Example 5.20 (Perfect refiner for set of disjoint subsets stabiliser and transporter; Figure 5.21). For every set of disjoint subsets $U := \{U_1, \ldots, U_k\}$, where $k \in \mathbb{N}_0$ and $U_i \subseteq \Omega$ for all $i \in \{1, \ldots, k\}$, let $\Gamma_U$ be the labelled digraph on $\Omega$ with arcs

$$\{(\alpha, \beta) \in \Omega \times \Omega : \alpha \neq \beta \text{ and } \{\alpha, \beta\} \subseteq U_i \text{ for some } i\},$$

where vertices in $U_1 \cup \cdots \cup U_k$ have label 1, and all other vertices and arcs have label 0. For every $S \in \text{DIGRAPHSTACKS}(\Omega)$, define $f_U(S) = [\Gamma_U]$.

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Let \( U \) and \( V \) be arbitrary sets of disjoint subsets of \( \Omega \). Then \((f_U, f_V)\) is a perfect refiner for the set \( \{ g \in \text{Sym}(\Omega) : U^g = V \} \) by Lemma 5.12, and by Corollary 5.13, \((f_U, f_U)\) is a perfect refiner for the group \( \{ g \in \text{Sym}(\Omega) : U^g = U \} \).

We demonstrate this in the case of \( U := \{\{1, 2\}, \{3\}\} \) and \( V := \{\{3, 4\}, \{2\}\} \), with the aim of describing the transporter set \( T := \{ g \in S_4 : U^g = V \} \). First, we build the labelled digraphs \( \Gamma_U \) and \( \Gamma_V \), which are shown in Figure 5.21. The function \( f_U \) has constant value \([\Gamma_U]\), and the function \( f_V \) has constant value \([\Gamma_V]\). Since \((f_U, f_V)\) is a perfect refiner for \( T \), we can describe \( T \) by describing \( \text{Iso}(\Gamma_U, [\Gamma_V]) = \text{Iso}(\Gamma_U, \Gamma_V) \). It is clear that \( (1 2) \) is the automorphism group of \( \Gamma_U \) induced by \( S_4 \), and that \( (1 3 2 4) \) induces an isomorphism from \( \Gamma_U \) to \( \Gamma_V \). Therefore, \( T \) is the right coset \( (1 2) \cdot (1 3 2 4) \) of \((1 2)\) in \( S_4 \).

![Figure 5.21: The labelled digraphs \( \Gamma_{\{1,2\} \cup \{3\}} \) and \( \Gamma_{\{3,4\} \cup \{2\}} \) from Example 5.20. The black vertices are those with label 0.](image)

An ordered partition of \( \Omega \) is a list of subsets of \( \Omega \), and an unordered partition of \( \Omega \) is a set of disjoint subsets of \( \Omega \). Therefore, Example 5.18 can be used to create a perfect refiner for the set of permutations that stabilises any particular ordered partition, or the set of permutations that transports one ordered partition to another. Similarly, Example 5.20 can be used to create perfect refiners for the analogous sets of permutations that involve unordered partitions.

### 5.2. Refiners given by a fixed sequence of stacks

We have seen that when creating a refiner for a set \( U \), it is necessary to construct a function \( f \) from \( \text{DigraphStacks}(\Omega) \) to itself that satisfies \( f(S^g) = f(S)^g \) for all \( S \in \text{DigraphStacks}(\Omega) \) and \( g \in U \). For many of the refiners that we wish to implement, such as those given in Section 5.1.1, this does not cause significant difficulty, especially when the value of the function \( f \) does not depend on its input. However, there are some refiners that we wish to define, especially refiners for an arbitrary subgroup of \( \text{Sym}(\Omega) \) specified by a generating set, or for a coset of such a subgroup, where satisfying the condition described above is difficult in practice. In this section, we give an example of this difficulty, and then present a general method for overcoming this problem.

**Example 5.22.** Let \( \Omega = \{1, \ldots, 6\} \), let \( G = \langle (1 2), (3 4), (5 6), (1 3 5)(2 4 6) \rangle \), let \( \Gamma \) be the labelled digraph on \( \Omega \) without arcs where vertex 1 has label \text{black}, vertex 2 has label \text{grey}, and the remaining vertices have label \text{white}, and define \( S = [\Gamma] \) and \( T = \left[\Gamma^{(135)(246)}\right] \).

Suppose that we are searching for the intersection \( D \) of a number of subsets of \( \text{Sym}(\Omega) \), one of which is \( G \), and suppose that \( \text{ Iso}(S, T) \) represents the current overestimate for the
solution. We wish to give a refiner for $G$ (which, by Lemma 5.4, has the form $(f,f)$ for some function $f$) that works by encoding relevant information about the orbit structure of $G$ into a new labelled digraph stack, since we know that the elements of $D$ respect the orbit structure of $G$ (which is not immediately of much use here, because $G$ is transitive).

However, there is further information that the refiner can use. Since $\text{Iso}(S,T)$ is an overestimate for $D$, we know that every element of $D$ induces an isomorphism from $S$ to $T$. In particular, if $\text{Fixed}$ is a fixed-point approximator, then every element of $D$ maps the list $\text{Fixed}(S)$ to the list $\text{Fixed}(T)$. A fixed-point approximator could give $\text{Fixed}(S) = [1,2]$ and $\text{Fixed}(T) = [3,4]$; suppose that this is the case. Since all elements of $D$ map $[1,2]$ to $[3,4]$ and are also contained in $G$, it follows that they are contained in $G_{[1,2]} \cdot h$, the right coset of the stabiliser of $[1,2]$ in $G$ determined by any permutation $h$ in $G$ that maps $[1,2]$ to $[3,4]$, such as, for example, $h := (1\ 3\ 5)(2\ 4\ 6) \in G$.

This means that we should be able to define $f(S)$ and $f(T)$ in terms of the orbits of the pointwise stabilisers of $[1,2]$ and $[3,4]$ in $G$, respectively, which are $G_{[1,2]} = \langle (3\ 4)(5\ 6) \rangle$ and $G_{[3,4]} = \langle (1\ 2)(5\ 6) \rangle$. Thus one option would be to define $f(S) = f_U(S)$ as in Example 5.20, for the set of orbits $U = \{\{1\},\{2\},\{3,4\},\{5,6\}\}$ of $G_{[1,2]}$ on $\Omega$, and to define $f(T)$ similarly for the set $V = \{\{1,2\},\{3\},\{4\},\{5,6\}\}$. This is valid, but it is not ideal, since permutations in $\text{Sym}(\Omega)$ can rearrange orbits of the same size arbitrarily while mapping $U$ to $V$, whereas elements of the right coset $G_{[1,2]} \cdot h$ can only map an orbit $O \in U$ to the orbit $O^h$. For instance, $(1\ 4)(2\ 3) \in \text{Sym}(\Omega)$ maps $U$ to $V$, but this permutation maps the orbit $\{1\}$ of $G_{[1,2]}$ to the orbit $\{4\}$ of $G_{[3,4]}$, and $\{4\} \neq \{1\}^h$.

Therefore, defining the refiner $(f,f)$ in this way does not discard some elements that, to us, are obviously not in $D$. This is unsatisfactory, so we would like to define $f(S) = f_U(S)$ as in Example 5.18, for some ordered list $U$ of the orbits $\{1\},\{2\},\{3,4\},\{5,6\}$ of $G_{[1,2]}$ on $\Omega$. But then how should we choose an ordering $V$ of the orbits $\{1,2\},\{3\},\{4\},\{5,6\}$ of $G_{[3,4]}$ on $\Omega$, in order to define the corresponding $f(T) (= f_V(T))$ so that $\text{Iso}(f(S),f(T))$ does not discard elements in $D$?

Without further techniques, we cannot answer this question.

To overcome this problem, we use a technique similar to that of Leon [13], where we explicitly pre-generate a list of fixed points and labelled digraph stacks, which are stored and then retrieved during the search, when needed. In essence, this allows us to make certain ordering choices in advance, so that during the search we can consult the fixed initial choice, and remain consistent with that. The mathematical foundation of this technique is described in the following lemma.

**Lemma 5.23.** Let $G \leq \text{Sym}(\Omega)$ and let $\text{Fixed}$ be a fixed-point approximator. For all $i \in N_0$, let $V_i$ be $\text{DIGRAPHSTACKS}(\Omega)$ be a labelled digraph stack on $\Omega$, and let $F_i$ be a list of points in $\Omega$, such that the stabiliser $\{g \in G : F_i^g = F_i\}$ is a subgroup of $\text{Aut}(V_i)$.

We define a function $f$ from $\text{DIGRAPHSTACKS}(\Omega)$ to itself as follows. For each $S \in \text{DIGRAPHSTACKS}(\Omega)$, let $a \in G$ be such that $a$ maps $F_{i[S]}$ to $\text{Fixed}(S)$ pointwise, if such an element exists, and otherwise let $a = \text{Fail}$, and set

$$f(S) = \begin{cases} \text{EMPTYSTACK}(\Omega) & \text{if } a = \text{Fail}, \\ (V_i[S])^a & \text{otherwise.} \end{cases}$$

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Then \((f, f)\) is a refiner for \(G\).

**Proof.** Note that \(f\) is well-defined: if \(S \in \text{DIGRAPHStacks}(\Omega)\) and \(a, b \in G\) both map \(F_{|S|}\) to \(\text{Fixed}(S)\), then \(ab^{-1}\) stabilises \(F_{|S|}\), and so \(ab^{-1} \in \text{Aut}(V_{|S|})\), and hence \((V_{|S|})^a = (V_{|S|})^b\).

Let \(S \in \text{DIGRAPHStacks}(\Omega)\) and \(g \in G\) be arbitrary. First note that \(|S| = |S^g|\). Let \(a\) be an element of \(G\) that maps \(F_{|S|}\) to \(\text{Fixed}(S)\), if such an element exists, and set \(a = \text{Fail}\) otherwise. Similarly, let \(b\) be an element of \(G\) that maps \(F_{|S|}\) to \(\text{Fixed}(S^g)\), if such an element exists, and set \(b = \text{Fail}\) otherwise. Note that \(a = \text{Fail}\) if and only if \(b = \text{Fail}\), since \(g \in G\) maps \(\text{Fixed}(S)\) to \(\text{Fixed}(S^g)\), by Definition 4.2(ii).

Thus, if \(a = \text{Fail}\), then \(f(S^g)\) and \(f(S)^g\) are both empty. Otherwise \(a \in G\), and so \(f(S) = (V_{|S|})^a\) and \(f(S^g) = (V_{|S|})^b\). It remains to prove in this case that \((V_{|S|})^{ag} = (V_{|S|})^b\), or equivalently that \(agb^{-1} \in \text{Aut}(V_{|S|})\). The choice of \(a, g\) and \(b\) implies that \(agb^{-1}\) fixes every entry of \(F_{|S|}\), and so \(agb^{-1} \in \text{Aut}(V_{|S|})\) by assumption.

Therefore \(f(S^g) = f(S)^g\) for all \(S \in \text{DIGRAPHStacks}(\Omega)\) and \(g \in G\), and so \((f, f)\) is a refiner for \(G\) by Lemma 5.5. \(\square\)

In isolation, Lemma 5.23 may seem very abstract. In particular, the lemma does not specify how the lists \(F_i\) and the stacks \(V_i\) should be chosen in the first place. We postpone these details until Section 7.3.2, because the real usefulness of this technique becomes apparent with the organisation of our forthcoming algorithms.

