Graph Isomorphism in Quasipolynomial Time

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Abstract

We show that the Graph Isomorphism (GI) problem and the related problems of String Isomorphism (under group action) (SI) and Coset Intersection (CI) can be solved in quasipolynomial (exp $((\log n)^{O(1)})$) time. The best previous bound for GI was $\exp(O(\sqrt{n \log n}))$), where n is the number of vertices (Luks, 1983); for the other two problems, the bound was similar, $\exp(\tilde{O}(\sqrt{n}))$, where n is the size of the permutation domain (Babai, 1983).

The algorithm builds on Luks's SI framework and attacks the barrier configurations for Luks's algorithm by group theoretic "local certificates" and combinatorial canonical partitioning techniques. We show that in a well-defined sense, Johnson graphs are the only obstructions to effective canonical partitioning.

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1 Introduction

1.1 Results and philosophy

1.1.1 Results: the String Isomorphism problem

Let G be a group of permutations of the set $[n] = \{1, \ldots, n\}$ and let $\mathfrak{x}, \mathfrak{y}$ be strings of length n over a finite alphabet. The String Isomorphism (SI) problem asks, given G, \mathfrak{x} , and \mathfrak{y} , does there exist an element of G that transforms \mathfrak{x} into \mathfrak{y} . (See the precise definition in Def. 3.2. Permutation groups are given by a list of generators.) A function f(n) is quasipolynomially bounded if there exist constants c, C such that $f(n) \leq \exp(C(\log n)^c)$ for all sufficiently large n. "Quasipolynomial time" refers to quasipolynomially bounded time.

We prove the following result.

Theorem 1.1. The String Isomorphism problem can be solved in quasipolynomial time.

The Graph Isomorphism (GI) Problem asks to decide whether or not two given graphs are isomorphic. The Coset Intersection (CI) problem asks, given cosets of two permutation groups over the same finite domain, do they have a nonempty intersection.

Corollary 1.2. The Graph Isomorphism problem and the Coset Intersection problem can be solved in quasipolynomial time.

The SI and CI problems were introduced by Luks [Lu82] (cf. [Lu93]) who also pointed out that these problems are polynomial-time equivalent (under Karp reductions) and GI easily reduces to either. For instance, GI for graphs with n vertices is identical, under obvious encoding, with SI for binary strings of length $\binom{n}{2}$ with respect to the induced action of the symmetric group of degree n on the set of $\binom{n}{2}$ unordered pairs.

The previous best bound for each of these three problems was $\exp(\tilde{O}(n^{1/2}))$ (the tilde hides polylogarithmic factors¹), where for GI, n is the number of vertices, for the two other problems, n is the size of the permutation domain. For GI, this bound was obtained in 1983 by combining Luks's group-theoretic algorithm [Lu82] with a combinatorial partitioning lemma by Zemlyachenko (see [ZKT, BaL, BaKL]). For SI and CI, additional group-theoretic observations were used ([Ba83], cf. [BaKL]). No improvement over either of these results was found in the intervening decades.

The actual results are slightly stronger: only the length of the largest orbit of G matters.

¹Accounting for those logs, the best bound for GI for three decades was $\exp(O(\sqrt{n \log n}))$, established by Luks in 1983, cf. [BaKL].

Theorem 1.3. The SI problem can be solved in time, polynomial in n (the length of the strings) and quasipolynomial in $n_0(G)$, the length of the largest orbit of G.

The first class of graphs studied using group theory was that of vertex-colored graphs (isomorphisms preserve color by definition) [Ba79a] (1979).

Corollary 1.4. The GI problem for vertex-colored graphs can be solved in time, polynomial in n (the number of vertices) and quasipolynomial in the largest color multiplicity.

1.1.2 Quasipolynomial complexity analysis, multiplicative cost

The analysis will be guided by the observation that if f(x) and q(x) are positive, monotone increasing functions and

$$f(n) \le q(n)f(9n/10) \tag{1}$$

then $f(n) \leq q(n)^{O(\log n)}$. In particular, if q(x) is quasipolynomially bounded then so is f(x). Here f(n) stands for the worst-case cost (number of group operations) on instances of size $\leq n$ and q(n) is the branching factor in the algorithm to which we refer as the "multiplicative cost" in reference to Eq. (1). So our goal will be to achieve a *significant reduction* in the problem size, say $n \leftarrow 9n/10$, at a quasipolynomial multiplicative cost. There is also an additive cost to the reduction, but this will typically be absorbed by the multiplicative cost.

Both in the group-theoretic and in the combinatorial arguments, we shall actually use double recursion. In addition to the input domain Ω of size $n = |\Omega|$, we shall also build an auxiliary set Γ and track its size $m = |\Gamma| \leq n$. Most of the action will occur on Γ . Significant progress will be deemed to have occurred if we significantly reduce Γ , say $m \leftarrow 9m/10$, while not increasing n. When m drops below a threshold $\ell(n)$ that is polylogarithmic in n, we perform brute force enumeration over the symmetric group $\mathfrak{S}(\Gamma)$ at a multiplicative cost of $\ell(n)$!. This eliminates the current Γ and significantly reduces n. Subsequently a new Γ , of size $m \leq n$, is introduced, and the game starts over. If $q_1(x)$ is the multiplicative cost of significantly reducing Γ then the overall cost estimate becomes $f(n) \leq q_1(x)^{\log^2 n}$.

1.1.3 Philosophy: local to global

We follow Luks's general framework [Lu82], developed for his celebrated polynomial-time algorithm to test isomorphism of graphs of bounded valence.

Luks's method meets a barrier when it encounters large primitive permutation groups without well-behaved subgroups of small index. By a 1981 result of Cameron [Cam81] these barrier groups are the "Johnson goups" (symmetric or alternating groups in their induced action on t-tuples). This much has been known for more than 35 years. Our contribution is in breaking this symmetry.

We achieve this goal via a new group-theoretic divide-and-conquer algorithm that handles Luks's barrier situation. The tools we develop include two combinatorial partitioning algorithms and a group-theoretic lemma. The latter serves as the main divide-and-conquer tool for the procedure at the heart of the algorithm.

Our strategy is an interplay between local and global symmetry, formalized through a technique we call *"local certificates."* We shall certify both the presence and the absence of

local symmetry. Locality in our context refers to logarithmic-size subdomains. If we don't find local symmetry, we infer global irregularity; if we do find local symmetry, we either build it up to global symmetry (find automorphisms) or use any obstacles to this attempt to infer local irregularity which we then synthesize to global irregularity. Building up symmetry means approximating the automorphism group from below; when we discover irregularity, we turn that into an effective upper bound on the automorphism group (by reducing the ambient group G using combinatorial partitioning techniques, including polylog-dimensional Weisfeiler-Leman refinement²). When the lower and the upper bounds on the automorphism group meet, we have found the automorphism group and solved the isomorphism problem.

The critical contribution of the group-theoretic LocalCertificates routine (Theorem 10.3) is the following, somewhat implausible, dichotomy: either the algorithm finds *global* automorphisms (automorphisms of the entire input string) that certify high *local symmetry*, or it finds a *local* obstruction to high local symmetry. We shall explain this in more specific terms.

1.2 Strategy

1.2.1 Notation, terminology. Giants, Johnson groups

For groups G, H we write $H \leq G$ to indicate that H is a subgroup of G.

For a set Γ we write $\mathfrak{S}(\Gamma)$ to denote the symmetric group acting on Γ , and $\mathfrak{A}(\Gamma)$ for the alternating group. We refer to these two subgroups of $\mathfrak{S}(\Gamma)$ as the *giants*. If $|\Gamma| = m$ then we also generically write \mathfrak{S}_m and \mathfrak{A}_m for the giants acting on m elements. We say that a homomorphism $\varphi : G \to \mathfrak{S}(\Gamma)$ is a *giant representation* if the image G^{φ} is a giant (i.e., $G^{\varphi} \geq \mathfrak{A}(\Gamma)$).

We write $\mathfrak{S}^{(t)}(\Gamma)$ for the induced action of $\mathfrak{S}(\Gamma)$ on the set $\binom{\Gamma}{t}$ of *t*-tuples of elements of Γ . We define $\mathfrak{A}^{(t)}(\Gamma)$ analogously. We call the groups $\mathfrak{S}^{(t)}(\Gamma)$ and $\mathfrak{A}^{(t)}(\Gamma)$ Johnson groups and also denote them by $\mathfrak{S}_m^{(t)}$ and $\mathfrak{A}_m^{(t)}$ if $|\Gamma| = m$. Here we assume $1 \le t \le m/2$.

The input to the String Isomorphism problem is a permutation group $G \leq \mathfrak{S}(\Omega)$ and two strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$ where Σ is a finite alphabet. For $\sigma \in \mathfrak{S}(\Omega)$, the string x^{σ} is obtained from \mathfrak{x} by permuting the positions of the entries via σ . The set $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ of *G*-isomorphisms of the strings $\mathfrak{x}, \mathfrak{y}$ consist of those $\sigma \in G$ that satisfy $\mathfrak{x}^{\sigma} = \mathfrak{y}$, and the *G*-automorphism group of \mathfrak{x} is the group $\operatorname{Aut}_G(\mathfrak{x}) = \operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$. The set $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ is either empty or a right coset of $\operatorname{Aut}_G(\mathfrak{x})$.

1.2.2 Local certificates

Luks's SI algorithm proceeds by processing the permutation group $G \leq \mathfrak{S}(\Omega)$ orbit by orbit. If G is transitive, it finds a minimal system Φ of imprimitivity (Φ is a G-invariant partition of the permutation domain Ω into maximal blocks), so the action $\mathfrak{G} \leq \mathfrak{S}(\Phi)$ is a primitive permutation group. The naive approach then is to enumerate all elements of \mathfrak{G} , each time reducing to the kernel of the $G \to \mathfrak{G}$ epimorphism.

²As far as I know, this paper is the first to derive analyzable gain from employing the k-dimensional WL method for unbounded values of k. We use it in the proof of the Design Lemma (Thm. 6.1). In our applications of the Design Lemma, the value of k is polylogarithmic (see Secc. 6.2, 10.2).

By Cameron's cited result, the barrier to efficient application of this method occurs when \mathfrak{G} is a Johnson group, $\mathfrak{S}_m^{(t)}$ or $\mathfrak{A}_m^{(t)}$, for some value *m* deemed too large to permit full enumeration of \mathfrak{G} . (Under brute force enumeration, the number *m* will go into the exponent of the complexity.) We shall set this threshold at $c \log n$ for some constant *c*.

It is easy to verify recursively whether or not $\operatorname{Aut}_G(\mathfrak{x})$ maps onto \mathfrak{G} , or a small-index subgroup of \mathfrak{G} ; and if the answer is positive, we can also find the *G*-isomorphisms of \mathfrak{x} and \mathfrak{y} via efficient recursion.

So our goal is to significantly reduce \mathfrak{G} unless $\operatorname{Aut}_G(\mathfrak{x})$ maps onto a large portion of \mathfrak{G} .