Given two lists of points in \(\Omega\) and a subgroup \(G \leq \text{Sym}(\Omega)\) given by a generating set, there exist efficient algorithms that either construct an element of \(G\) that maps the first list of points to the second, or determine that no such element exists. In GAP [3], this can be achieved via the function \texttt{RepresentativeAction}.

Note that, in combination with Lemma 5.6, Lemma 5.23 may be used to build a refiner for any coset for which we have a representative.

6. Distributing stack isomorphisms across new stacks

In backtrack search, when it is not readily apparent how to further prune a search space, it is necessary to divide the search across a number of subproblems, each of which, being smaller, can be solved more easily. We call this process *splitting*.

In order to organise a backtrack search around stacks of labelled digraphs, therefore, we need to be able to implement a version of splitting for labelled digraph stacks. In other words, we need to be able to take a pair of labelled digraph stacks that represents a potentially large search space, and define new pairs of stacks that divide the search space amongst themselves in a sensible way. Since the search space that a pair of stacks represents is the overestimated set of isomorphisms from the first stack to the second, it follows that we need to be able to take one pair of stacks and define new pairs, such that the originally estimated set of isomorphisms is subdivided across these new pairs.

In this section, we define and discuss the notion of a splitter for labelled digraph stacks.
Definition 6.1. A splitter for an isomorphism approximator \textup{APPROX} is a function \textup{SPLIT} that maps one pair of labelled digraph stacks on \( \Omega \) to a finite list of pairs of stacks, such that for all \( S, T \in \text{DIGRAPHSTACKS}(\Omega) \) with \(|\text{APPROX}(S, T)| \geq 2\),

\[
\text{SPLIT}(S, T) = [(S_1, T_1), (S_2, T_2), \ldots, (S_m, T_m)]
\]

for some \( m \in \mathbb{N}_0 \) and \( S_1, \ldots, S_m, T_1, \ldots, T_m \in \text{DIGRAPHSTACKS}(\Omega) \), and:

(i) \( \text{Iso}(S, T) = \text{Iso}(S\|S_1, T\|T_1) \cup \cdots \cup \text{Iso}(S\|S_m, T\|T_m) \) (a disjoint union).

(ii) \(|\text{APPROX}(S\|S_i, T\|T_i)| < |\text{APPROX}(S, T)|\) for all \( i \in \{1, \ldots, m\} \).

(iii) If \( S = T \), then \( S_1 = T_1 \).

(iv) For all \( U \in \text{DIGRAPHSTACKS}(\Omega) \) with \(|\text{APPROX}(S, U)| \geq 2\), there exists some \( n \in \mathbb{N} \) and \( U_1, U_2, \ldots, U_n \in \text{DIGRAPHSTACKS}(\Omega) \) for all \( i \in \{1, \ldots, n\} \) such that

\[
\text{SPLIT}(S, U) = [(S_1, U_1), (S_2, U_2), \ldots, (S_1, U_n)].
\]

We briefly explain the purpose of the conditions in Definition 6.1, retaining its notation. In Definition 6.1, we do not restrict the behaviour of a splitter when given stacks \( S \) and \( T \) with \(|\text{APPROX}(S, T)| \leq 1\), since this situation never occurs in the algorithms of Section 7. Throughout the following explanation, we assume that \(|\text{APPROX}(S, T)| \geq 2\).

The new subproblems to which the splitter gives rise are the pairs of stacks of the form \((S\|S_i, T\|T_i)\) for each \( i \in \{1, \ldots, m\} \). Definition 6.1(i) ensures that the set of isomorphisms induced by \( \text{Sym}(\Omega) \) from \( S \) to \( T \) is shared amongst these new pairs of stacks. In other words, each \( g \in \text{Iso}(S, T) \) belongs to a unique set \( \text{Iso}(S\|S_i, T\|T_i) \) for some \( i \in \{1, \ldots, m\} \), and so \( g \) belongs to the unique set \( \text{Iso}(S\|S_i, T\|T_i) \) for the same \( i \). This means that each solution to a search problem appears in exactly one branch of the search tree, and so we do not waste resources by repeatedly discovering the same solution. Definition 6.1(i) also implies that no new isomorphisms are introduced by splitting.

Definition 6.1(ii) ensures that each new pair of stacks gives rise to a strictly smaller subproblem than does the original pair of stacks, which will be required to show that our algorithms terminate. It would be ideal for each new approximation of the form \( \text{APPROX}(S\|S_i, T\|T_i) \) to be disjoint from the other new approximations, but we do not need to require this.

Definition 6.1(iii) and (iv) are technical conditions, not of deep mathematical importance, but they are used in Sections 7.2 and 7.3. Definition 6.1(iii) is useful in a notational sense when it comes to describing an algorithm to search for a generating set for a subgroup. Definition 6.1(iv) implies that \( S_1 = S_2 = \cdots = S_m \). This is useful when it comes to applying refiners of the kind introduced in Section 5.2.

The following lemma shows a way of giving a splitter by specifying its behaviour on the left stack that it is given.

Lemma 6.2. Let \textup{APPROX} be an isomorphism approximator, and let \( f \) be any function from \text{DIGRAPHSTACKS}(\Omega) to itself such that, for all \( S \in \text{DIGRAPHSTACKS}(\Omega) \):

\[
\text{if } |\text{APPROX}(S)| \geq 2, \text{ then } |\text{APPROX}(S\|f(S))| < |\text{APPROX}(S)|.
\]
Let $S, T \in \text{DIGRAPHSTACKS}(\Omega)$. If $|\text{APPROX}(S, T)| \leq 1$, then we define $\text{SPLIT}(S, T)$ to be empty. Otherwise, we choose a fixed enumeration $T_1, \ldots, T_m$ of $\{f(S)^g : g \in \text{APPROX}(S, T)\}$, in particular we set $T_1 = f(S) = f(S)^{\text{id}}$ if $S = T$, and we set $\text{SPLIT}(S, T) = [(f(S), T_1), \ldots, (f(S), T_m)]$. Then $\text{SPLIT}$ is a splitter for $\text{APPROX}$.

**Proof.** Let $S, T \in \text{DIGRAPHSTACKS}(\Omega)$ with $|\text{APPROX}(S, T)| \geq 2$, and assume that $\text{SPLIT}(S, T)$ and $[(f(S), T_1), \ldots, (f(S), T_m)]$ are defined as in the statement of the lemma.

We first prove that the equation in Definition 6.1(i) holds. Since $|S| = |T|$ by Definition 4.1(ii), it follows from Remark 3.1 that the left hand side of this equation contains the right hand side, so it remains to show the reverse inclusion, and that the right hand side is a disjoint union. Let $g \in \text{Iso}(S, T) \subseteq \text{APPROX}(S, T)$ be arbitrary. Since $f(S)^g = T_i$ for some $i \in \{1, \ldots, m\}$, it follows that $g \in \text{Iso}(S||f(S), T||T_i)$. If there exists some $h \in \text{Iso}(S||f(S), T||T_i) \cap \text{Iso}(S||f(S), T||T_j)$ for some $i, j \in \{1, \ldots, m\}$, then in particular $T_i = f(S)^h = T_j$, and so $i = j$.

To show that Definition 6.1(ii) holds, let $i \in \{1, \ldots, m\}$. If $\text{APPROX}(S||f(S), T||T_i) = \emptyset$, then we are done, so suppose otherwise. By Definition 4.1(iii) and by assumption,

$$|\text{APPROX}(S||f(S), T||T_i)| = |\text{APPROX}(S||f(S))| < |\text{APPROX}(S)| = |\text{APPROX}(S, T)|,$$

as required. Definition 6.1(iii) and (iv) hold by construction. \hfill $\Box$

Let the notation of Lemma 6.2 hold. Note that we imposed no further conditions in Lemma 6.2 on the enumeration of $\{f(S)^g : g \in \text{APPROX}(S, T)\}$ beyond the condition when $S = T$, because there is no mathematical need to, as long as it is consistent. This set can be computed via the orbit of $f(S)$ under the action of $\text{APPROX}(S)$. Indeed, if $h \in \text{APPROX}(S, T)$, then

$$\{f(S)^g : g \in \text{APPROX}(S, T)\} = \{f(S)^g : g \in \text{APPROX}(S) \cdot h\}$$

$$= \{f(S)^x : x \in \text{APPROX}(S)\}^h$$

$$= \left(f(S)^{\text{APPROX}(S)}\right)^h,$$

by Definition 4.1(iii). In particular, $|\text{SPLIT}(S, T)| = |f(S)^{\text{APPROX}(S)}|$.

In the following definition, we give a specific instance of a splitter that can be obtained with Lemma 6.2. Here, still using the notation of Lemma 6.2, appending the stack $f(S)$ to the stack $S$ corresponds to stabilising $f(S)$ in the current approximation of $\text{Aut}(S)$; the stacks of the form $T_i$ correspond to the images of $f(S)$ under $\text{APPROX}(S, T)$.

**Definition 6.3** (Fixed point splitter). For all $\alpha \in \Omega$, let $\Gamma_\alpha = (\Omega, \emptyset, \text{LABEL})$ be the labelled digraph on $\Omega$ where $\text{LABEL}(\alpha) = 1$ and $\text{LABEL}(\beta) = 0$ for all $\beta \in \Omega \setminus \{\alpha\}$. Note that $\Gamma_\alpha^\beta = \Gamma_\alpha^\beta$ for all $g \in \text{Sym}(\Omega)$. Let $\text{APPROX}$ be any isomorphism approximator such that $\text{APPROX}(U||\Gamma_\alpha) \leq \text{APPROX}(U) \cap \{g \in \text{Sym}(\Omega) : \alpha^g = \alpha\}$ for all $\alpha \in \Omega$ and $U \in \text{DIGRAPHSTACKS}(\Omega)$. We define a function $f$ from $\text{DIGRAPHSTACKS}(\Omega)$ to itself by

$$f(S) = \begin{cases} \text{EMPTYSTACK}(\Omega) & \text{if } |\text{APPROX}(S)| \leq 1, \\ [\Gamma_\alpha] & \text{otherwise, where } \alpha := \min(\min(\mathcal{O}) : \mathcal{O} \text{ is an orbit of } \text{APPROX}(S) \text{ of minimal size, subject to } |\mathcal{O}| \geq 2), \end{cases}$$

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for all \( S \in \text{DIGRAPHSTACKS}(\Omega) \). Finally, define \( \text{_SPLIT} \) as in Lemma 6.2, for the isomorphism approximator \( \text{APPROX} \) and the function \( f \).

The following corollary holds by Lemma 6.2. The crucial step is showing that the function \( f \) has the required property; this follows by the careful choice of isomorphism approximator in Definition 6.3.

**Corollary 6.4.** The function \( \text{_SPLIT} \) from Definition 6.3 is a splitter for any isomorphism approximator that satisfies the condition in Definition 6.3.

7. The search algorithm

In this section, we present our main algorithms, which combine the tools from Sections 3–6 to solve search problems in \( \text{Sym}(\Omega) \). A version of our algorithms is implemented in the GRAPHBACKTRACKING [7] package for GAP [3].

Let \( U_1, \ldots, U_k \subseteq \text{Sym}(\Omega) \), and suppose that we have a collection of refiners for these subsets, an isomorphism approximator, and a corresponding splitter. The section proceeds as follows: in Section 7.1 we show how it is possible to use these refiners, the approximator, and the splitter to perform a backtrack search that finds one or all elements of the intersection \( U_1 \cap \cdots \cap U_k \). In Section 7.2, we describe how, when the result is known to form a subgroup of \( \text{Sym}(\Omega) \), it is possible to search for a base and strong generating set for the subgroup (see for example [2, p. 101]), rather than for the set of all its elements. This is also useful when searching for a coset of a subgroup. Finally, in Section 7.3, we explain the use of the refiners described in Section 5.2.

7.1. The basic procedure

What follows is a high-level description of Algorithm 7.1, which is the main algorithm of this section. This algorithm comprises the \text{SEARCH} and \text{REFINE} procedures, and begins with a call to the \text{SEARCH} procedure on line 20. We say that the algorithm \text{backtracks} when it finishes executing one recursive call to the \text{SEARCH} procedure, and goes back to the point where it was initiated, in order to continue.

Each subset of \( \text{Sym}(\Omega) \) given as input to Algorithm 7.1 should be specified in such a way that it is computationally inexpensive to test whether or not an arbitrary element of \( \text{Sym}(\Omega) \) belongs to the set. For example, the set could be a subgroup specified by a generating set, or it could be defined as the subset of elements of \( \text{Sym}(\Omega) \) that conjugate the subgroup \( G \) to the subgroup \( H \), where \( G \) and \( H \) are given by generating sets. Note that the number of subsets given as input does not need to equal the number of given refiners. For instance, a subset could have multiple refiners, or none.

At any point during the execution of the algorithm, we have a pair of labelled digraph stacks \((S, T)\) whose corresponding set \( \text{Iso}(S, T) \) overestimates the set of solutions to the current problem. (The current problem might be the full problem, or it might be a subproblem produced by a splitter.) However, since we do not necessarily wish to calculate \( \text{Iso}(S, T) \) exactly, in practice we only have access to \( \text{APPROX}(S, T) \), an overestimate for \( \text{Iso}(S, T) \).
Algorithm 7.1 A recursive algorithm using labelled digraph stacks to search in $\text{Sym}(\Omega)$.

**Input:** a sequence of subsets $U_1, \ldots, U_k \subseteq \text{Sym}(\Omega)$ in which membership is easily tested; a sequence $(f_{L,1}, f_{R,1}), \ldots, (f_{L,m}, f_{R,m})$, where each pair is a refiner for some $U_j$; an isomorphism approximator $\text{APPROX}$ and a splitter $\text{SPLIT}$ for $\text{APPROX}$.

**Output:** all elements of the intersection $U_1 \cap \cdots \cap U_k$, which we refer to as ‘solutions’.

1: **procedure** Search($S, T$)  
   $\triangleright$ The main recursive search procedure.
2:  $(S, T) \leftarrow \text{Refine}(S, T)$  
   $\triangleright$ Refine the given stacks.
3:  **case** $\text{APPROX}(S, T) = \emptyset$:  
   $\triangleright$ Nothing found in the present branch: backtrack.
4:   **return** $\emptyset$
5:  **case** $\text{APPROX}(S, T) = \{h\}$ for some $h$:  
   $\triangleright$ $h$ is the sole potential solution here.
6:   **if** $S^h = T$ and $h \in U_1 \cap \cdots \cap U_k$ **then**
7:      **return** $\{h\}$  
   $\triangleright$ $h$ is a solution in $\text{Iso}(S, T)$: backtrack.
8:   **else**
9:      **return** $\emptyset$  
   $\triangleright$ $h$ is not a solution in $\text{Iso}(S, T)$: backtrack.
10: **case** $|\text{APPROX}(S, T)| \geq 2$:  
   $\triangleright$ Multiple potential solutions.
11: **return** $\bigcup_{(S, T_i) \in \text{SPLIT}(S, T)} \text{Search}(S \parallel S_i, T \parallel T_i)$  
   $\triangleright$ Split, and search recursively.
12: **procedure** Refine($S, T$)  
   $\triangleright$ Attempt to remove non-solutions from $\text{Iso}(S, T)$.
13:  **while** $\text{APPROX}(S, T) \neq \emptyset$ **do**  
   $\triangleright$ Proceed while there are potential solutions.
14:     $(S', T') \leftarrow (S, T)$  
   $\triangleright$ Save the stacks before the next round of refinements.
15:     **for** $i \in \{1, \ldots, m\}$ **and while** $|S| = |T|$ **do**
16:        $(S, T) \leftarrow (S \parallel f_{L,i}(S), T \parallel f_{R,i}(T))$  
   $\triangleright$ Apply each refiner in turn.
17:     **if** $|\text{APPROX}(S, T)| \not< |\text{APPROX}(S', T')|$ **then**
18:        **return** $(S', T')$  
   $\triangleright$ Stop: the last refinements seemingly made no progress.
19:     **return** $(S, T)$  
   $\triangleright$ Stop: $\text{APPROX}(S, T) = \emptyset$: no solutions in this branch.
20: **return** Search(EmptyStack($\Omega$), EmptyStack($\Omega$))

The Search procedure is first called on line 20, and later it may be called recursively on line 11. As we prove in Lemma 7.5, this procedure takes a pair of labelled digraph stacks $S$ and $T$, and returns the set of all elements in $U_1 \cap \cdots \cap U_k$ that induce isomorphisms from $S$ to $T$. It does so by first using the Refine procedure to refine the pair of stacks that it is given.

Roughly speaking, the Refine procedure uses refiners to encode information about the search problem into the stacks $S$ and $T$, thereby potentially reducing the size of the remaining search space, without losing any valid solutions. We state and prove this in a precise way in Lemma 7.4.

The Refine procedure repeatedly applies each refiner in turn, until either it determines that there are no induced isomorphisms from the current first stack to the current second stack (and hence there are no solutions to the current problem), or it realises that the most recent round of refiner applications failed to lead to a smaller approximation.
(which we interpret as an indication that the refiners are unable to encode further useful information into the stacks).

The next step of the SEARCH procedure is determined by the value of the isomorphism approximator. The algorithm has reached a leaf of the search tree if the isomorphism approximator determines that there is at most one solution to the current problem, in which case the SEARCH procedure takes the appropriate behaviour, and backtracks. Otherwise, the SEARCH procedure uses a splitter to divide the current problem into smaller subproblems. In more detail:

- If the approximator determines that the pair of stacks is non-isomorphic, then the algorithm backtracks, because it has proved that there are no solutions to the current problem.

- If the approximator estimates that there is a single potential isomorphism from the first stack to the second, then the SEARCH procedure tests whether this element is both an isomorphism and a solution to the search problem, and returns it if so. The algorithm then backtracks, since the current problem has been exhaustively searched.

- If the approximator estimates that there are at least two isomorphisms from the first stack to the second (and therefore, there are at least two potential solutions), then the SEARCH procedure uses a splitter to produce pairs of labelled digraph stacks that represent smaller subproblems, and the SEARCH procedure is then called recursively on these new pairs. This constructs the set of solutions to each of these subproblems, and the union of these sets is the set of solutions to the current problem.

It remains to prove that, given a valid combination of inputs, and after a finite number of steps (Lemma 7.3), Algorithm 7.1 returns the stated output (Theorem 7.6). First, the definition of the REFINE procedure yields the following lemma:

**Lemma 7.2.** Let \( \text{Approx} \) and the REFINE procedure be defined as in Algorithm 7.1. Then \( |\text{Approx}(\text{Refine}(S,T))| \leq |\text{Approx}(S,T)| \) for all \( S, T \in \text{DigraphStacks}(\Omega) \).

**Lemma 7.3.** Given valid input, Algorithm 7.1 terminates after a finite number of steps.

**Proof.** We assume that computing the value of a refiner, the isomorphism approximator, or the splitter each counts as a single step in the execution of Algorithm 7.1.

We first prove that the REFINE procedure, given the pair of stacks \((S, T)\), terminates after a finite number of steps. If \( \text{Approx}(S,T) = \emptyset \), then the procedure terminates immediately. Otherwise, the procedure runs the loop on lines 13–18. We will show that this loop terminates.

As in line 14 of Algorithm 7.1, let \((S', T')\) denote the pair of stacks at the beginning of the first iteration of the loop, and let \((S, T)\) be the pair of stacks at the end of this iteration, after applying the refiners. The loop will iterate again if and only if

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0 < \|\text{APPROX}(S, T)\| < \|\text{APPROX}(S', T')\|$. Note that an isomorphism approximator gives a subset of $\text{Sym}(\Omega)$, which is finite by definition. Define $t = \|\text{APPROX}(S, T)\| \in \mathbb{N}_0$.

In the case that the loop iterates again, then at the beginning of its next iteration, we redefine $(S', T') := (S, T)$ on line 14, and we obtain the new pair of stacks $(S, T)$ by applying the refiners again. Now, the loop will iterate again if and only if $0 < \|\text{APPROX}(S, T)\| < t$. By continuing to argue in this way, we see that for every iteration of the loop, we can add an entry to a strictly decreasing sequence of non-negative integers that begins with $t$. Therefore, the loop iterates only a finite number of times.

To complete the proof, we prove by induction that, for all $n \in \mathbb{N}_0$, the \text{Search} procedure terminates when given stacks $S, T \in \text{DigraphStacks}(\Omega)$ with $\|\text{APPROX}(S, T)\| = n$. Recall that an isomorphism approximator always gives a finite subset, by definition.

In the inductive base case of $\|\text{APPROX}(S, T)\| = 0$, the pair $(S, T)$ is replaced on line 2 by another pair of stacks $(S, T) = (S, T) = \emptyset$ (Lemma 7.2) and the procedure terminates on line 4. Let $n \in \mathbb{N}$, assume that \text{Search}(S, T) terminates for all $S, T \in \text{DigraphStacks}(\Omega)$ with $\|\text{APPROX}(S, T)\| < n$, and let $S, T \in \text{DigraphStacks}(\Omega)$ be such that $\|\text{APPROX}(S, T)\| = n$. On line 2, the pair $(S, T)$ is replaced by another pair of stacks $(S, T)$ with $\|\text{APPROX}(S, T)\| \leq n$ (Lemma 7.2). If $\|\text{APPROX}(S, T)\| \in \{0, 1\}$, then the \text{Search} procedure terminates on one of lines 4, 7, or 9. Otherwise, on line 11, the splitter is used to create a finite list of new pairs of labelled digraph stacks. For each such pair $(S_i, T_i)$, it follows by Definition 6.1(ii) that

$$\|\text{APPROX}(S, S_i, T)\| < n.$$

Therefore, each call \text{Search}(S, S_i, T) terminates by the inductive hypothesis. Since there are only finitely many of these calls to \text{Search} on line 11, and since this is the last line of the \text{Search} procedure, it follows that \text{Search}(S, T) as a whole terminates.

Therefore the call to \text{Search} on line 20 – and thus Algorithm 7.1 – terminates.

**Lemma 7.4.** Let $S, T \in \text{DigraphStacks}(\Omega)$, and let the notation of Algorithm 7.1 hold. Then $(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T) = (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(\text{Refine}(S, T))$.