First we note that our Johnson group \mathfrak{G} , a quotient of G, is isomorphic to a symmetric or alternating group, \mathfrak{S}_m or \mathfrak{A}_m , so G has a giant representation $\varphi : G \to \mathfrak{S}(\Gamma)$ for some domain Γ of size $|\Gamma| = m$.

Virtually all the action in our algorithm will occur on the set Γ . By "locality" we shall refer to logarithmic-size subsets of Γ which we call *test sets*. If $A \subseteq \Gamma$ is a test set, we say that A is *full* if all permutations in $\mathfrak{A}(A)$ lift to G-automorphisms of the input string \mathfrak{x} .

One of our main technical result says, somewhat surprisingly, that we can efficiently decide local symmetry (fullness of a test set): in quasipolynomial time we are able to reduce the question of fullness to N-isomorphism questions, where the groups N have no orbit larger than n/m.

This is a significant reduction, it permits efficient application of Luks's recurrence.

Our test sets (small subsets of Γ) have corresponding portions of the input (defined on subsets of Ω); we refer to elements of G that respect such a portion of the input as *local automorphisms*. The obstacles to local symmetry we find are local (they already block local automorphisms from being sufficiently rich), so our certificates to non-fullness will be local. Fullness certificates, however, by definition cannot be local: we need global automorphisms (that respect the full input) to certify fullness. The surprising part is that from a sufficiently rich set of local automorphisms we are able to infer global automorphisms (automorphisms of the full string).

The nature of these certificates is outlined in Sec. 1.3.2.

1.2.3 Aggregating the local certificates

The next phase is that we aggregate these $\binom{m}{k}$ local certificates (where k = |A| is the size of the test sets; we shall choose k to be $O(\log n)$) into global information. In fact, not only do we study test sets A but compare pairs A, A' of test sets, and we also compare test sets for the input \mathfrak{x} and for the input \mathfrak{y} , so our data for the aggregation procedures take about $\binom{m}{k}^2$ items of local information as input.

Aggregating the positive certificates is rather simple; these are subgroups of the automorphism group, so we study the group F they generate, and the structure of its projection F^{Γ} into $\mathfrak{S}(\Gamma)$. If this group is all of $\mathfrak{S}(\Gamma)$ then \mathfrak{x} and \mathfrak{y} are G-isomorphic if and only if they are N-isomorphic where $N = \ker(\varphi)$. The situation is not much more difficult when F^{Γ} acts as a giant on a large portion of Γ (Section 9).

Otherwise, if F^{Γ} has a large support in Γ but is not a giant on a large orbit of this support, then we can take advantage of the structure of F^{Γ} (orbits, domains of imprimitivity) to obtain the desired split of Γ (Section 10.2). The aggregate of the negative certificates will be a canonical k-ary relational structure on Γ and the subject of our combinatorial reduction techniques (Design Lemma, Sec. 6, and Split-or-Johnson algorithm, Sec. 7) which, in combination, will achieve the desired reduction of Γ .

1.2.4 Group theory required

The algorithm heavily depends on the Classification of Finite Simple Groups (CFSG) through Cameron's classification of large primitive permutation groups. Another instance where we rely on CFSG occurs in the proof of Lemma 8.5 that depends on "Schreier's Hypothesis" (that the outer automorphisms group of a finite simple group is solvable), a consequence of CFSG.

No deep knowledge of group theory is required for reading this paper. The cited consequences of the CFSG are simple to state, and aside from these, we only use elementary group theory.

We should also note that we are able to dispense with Cameron's result using our combinatorial partitioning technique, significantly reducing the dependence of our analysis on the CFSG. We comment on this in Section 13.1.

1.3 The ingredients

The algorithm is based on Luks's classical framework. It has four principal new ingredients: a group-theoretic result, a group-theoretic divide-and-conquer algorithm, and two combinatorial partitioning algorithms. Both the group-theoretic algorithm and part of one of the combinatorial partitioning algorithms implement the idea of "local certificates."

1.3.1 The group-theoretic divide-and-conquer tool

In this section we describe our main group theoric tool.

Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group. Recall that we say that a homomorphism $\varphi: G \to \mathfrak{S}_k$ is a giant representation of G if G^{φ} (the image of G under φ) contains \mathfrak{A}_k . We say that an element $x \in \Omega$ is affected by φ if $G_x^{\varphi} \not\geq \mathfrak{A}_k$, where G_x denotes the stabilizer of x in G. Note that if x is affected then every element of the orbit x^G is affected. So we can speak of affected orbits.

Theorem 1.5. Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and let n_0 denote the length of the largest orbit of G. Let $\varphi : G \to \mathfrak{S}_k$ be a giant representation. Let $U \subseteq \Omega$ denote the set of elements of Ω not affected by φ . Then the following hold.

- (a) (Unaffected Stabilizer Theorem) Assume $k > \max\{8, 2 + \log_2 n_0\}$. Then φ maps $G_{(U)}$, the pointwise stabilizer of U, onto \mathfrak{A}_k or \mathfrak{S}_k (so $\varphi : G_{(U)} \to \mathfrak{S}_k$ is still a giant representation). In particular, $U \neq \Omega$ (at least one element is affected).
- (b) (Affected Orbits Lemma) Assume $k \geq 5$. If Δ is an affected G-orbit, i. e., $\Delta \cap U = \emptyset$, then ker(φ) is not transitive on Δ ; in fact, each orbit of ker(φ) in Δ has length $\leq |\Delta|/k$.

This result is a combination of Theorem 8.11 and Corollary 8.13 proved in Section 8.

Remark 1.6. We note that part (a) becomes false if we relax the condition $k > 2 + \log_2 n_0$ to $k \ge 2 + \log_2 n_0$. In Remark 8.6 we exhibit infinitely many transitive groups with giant actions with $k = 2 + \log_2 n$ where none of the elements is affected (and the kernel is transitive).

The affected/not affected dichotomy is our *principal divide-and-conquer* tool.

These results are employed in Procedure LocalCertificates, the heart of the entire algorithm, in Section 10. It is Theorem 1.5 that allows us to build up local symmetry to global automorphism unless an explicit obstacle is found.

1.3.2 The group-theoretic divide-and-conquer algorithm

We sketch the LocalCertificates procedure, to be formally described in Section 10. The procedure takes a logarithmic size "test set" $A \subseteq \Gamma$, |A| = k, and tries to build automorphisms corresponding to arbitrary (even) permutations of A. This is an iterative process: first we ignore the input string \mathfrak{x} , so we have the group G_A (setwise stabilizer of A). Then we begin "growing a beard" which at first consists of those elements of Ω that are affected by φ . Now we take the segment of \mathfrak{x} that falls in the "beard" into account, so the automorphism group shrinks, more points will be affected; we include them in the next layer of the growing beard, etc.

We stop when either the action of the current automorphism group (of the segment of the input that belongs to the beard) on A is no longer giant, or the affected set (the beard) stops growing.

In the former case we found a canonical k-ary relation on A; after aggregating these over all test sets, we hand over the process to the combinatorial partitioning techniques of the next section (Design Lemma, Split-or-Johnson algorithm).

In the latter case we pointwise stabilize all non-affected points; we still have a giant action on A and this time the reduced group consists of automorphisms of the entire string \mathfrak{r} (since it does not matter what letter of the alphabet is assigned to fixed points of the group). Then we analyze the action on Γ of the group of automorphisms obtained from the positive local certificates (Sec. 10.2).

The procedure described is to be used when G is transitive and imprimitive. If G is intransitive, we apply Luks's Chain Rule (orbit-by-orbit processing, Prop. 3.7). If G is primitive, we may assume G is a Johnson group $\mathfrak{S}_m^{(t)}$ or $\mathfrak{A}_m^{(t)}$, so the situation is that of an edge-colored *t*-uniform hypergraph on m vertices. We use the Extended Design Lemma (Theorem 7.12) to either canonically partition k or to reduce \mathfrak{A}_m to a much smaller Johnson group acting on $\leq m$ points, see Sec. 12.

1.3.3 Combinatorial partitioning; discovery of a canonically embedded large Johnson graph

The partitioning algorithms take as input a set Ω related in some way to a structure X. The goal is either to establish high symmetry of X or to find a canonical structure on Ω that represents and explicit obstacle to such high symmetry.

Significant partitioning is expected at modest "multiplicative cost" (explained below). Favorable outcomes of the partitioning algorithms are (a) a canonical coloring of Ω where each color-class has size $\leq 0.9n$ $(n = |\Omega|)$, or (b) a canonical equipartition of a canonical subset of Ω of size $\geq 0.9n$.

A Johnson graph J(v,t) has $n = {v \choose t}$ vertices labeled by the t-subsets $T \subseteq [v]$. The tsubsets T_1, T_2 are adjacent if $|T_1 \setminus T_2| = 1$. Johnson graphs do not admit a coloring/partition as described, even at quasipolynomial multiplicative cost, if t is subpolynomial in v (i.e., $t = v^{o(1)}$). (Johnson graphs with t = 2 have been the most notorious obstacles to breaking the $\exp(\tilde{O}(\sqrt{n}))$ bound on GI.) One of the main results of the paper is that in a well-defined sense, Johnson graphs are the only obstructions to effective partitioning: either partitioning succeeds as desired or a canonically embedded Johnson graph on a subset of size $\geq 0.9n$ is found. Here is a corollary to the result.

Theorem 1.7. Let X = (V, E) be a nontrivial regular graph (neither complete, nor empty) with n vertices. At a quasipolynomial multiplicative cost we can find one of the following structures. We call the structure found Y.

- (a) A coloring of V with no color-class larger than 0.9n;
- (b) A coloring of V with a color-class C of size $\geq 0.9n$ and a nontrivial equipartition of C (the blocks of the partition are of equal size ≥ 2 and there are at least two blocks);
- (c) A coloring of V with a color-class C of size $\geq 0.9n$ and a Johnson graph J(v,t) $(t \geq 2)$ with vertex-set C,

such that the index of the subgroup $\operatorname{Aut}(X) \cap \operatorname{Aut}(Y)$ in $\operatorname{Aut}(X)$ is quasipolynomially bounded.

The index in question (and its natural extension to isomorphisms) represents the multiplicative cost incurred. The full statement can be found in Theorem 7.10.

The same is true if X is a k-ary relational structure that does not admit the action of a symmetric group of degree $\geq 0.9n$ on its vertex set (has "symmetry defect" $\geq 0.1n$, see Def. 2.14) assuming k is polylogarithmically bounded. The reduction from k-ary relations $(k \geq 3)$ to regular graphs (and to highly regular binary relational structures called "uniprimitive coherent configurations" or UPCCs) is the content of the Design Lemma (Theorem 6.1).

Note that the Johnson graph will not be a subgraph of X; but it will be "canonically embedded" relative to an arbitrary choice from a quasipolynomial number of possibilities, with the consequence of not reducing the number of automorphisms/isomorphisms by more than a quasipolynomial factor.