**Proof.** The \text{Refine} procedure returns a pair of labelled digraph stacks that is obtained from the original pair $(S, T)$ only by the application of refiners on line 16 to stacks of equal lengths. Therefore, it suffices to show that if $i \in \{1, \ldots, m\}$ and $|S| = |T|$, then

$$(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T) = (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S; f_{L,i}(S), T; f_{R,i}(T)). \quad \ast$$

If $\text{Iso}(S, T) = \emptyset$, then since $|S| = |T|$, Remark 3.1 implies that $\text{Iso}(S; f_{L,i}(S), T; f_{R,i}(T))$ is empty, and so $(\ast)$ holds. Otherwise, since there exists $j \in \{1, \ldots, k\}$ such that $(f_{L,i}, f_{R,i})$ is a refiner for the set $U_j$, it follows by Lemma 5.2(ii) that

$$U_j \cap \text{Iso}(S, T) = U_j \cap \text{Iso}(S; f_{L,i}(S), T; f_{R,i}(T)).$$

Since $U_1 \cap \cdots \cap U_k \subseteq U_j$, it follows that $(\ast)$ holds, as required. \qed
Lemma 7.5. Let $S, T \in \text{DigraphStacks}(\Omega)$, and let the notation of Algorithm 7.1 hold. Then

$$\text{Search}(S, T) = (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T).$$

In particular, $\text{Search}(S, S) = (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(S)$, and so if $U_1 \cap \cdots \cap U_k$ is a subgroup of $\text{Sym}(\Omega)$, then $\text{Search}(S, S)$ is a subgroup of $\text{Sym}(\Omega)$, too.

Proof. We proceed by induction on $|\text{Approx}(S, T)|$, as in the proof of Lemma 7.3. If $|\text{Approx}(S, T)| = 0$, then $\text{Iso}(S, T) = \emptyset$ by Definition 4.1(i), and so $(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T) = \emptyset$. Furthermore, if $|\text{Approx}(S, T)| = 0$, then Search$(S, T)$ returns $\emptyset$ on line 4. Thus we have established the base case.

Let $n \in \mathbb{N}$, assume that the statement holds for all $S, T \in \text{DigraphStacks}(\Omega)$ with $|\text{Approx}(S, T)| < n$, and let $S, T \in \text{DigraphStacks}(\Omega)$ with $|\text{Approx}(S, T)| = n$. Note that $|\text{Approx}(\text{Refine}(S, T))| \leq n$ by Lemma 7.2, and that

$$(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T) = (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(\text{Refine}(S, T))$$

by Lemma 7.4. On line 2, the pair $(S, T)$ is replaced by the value of $\text{Refine}(S, T)$, which by the above equation leaves the value of $(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T)$ unchanged.

If $|\text{Approx}(S, T)| = 0$, then as above, the procedure correctly returns $\emptyset$ on line 4.

If $\text{Approx}(S, T) = \{h\}$ for some $h \in \text{Sym}(\Omega)$, then $(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T)$ is either empty or equal to $\{h\}$ by Definition 4.1(i). This is decided on line 6, and the correct answer is returned on line 7 or 9, as required.

In the final case, $|\text{Approx}(S, T)| \geq 2$, and on line 11 the procedure uses the splitter to produce a list of pairs of new labelled digraph stacks $[(S_1, T_1), \ldots, (S_t, T_t)]$ for some $t \in \mathbb{N}$, and it returns the union of the sets $\text{Search}(S || S_1, T || T_1), \ldots, \text{Search}(S || S_t, T || T_t)$. It suffices to prove that this union is equal to $(U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T)$. Recall that

$$\text{Iso}(S, T) = \text{Iso}(S || S_1, T || T_1) \cup \cdots \cup \text{Iso}(S || S_t, T || T_t),$$

by Definition 6.1(i), and that $|\text{Approx}(S || S_i, T || T_i)| < |\text{Approx}(S, T)| \leq n$ for all $i \in \{1, \ldots, t\}$ by Definition 6.1(ii). By the inductive hypothesis, it follows that

$$\text{Search}(S || S_i, T || T_i) = (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S || S_i, T || T_i).$$

for all $i \in \{1, \ldots, t\}$, and so

$$\text{Search}(S, T) = \text{Search}(S || S_1, T || T_1) \cup \cdots \cup \text{Search}(S || S_t, T || T_t)
= (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S || S_1, T || T_1) \cup \cdots \cup (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S || S_t, T || T_t)
= (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(S, T).$$

Theorem 7.6. Algorithm 7.1 is correct. In other words, using the notation of Algorithm 7.1, $\text{Search}(\text{EmptyStack}(\Omega), \text{EmptyStack}(\Omega)) = (U_1 \cap \cdots \cap U_k)$.

Proof. The result follows by setting $S = T = \text{EmptyStack}(\Omega)$ in Lemma 7.5.
Note that Algorithm 7.1 finds and returns all elements of its output, as proved in Theorem 7.6. To search for a single element of the desired intersection, one needs to modify the SEARCH procedure to terminate on line 7 as soon as the first solution to the search problem is found.

**Definition 7.7.** Define SEARCHSINGLE to be the procedure obtained from the SEARCH procedure of Algorithm 7.1 by completely terminating the recursion with a solution to the search problem the first time that it finds one (line 7), and by recursively calling SEARCHSINGLE on line 11 rather than SEARCH.

**Corollary 7.8.** Let the notation of Algorithm 7.1 and Definition 7.7 hold. Then

\[
\text{SEARCHSINGLE}(\text{EMPTYSTACK}(\Omega), \text{EMPTYSTACK}(\Omega)) = \begin{cases} 
\emptyset & \text{if } U_1 \cap \cdots \cap U_k = \emptyset, \\
\{g\} & \text{if } U_1 \cap \cdots \cap U_k \neq \emptyset,
\end{cases}
\]

where \(g\) is the first element of \(U_1 \cap \cdots \cap U_k\) found during the search, in the case that this intersection is non-empty.

**Proof.** Termination and correctness follow almost exactly as in Lemmas 7.3 and 7.5. \(\square\)

### 7.2. Searching for a generating set of a subgroup

In Theorem 7.6 we showed that Algorithm 7.1 can be used to find the set of all solutions to a given problem, and in Corollary 7.8 we showed that a slightly adapted version of Algorithm 7.1 can be used to search for a single solution in the case that one exists, and to return \(\emptyset\) otherwise.

Searching for a single solution is especially useful when one wishes to find an isomorphism from one combinatorial structure to another, or to prove that none exists.

It is typically most efficient to compute with a permutation group when it is specified by a base and strong generating set. In this section, we show how it is possible to modify Algorithm 7.1 (resulting in Algorithm 7.11) to search for a base and strong generating set, in the case that the intersection of the given subsets of \(\text{Sym}(\Omega)\) is a subgroup of \(\text{Sym}(\Omega)\). We also show how the partially-constructed generating set can be used to prune the search tree as the algorithm progresses.

This algorithm is also useful when searching for an intersection of (right) cosets. Suppose that \(k, m \in \mathbb{N}\) and that \(U_1, \ldots, U_k\) is a list of right cosets of subgroups of \(\text{Sym}(\Omega)\), and that \((f_{L,1}, f_{R,1}), \ldots, (f_{L,m}, f_{R,m})\) is a list of refiners for some of those cosets. In order to compactly describe their intersection, we can first use the SEARCHSINGLE procedure as shown in Corollary 7.8: this either shows that \(U_1 \cap \cdots \cap U_k\) is empty, or it produces a representative element \(g \in U_1 \cap \cdots \cap U_k\). In this latter case, then for all \(i \in \{1, \ldots, k\}\), it follows that \(U_i g^{-1}\) is a subgroup of \(\text{Sym}(\Omega)\), and Lemma 5.6 implies that \((f_{L,i}, f_{R,i})\) is a refiner for \(U_i g^{-1}\). Note that we can easily test for membership in \(U_i g^{-1}\) if and only if we can easily test for membership in \(U_i\). Therefore we may use Algorithm 7.11 to search for a generating set of \(U_1 g^{-1} \cap \cdots \cap U_k g^{-1}\). Since

\[
U_1 \cap \cdots \cap U_k = (U_1 g^{-1} g) \cap \cdots \cap (U_k g^{-1} g) = (U_1 g^{-1} \cap \cdots \cap U_k g^{-1}) g,
\]
it follows that this generating set, along with the representative element $g$, gives a compact description for the intersection $U_1 \cap \cdots \cap U_k$.

The correctness of Algorithm 7.11 relies on the following rather technical lemmas. Algorithm 7.11 applies Lemma 7.10 recursively to find a base and strong generating set.

**Lemma 7.9.** Let the notation of Algorithm 7.1 hold, suppose that $U_1 \cap \cdots \cap U_k$ is a subgroup of $\text{Sym}(\Omega)$, and let $S \in \text{DIGRAPHSTACKS}(\Omega)$ be arbitrary. Then the following hold:

(i) $\text{Refine}(S, S) = (T, T)$ for some $T \in \text{DIGRAPHSTACKS}(\Omega)$.

(ii) $\{\text{id}_\Omega\} \subseteq \text{Approx}(T)$.

(iii) If $\text{Approx}(T) = \{\text{id}_\Omega\}$, then $\text{Search}(S, S) = \{\text{id}_\Omega\}$.

(iv) If $|\text{Approx}(T)| \geq 2$, then there exists $t \in \mathbb{N}$ and $S_1, \ldots, S_t \in \text{DIGRAPHSTACKS}(\Omega)$ such that $\text{Split}(T, T) = [(S_1, S_1), (S_1, S_2), \ldots, (S_1, S_t)]$.

**Proof.** (i) Lemma 5.4 implies that every refiner given as input to Algorithm 7.1 is a pair of equal functions. Therefore $\text{Refine}$ maps pairs of equal stacks to pairs of equal stacks.

(ii) By Lemmas 7.4 and 7.5 and Definition 4.1(i), it follows that

$$\{\text{id}_\Omega\} \subseteq \text{Search}(S, S) = (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(S)$$
$$= (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(\text{Refine}(S, S))$$
$$= (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(T)$$
$$\subseteq \text{Aut}(T) \subseteq \text{Approx}(T).$$

(iii) Here the containments in the proof of (ii) become equalities, and the result follows.

(iv) This follows by Definition 6.1(iii) and (iv).

**Lemma 7.10.** Let the notation of Algorithm 7.1 hold, assume that $U_1 \cap \cdots \cap U_k$ is a subgroup, let $S \in \text{DIGRAPHSTACKS}(\Omega)$ with $|\text{Approx}(\text{Refine}(S, S))| \geq 2$, and define $(T, T) = \text{Refine}(S, S)$ and $\text{Split}(T, T) = [(S_1, S_1), \ldots, (S_1, S_t)]$ as in Lemma 7.9.

(i) $\text{Search}(T\|S_1, T\|S_1)$ is the stabiliser of $S_1$ in $\text{Search}(S, S)$.

(ii) For all $i \in \{2, \ldots, t\}$, either the set $\text{Search}(T\|S_1, T\|S_i)$ is empty, or it is a right coset of $\text{Search}(T\|S_1, T\|S_1)$ in $\text{Search}(S, S)$.