The number 0.9 is arbitrary; the result would remain valid for any constant $0.5 < \alpha < 1$ in place of 0.9.

We note that the *existence* of such a structure Y can be deduced from the Classification of Finite Simple Groups. We not only assert the existence but also find such a structure in quasipolynomial time, and the analysis is almost entirely combinatorial, with a modest use of elementary group theory.

The structure Y is "canonical relative to an arbitrary choice" from a quasipolynomial number of possibilities. These arise by individualizing a polylogarithmic number of "ideal points" of Y. An "ideal point" of X is a point of a structure X' canonically constructed from X, much like "ideal points" of an affine plane are the "points at infinity." Individualizing a point at infinity means individualizing a parallel class of lines in the affine plane.

Canonicity means being preserved under isomorphisms in a category of interest. This category is always very small, it often has just two objects (the two graphs or strings of which we wish to decide isomorphism); sometimes it has a quasipolynomial number of objects (when checking local symmetry, we need to compare every pair of polylogarithmic size subsets of the domain). In any case, this notion of canonicity does not require canonical forms for the class of all graphs or strings, a problem we do not address in this paper. We say that we incur a "multiplicative cost" τ if a choice is made from τ possibilities. This indeed makes the algorithm branch τ ways, giving rise to a factor of τ in the recurrence.

Canonicity and "relative canonicity at a multiplicative cost" are formalized in the language of functors in Section 4.

2 Preliminaries

2.1 Fraktur

We list the Roman equivalents of the letters in Fraktur we use:

2.2 Permutation groups

All groups in this paper are finite. Our principal reference for permutation groups is the monograph by Dixon and Mortimer [DiM]. Wielandt's classic [Wi] is a sweet introduction. Cameron's article [Cam81] is very informative. For the basics of permutation group algorithms we refer the reader to Seress's monograph [Se]. Even though we summarize Luks's method in our language in Sec. 3.1, Luks's seminal paper [Lu82] is a prerequisite for this one.

For a set Ω we write $\mathfrak{S}(\Omega)$ for the symmetric group consisting of all permutations of Ω and $\mathfrak{A}(\Omega)$ for the alternating group on Ω (set of even permutations of Ω). We write \mathfrak{S}_n for $\mathfrak{S}([n])$ and \mathfrak{A}_n for $\mathfrak{A}([n])$ where $[n] = \{1, \ldots, n\}$. We also use the symbols \mathfrak{S}_n and \mathfrak{A}_n when the permutation domain is not specified (only its size). For a function f we usually write x^f for f(x). In particular, for $\sigma \in \mathfrak{S}(\Omega)$ and $x \in \Omega$ we denote the image of x under σ by x^{σ} . For $x \in \Omega, \sigma \in \mathfrak{S}(\Omega), \Delta \subseteq \Omega$, and $H \subseteq \mathfrak{S}(\Omega)$ we write

$$x^{H} = \{x^{\sigma} \mid \sigma \in H\} \text{ and } \Delta^{\sigma} = \{y^{\sigma} \mid y \in \Delta\} \text{ and } \Delta^{H} = \{\Delta^{\sigma} \mid \sigma \in H\}.$$
 (2)

For groups G, H we write $H \leq G$ to indicate that H is a subgroup of G. The expression |G:H| denotes the *index* of H in G. Subgroups $G \leq \mathfrak{S}(\Omega)$ are the *permutation groups* on the domain Ω . The size of the permutation domain, $|\Omega|$, is called the *degree* of G while |G| is the *order* of G. We refer to $\mathfrak{S}(\Omega)$ and $\mathfrak{A}(\Omega)$, the two largest permutation groups on Ω , as the *giants*.

By a representation of a group G we shall always mean a permutation representation, i.e., a homomorphism $\varphi: G \to \mathfrak{S}(\Omega)$. We also say in this case that G acts on Ω (via φ). We say that Ω is the *domain* of the representation and $|\Omega|$ is the *degree* of the representation. If φ is evident from the context, we write x^{π} for $x^{\pi^{\varphi}}$. For $x \in \Omega$, $\sigma \in G$, $\Delta \subseteq \Omega$, and $H \subseteq G$, we define x^{H} and Δ^{σ} and Δ^{H} by Eq. (2).

We denote the image of G under φ by G^{φ} , so $G^{\varphi} \cong G/\ker(\varphi)$. If $G^{\varphi} \ge \mathfrak{A}(\Omega)$ we say φ is a *giant action* and G acts on Ω "as a giant."

A subset $\Delta \subseteq \Omega$ is *G*-invariant if $\Delta^G = \Delta$.

Notation 2.1. If $\Delta \subseteq \Omega$ is *G*-invariant then G^{Δ} denotes the image of the representation $G \to \mathfrak{S}(\Delta)$ defined by restriction to Δ . So $G^{\Delta} \leq \mathfrak{S}(\Delta)$.

The stabilizer of $x \in \Omega$ is the subgroup $G_x = \{\sigma \in G \mid x^{\sigma} = x\}$. The orbit of $x \in \Omega$ is the set $x^G = \{x^{\sigma} \mid \sigma \in G\}$. The orbits partition Ω . A simple bijection shows that

$$|x^G| = |G:G_x|. aga{3}$$

For $T \subseteq \Omega$ and $G \leq \mathfrak{S}(\Omega)$ we write G_T for the setwise stabilizer of T and $G_{(T)}$ for the pointwise stabilizer of T, i. e.,

$$G_T = \{ \alpha \in G \mid T^\alpha = T \}$$
(4)

and

$$G_{(T)} = \{ \alpha \in G \mid (\forall x \in T) (x^{\alpha} = x) \}.$$
(5)

So $G_{(T)}$ is the kernel of the $G_T \to \mathfrak{S}(T)$ homomorphism obtained by restriction to T; in particular, $G_{(T)} \triangleleft G_T$.

For $t \ge 0$ we write $\binom{\Omega}{t}$ to denote the set of t-subsets of Ω . So if $|\Omega| = k$ then $\left|\binom{\Omega}{t}\right| = \binom{k}{t}$. A permutation group $G \le \mathfrak{S}(\Omega)$ naturally acts on $\binom{\Omega}{t}$; we refer to this as the *induced action* on t-sets and denote the resulting subgroup of $\mathfrak{S}\binom{\Omega}{t}$ by $G^{(t)}$. This in particular defines the notation $\mathfrak{S}_k^{(t)}$ and $\mathfrak{A}_k^{(t)}$; these are subgroups of $\mathfrak{S}\binom{k}{t}$. We refer to $\mathfrak{S}_k^{(t)}$ and $\mathfrak{A}_k^{(t)}$ as Johnson groups since they act on the "Johnson schemes" (see below) ³.

The group G is *transitive* if it has only one orbit, i.e., $x^G = \Omega$ for some (and therefore any) $x \in \Omega$. The G-invariant sets the unions of orbits.

A *G*-invariant partition of Ω is a partition $\{B_1, \ldots, B_m\}$ where the B_i are nonempty, pairwise disjoint subsets of which the union is Ω such that *G* permutes these subsets, i.e., $(\forall \sigma \in G)(\forall i)(\exists j)(B_i^{\sigma} = B_j)$. The B_i are the *blocks* of this partition.

A nonempty subset $B \subseteq \Omega$ is a block of imprimitivity for G if $(\forall g \in G)(B^g = B \text{ or } B^g \cap B = \emptyset)$. A subset $B \subseteq \Omega$ is a block of imprimitivity if and only if it is a block in an invariant partition.

A system of imprimitivity for G is a G-invariant partition $\mathcal{B} = \{B_1, \ldots, B_m\}$ of a G-invariant subset $\Delta \subseteq \Omega$ such that G acts transitively on \mathcal{B} . (So $\Delta = \bigcup_i B_i$; we assume here that $(\forall i)(B_i \neq \emptyset)$). The B_i are then blocks of imprimitivity, and every system of imprimitivity arises as the set of G-images of a block of imprimitivity. The group G acts on \mathcal{B} by permuting the blocks; this defines a representation $G \to \mathfrak{S}_m$.

³ "Johnson schemes" is a standard term; we introduce the term "Johnson groups" for convenience.

A maximal system of imprimitivity for G is a system of imprimitivity of blocks of size ≥ 2 that cannot be refined, i.e., where the blocks are minimal (do not properly contain any block of imprimitivity of size ≥ 2).

 $G \leq \mathfrak{S}(\Omega)$ is primitive if $|G| \geq 2$ and G has no blocks of imprimitivity other than Ω and the singletons (sets of one element). In particular, a primitive group is transitive. Examples of primitive groups include the cyclic group of prime order p acting naturally on a set of p elements, and the Johnson groups $\mathfrak{S}_k^{(t)}$ and $\mathfrak{A}_k^{(t)}$ for $t \geq 1$ and $k \geq 2t + 1$. A group $G \leq \mathfrak{S}(\Omega)$ is doubly transitive if its induced action on the set of n(n-1) ordered

A group $G \leq \mathfrak{S}(\Omega)$ is *doubly transitive* if its induced action on the set of n(n-1) ordered pair is transitive (where $n = |\Omega|$).

Definition 2.2. The support of a permutation $\sigma \in \mathfrak{S}(\Omega)$ is the set of elements that σ moves: $\operatorname{supp}(\sigma) = \{x \in \Omega \mid x^{\sigma} \neq x\}$. The degree of σ is the size of its support. The minimal degree of a permutation group G is $\min_{\sigma \in G, \sigma \neq 1} |\operatorname{supp}(\sigma)|$.

The following 19th-century gem will be used in the proof of Claim 2b1 in Sec. 10.2. It appears in [Bo97]. We quote if from [DiM, Thm. 5.4A].

Theorem 2.3 (Bochert, 1897). If G is a doubly transitive group of degree n other than \mathfrak{A}_n or \mathfrak{S}_n then its minimal degree is at least n/8. If $n \ge 217$ then the minimal degree is at least n/4.

2.3 Relational structures, k-ary coherent configurations

A k-ary relation on the set Ω is a subset $R \subseteq \Omega^k$. A relational structure $\mathfrak{X} = (\Omega; \mathcal{R})$ consists of Ω , the set of vertices, and $\mathcal{R} = (R_1, \ldots, R_r)$, a list of relations on Ω . We write $\Omega = V(\mathfrak{X})$. We say that \mathfrak{X} is a k-ary relational structure if each R_i is k-ary. Let $\mathfrak{X}' = (\Omega'; \mathcal{R}')$ where $\mathcal{R}' = (R'_1, \ldots, R'_r)$. A bijection $f : \Omega \to \Omega'$ is an $\mathfrak{X} \to \mathfrak{X}'$ isomorphism if $(\forall i)(R_i^f = R'_i)$, i.e., for $x_i \in \Omega$ we have $(x_1, \ldots, x_k) \in R_i \iff (x_1^f, \ldots, x_k^f) \in R'_i)$. We denote the set of $\mathfrak{X} \to \mathfrak{X}'$ isomorphisms by $\operatorname{Iso}(\mathfrak{X}, \mathfrak{X}')$ and write $\operatorname{Aut}(\mathfrak{X}) = \operatorname{Iso}(\mathfrak{X}, \mathfrak{X})$ for the automorphism group of \mathfrak{X} .