(iii) The subgroup $\text{Search}(S, S)$ is generated by any of its subsets that contains a generating set for $\text{Search}(T\|S_1, T\|S_1)$ and an element from each of the non-empty sets amongst

$$\text{Search}(T\|S_1, T\|S_2), \ldots, \text{Search}(T\|S_1, T\|S_t).$$
(iv) Let \( \{ j_1, \ldots, j_l \} \subseteq \{ 2, \ldots, t \} \). Suppose that, for each \( j \in \{ j_1, \ldots, j_l \} \), either we have fixed some element \( y_j \in \text{SEARCH}(T \| S_1, T \| S_j) \), or we have determined that \( \text{SEARCH}(T \| S_1, T \| S_j) \) is empty. Let \( Y_0 \) be the set of elements \( y_j \) that we fixed when \( \text{SEARCH}(T \| S_1, T \| S_j) \neq \emptyset \), let \( Y \) be any generating set for \( \text{SEARCH}(T \| S_1, T \| S_1) \), and define \( X = Y \cup Y_0 \). If there exists some \( g \in \langle X \rangle \), \( i \in \{ 2, \ldots, t \} \setminus \{ j_1, \ldots, j_l \} \), and \( j \in \{ j_1, \ldots, j_l \} \) such that \( S_i = S_j^g \), then \( \text{SEARCH}(T \| S_1, T \| S_i) \subseteq \langle X \rangle \).

**Proof.**

(i) By Lemmas 7.4 and 7.5, Remark 3.1, and as in the proof of Lemma 7.9(ii),

\[
\text{SEARCH}(T \| S_1, T \| S_1) = (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(T \| S_1)
\]

\[
= (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(T) \cap \text{Aut}(S_1)
\]

\[
= (U_1 \cap \cdots \cap U_k) \cap \text{Iso} (\text{REFINE}(S, S)) \cap \text{Aut}(S_1)
\]

\[
= \text{SEARCH}(S, S) \cap \text{Aut}(S_1).
\]

(ii) Let \( i \in \{ 2, \ldots, t \} \). By inspecting the Search procedure, it is clear that

\[
\text{SEARCH}(S, S) = \text{SEARCH}(T \| S_1, T \| S_1) \cup \cdots \cup \text{SEARCH}(T \| S_1, T \| S_t).
\]

Hence \( \text{SEARCH}(T \| S_1, T \| S_i) \subseteq \text{SEARCH}(S, S) \). Suppose there exists some element \( x \in \text{SEARCH}(T \| S_1, T \| S_i) \). By Lemma 7.5 and the assumption that \( U_1 \cap \cdots \cap U_k \) is a subgroup of \( \text{Sym}(\Omega) \) containing \( x \), it follows that

\[
\text{SEARCH}(T \| S_1, T \| S_1) \cdot x = ((U_1 \cap \cdots \cap U_k) \cap \text{Aut}(T \| S_1)) \cdot x
\]

\[
= (U_1 \cap \cdots \cap U_k) \cap \text{Iso}(T \| S_1, T \| S_i)
\]

\[
= \text{SEARCH}(T \| S_1, T \| S_i).
\]

(iii) This follows from (ii).

(iv) Let \( g \in \langle X \rangle \), \( i \in \{ 2, \ldots, t \} \setminus \{ j_1, \ldots, j_l \} \), and \( j \in \{ j_1, \ldots, j_l \} \) be such that \( S_i = S_j^g \). Note that \( X \subseteq \text{SEARCH}(S, S) \) by (i) and (ii), and so in particular, \( g \in (U_1 \cap \cdots \cap U_k) \cap \text{Aut}(T) \) by Lemmas 7.4 and 7.5. Therefore \( g \in \text{Iso}(T \| S_j, T \| S_i) \), and so \( \text{Iso}(T \| S_1, T \| S_i) \cdot g = \text{Iso}(T \| S_1, T \| S_i) \). It then follows similarly as in the end of the proof of (ii) that

\[
\text{SEARCH}(T \| S_1, T \| S_j) \cdot g = \text{SEARCH}(T \| S_1, T \| S_i).
\]

Thus, if \( \text{SEARCH}(T \| S_1, T \| S_j) \neq \emptyset \), and so \( y_j \in X \cap \text{SEARCH}(T \| S_1, T \| S_j) \), then

\[
\text{SEARCH}(T \| S_1, T \| S_i) = \text{SEARCH}(T \| S_1, T \| S_j) \cdot g
\]

\[
= (\text{SEARCH}(T \| S_1, T \| S_1) \cdot y_j) \cdot g
\]

\[
= \langle Y \rangle \cdot (y_j g) \subseteq \langle X \rangle.
\]

Let the notation of Algorithms 7.1 and 7.11 hold. We briefly explain how the Search-Gens procedure has been obtained from the Search procedure of Algorithm 7.1. Given
Algorithm 7.11 Search for a base and strong generating set of a subgroup of $\text{Sym}(\Omega)$.

**Input:** as in Algorithm 7.1, plus the assumption that $U_1 \cap \cdots \cap U_k$ is a subgroup.

**Output:** a base and strong generating set for the subgroup $U_1 \cap \cdots \cap U_k$.

1: $\text{BASE} \leftarrow []$ \Comment{The base is initialised as an empty list.}
2: return $\{\text{SEARCHGENS}(\text{EMPTYSTACK}(\Omega)), \text{BASE}\}$
3: procedure SEARCHGENS($S$)
4: $(T, T) \leftarrow \text{Refine}(S, S)$ \Comment{Refine the given stacks.}
5: case $\text{APPROX}(T) = \{\text{id}_\Omega\}$:
6: return $\{\text{id}_\Omega\}$ \Comment{Lemma 7.9(iii)}
7: case $|\text{APPROX}(T)| \geq 2$:
8: $[(S_1, S_1), \ldots, (S_1, S_t)] \leftarrow \text{SPLIT}(T, T)$ \Comment{Lemma 7.9(iv)}
9: $\text{BASE} \leftarrow \text{BASE} \parallel [S_1] \Comment{Add the stack $S_1$ to the base.}$
10: $X \leftarrow \text{SEARCHGENS}(T \parallel S_1)$ \Comment{Recursively find generators for a subgroup.}$
11: for $i \in \{2, \ldots, t\}$ do
12: if $S_i \notin S_j^{(X)}$ for any $j \in \{1, \ldots, i-1\}$ then \Comment{Pruning; Lemma 7.10(iv)}
13: $X \leftarrow X \cup \text{SEARCHSINGLE}(T \parallel S_1, T \parallel S_i)$ \Comment{Search for a coset rep.}$
14: return $X$
15: procedure Refine($S, T$) \Comment{The Refine procedure from Algorithm 7.1.}$
16: procedure SEARCHSINGLE($S, T$) \Comment{The procedure from Definition 7.7.}$

the validity of these modifications, the correctness of the SEARCHGENS procedure then follows from the correctness of the SEARCH procedure (Lemma 7.5).

Lemma 7.9(ii) implies that the condition on line 3 of the SEARCH procedure is never satisfied when $U_1 \cap \cdots \cap U_k$ is a subgroup and the stacks in question are equal, and so it is unnecessary to include this case in SEARCHGENS. From the same result, it also follows that the condition on line 5 of the SEARCH procedure can be restated as on line 5 of SEARCHGENS, since $|\text{APPROX}(T)| = 1$ if and only if $\text{APPROX}(T) = \{\text{id}_\Omega\}$. Note that $\text{id}_\Omega$ is contained in $U_1 \cap \cdots \cap U_k$ by assumption and in $\text{Aut}(T)$ by definition, which explains the remaining simplification of this case. Finally, it follows from Lemmas 7.9 and 7.10 and the correctness of the SEARCHSINGLE procedure (Corollary 7.8) that line 11 of SEARCH can be replaced by lines 8–14 in SEARCHGENS. Thus we have proved the following lemma:

**Lemma 7.12.** Let $S \in \text{DIGRAPHSTACKS}(\Omega)$ and let the notation of Algorithm 7.11 hold. Then SEARCHGENS($S$) is a generating set for $U_1 \cap \cdots \cap U_k \cap \text{Aut}(S) = \text{SEARCH}(S, S)$.

That Algorithm 7.11 terminates given any valid input can be proved in a very similar way to Lemma 7.3. Thus we present the main result of this section.

**Theorem 7.13.** In the notation of Algorithm 7.11, SEARCHGENS(EMPTYSTACK($\Omega$)) is a strong generating set for $U_1 \cap \cdots \cap U_k$ relative to the base BASE. In other words, Algorithm 7.11 returns a base and strong generating set for its input.
Proof. Given Lemma 7.12, \(\text{SEARCHGENS}(\text{EMPTYSTACK}(\Omega))\) is a generating set for the subgroup \(U_1 \cap \cdots \cap U_k\), so it remains to show that \(\text{BASE}\) is a base, relative to which the generating set is strong.

Firstly, if \(\text{APPROX}(\text{REFINE}(\text{EMPTYSTACK}(\Omega), \text{EMPTYSTACK}(\Omega))) = \{\text{id}_\Omega\}\), then \(\text{SEARCHGENS}(\text{EMPTYSTACK}(\Omega))\) returns the generating set \(\{\text{id}_\Omega\}\) without modifying the variable \(\text{BASE}\), which is therefore still an empty list. This is a base and strong generating set for the trivial subgroup of \(\text{Sym}(\Omega)\), and so this case is complete.

Otherwise, if \(|\text{APPROX}(\text{REFINE}(\text{EMPTYSTACK}(\Omega), \text{EMPTYSTACK}(\Omega)))| \geq 2\), then we define \(T_0 = S_{1,0} = \text{EMPTYSTACK}(\Omega)\), and iteratively define \(T_{i+1}\) and \(S_{1,i+1}\) for \(i = 0, 1, \ldots\), so long as \(|\text{APPROX}(\text{REFINE}(T_i||S_{1,i}, T_i||S_{1,i+1}))| \geq 2\), via \((T_{i+1}, T_{i+1}) = \text{REFINE}(T_i||S_{1,i}, T_i||S_{1,i+1})\) and \(\text{SPLIT}(T_{i+1}, T_{i+1}) = [(S_{1,i+1}, S_{1,i+1}), \ldots]\). Thus \(T_{i+1}\) is the stack obtained by refining \(T_i||S_{1,i}\), and \(S_{1,i+1}\) is the left-hand stack obtained by splitting \(T_{i+1}\). Let \(r \in \mathbb{N}\) be the maximum value for which we defined \(T_r\), which means that \(\text{APPROX}(\text{REFINE}(T_r||S_{1,r}, T_r||S_{1,r})) = \{\text{id}_\Omega\}\).

It is straightforward to see that the sequence of stacks \(T_0||S_{1,0}, T_1||S_{1,1}, \ldots, T_r||S_{1,r}\) is exactly the sequence of stacks upon which the recursive procedure \(\text{SEARCHGENS}\) is called during the execution of Algorithm 7.11, on line 10. Therefore

\[
\{\text{id}_\Omega\} = \text{SEARCHGENS}(T_r||S_{1,r}) \subseteq \cdots \subseteq \text{SEARCHGENS}(T_1||S_{1,1}) \subseteq \text{SEARCHGENS}(T_0||S_{1,0}) = \text{SEARCHGENS}(\text{EMPTYSTACK}(\Omega)),
\]

and so

\[
\{\text{id}_\Omega\} = \langle \text{SEARCHGENS}(T_r||S_{1,r}) \rangle \leq \cdots \leq \langle \text{SEARCHGENS}(T_1||S_{1,1}) \rangle \leq \langle \text{SEARCHGENS}(T_0||S_{1,0}) \rangle = U_1 \cap \cdots \cap U_k.
\]

Lemma 7.10(i) and Lemma 7.12 imply that \(\langle \text{SEARCHGENS}(T_r||S_{1,i}) \rangle\) is the stabiliser of \(S_{1,i}\) in \(\langle \text{SEARCHGENS}(T_{i-1}||S_{1,i-1}) \rangle\) for each \(i \in \{1, \ldots, r\}\). In other words, Algorithm 7.11 constructs a stabiliser chain for \(U_1 \cap \cdots \cap U_k\) relative to \(\text{BASE}\). This proves the result.