Definition 2.4 (Induced substructure). Let $\Delta \subseteq \Omega$ and let $\mathfrak{X} = (\Omega; R_1, \ldots, R_r)$ be a k-ary relational structure. Let $R_i^{\Delta} = R_i \cap \Delta^k$. We define the *induced substructure* $\mathfrak{X}[\Delta]$ of \mathfrak{X} on Δ as $\mathfrak{X}[\Delta] = (\Delta; R_1^{\Delta}, \ldots, R_r^{\Delta})$.

Definition 2.5 (s-skeleton). For $R \subseteq \Omega^k$ and $t \leq k$ let $R^{(s)} = \{(x_1, \ldots, x_s) \mid (x_1, \ldots, x_s, x_s, \ldots, x_s) \in R\}$. We define the *t*-skeleton $\mathfrak{X}^{(t)} = (\Omega; \mathcal{R}^{(t)})$ of the *k*-ary relational structure $\mathfrak{X} = (\Omega; \mathcal{R}) = (\Omega; R_1, \ldots, R_r)$ by setting $\mathcal{R}^{(s)} = (R_1^{(s)}, \ldots, R_r^{(s)})$.

The group \mathfrak{S}_k acts naturally on Ω^k by permuting the coordinates.

Notation 2.6 (Substitution). For $\vec{x} = (x_1, \ldots, x_k) \in \Omega^k$ and $y \in \Omega$ let $\vec{x}_i^y = (x'_1, \ldots, x'_k)$ where $x'_i = x_j$ for all $j \neq i$ and $x'_i = y$.

We shall especially be interested in the case when the R_i partition Ω^k . This is equivalent to coloring Ω^k ; if $\vec{x} = (x_1, \ldots, x_k) \in R_i$ then we call *i* the *color* of the *k*-tuple \vec{x} and write $c(\vec{x}) = i$. **Definition 2.7** (Configuration). We say that the k-ary relational structure \mathfrak{X} is a k-ary configuration if the following hold:

(i) the R_i partition Ω^k and all the R_i are nonempty;

(ii) if
$$c(x_1,\ldots,x_k) = c(x'_1,\ldots,x'_k)$$
 then $(\forall i,j \le k)(x_i = x_j \iff x'_i = x'_j);$

(iii) $(\forall \pi \in \mathfrak{S}_k) (\forall i \le k) (\exists j \le k) (R_i^{\pi} = R_j).$

Here R^{π} denotes the relation $R^{\pi} = \{(x_{1^{\pi}}, \ldots, x_{k^{\pi}}) \mid (x_1, \ldots, x_k) \in R\}.$

We call r the rank of the configuration. We note that the t-skeleton of a configuration of rank r is a configuration of rank $\leq r$ (we keep only one copy of identical relations).

Vertex colors are the colors of the diagonal elements: c(x) = c(x, ..., x). We say that the configuration \mathfrak{X} is *homogeneous* if all vertices have the same color. We note that the *s*-skeleton of a *k*-ary homogeneous configuration is homogeneous.

Definition 2.8 (*k*-ary coherent configurations). We call a *k*-ary configuration $\mathfrak{X} = (\Omega; R_1, \ldots, R_r)$ coherent if, in addition to items (i)–(iii), the following holds:

(iv) For all $i_0, \ldots, i_k \leq r$ there exist nonnegative integer structure constants $p(i_0, \ldots, i_k)$ such that for all j $(1 \leq j \leq k)$ and all $\vec{x} \in R_{i_0}$ we have

$$|\{y \in \Omega \mid c(\vec{x}_{j}^{y}) = i_{j}\}| = p(i_{0}, \dots, i_{k})).$$
(6)

These are the stable configurations under the k-dimensional Weisfeiler-Leman canonical refinement process (Sec. 2.9).

Observation 2.9. For all $s \le k$, the *s*-skeleton of a *k*-ary coherent configuration is an *s*-ary coherent configuration.

2.4 Twins, symmetry defect

Convention 2.10. Let $\Psi \subseteq \Omega$. We view $\mathfrak{S}(\Psi)$ as a subgroup of $\mathfrak{S}(\Omega)$ by extending each element of $\mathfrak{S}(\Psi)$ to act trivially on $\Omega \setminus \Psi$.

Definition 2.11 (Twins). Let $G \leq \mathfrak{S}(\Omega)$ and $x, y \in \Omega$. We say that vertices $x \neq y$ are strong twins if the transposition $\tau = (x, y)$ belongs to $\operatorname{Aut}(\mathfrak{X})$. We say that vertices $x \neq y$ are weak twins if either they are strong twins or there exists $z \notin \{x, y\}$ such that the 3-cycle $\sigma = (x, y, z)$ belongs to $\operatorname{Aut}(\mathfrak{X})$.

We observe that both the "strong twin or equal" and the "weak twin or equal" relations are equivalence relations on Ω . We call the nontrivial (non-singleton) equivalence classes of these relations the *strong/weak-twin-equivalence classes* of G, respectively.

Definition 2.12 (Symmetrical sets). Let $G \leq \mathfrak{S}(\Omega)$ where $|\Omega| = n$. Let $\Psi \subseteq \Omega$. We say that Ψ is a *strongly/weakly symmetrical set* for Ω if $|\Psi| \geq 2$ and all pairs of points in Ψ are strong/weak twins, resp.

Observation 2.13. $\Psi \subseteq \Omega$ is a strongly symmetrical set exactly if $\mathfrak{S}(\Psi) \leq G$. $\Psi \subseteq \Omega$ is a weakly symmetrical set exactly if either $|\Psi| \geq 3$ and $\mathfrak{A}(\Psi) \leq G$, or $|\Psi| = 2$ and $\mathfrak{S}(\Psi) \leq G$, or $|\Psi| = 2$ and there exists a proper superset $\Psi' \supset \Psi$ such that $\mathfrak{A}(\Psi') \leq G$.

Definition 2.14. Let $T \subseteq \Omega$ be a smallest subset of Ω such that $\Omega \setminus T$ is a weakly symmetrical set. We call |T| the symmetry defect of G and the quotient |T|/n the relative symmetry defect of G, where $n = |\Omega|$.

Definition 2.15. Let $\mathfrak{X} = (\Omega; \mathcal{R})$ be a relational structure. We say that $x, y \in \Omega$ are strong twins for \mathfrak{X} if they are strong twins for $\operatorname{Aut}(\mathfrak{X})$. We analogously transfer all concepts introduced in this section from groups to structures via their automorphism groups (weak twins, strongly/weakly symmetrical sets, symmetry defect). For instance, the (relative) symmetry defect of \mathfrak{X} is the (relative) symmetry defect of $\operatorname{Aut}(\mathfrak{X})$.

Observation 2.16. Given an explicit relational structure \mathfrak{X} with vertex set Ω , one can find the maximal weakly symmetrical subsets of Ω in polynomial time. Consequently, the (relative) symmetry defect of \mathfrak{X} can also be determined in polynomial time.

Proof. Test, for each transposition and 3-cycle $\sigma \in \mathfrak{S}(\Omega)$, whether or not $\sigma \in \operatorname{Aut}(\mathfrak{X})$. Join two elements x, y of Ω by an edge if the transposition $(x, y) \in \operatorname{Aut}(\mathfrak{X})$ or there exists $z \in \Omega$ such that the 3-cycle $(x, y, z) \in \operatorname{Aut}(\mathfrak{X})$. The connected components of this graph are the maximal symmetrical sets.

Proposition 2.17. Let \mathfrak{X} be a k-ary relational structure on the vertex set Ω and $\Psi \subset \Omega$ such that $|\Psi| \ge k+2$. If Ψ is weakly symmetrical then Ψ is strongly symmetrical. In other words, any k+2 vertices that are pairwise weak twins are pairwise strong twins.

Proof. We need to show that if $\mathfrak{A}(\Psi) \leq \operatorname{Aut}(\mathfrak{X})$ then $\mathfrak{S}(\Psi) \leq \operatorname{Aut}(\mathfrak{X})$. Let $x, y \in \Psi, x \neq y$, and let $\tau = (x, y)$ be the corresponding transposition. Suppose for a contradiction that $\tau \notin \operatorname{Aut}(\mathfrak{X})$ and let $i \leq r$ and $\vec{x} = (x_1, \ldots, x_k) \in R_i$ be a witness of this, i.e., $\vec{x}^{\tau} \notin R_i$. Let $u, v \in \Psi \setminus \{x_1, \ldots, x_k\} \ u \neq v$, and let $\sigma = (x, y)(u, v)$ (product of two transpositions). So $\sigma \in \mathfrak{A}(\Psi)$ and therefore $\sigma \in \operatorname{Aut}(\mathfrak{X})$. But $\vec{x}^{\sigma} = \vec{x}^{\tau} \notin R_i$, a contradiction.

Definition 2.18. A digraph is a pair X = (V, E) where $E \subseteq V \times V$ is a binary relation on V. The out-degree of vertex $u \in V$ is the number of $v \in V$ such that $(u, v) \in E$. Indegree is defined analogously. X is biregular if all vertices have the same in-degree and the same out-degree (so these two number are also equal). The diagonal of V is the set $\operatorname{diag}(V) = \{(x, x) \mid x \in V\}$. X is irreflexive if $E \cap \operatorname{diag}(V) = \emptyset$. The irreflexive complement of an irreflexive digraph X = (V, E) is X' = (V, E') where $E' = V \times V \setminus (\operatorname{diag}(V) \cup E)$. X is trivial if $\operatorname{Aut}(X) = \mathfrak{S}(V)$, i. e., E is one of the following: the empty set, $V \times V$, $\operatorname{diag}(V)$, or $V \times V \setminus \operatorname{diag}(V)$. A subset of $A \subseteq V$ is independent if it spans no edges, i. e., $E \cap A \times A = \emptyset$. Note that an independent set cannot contain a self-loop, i. e., a vertex x such that $(x, x) \in E$.

The following observation is well known. It will be used directly in Case 3a2 in Section 7.8 and indirectly through Cor. 2.20 below.

Proposition 2.19. Let X = (V, E) be a nontrivial biregular digraph. Then X has no independent set of size greater than n/2 where n = |V|.

Proof. Let $A \subseteq V$ be an independent set. Then $V \setminus A$ has to absorb all edges emanating from A,

The following corollary will be used in item 2b2 of the algorithm described in Section 10.2.

Corollary 2.20. Let X = (V, E) be a nontrivial irreflexive biregular digraph with $n \ge 4$ vertices. Then the relative symmetry defect of X is $\ge 1/2$.

Proof. Let $A \subseteq V$ be a (weakly) symmetrical set with ≥ 3 vertices. So Aut $(X) \geq \mathfrak{A}(A)$. Then A is either an independent set in X, or independent in the irreflexive complement of X. In both cases, Prop. 2.19 guarantees that $|A| \leq n/2$.

2.5 Classical coherent configurations, UPCCs

Continuing our discussion of k-ary coherent configurations (Sec. 2.3), we now turn to the classical case, k = 2. A *(classical) coherent configuration* is a binary (2-ary) coherent configuration. If we don't specify arity, we mean the classical case and usually omit the adjective "classical." Coherent configurations are the stable configurations of the classical Weisfeiler-Leman canonical refinement process [WeL, We] see Sec. 2.9.

Let us review the definition, starting with binary configurations.

Recall that diag $(\Omega) = \{(x,x) \mid x \in \Omega\}$ denotes the diagonal of the set Ω . For a relation $R \subseteq \Omega \times \Omega$ let $R^{-1} = \{(y,x) \mid (x,y) \in R\}$.

We call a binary relational structure $\mathfrak{X} = (\Omega; R_1, \ldots, R_r)$ $(R_i \subseteq \Omega \times \Omega)$ a binary configuration if

- (i) the R_i are nonempty and partition $\Omega \times \Omega$
- (ii) $(\forall i)(R_i \subseteq \operatorname{diag}(\Omega) \text{ or } R_i \cap \operatorname{diag}(\Omega) = \emptyset$
- (iii) $(\forall i)(\exists j)(R_i^{-1} = R_j)$

(This is the binary case of the k-ary configurations defined in Section 2.3.) The rank of \mathfrak{X} is r; so if $|\Omega| \ge 2$ then $r \ge 2$. If $(x, y) \in R_i$ we say that the color of the pair (x, y) is c(x, y) = i. We designate c(x, x) to be the color of the vertex x.

We call the digraphs $X_i = (\Omega, R_i)$ the constituents of \mathfrak{X} .

In accordance with Sec. 2.3, we say that the configuration \mathfrak{X} is *coherent* if

(iv)
$$(\forall i, j, k \leq r) (\exists p_{ij}^k) (\forall (x, y) \in R_k) (|\{z \mid (x, z) \in R_j \text{ and } (z, y) \in R_j\}| = p_{ij}^k$$

For the rest of this section, let $\mathfrak{X} = (\Omega; R_1, \ldots, R_r)$ be a coherent configuration. Let $n = |\Omega|$.

A graph X = (V, E) can be viewed as a configuration $\mathfrak{X}(X) = (V; \operatorname{diag}(V), E, \overline{E})$ where the edge set E is viewed as an irreflexive, symmetric relation and $\overline{E} = V \times V \setminus (\operatorname{diag}(V) \cup E)$ is the set of edges of the complement of X.

The configuration $\mathfrak{X}(X)$ has rank 3 unless X is the empty or the complete graphs (empty relations are omitted), in which case it has rank 2.

The configuration $\mathfrak{X}(X)$ is coherent if and only if X is a strongly regular graph.

Definition 2.21. The clique configuration $\mathfrak{X}(K_n)$ has *n* vertices and rank 2: the constituents are the diagonal diag $(\Omega) = \{(x, x) \mid x \in \Omega\}$, and the rest: $\Omega \times \Omega \setminus \text{diag}(\Omega)$. We also refer to the clique configuration as the *trivial configuration*.

Alternatively, the clique configuration can be defined as the unique (up to naming the relations) configuration of which \mathfrak{S}_n is the automorphism group.

Since diagonal and off-diagonal colors must be distinct, the rank is $r \ge 2$ (assuming $n \ge 2$). The only rank-2 configuration is the clique configuration.

Recall that the color of a vertex x is defined as c(x) = c(x, x). Let C_1, \ldots, C_s be the vertex color classes; they partition Ω . The following observation will be useful.

Proposition 2.22 (Induced subconfiguration). Let $\Delta \subseteq \Omega$ be the union of some of the vertex color-classes and let \mathfrak{X}^{Δ} denote the subconfiguration induced in Δ . Then \mathfrak{X}^{Δ} is coherent.

Note that for $x, y \in \Omega$, the color c(x, y) determines the colors c(x) and c(y).

We call the digraph $X_i = (V, R_i)$ the color-*i* constituent digraph of \mathfrak{X} . It follows from the previous paragraph that either all vertices of X_i have the same color (" X_i is homogeneous") or they belong to two color classes, say C_j and C_ℓ , $j \neq \ell$, and $R_i \subseteq C_j \times C_\ell$ (" X_i is bipartite").

Definition 2.23 (Equipartition). An *equipartition* of a set Ω is a partition of Ω into blocks of equal size.

Proposition 2.24 (Bipartite connected components). If X_i is a constituent digraph with vertices in color classes C_j and C_ℓ then X_i is biregular (all vertices in C_j have the same degree and the same holds for C_ℓ) and the weakly connected components of X_i equipartition each of the two color classes. In particular, all weakly connected components of X_i have the same number of vertices.

Proposition 2.25 (Homogeneous connected components). If X_i is a homogeneous constituent in color class C_j then each weakly connected component of X_i is strongly connected, and the connected components equipartition C_j .

Corollary 2.29 below will be used in the justification of one of our main algorithms, see Lemma 7.17. We start with three preliminary lemmas.

Lemma 2.26 (Neighborhood of connected component of constituent). Let $\mathfrak{X} = (\Omega; \mathcal{R})$ be a coherent configuration. Let C_1 and C_2 be two distinct vertex-color classes. Let B_1, \ldots, B_m be the connected components of the homogeneous constituent digraph $X_3 = (C_1, R_3)$ in C_1 and let $X_4 = (C_1, C_2; R_4)$ be a bipartite constituent between C_1 and C_2 . For $j = 1, \ldots, m$ let M_j denote the set of vertices $v \in C_2$ such that there exists $w \in C_1$ such that c(w, v) = 4. Then $|M_1| = \cdots = |M_m|$.

Proof. Let $J = \{j \mid (\exists u \in C_1, v \in C_2) (c(u, v) = j)\}$. For each color j, the number $d_j = p(1, j, j^{-1})$ is the out-degree of each vertex in C_1 in the constituent $X_j = (C_1, C_2; R_j)$. Let $x \in B_i$. Let $N_j(x) = \{y \in C_2 \mid c(x, y) = j\}$. So $|N_j(x)| = d_j$. For $y \in N_j(x)$, let f(k, j) denote the number of walks of length k starting from x, ending at y, and consisting of k - 1 steps of color 3 and one step of color 4. By coherence, this number does not depend on the

choice of either x or y, only on the color j = c(x, y), justifying the notation f(k, j). Such a walk stays in B_i for the first k-1 steps, and moves to C_2 along an edge of color 4 in the last step. Let K be the set of those j for which $(\exists k)(f(k, j)) > 0$. Clearly, $M_i = \bigcup_{j \in K} N_j(x)$ and therefore $|M_i| = \sum_{j \in K} d_j$. This number does not depend on i.

Lemma 2.27. Using the notation of Lemma 2.26, let $x \in C_1$ and $y \in C_2$ such that c(x, y) = 4. Assume $x \in B_i$. Let $M(x, y) = \{z \in B_i \mid c(z, y) = 4\}$. Then |M(x, y)| does not depend on the choice of x and y.

Proof. Let *L* be the set of those colors *j* for which $p(j, 4, 4^{-1}) > 0$ and for which there exists a pair (u, v) of vertices such that c(u, v) = j and there exists a walk from *u* to *v* solely along steps of color 3. The existence of such a walk does not depend on the choice of *u* and *v*, only on c(u, v). Therefore, $M(x, y) = \bigcup \{N_j(x) \mid j \in M\}$ and so $|M(x, y)| = \sum_{j \in L} d_j$, independent of the choice of *x* and *y*.

Lemma 2.28. Using the notation of Lemma 2.26, for $y \in C_2$ let E(y) denote the set of those *i* for which there exists $x \in B_i$ satisfying c(x, y) = 4. Then |E(y)| does not depend on y.

Proof. Let q = |M(x,y)| > 0 be the quantity shown not to depend on x, y in Lemma 2.27 (c(x,y) = 4). Now $d_{4^{-1}} = q|E(y)|$ by Lemma 2.27.

Corollary 2.29 (Contracting components). Using the notation of Lemma 2.26, let Y be the graph $Y = (C_2, [m]; E)$ where $(y, i) \in E$ if $(\exists x \in B_i)(c(x, y) = 4)$. Then Y is biregular.

Proof. Regularity on the [m] side is the content of Lemma 2.26. Regularity on the C_2 side is the content of Lemma 2.28.

Next we formalize the statement that \mathfrak{X} is "aware" of the "strong twin" relation.

- **Proposition 2.30.** (i) If x, y are strong twins and c(x, y) = c(u, v) then u, v are strong twins.
- (ii) Every strong-twin-equivalence class is homogeneous (all of its vertices have the same color).
- (iii) Let C be a vertex-color class. Then the pairs of strong twins in C form a constituent digraph R_i .
- (iv) Every vertex-color class that includes strong twins is equipartitioned by its strong-twinequivalence classes.
- (v) If $x, y, z, w \in \Omega$ are pairwise weak twins then they are pairwise strong twins.

Proof. The statement "x, y are strong twins" is equivalent to " $(\forall z \notin \{x, y\})(c(z, x) = c(z, y)$." If $c(x, y) = i_0$ then this is equivalent to saying that $(\forall i_1, i_2 \leq r)(p(i_0, i_1, i_2) \neq 0 \implies i_1 = i_2)$. So the validity of this statement only depends on i_0 . This proves item (i).

Item (ii) holds because automorphisms preserve vertex color. Item (iii) follows from item (i) and the fact that automorphisms preserve edge color. Item (iv) now follows from Prop. 2.25. Item (v) is a special case of Prop. 2.17 (case k = 2).

Remark 2.31. It is easy to see that ternary (3-ary) coherent configurations are "aware" of the "weak twin" relation. More precisely, if \mathfrak{X} is a ternary coherent configuration then items (i)–(iv) hold. (Recall that c(x, y) := c(x, y, y).)

Recall that \mathfrak{X} is *homogeneous* if all vertices have the same color.

Definition 2.32. \mathfrak{X} is *primitive* if it is homogeneous and all constituent digraphs other than the diagonal are connected. \mathfrak{X} is *uniprimitive* if it is primitive and has rank ≥ 3 , i.e., it is not the clique configuration.

Notation 2.33. We abbreviate "uniprimitive coherent configuration" as UPCC.

Combinatorial properties of UPCCs have been studied by the author in [Ba81] and in great depth by Sun and Wilmes in [SuW]. UPCCs play a important role in the study of GI as the obstacles to a natural combinatorial partitioning approach. One of the main technical contributions of this paper is that we overcome this obstacle (Section 7).

2.6 Association schemes, Johnson schemes

We say that the coherent configuration \mathfrak{X} is an association scheme if c(x, y) = c(y, x) for every $x, y \in \Omega$. It follows that association schemes are homogeneous.

A particular class of association schemes will be of great interest to us.