Typically, a base for a subgroup of \(\text{Sym}(\Omega)\) is assumed to be a list of points in \(\Omega\) itself, as opposed to a list of arbitrary objects upon which the group acts. This latter more general definition is the one that we have used so far in this paper. In order to use Algorithm 7.11 to obtain a base consisting of points in \(\Omega\), one can use the splitter from Definition 6.3: using the notation of this definition and an arbitrary \(\alpha \in \Omega\), a permutation stabilises the stack \([\Gamma_\alpha]\) if and only if it stabilises the point \(\alpha\). Therefore, a generating set for a subgroup of \(\text{Sym}(\Omega)\) is strong with respect to the list of stacks \([\Gamma_{\alpha_1}], \ldots, [\Gamma_{\alpha_r}]\) if and only if it is strong with respect to \([\alpha_1, \ldots, \alpha_r]\).

7.3. Computing with a fixed sequence of left-hand stacks
In this section, we discuss a consequence of the setup of our definitions and algorithms, which enables a significant performance optimisation, and through which the usefulness and practicality of the refiners from Section 5.2 becomes apparent. This idea was inspired by, and is closely related to, the \(\mathcal{R}\)-base technique of Jeffrey Leon [13, Section 6] for partition backtrack search, although we present the idea quite differently.

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Roughly speaking, we observe that any time Algorithm 7.1 or 7.11 is executed to solve a problem, then the left-hand stack of the ever-present pair is modified with the same sequence of changes in every branch of the search. In other words, every branch of search has the same sequence of left-hand stacks, up until the point that the branch ends (different branches can have different lengths). This means that any entry in this fixed sequence of left-hand stacks only ever needs to be computed once, and then stored and recalled for later use. Furthermore, these stacks can give rise to the fixed stacks and lists of points required by the refiners of Section 5.2.

This behaviour emerges, in essence, because a refiner is a pair of functions of one variable, rather than a single function of two variables (Definition 5.1); because a non-empty value of an isomorphism approximator is a coset of a subgroup, where the subgroup depends only on the given left-hand stack (Definition 4.1(iii)); and because the left-hand stacks produced by a splitter depend only on the left-hand stack that it is given (Definition 6.1(iv)).

7.3.1. A performance improvement by using a fixed sequence of left-hand stacks

**Lemma 7.14.** Let the notation of Algorithm 7.1 hold, and let $S \in \text{DigraphStacks}(\Omega)$. Then there exist $n, r \in \mathbb{N}$ and a fixed sequence of at most $mn$ modifications to $S$ such that, for all $V \in \text{DigraphStacks}(\Omega)$, either:

(i) $\text{Refine}(S, V)$ executes line 16 of Algorithm 7.1 some $i \in \{0, \ldots, mn\}$ times, performing the first $i$ modifications to $S$ in turn, and $\text{APPROX}(\text{Refine}(S, V)) = \emptyset$; or

(ii) $\text{Refine}(S, V)$ executes line 16 of Algorithm 7.1 exactly $mn$ times, performing all $mn$ modifications to $S$ in turn, and $|\text{APPROX}(\text{Refine}(S, V))| = r$.

**Proof.** The $\text{Refine}$ procedure from Algorithm 7.1 modifies its pair of stacks only on line 16, and the number of modifications that it makes is equal to the number of times that line 16 is executed. If the pair of stacks given to the $\text{Refine}$ procedure is $(S, T)$, for instance, then the left-hand stack could be modified with the sequence of moves:

$$S \rightarrow S \parallel f_{L,1}(S) \rightarrow (S \parallel f_{L,1}(S)) \parallel f_{L,2}(S) \parallel f_{L,1}(S) \rightarrow \cdots$$

up to some point, and the right-hand stack would be modified in the corresponding way:

$$T \rightarrow T \parallel f_{R,1}(T) \rightarrow (T \parallel f_{R,1}(T)) \parallel f_{R,2}(T) \parallel f_{R,1}(T) \rightarrow \cdots$$

If the $m$-fold for loop on lines 15 and 16 is interrupted because the condition $|S| = |T|$ fails to be satisfied at some point, then $\text{APPROX}(S, T) = \emptyset$ by Definition 4.1(ii). In this case, neither the condition on line 17 nor the condition on line 13 is satisfied, and so the procedure returns its pair of stacks $(S, T)$ on line 19, without further modification.

Otherwise, the $\text{Refine}$ procedure returns after completing some number (perhaps zero) of repetitions of the full for loop from lines 15 and 16. The procedure returns because either the condition on line 17 is satisfied, or the condition on line 13 is not.
Definition 6.1(iv). \textit{Recursion happens} is independent of the right-hand stack. Furthermore, Lemma 7.15 shows that, if the call on line 20, and ending at some depth of the recursion by backtracking on one of lines 4, 7, or 9, Lemmas 7.14 and 7.15 show that, if the \textit{search procedure} at some depth of the recursion is given the left-hand stack \(S\) and any right-hand stack, then the sequence of modifications made to the left-hand stack (until either backtracking or recursion happens) is independent of the right-hand stack. Furthermore, Lemma 7.15

Let \(V_1 \in \text{DigraphStacks}(\Omega)\), and suppose that the \textit{Refine} procedure, when given the \(n\text{th}\) full iteration of \textit{for loop}, has completed its \(n\text{th}\) full iteration of the \textit{for loop} for some \(n \in \mathbb{N}\), and suppose that the condition on line 17 is satisfied. Let \((S', V'_1)\) denote the pair of stacks immediately before the \(n\text{th}\) iteration of the \textit{for loop}, and let \((S^*, V^*_1)\) denote the pair of stacks immediately after it. It follows that \(0 < r := |\text{Approx}(S', V'_1)| \leq |\text{Approx}(S^*, V^*_1)|\), and so \(\text{Refine}(S, V_1) = (S', V'_1)\).

Next, let \(V_2 \in \text{DigraphStacks}(\Omega)\) and suppose that the \textit{Refine} procedure, when given the \(n\text{th}\) full iteration of the \textit{for loop}. By the earlier arguments, the procedure has modified the \(n\text{th}\) iteration of the \textit{left-hand stack} with the exact same sequence of modifications as before, and so there exist stacks \(V'_2, V^*_2 \in \text{DigraphStacks}(\Omega)\) such that \((S', V^*_2)\) is the pair of stacks immediately before the \(n\text{th}\) iteration of the \textit{for loop}, and \((S^*, V^*_2)\) is the pair of stacks immediately after it. If \(\text{Approx}(S^*, V^*_2) = \emptyset\), then the procedure returns on line 19. Otherwise, Definition 4.1(iii) implies that

\[
|\text{Approx}(S^*, V^*_2)| = |\text{Approx}(S^*)| = |\text{Approx}(S^*, V^*_1)|, \quad \text{and that} \quad |\text{Approx}(S', V'_2)| = |\text{Approx}(S')| = |\text{Approx}(S', V'_1)|.
\]

In particular \(0 < |\text{Approx}(S', V'_2)| \leq |\text{Approx}(S^*, V^*_2)|\). Thus the condition on line 17 is satisfied in this case, and \(\text{Refine}(S, V_2) = (S', V'_2)\) with \(|\text{Approx}(S', V'_2)| = r\).

Lemma 7.15. Let the notation of Algorithm 7.1 hold and let \(S \in \text{DigraphStacks}(\Omega)\). Then there exists some \(r \in \mathbb{N} \setminus \{1\}\) and fixed stacks \(S', S'_1 \in \text{DigraphStacks}(\Omega)\) such that, for all \(V \in \text{DigraphStacks}(\Omega)\), either:

(i) \(|\text{Approx}(\text{Refine}(S, V))| \leq 1\), and \(\text{Search}(S, V)\) backtracks on either line 4, 7, or 9 of Algorithm 7.1; or

(ii) \(|\text{Approx}(\text{Refine}(S, V))| = r\), \(\text{Refine}(S, V) = (S', V')\) for some labelled digraph \(S'\), and \(\text{Search}(S, V)\) recursively calls \(\text{Search}\) on line 11 of Algorithm 7.1, always with first argument \(S'||S'_1\).

Proof. When studying the \(\text{Search}\) procedure from Algorithm 7.1, it becomes clear that (i) is a possibility. We see that (ii) is the remaining possibility, by noticing that \(r\) and the fixed stack \(S'\) exist by Lemma 7.14 (in the notation of Lemma 7.14, \(S'\) is obtained by applying the first \(m(n-1)\) modifications to \(S\)), and the stack \(S'_1\) is fixed by Definition 6.1(iv).

Corollary 7.16. In each branch of search, Algorithm 7.1 modifies its left-hand stack with the same sequence of moves, until the branch ends and the algorithm backtracks.

Proof. A branch consists of a sequence of recursive calls to \(\text{Search}\), beginning with the call on line 20, and ending at some depth of the recursion by backtracking on one of lines 4, 7, or 9. Lemmas 7.14 and 7.15 show that, if the \(\text{Search}\) procedure at some depth of the recursion is given the left-hand stack \(S\) and any right-hand stack, then the sequence of modifications made to the left-hand stack (until either backtracking or recursion happens) is independent of the right-hand stack. Furthermore, Lemma 7.15
shows that at any given depth of recursion, the Search procedure is recursively called with the same left-hand stack. The result follows.

By very similar arguments, Algorithm 7.11 also modifies its left-hand stack with the exact same sequence of moves in each branch of search, until the algorithm backtracks.

Corollary 7.16 shows that we may store the modifications to the left-hand stacks the first time that they are made, and then we can simply recall a result whenever it is needed again. This means that on most occasions, when applying a refiner, we need only compute the value of the right-hand stack under the refiner, since we can simply look up the result for the left-hand stack. This leads to a performance speedup of roughly 50%.

7.3.2. Constructing and applying a refiner via the fixed sequence of left-hand stacks

We discuss how to use Lemma 5.23 to build a refiner for a group $G$ via the fixed sequence of left-hand stacks. Using the notation of this lemma, in order to define the function $f$ such that $(f, f)$ is a refiner for $G$, for each $i \in \mathbb{N}_0$ we must create labelled digraph stacks $V_i$, and lists $F_i$ that consist of points in $\Omega$. We start with $V_i$ and $F_i$ being undefined for all $i \in \mathbb{N}_0$, and we define $V_i$ and $F_i$ on-demand as we apply the refiner during the execution of Algorithm 7.1 or 7.11.

Let $S, T \in \text{DigraphStacks}(\Omega)$ have equal lengths. We apply the refiner as follows.

If $V_{|S|}$ and $F_{|S|}$ have already been defined, then we can look up and return the stored value of $f(S)$ (if it is already known), and we can compute $f(T)$ (and $f(S)$, if it is not already known) as specified in Lemma 5.23. Since we compute with the same sequence of left-hand stacks in every branch of search, as discussed above, then it is likely that $f(S)$ has already been computed.