Let $t \geq 2$ and $k \geq 2t + 1$. The Johnson scheme $\mathfrak{J}(k,t) = (\Omega; R_0, \ldots, R_t)$ is an association scheme with $\binom{k}{t}$ vertices corresponding to the *t*-subsets of an *k*-set Γ . We identify Ω with the set $\Omega = \binom{\Gamma}{t}$. The relation R_i consists of those pairs (T_1, T_2) $(T_j \subset \Gamma, |T_j| = t)$ with $|T_1 \setminus T_2| = i$.

An important functor (see Section 4) maps the category of k-sets to the category of Johnson schemes $\mathfrak{J}(k,t)$. This functor is *surjective* (on $\mathrm{Iso}(\mathfrak{X},\mathfrak{Y})$ for any pair $(\mathfrak{X},\mathfrak{Y})$ of objects). The principal content of this nontrivial statement is the following.

Proposition 2.34. If $t \ge 2$ and $m \ge 2t + 1$ then $\operatorname{Aut}(\mathfrak{J}(m, t)) = \mathfrak{S}^{(t)}(\Gamma)$.

2.7 Hypergraphs

2.7.1 Basic terminology

A hypergraph $\mathcal{H} = (V, \mathcal{E})$ consists of a vertex set V and a subset \mathcal{E} of the power-set of V. We say that \mathcal{H} is *d*-uniform if |E| = d for all $E \in \mathcal{E}$.

We say that \mathcal{H} is an *empty hypergraph* if $\mathcal{E} = \emptyset$. The *complete d-uniform hypergraph* has edge set $\mathcal{E} = \begin{pmatrix} V \\ d \end{pmatrix}$. The *trivial d*-uniform hypergraphs are the empty and the complete ones. In other words, a *d*-uniform hypergraph is trivial if its automorphism group is $\mathfrak{S}(V)$.

The degree of a vertex $x \in V$ is the number of edges containing x. \mathcal{H} is r-regular if every vertex has degree r.

Definition 2.35 (Induced subhypergraph). For a subset $W \subseteq V$ we define the *induced* subhypergraph $\mathcal{H}[W]$ as follows: the vertex set of $\mathcal{H}[W]$ is W and $E \in \mathcal{E}$ is an edge of $\mathcal{H}[W]$ if and only if $E \subseteq W$.

In particular, every induced subhypergraph of a *d*-uniform hypergraph is *d*-uniform.

Definition 2.36 (Trace of hypergraph). Let $\mathcal{H} = (V, \mathcal{E})$ be a hypergraph. The *trace* \mathcal{H}_S on the set $S \subseteq V$ is the set $\{E \cap S \mid E \in \mathcal{E}\}$.

We can treat *d*-uniform hypergraphs as *d*-ary relational structures (V, R) with a symmetric relation $R \subseteq \Omega^d$, i. e., $(\forall \pi \in \mathfrak{S}_k)(R^{\pi} = R)$, with the additional condition that if $(x_1, \ldots, x_d) \in$ R then all the x_i are distinct. So some results on *d*-ary relational structures apply to *d*uniform hypergraphs. We shall in particular apply the Design Lemma (Theorem 6.1) to uniform hypergraphs.

2.7.2 Random hypergraphs

Let |V| = n, $d \leq n$, and $m \leq {n \choose d}$. Following Erdős and Rényi, by a random d-uniform hypergraph with n vertices and m edges we mean a uniform random member of the set $\operatorname{Hyp}_d(n,m) = {\binom{V}{d}}$. We are concerned with very sparse hypergraphs. For $X \in \operatorname{Hyp}_d(n,m)$, let U(X) denote the union of all edges of X. We call U(X) the support of X. Obviously $|U(X)| \leq md$. The following observation will be used in Section 7.11 to justify a subroutine.

Proposition 2.37. For a random d-uniform hypergraph X with n vertices and m edges, the probability that its support has size |U(X)| < md is less than $(md)^2/n$.

It follows that if md = o(n) then the edges of a typical hypergraph with these parameters are pairwise disjoint.

Proof. Let the edges of X be E_1, \ldots, E_m (numbered uniformly at random). Let us say that $v \in V$ is a *unique vertex of* E_i if $v \in E_i \setminus W_i$ where $W_i = \bigcup_{j:j \neq i} E_j$. Let ξ_i denote the number of unique vertices of E_i . So $|U(X)| \geq \sum \xi_i$. Let \mathbb{E} stand for expected value.

Claim. $\mathbb{E}(\xi_i) \ge d - (m-1)d^2/n$.

Proof. Let $\eta_i = d - \xi_i = |E_i \cap W_i|$. So our claim says that $\mathbb{E}(\eta_i) \leq (m-1)d^2/n$. Let us fix the set $\mathcal{E}_i = \{E_j \mid 1 \leq j \leq m, j \neq i\}$ edges other than E_i and let η denote η_i conditioned on the given choice of \mathcal{E}_i .

We claim that for every \mathcal{E}_i we have $\mathbb{E}(\eta) \leq (m-1)d^2/n$.

The edge E_i is chosen uniformly at random from $\binom{V}{d} \setminus \mathcal{E}_i$. Let F be chosen uniformly at random from $\binom{V}{d}$ and let $\zeta = |F \cap W_i|$. Now if $F \in \mathcal{E}_i$ then $\zeta = d$, so $\mathbb{E}(\zeta) = \epsilon d + (1 - \epsilon)\mathbb{E}(\eta) > E(\eta)$, where $\epsilon = (m-1)/\binom{n}{d}$. We claim that $E(\zeta) \leq (m-1)d^2/n$. Indeed, we have $\mathbb{E}(|F \cap W_i|) = |F||W_i|/n \leq (m-1)d^2/n$.

It follows from the Claim that $\mathbb{E}(|U(X)|) \geq \sum_i \mathbb{E}(\xi_i) \geq md - m(m-1)d^2/n$. Let $\theta = md - |U(X)|$. So $\mathbb{E}(\theta) \leq m(m-1)d^2/n$. But $\theta \geq 0$, so by Markov's inequality, $\mathbb{P}(\theta \geq 1) \leq \mathbb{E}(\theta) \leq m(m-1)d^2/n < (md)^2/n$.

2.7.3 Twins, symmetry defect

In Section 2.4 we defined concepts of weak/strong twins, weakly/strongly symmetrical sets, (relative) symmetry defect for relational structures via their automorphism groups. We make the analogous definitions for hypergraphs, so for instance the symmetry defect of the hypergraph \mathcal{H} is the symmetry defect of Aut(\mathcal{H}).

Proposition 2.38 (Weak is strong). Let $\mathcal{H} = (V, \mathcal{E})$ be a hypergraph and $x, y \in V$, $x \neq y$. If x and y are weak twins then they are strong twins.

Proof. Let $\sigma = (x, y, z)$ be a 3-cycle in $\mathfrak{S}(V)$ and let $\tau = (x, y)$ (transposition). We need to show that if $\sigma \in \operatorname{Aut}(\mathcal{H})$ then $\tau \in \mathcal{H}$. Suppose otherwise; let $E \in \mathcal{E}$ be a witness to this, i. e., $E^{\tau} \notin \mathcal{E}$ but $E^{\sigma} \in \mathcal{E}$ and $E^{\sigma^2} \in \mathcal{E}$. It follows that one of x and y is in E and the other is not, say $x \in E$ and $y \notin E$. Now if $z \notin E$ then $E^{\tau} = E^{\sigma} \in \mathcal{E}$, a contradiction. If $z \in E$ then $E^{\tau} = E^{\sigma^2} \in \mathcal{E}$, again a contradiction.

So for hypergraphs, we can omit the adjectives "strong/weak" when talking about twins and about symmetrical sets.

2.7.4 Skeletons

The "Skeleton defect lemma" (Lemma 2.42) below will play an important role in the analysis of the Split-or-Johnson routine (see Section 7.8, Case 3b).

Definition 2.39. The *t*-skeleton of the hypergraph $\mathcal{H} = (V, \mathcal{E})$ is the *t*-uniform hypergraph $\mathcal{H}^{(t)} = (V, \mathcal{E}^{(t)})$ where $F \in {V \choose t}$ belongs to $\mathcal{E}^{(t)}$ exactly if there exists $E \in \mathcal{E}$ such that $F \subseteq E$.

Note that for d-uniform hypergraphs, viewed as d-ary relational structures, this definition does not agree with Def. 2.5, although it is similar in spirit.

Proposition 2.40. Let \mathcal{H} be a nontrivial d-uniform hypergraph with n vertices and m edges, where $d \leq n/2$. Then there exists $t \leq \min\{d, 1 + \log_2 m\}$ such that the t-skeleton $\mathcal{H}^{(t)}$ is nontrivial.

Proof. Choose t = d if $d \leq 1 + \log_2 m$. Otherwise let $t = 1 + \lfloor \log_2 m \rfloor$. Let x_1, \ldots, x_t be independently uniformly selected vertices of \mathcal{H} . The probability that all of them belong to an edge $E \in \mathcal{E}$ is $(|E|/n)^t \leq 1/2^t$. The probability that there exists an edge to which all the x_i belong is less than $m/2^t$ which is less than 1 if $t > \log_2 m$. So $\mathcal{H}^{(t)}$ is not complete. It is also not empty since $t \leq d$.

Proposition 2.41. Let $\mathcal{H} = (V, \mathcal{E})$ be a nonempty, regular, d-uniform hypergraph. Let $S \subseteq V$. Let $\alpha = |S|/|V|$. Then there is an edge $E \in \mathcal{E}$ such that $|E \cap S| \ge \alpha d$.

Proof. Let |V| = n and $|\mathcal{E}| = m$. Each vertex belongs to md/n edges, so for each vertex x, the probability that $x \in E$ for a randomly selected edge is d/n. Therefore the expected number of vertices in $|S \cap E|$ for a random edge E is $|S|d/n = \alpha d$.

Lemma 2.42 (Skeleton defect lemma). Let $\mathcal{H} = (V, \mathcal{E})$ be a nontrivial, regular, d-uniform hypergraph with n vertices and m edges where $d \leq n/2$. Let $(7/4) \log_2 m \leq t \leq (3/4)d$. Then the symmetry defect of the t-skeleton $\mathcal{H}^{(t)}$ is greater than 1/4.

Proof. Let $S \subseteq V$ be a symmetrical subset. Assume for a contradiction that $|S| \geq 3n/4$. Then, by Prop. 2.41, there is an edge $E \in \mathcal{E}$ such that $|S \cap E| \geq (3/4)d \geq t$. Let $T \subseteq S \cap E$, |T| = t. So $T \in \mathcal{E}^{(t)}$. Since S is a symmetrical set, it follows that $\binom{S}{t} \subseteq \mathcal{E}^{(t)}$. Since every edge of \mathcal{H} contains at most $\binom{d}{t}$ of these t-sets, it follows that

$$m \ge \frac{\binom{|S|}{t}}{\binom{d}{t}} > \left(\frac{3n/4}{d}\right)^t \ge \left(\frac{3}{2}\right)^t > m,\tag{7}$$

a contradiction.