Otherwise, if $V_{|S|}$ and $F_{|S|}$ are still undefined, then we define $F_{|S|} = \text{Fixed}(S)$, and we define $V_{|S|}$ to be some arbitrary labelled digraph stack that is preserved by $G_{\text{Fixed}(S)}$, the stabiliser of $\text{Fixed}(S)$ in $G$. For example, if we want our refiner to exploit the orbit data of $G_{\text{Fixed}(S)}$, then we could define $V_{|S|}$ to be the stack $[\Gamma]$, where $\Gamma$ is a labelled digraph on $\Omega$ without arcs in which two vertices share a label if and only if they belong to the same orbit of $G_{\text{Fixed}(S)}$ on $\Omega$. Alternatively, $V_{|S|}$ could be a list of all, or some, of the orbital graphs of $G_{\text{Fixed}(S)}$ on $\Omega$, represented as labelled digraphs. Given $V_{|S|}$ and $F_{|S|}$, then $f(S) = V_{|S|}$ (and we store its value), and we compute $f(T)$ as in Lemma 5.23.

In order to construct a refiner for the coset $Gh$, for some $h \in \text{Sym}(\Omega)$, we construct the function $f$ as above; the corresponding refiner is $(f, g)$, where $g(S) = f(S^{h^{-1}})^h$ for all $S \in \text{DigraphStacks}(\Omega)$ (see Lemma 5.6).

In essence, this technique lets us use the fixed sequence of left-hand stacks to arbitrarily order objects like orbits and orbital graphs, for use in refiners. This addresses the problem discussed in Example 5.22, and thus can lead to more effective refinement.

8. Experiments

In this section, we provide experimental data comparing the behaviour of our algorithms against partition backtrack, in order to highlight the potential of our techniques.
In particular, we repeat the experiments of [9, Section 6] (by the first three authors of the present paper), which showed how orbital graphs can significantly improve the partition backtrack algorithm when computing various kinds of set stabilisers and subgroup intersections. We also investigate some additional challenging problems.

It would not be useful to investigate classes of problems where partition backtrack already performs very well, and for which there is no necessary or realistic scope for further improvement. In addition, there are other classes of problems, such as those that involve searching for highly-transitive groups, where we would expect all techniques (including ours) to perform badly, and so it also makes sense to avoid such problems. Instead, we have chosen to investigate problems that are interesting and important in their own right, including ones that we expect to be hard for many search techniques.

At the time of writing, we have focused on the mathematical theory of our algorithms, rather than on the speed of our implementations. Because of this, we would expect our current implementations to perhaps unfairly struggle in time comparisons against implementations of partition backtrack, and so such comparisons would be inappropriate at this point.

Therefore, whereas the experiments in [9, Section 6] analyse the time required by an algorithm to solve a problem, here we analyse the size of the search required by the algorithm to solve it. We define a search node of a search to be an instance of the main searching procedure being called recursively during its execution; the size of a search is then its number of search nodes. If an algorithm requires 0 search nodes to solve a problem, then this means that the algorithm solved the problem without entering recursion. For the algorithms that we compare, this can only be achieved with a search problem that has either no solutions, or exactly one.

In general, a backtrack search algorithm spends effort at each node to prune the search tree and organise the search. The size of a search is not obviously related to the time taken to complete it, since a smaller search typically comes at the cost of spending more effort at each node. However, the computations at each node of our algorithms are largely digraph-based, and the very high performance of digraph-based computer programs such as Bliss [11] and Nauty [14] suggests that, in practice, such computations could potentially be cheap. Therefore, with further development, we have reason to believe that, for problems where our techniques require significantly smaller searches, the increased time spent at each node could be out-weighed by the smaller number of nodes in total, giving faster searches.

For the problems that we investigate in Sections 8.1–8.3, we compare the following techniques:

(i) LEON: Standard partition backtrack search, as described by Jeffrey Leon [12, 13].

(ii) ORBITAL: Partition backtrack search with orbital graph refiners, as described in [9].

(iii) STRONG: Backtrack search with labelled digraphs, using the isomorphism and fixed-point approximators from Definition 4.10 and the splitter from Definition 6.3.
Full: Backtrack search with labelled digraphs, using the isomorphism and fixed-point approximators from Definition 4.4 and the splitter from Definition 6.3.

The Leon technique is roughly the same as backtrack search with labelled digraphs, where the labelled digraphs in the stack have no arcs. The Orbital technique is essentially the same as backtrack search with labelled digraphs, using the 'weak equitable labelling’ isomorphism and fixed-point approximators from Definition 4.11. The Strong technique considers all labelled digraphs in the stack simultaneously to make its approximations, while the Full technique, which completely calculates rather than just approximates, is in principle the most expensive of the four methods.

We performed our experiments using the GraphBacktracking [7] and BacktrackKit [8] packages for GAP [3]. BacktrackKit provides a simple implementation of the algorithms in [9, 13], and provides a base for GraphBacktracking. Where we reproduce experiments from [9], we ensure that we find the same sized searches.

8.1. Set stabilisers and partition stabilisers in grid groups

We first explore the behaviour of our techniques on stabiliser problems in grid groups. This setting was previously considered in [9, Section 6.1], and as mentioned there, these kinds of problems arise in numerous real-world situations.

Definition 8.1 (Grid group [9, Definition 36]). Let \( n \in \mathbb{N} \) and \( \Omega = \{1, \ldots, n\} \). The direct product \( \text{Sym}(\Omega) \times \text{Sym}(\Omega) \) acts faithfully on the Cartesian product \( \Omega \times \Omega \) via \( (\alpha, \beta)(g, h) = (\alpha^g, \beta^h) \) for all \( \alpha, \beta \in \Omega \) and \( g, h \in \text{Sym}(\Omega) \). The \( n \times n \) grid group is the image of the embedding of \( \text{Sym}(\Omega) \times \text{Sym}(\Omega) \) into \( \text{Sym}(\Omega \times \Omega) \) defined by this action.

Let \( n \in \mathbb{N} \) and \( \Omega = \{1, \ldots, n\} \), and let \( G \leq \text{Sym}(\Omega \times \Omega) \) be the \( n \times n \) grid group. If we consider \( \Omega \times \Omega \) to be an \( n \times n \) grid, where the sets of the form \( \{\alpha, \beta\} : \beta \in \Omega \) and \( \{(\beta, \alpha) : \beta \in \Omega\} \) for each \( \alpha \in \Omega \) are the rows and columns of the grid, respectively, then \( G \) is the subgroup of \( \text{Sym}(\Omega \times \Omega) \) that preserves the set of rows and the set of columns of the grid. Note that the \( n \times n \) grid group is 2-closed, which means that it is well suited to the techniques of this paper.

The experiments in [9] solved two kinds of set stabiliser problems in grid groups. We repeat these problems here, along with an unordered partition stabiliser problem:

(i) Compute the stabiliser in \( G \) of a subset of \( \Omega \times \Omega \) of size \( \lfloor n^2/2 \rfloor \).

(ii) Compute the stabiliser in \( G \) of a subset of \( \Omega \times \Omega \) that has \( \lfloor n/2 \rfloor \) entries from each grid-row.

(iii) If \( 2 \mid n \), then compute the stabiliser in \( G \) of an unordered partition of \( \Omega \times \Omega \) that has two cells, each of size \( n^2/2 \).

As in [9, Section 6.1], we compute with the \( n \times n \) grid group as a subgroup of \( S_n \) rather than as a subgroup of \( \text{Sym}(\{1, \ldots, n\} \times \{1, \ldots, n\}) \). The algorithms have no prior knowledge of the grid structure that the group preserves. Tables 8.2 and 8.3 show the
results concerning the search size required by the different techniques to solve 50 random problems each of types (i), (ii), and (iii) in a grid group. An entry in the ‘Zero%’ column shows the percentage of problems that an algorithm solved with a search of size zero. These columns are omitted when they are all-zero.

| n  | Leon Median | Leon Median | Leon Median | Orbital Median | Orbital Median | Orbital Median | Leon Median | Leon Median | Leon Median |
|----|-------------|-------------|-------------|----------------|----------------|----------------|-------------|-------------|-------------|
| 3  | 4           | 2           | 22          | 7              | 2              | 0              | 2           | 2           | 0           |
| 4  | 8           | 0           | 50          | 8              | 2              | 0              | 8           | 2           | 0           |
| 5  | 16          | 2           | 44          | 13             | 2              | 0              | 13          | 2           | 0           |
| 6  | 23          | 0           | 68          | 34             | 2              | 20             | 34          | 2           | 20          |
| 7  | 34          | 0           | 74          | 41             | 0              | 54             | 41          | 0           | 54          |
| 8  | 46          | 0           | 90          | 92             | 0              | 68             | 92          | 0           | 68          |
| 9  | 58          | 0           | 92          | 108            | 0              | 54             | 108         | 0           | 54          |
| 10 | 75          | 0           | 88          | 290            | 0              | 86             | 290         | 0           | 86          |
| 11 | 107         | 0           | 94          | 262            | 0              | 90             | 262         | 0           | 90          |
| 12 | 124         | 0           | 100         | 1085           | 0              | 92             | 1085        | 0           | 92          |
| 13 | 155         | 0           | 100         | 788            | 0              | 98             | 788         | 0           | 98          |
| 14 | 185         | 0           | 96          | 21774          | 0              | 96             | 21774       | 0           | 96          |
| 15 | 216         | 0           | 98          | 2471           | 0              | 100            | 2471        | 0           | 100         |

Table 8.2: Search sizes for 50 instances of Problems (i) and (ii) in the $n \times n$ grid group.

Table 8.3: Search sizes for 50 instances of Problem (iii) in the $n \times n$ grid group.

In [9, Section 6.1], the Orbital algorithm was much faster than the classical Leon algorithm at solving problems of types (i) and (ii). In Table 8.2, we see why: Orbital typically requires no search for these problems. Leon used a total of 65,834 nodes to solve all problems in Problem (i), and 37,882,616 nodes for Problem (ii), while Orbital required 567 for Problem (i) and 1073 for Problem (ii). The same numbers of nodes were also required for both Strong and Full, since there is no possible improvement.

In Table 8.3, however, we clearly see the benefits of our new techniques with unordered partition stabilisers. For these problems, partition backtrack – Leon and Orbital – takes an increasing number of search nodes, with 140,177 nodes required for Leon and
57,120 nodes for ORBITAL to solve all instances of Problem (iii). The STRONG algorithm, on the other hand, is powerful enough in almost all cases to solve these same problems without search, requiring only 450 nodes to solve all problem instances.

8.2. Intersections of primitive groups with symmetric wreath products

As in [9, Section 6.2], we next investigate the behaviours that the various search techniques have when intersecting primitive groups with wreath products of symmetric groups. This gives difficult but interesting examples of subgroup intersections. To construct these problems, we use the primitive groups library, which is included in the PrimGrp [6] package for GAP.

For a given a composite \( n \in \{6, \ldots, 80\} \), we create the following problems: for each primitive subgroup \( G \leq S_n \) that is neither the symmetric group nor the natural alternating subgroup of \( S_n \), and for each proper divisor \( d \) of \( n \), we construct the wreath product \( S_{n/d} \wr S_d \) as a subgroup of \( S_n \), which we then conjugate by a randomly chosen element of \( S_n \). Finally, we use each of the algorithms in turn to compute the intersection of \( G \) with the conjugated wreath product. We create 50 such intersection problems for each \( n, G, \) and \( d \).

For each \( k \in \{6, \ldots, 80\} \), we record the cumulative number of search nodes that each algorithm requires to solve all of the intersection problems for all composite \( n \in \{6, \ldots, k\} \). We display these cumulative totals in Figures 8.4 and 8.5. As in [9, Section 6.2], we separate the 2-transitive groups from those primitive groups that are not 2-transitive. Note that there exist quite a few values of \( n \in \{6, \ldots, 80\} \) for which every primitive subgroup of \( S_n \) is 2-transitive.

![Figure 8.4: Cumulative nodes required to intersect primitive (but not 2-transitive) groups with wreath products of symmetric groups, for all problems with \( n \in \{6, \ldots, k\} \).](image)

For the primitive but not 2-transitive groups, the total number of search nodes required by the LEON algorithm is 3,239,403. The ORBITAL algorithm reduces this to-
tal search size by approximately 35%, to 2,079,356, but the cumulative search size for \texttt{Strong} is much smaller, at only 3,248 nodes, and for \texttt{Full} the cumulative search size is even smaller, at only 2,140 nodes.

This huge reduction in search size is because the \texttt{Strong} and \texttt{Full} algorithms solve almost every problem without any search. Out of 40,150 experiments, the \texttt{Strong} algorithm required search for only 703, and the \texttt{Full} algorithm required search for only 654. On the other hand, the \texttt{Leon} and \texttt{Orbital} algorithms required search for every single problem.

![Cumulative nodes required to intersect 2-transitive groups with wreath products of symmetric groups, for all problems with $n \in \{6, \ldots, k\}$. The line for Full is omitted, since at this scale, it is indistinguishable from the line for Strong.](image)

**Figure 8.5:** Cumulative nodes required to intersect 2-transitive groups with wreath products of symmetric groups, for all problems with $n \in \{6, \ldots, k\}$. The line for \texttt{Full} is omitted, since at this scale, it is indistinguishable from the line for \texttt{Strong}.

For the intersection problems involving groups that are at least 2-transitive, the improvement of the new techniques over the partition backtrack algorithms is much smaller, and all of the algorithms require a non-zero search size to solve every problem. This stems from the fact that a 2-transitive group has a unique orbital graph, which is a complete digraph.

The \texttt{Leon} algorithm needs roughly 359 million search nodes, while the \texttt{Orbital} algorithm requires roughly 9.23 million, the \texttt{Strong} algorithm requires roughly 5.72 million, and the \texttt{Full} algorithm requires roughly 5.59 million. Therefore the \texttt{Strong} and \texttt{Full} algorithms still require almost 40% fewer nodes than the \texttt{Orbital} algorithm. Out of the 25,600 total experiments, \texttt{Orbital} is better than \texttt{Leon} in 22,178 instances. Of these, \texttt{Strong} is better than \texttt{Orbital} in 2,554 instances, and of these, \texttt{Full} is better than \texttt{Strong} 236 times. This shows that for 2-transitive groups, there are a relatively small number of problems where \texttt{Strong} and \texttt{Full} improve upon \texttt{Orbital}. 
8.3. Intersections of cosets of intransitive groups

In this section, we go beyond the experiments of [9, Section 6], and investigate the behaviour of the algorithms when intersecting cosets of intransitive groups that have identical orbits, and where all orbits have the same size. We chose these kinds of problems because there should be many instances that all of the algorithms find difficult, because of this regularity of orbit structure.

We intersect right cosets of subdirect products of transitive groups of equal degree. Although we create them in a random way, we do not make any claims about their distribution. Given \( k, n \in \mathbb{N} \), we randomly choose \( k \) transitive subgroups of \( S_n \) from the transitive groups library TransGrp [5], each of which we conjugate by a random element of \( S_n \), and we create their direct product, \( G \), which we regard as a subgroup of \( S_{kn} \). Then, we randomly sample elements of \( G \) until the subgroup that they generate is a subdirect product of \( G \). If this subdirect product is equal to \( G \), then we abandon the process and start again. Otherwise, the result is a generating set for what we call a proper \((k, n)\)-subdirect product.

In our experiments, for various \( k, n \in \mathbb{N} \), we explore the search space required to determine whether the intersections of pairs of right cosets of different \((k, n)\)-subdirect products are empty. To make the problems as hard as possible, we choose coset representatives that preserve the orbit structure of the \((k, n)\)-subdirect product.

We performed 50 random instances for each pair \((k, n)\), for all \( k, n \in \{2, \ldots, 10\} \), and we show a representative sample of this data in Tables 8.6 and 8.7 and Figure 8.8. Table 8.6 shows all results for each \( n \), and Table 8.7 gives a more in-depth view for two values of \( k \). The tables omit data for the \textit{Full} algorithm, because it was mostly identical to the data for the \textit{Strong} algorithm, and it varied in only one instance by more than 1%.

| \( n \) | \textbf{Leon} Mean | \textbf{Leon} Median | \textbf{Orbital} Mean | \textbf{Orbital} Median | \textbf{Orbital} Zero\% | \textbf{Strong} Mean | \textbf{Strong} Median | \textbf{Strong} Zero\% |
|---|---|---|---|---|---|---|---|---|
| 2 | 3 | 2 | 2 | 2 | 14 | 2 | 2 | 14 |
| 3 | 1418 | 7 | 19 | 0 | 58 | 19 | 0 | 59 |
| 4 | 1250 | 12 | 71 | 0 | 69 | 62 | 0 | 70 |
| 5 | 37924 | 30 | 15576 | 10 | 14 | 8803 | 0 | 54 |
| 6 | 584 | 12 | 254 | 6 | 36 | 139 | 0 | 86 |
| 7 | 53612 | 28 | 43555 | 14 | 0 | 8982 | 0 | 70 |
| 8 | 1142 | 8 | 997 | 8 | 15 | 4 | 0 | 98 |
| 9 | 6547 | 9 | 5562 | 9 | 2 | 7 | 0 | 95 |
| 10 | 8350 | 10 | 6959 | 10 | 1 | 7 | 0 | 97 |

Table 8.6: Search sizes for \((k, n)\)-subdirect product coset intersection problems, where for each \( n \), we ran 50 experiments for each \( k \in \{2, \ldots, 10\} \).

The \textit{Strong} algorithm solved a large proportion of problems with zero search. As \( n \) and \( k \) increase, we find that \textit{Strong} is also able to solve almost all problems without search, and the remaining problems with very little search. The only problems where \textit{Strong} does not perform significantly better are those involving orbits of size 2 \((n = 2)\).
Table 8.7: Search sizes for 50 \((k, n)\)-subdirect product coset intersection problems.

| k  | n  | LEON Mean | LEON Median | ORBITAL Mean | ORBITAL Median | ORBITAL Zero% | STRONG Mean | STRONG Median | STRONG Zero% |
|----|----|-----------|-------------|--------------|---------------|-------------|-------------|---------------|-------------|
| 4  | 5  | 13683     | 30          | 6356         | 11            | 8           | 6176        | 5            | 40          |
| 4  | 6  | 376       | 18          | 335          | 6             | 8           | 87          | 0            | 76          |
| 4  | 7  | 8612      | 49          | 7065         | 43            | 0           | 6494        | 0            | 54          |
| 4  | 8  | 1133      | 8           | 365          | 8             | 14          | 0           | 0            | 100         |
| 4  | 9  | 1947      | 9           | 621          | 9             | 0           | 0           | 0            | 96          |
| 4  | 10 | 458       | 10          | 410          | 10            | 2           | 0           | 0            | 98          |
| 8  | 5  | 11956     | 130         | 42885        | 30            | 17          | 36888       | 0            | 58          |
| 8  | 6  | 70        | 12          | 25           | 0             | 56          | 67          | 0            | 98          |
| 8  | 7  | 19731     | 49          | 11154        | 43            | 0           | 167         | 0            | 86          |
| 8  | 8  | 209       | 8           | 58           | 8             | 12          | 0           | 0            | 100         |
| 8  | 9  | 152       | 9           | 144          | 9             | 2           | 0           | 0            | 100         |
| 8  | 10 | 138       | 10          | 64           | 10            | 2           | 0           | 0            | 100         |

This is not surprising as there are very few possible orbital graphs for such groups. We note that the problems with \(n = 5\) and \(7\) seem particularly difficult. This is because transitive groups of prime degree are primitive, and sometimes even 2-transitive, in which case they do not have useful orbital graphs.

On the other hand, ORBITAL solved a lot fewer problems without search, and LEON solved none in this way. Although the relatively low medians show that all of the algorithms performed quite small searches for many of the problems, we see a much starker difference in the mean search sizes. These means are typically dominated by a few problems; see Figure 8.8.

Figure 8.8: Search sizes for 50 \((7,7)\)-subdirect product coset intersection problem instances. The data for FULL is almost identical to the data for STRONG, and is omitted.
To give a more complete picture of how the algorithms perform, Figure 8.8 shows the search sizes for all 50 intersections problem that we considered for $n = k = 7$, sorted by difficulty. The data that we collected in this case was fairly typical. Figure 8.8 shows that Strong solves almost all problems with very little or no search, and it only requires more than 50 search nodes for the three hardest problems. On the other hand, Leon and Orbital need more than 50 nodes for the 18 hardest problems. All algorithms found around 30% of the problems easy to solve. This is because our problem generator randomly produces easy problems, sometimes.

9. Conclusions and directions for further work

We have introduced and discussed new data structures and algorithms, using labelled digraphs, which can be used to substantially reduce the size of a search required to solve a large range of group and coset problems in Sym($\Omega$). This work builds on the earlier partition backtrack framework of Leon [12, 13], and also provides an alternative way of viewing that earlier work.

Our new algorithms often reduce problems that previously involved searches of hundreds of thousands of nodes into problems that require no search, and can instead be solved by applying strong equitable labelling to a pair of stacks. There already exists a significant body of work on efficiently implementing equitable partitioning and automorphism finding on digraphs [11, 14], which we believe can be generalised to work incrementally with labelled digraph stacks that grow in length.

We therefore believe there is room for significant performance improvement over the current state of the art, if time is spent on optimising the implementation of the algorithms that we have presented here. In future work, we will show how the algorithms described in this paper can be implemented efficiently, and compare the speed of various methods for hard search problems. In particular, we aim for a better understanding of when partition backtrack is already the best method available, and when it is worth using our methods. Further, earlier work which used orbital graphs [9] showed that there are often significant practical benefits to using only some of the possible orbital graphs in a problem, rather than all of them. We will investigate whether a similar effect occurs in our methods.

Another direction of research is the development and analysis of new types of refiners, along with an extension of our methods. For example, we could allow more substantial changes to the digraphs, such as adding new vertices outside of $\Omega$. One obvious major area not addressed in this paper is normaliser and group conjugacy problems, and we plan to look for new refiners for normaliser calculations.

While the step from ordered partitions to labelled digraphs already adds some difficulty, we still think that it is worth considering even more intricate structures. Why not generalise our ideas to stacks of more general combinatorial structures defined on a set $\Omega$? The definitions of a splitter, of an isomorphism approximator, and of a refiner were essentially independent of the notion of a labelled digraph, and so they – and therefore the algorithms – could work for more general objects around which a search method could be organised.
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