2.8 Individualization and canonical refinement

Let \mathfrak{X} be a structure such as a graph, digraph, k-ary relational structure, hypergraph, with colored elements (vertices, edges, k-tuples, hyperedges). The colors form an ordered list. A *refinement* of the coloring c is a new coloring c' of the same elements such that if c'(x) = c'(y)for elements x, y then c(x) = c(y); this results in the refined structure \mathfrak{X}' . We say that the refinement is *canonical* with respect to a set $\{\mathfrak{X}_i \mid i \in I\}$ of objects of the same type if it is executed simultaneously on each \mathfrak{X}_i and for all $i, j \in I$ we have

$$\operatorname{Iso}(\mathfrak{X}'_{i},\mathfrak{X}'_{j}) = \operatorname{Iso}(\mathfrak{X}_{i},\mathfrak{X}_{j}).$$
(8)

(This is consistent with the functorial notion of canonicity explained in Sec. 4.) Naive vertex refinement (refine vertex colors by number of neighbors of each color) has been the basic isomorphism rejection heuristic for ages. More sophisticated canonical refinement methods are explained in the next section.

Another classical heuristic is *individualization:* the assignment of a unique color to an element. Let \mathfrak{X}_x denote \mathfrak{X} with the element x individualized. If the number of elements of the given type is m then individualization incurs a multiplicative cost of m: when testing isomorphism of structures \mathfrak{X} and \mathfrak{Y} , if we individualize $x \in \mathfrak{X}$, we need compare \mathfrak{X}_x with all \mathfrak{Y}_y for $y \in \mathfrak{Y}$: for any $x \in \mathfrak{X}$ we have

$$\operatorname{Iso}(\mathfrak{X},\mathfrak{Y}) = \bigcup_{y \in \mathfrak{Y}} \operatorname{Iso}(\mathfrak{X}_x,\mathfrak{Y}_y).$$
(9)

(Compare this with the more general categorical concept in Sec. 4.)

The individualization/refinement method (I/R) (individualization followed by refinement) is a powerful heuristic and has also been used to proven advantage (see e. g., [Ba79a, Ba81, BaL, BaCo, BaW1, CST, BaCh+]), even though strong limitations of its isomorphism rejection capacity have also been proven [CaiFI]. I/R combines well with the group theory method and the combination is not subject to the CFI limitations ([Ba79a, BaL, BaCo, BaCh+]). This power of this combination is further explored in this paper.

2.9 Weisfeiler-Leman canonical refinement

2.9.1 Classical WL refinement

The classical Weisfeiler-Leman ⁴ (WL) refinement [WeL, We] takes as input a binary configuration and refines it to a coherent configuration (see Sec. 2.5) as follows. The process proceeds in rounds. Let \mathfrak{X} be the input to a round of refinement. For $(x, y) \in \Omega \times \Omega$, we encode in the new color c'(x, y) the following information: the old color c(x, y), and for all $j, k \leq r$, the number $|\{z \in \Omega \mid c(x, z) = j \text{ and } c(z, y) = k\}|$. These data form a list, naturally ordered. To each list we assign a new color; these colors are sorted lexicographically.

This gives a refined coloring that defines a new configuration \mathfrak{X}' . We stop when we reach a stable configuration ($\mathfrak{X} = \mathfrak{X}'$, i. e., no refinement occurs, i. e., no R_i is split).

Observation 2.43. The stable configurations under WL refinement are precisely the coherent configurations.

The process is clearly *canonical* in the following sense. Let \mathfrak{X} and \mathfrak{Y} be configurations. We simultaneously execute each round of refinement (merging the lists of refined colors). Let \mathfrak{X}^* and \mathfrak{Y}^* be the coherent configurations obtained. then

$$. \operatorname{Iso}(\mathfrak{X}, \mathfrak{Y}) = \operatorname{Iso}(\mathfrak{X}^*, \mathfrak{Y}^*).$$
(10)

In particular, if one of the colors of \mathfrak{X}^* does not occur in \mathfrak{Y}^* then \mathfrak{X} and \mathfrak{Y} are not isomorphic, so WL gives an isomorphism rejection tool.

2.9.2 k-dimensional WL refinement

The k-ary version of this process, referred to as "k-dimensional WL refinement," was introduced by Mathon and this author [Ba79b] in 1979 and independently by Immerman and Lander [ImL] in the context of counting logic, cf. [CaiFI]. The refinement step is defined as follows. Let $\mathfrak{X} = (\Omega; R_1, \ldots, R_r)$ be a k-ary configuration (Sec. 2.3). For $\vec{x} = (x_1, \ldots, x_k) \in \Omega^k$ we encode in the new color $c'(\vec{x})$ the following information: the old color $c(\vec{x})$, and for all $i_1, \ldots, i_k \leq r$, the number $|\{y \in \Omega \mid (\forall j \leq r)(c(\vec{x}_j^y) = i_j)\}$. As before, these data form a list, naturally ordered. To each list we assign a new color; these colors are sorted lexicographically. This gives a refined coloring that defines a new configuration \mathfrak{X}' . We stop when we reach a stable configuration ($\mathfrak{X} = \mathfrak{X}'$). Observation 2.43 remains valid, as is the canonicity of the stable configuration stated in Eq. (10).

As far as I know, this paper is the first to derive analyzable gain from employing the k-dimensional WL method for unbounded values of k (or any value k > 4). (In fact, I am only aware of one paper that goes beyond k = 2 [BaCh+].) We use k-dimensional WL in the proof of the Design Lemma (Thm. 6.1). In our applications of the Design Lemma, the value of k is polylogarithmic (see Secc. 6.2, 10.2).

⁴Weisfeiler's book [We] transliterates Leman's name from the original Russian as "Lehman." However, Leman himself omits the "h." (Source: private communication by Mikhail Klin, Aug. 2006.)

2.9.3 Complexity of WL refinement.

The stable refinement (k-ary coherent configuration) can trivially be computed in time $O(k^2n^{2k+1})$ and nontrivially in time $O(k^2n^{k+1}\log n)$ [ImL, Sec. 4.9].

3 Algorithmic setup

3.1 Luks's framework

In this section we review Luks's framework using notation and terminology that better suits our purposes.

Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group acting on the domain Ω . G will be represented concisely by a list of generators; if $|\Omega| = n$ then every minimal set of generators has $\leq 2n$ elements [Ba86].

Let Σ be a finite alphabet. We consider the set of strings \mathfrak{x} over the alphabet Σ indexed by Ω , i.e., mappings $\mathfrak{x} : \Omega \to \Sigma$. For $\tau \in \mathfrak{S}(\Omega)$ and $\mathfrak{x} : \Sigma \to \Omega$ we define the string \mathfrak{x}^{τ} by setting $\mathfrak{x}^{\tau}(u) = \mathfrak{x}(u^{\tau^{-1}})$ for all $u \in \Omega$. In other words, for all $u \in \Omega$ and $\tau \in \mathfrak{S}(\Omega)$,

$$\mathfrak{x}^{\tau}(u^{\tau}) = \mathfrak{x}(u). \tag{11}$$

(The purpose of the inversion is to ensure that $\mathfrak{x}^{\sigma\tau} = (\mathfrak{x}^{\sigma})^{\tau}$ for $\sigma, \tau \in \mathfrak{S}(\Omega)$.)

For $K \subseteq \mathfrak{S}(\Omega)$ we say that τ is a *K*-isomorphism of strings \mathfrak{x} and \mathfrak{y} if $\tau \in K$ and $\mathfrak{x}^{\tau} = \mathfrak{y}$. Let $\operatorname{Iso}_K(\mathfrak{x}, \mathfrak{y})$ denote the set of *K*-isomorphisms of \mathfrak{x} to \mathfrak{y} :

$$\operatorname{Iso}_{K}(\mathfrak{x},\mathfrak{y}) = \{\tau \in K \mid \mathfrak{x}^{\tau} = \mathfrak{y}\} = \{\tau \in K \mid (\forall u \in \Omega)(\mathfrak{x}(u) = \mathfrak{y}(u^{\tau})\}$$
(12)

and let $\operatorname{Aut}_K(\mathfrak{x}) = \operatorname{Iso}_K(\mathfrak{x}, \mathfrak{x})$ denote the set of K-automorphisms of \mathfrak{x} .

Remark 3.1. The only context in which we use this concept is when K is a coset. However, the general principles are more transparent in this more general context.

In the Introduction we stated the String Isomorphism decision problem: "Is $\text{Iso}_G(\mathfrak{x}, \mathfrak{y})$ not empty?" In the rest of the paper we shall use the term "String Isomorphism problem" for the computation version (compute the set $\text{Iso}(\mathfrak{x}, \mathfrak{y})$). The decision and computation versions are polynomial-time equivalent (under Cook reductions).

Definition 3.2 (String Isomorphism Problem).

generators of the group $\operatorname{Aut}_G(\mathfrak{x})$ and a coset representative $\sigma \in \operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$.

For $K \subseteq \mathfrak{S}(\Omega)$ and $\sigma \in \mathfrak{S}(\Omega)$ we note the *shift identity*

$$\operatorname{Iso}_{K\sigma}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{K}(\mathfrak{x},\mathfrak{y}^{\sigma^{-1}})\sigma.$$
(13)

For the purposes of recursion we need to introduce one more variable, a subset $\Delta \subseteq \Omega$ to which we shall refer as the *window*.

Definition 3.3 (Window isomorphism). Let $\Delta \subseteq \Omega$ and $K \subset \mathfrak{S}(\Omega)$. Let

$$\operatorname{Iso}_{K}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \{\tau \in K \mid (\forall u \in \Delta)(\mathfrak{x}(u) = \mathfrak{y}(u^{\tau}))\}.$$
(14)

For $K \subseteq \mathfrak{S}(\Omega)$ and $\sigma \in \mathfrak{S}(\Omega)$ we again have the *shift identity*:

$$\operatorname{Iso}_{K\sigma}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{K}^{\Delta}(\mathfrak{x},\mathfrak{y}^{\sigma^{-1}})\sigma.$$
(15)

Remark 3.4 (Alignment). Applying Eq. (13) to a subgroup $K = G \leq \mathfrak{S}(\Omega)$, we see that the isomorphism problem for the pair $(\mathfrak{x}, \mathfrak{y})$ of strings with respect to a coset $G\sigma$ is the same as the isomorphism problem for $(\mathfrak{x}, \mathfrak{y}^{\sigma^{-1}})$ with respect to the group G. In view of Eq. (15), the same holds for window-isomorphism. The shift $\mathfrak{y} \leftarrow \mathfrak{y}^{\sigma^{-1}}$ is an important **alignment step** that will accompany every reduction of the ambient group G.

Remark 3.5. When applying the concept of window-isomorphism, we shall always assume that the window is *invariant* under the group $G \leq \mathfrak{S}(\Omega)$, and K is a coset, $K = G\sigma$ for some $\sigma \in \mathfrak{S}(\Omega)$. Under these circumstances we make the following observations.

(i) $\operatorname{Aut}_{G}^{\Delta}(\mathfrak{x})$ is a subgroup of $\mathfrak{S}(\Omega)$

(ii) $\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x},\mathfrak{y})$ is either empty or a right coset of $\operatorname{Aut}_{G}^{\Delta}(\mathfrak{x})$, namely,

$$\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \operatorname{Aut}_{G}^{\Delta}(\mathfrak{x})\sigma \quad \text{for any} \quad \sigma \in \operatorname{Iso}(\mathfrak{x},\mathfrak{y})$$
(16)

However, again, the general principles are more transparent in the more general context where K is an arbitrary subset of $\mathfrak{S}(\Omega)$ and Δ is an arbitrary subset of Ω .

The following straightforward identity plays a central role in Luks's method. Let $K, L \subseteq \mathfrak{S}(\Omega)$ and $\Delta \subseteq \Omega$. Then

$$\operatorname{Iso}_{K\cup L}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{K}^{\Delta}(\mathfrak{x},\mathfrak{y}) \cup \operatorname{Iso}_{L}^{\Delta}(\mathfrak{x},\mathfrak{y})$$
(17)

Next we describe Luks's group-theoretic divide-and-conquer strategies.

Proposition 3.6 (Weak Luks reduction). Let $H \leq G$. Then finding $\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x}, \mathfrak{y})$ reduces to |G:H| instances of finding $\operatorname{Iso}_{H}^{\Delta}(\mathfrak{x}, \mathfrak{y}^{\sigma})$ for various $\sigma \in G$.

Proof. We can write $G = \bigcup_{\sigma} H\sigma$ where σ ranges over a set of right coset representatives of H in G. Apply Eq. (17) to this decomposition, we obtain

$$\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \bigcup_{\sigma} \operatorname{Iso}_{H\sigma}^{\Delta}(\mathfrak{x},\mathfrak{y}) = \bigcup_{\sigma} \operatorname{Iso}_{H}^{\Delta}(\mathfrak{x},\mathfrak{y}^{\sigma^{-1}})\sigma$$
(18)

where we also employed the shift identity, Eq. (15).

The following identity describes Luks's basic recurrence for sequential processing of windows. **Proposition 3.7** (Chain Rule). Let Δ_1 and Δ_2 be *G*-invariant subsets of Ω and let $\operatorname{Iso}_G^{\Delta_1}(\mathfrak{x}, \mathfrak{y}) = G_1 \sigma$, where $\sigma \in G$ and $G_1 \leq G$. Then

$$\operatorname{Iso}_{G}^{\Delta_{1}\cup\Delta_{2}}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{G_{1}\sigma}^{\Delta_{2}}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{G_{1}}^{\Delta_{2}}(\mathfrak{x},\mathfrak{y}^{\sigma^{-1}})\sigma.$$
(19)

Proof. The first equation is immediate from the definitions. The second equation uses the shift identity, Eq. (15).

We can now describe what we call "strong Luks reduction." Recall the restriction notation G^{Δ} (Notation 2.1).

Theorem 3.8 (Strong Luks reduction). Let $G \leq \mathfrak{S}(\Omega)$ and let $\Delta \subseteq \Omega$ be a *G*-invariant subset. Let $\{B_1, \ldots, B_m\}$ be a *G*-invariant partition of Δ . Let $\psi : G \to \overline{G} \leq \mathfrak{S}_m$ be the induced action of *G* on the set of blocks and let $N = \ker(\psi)$. Then finding $\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x}, \mathfrak{y})$ reduces to $m|\overline{G}| = m|G/N|$ instances of finding $\operatorname{Iso}_{M_i}^{B_i}(\mathfrak{x}, \mathfrak{y}^{\sigma_i})$ for the blocks B_i and certain subgroups $M_i \leq N$ and $\sigma_i \in G$.

(The cost of the reduction is polynomial per instance.)

Proof. First apply weak Luks reduction with $H = N = \ker \psi$. Then consider each B_i to be the window in succession, reducing the group at each round, following the Chain Rule. In the end, combine all the results into a single coset.

Following Luks, the way this reduction is typically used is by taking a minimal system of imprimitivity (a system with at least two blocks that cannot be made coarser, i. e., the blocks are maximal) so \overline{G} is a primitive group. Therefore the order of primitive groups involved in G (action of subgroups on a system of blocks of imprimitivity of the subgroup) is a critical parameter of the performance of Luks reduction.

A final observation: when trying to determine $\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x},\mathfrak{y})$, it suffices to consider the case $\Delta = \Omega$ (Obs. 3.10 below).

Definition 3.9 (Straight-line program). Given a group G by a list S of generators, a *straight-line program* of length ℓ in G is a sequence of length ℓ of elements of G such that each element in the sequence is either one of the generators or is a product of two elements earlier in the sequence or is the inverse of an element earlier in the sequence. We say that the straight-line program *computes* a set T of elements if the elements of T appear in the sequence and are marked as belonging to T. A subgroup is computed if a set of generators of the subgroup is computed.

Observation 3.10 (Reducing to the window). Let $G \leq \mathfrak{S}(\Omega)$ and let Δ be a *G*-invariant subset of Ω . Let \mathfrak{x}^{Δ} and \mathfrak{y}^{Δ} be the restriction of \mathfrak{x} and \mathfrak{y} to Δ , respectively. Given a straightline program of length ℓ that computes $\operatorname{Iso}_{G^{\Delta}}(\mathfrak{x}^{\Delta},\mathfrak{y}^{\Delta})$, we can, in time $O(n\ell) + \operatorname{poly}(n)$, compute $\operatorname{Iso}_{G}^{\Delta}(\mathfrak{x},\mathfrak{y})$ (where $n = |\Omega|$). *Proof.* While we concentrate on he action of the elements of G on the window, we maintain their "tails" – their action on the rest of the permutation domain. In the end we obtain a set S of elements of G that generate the reduced group $\operatorname{Aut}_{G}^{\Delta}(\mathfrak{x})$; we add to S a set of generators of the kernel of the G-action on Δ .

Once again we stress that everything in this section was a review of Luks's work.

3.2 Johnson groups are the only barriers

The barriers to efficient application of Luks's reductions are large primitive groups involved in G.

The following result reduces the Luks barriers to the class of Johnson groups at a multiplicative cost of $\leq n$.

Theorem 3.11. Let $G \leq \mathfrak{S}_n$ be a primitive group of order $|G| \geq 2^{1+\log_2 n}$ where n is greater than some absolute constant. Then G has a normal subgroup N of index $\leq n$ such that N has a system of imprimitivity on which N acts as a Johnson group $\mathfrak{A}_k^{(t)}$ with $k \geq \log_2 n$. Moreover, N and the system of imprimitivity in question can be found in polynomial time.

The mathematical part of this result is an immediate consequence of Cameron's classification of large primitive groups which we state below.

The *socle* Soc(G) of the group G is defined as the product of its minimal normal subgroups. Soc(G) can be written as $Soc(G) = R_1 \times \cdots \times R_s$ where the R_i are isomorphic simple groups.

Definition 3.12. $G \leq \mathfrak{S}_n$ is a *Cameron group* with parameters $s, t \geq 1$ and $k \geq \max(2t, 5)$ if for some $s, t \geq 1$ and k > 2t we have $n = \binom{k}{t}^s$, the socle of G is isomorphic to \mathfrak{A}_k^s , and $(\mathfrak{A}_k^{(t)})^s \leq G \leq \mathfrak{S}_k^{(t)} \wr \mathfrak{S}_s$ (wreath product, product action), moreover the induced action $G \to \mathfrak{S}_s$ on the direct factors of the socle is transitive.

Note that for $k \geq 5$ the Johnson groups $\mathfrak{S}_k^{(t)}$ and $\mathfrak{A}_k^{(t)}$ are exactly the Cameron groups with s = 1.

Theorem 3.13 (Cameron [Cam81], Maróti [Mar]). For $n \ge 25$, if G is primitive and $|G| \ge n^{1+\log_2 n}$ then G is a Cameron group.

We can further reduce Cameron groups to Johnson groups.

Proposition 3.14. If $G \leq \mathfrak{S}_n$ is a Cameron group with parameters k, t, s then $ts \leq \log_2 n$. Moreover, $s \leq \log n / \log k \leq \log n / \log 5$.

Proof. We have
$$n = {\binom{k}{t}}^s \ge (k/t)^{ts} \ge 2^{ts}$$
. Moreover, $n = {\binom{k}{t}}^s \ge k^s$.

Proposition 3.15. If $G \leq \mathfrak{S}_n$ is a Cameron group with parameters k, t, s and $|G| \geq n^{1+\log_2 n}$ then $k \geq \log_2 n$ and s! < n, assuming n is greater than an absolute constant.

Proof. As before, we have $n \geq k^s$. On the other hand $n^{1+\log_2 n} \leq |G| \leq (k!)^s s! < k^{ks} s! \leq n^k s! < n^k (\log_2 n)^{\log_2 n} = n^{k+\log_2 \log_2 n}$. Therefore $k > \log_2 n - \log_2 \log_2 n > \log_2 n / \log 5 \geq s$. Hence, $s! < s^s \leq k^s \leq n$. Moreover, $n^{1+\log_2 n} < n^k s! < n^{k+1}$, hence $k \geq \log_2 n$.

This completes the proof of the mathematical part of Theorem 3.11. The algorithmic part is well known: Cameron groups can be recognized and their structure mapped out in polynomial time (and even in NC [BaLS]).

3.3 Reduction to Johnson groups

We summarize the reduction to Johnson groups.

Procedure Reduce-to-Johnson

Input: group $G \leq \mathfrak{S}(\Omega)$, strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$

Output: Iso_G($\mathfrak{x}, \mathfrak{y}$) or updated $\Omega, G, \mathfrak{x}, \mathfrak{y}, G$ transitive, with set \mathcal{B} of blocks on which G acts as Johnson group $\mathfrak{G} \leq \mathfrak{S}(\mathcal{B})$

1. if $G \leq \operatorname{Aut}(\mathfrak{x})$ then

if $\mathfrak{x} = \mathfrak{y}$ then return $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y}) = G$, exit else return $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y}) = \emptyset$, exit

- 2. if $|G| < C_0$ for some absolute constant C_0 then compute $\operatorname{Iso}_G(\mathfrak{x},\mathfrak{y})$ by brute force, exit
- 3. if G intransitive then apply Chain Rule
- 4. (: *G* transitive :) Find minimal block system \mathcal{B} . Let $m = |\mathcal{B}|$. Let $\mathfrak{G} \leq \mathfrak{S}(\mathcal{B})$ be the induced *G*-action on \mathcal{B} and *N* the kernel of the $G \to \mathfrak{G}$ epimorphism (: \mathfrak{G} is a primitive group :)
- 5. if $|\mathfrak{G}| < m^{1 + \log_2 m}$ then reduce G to N via strong Luks reduction
- 6. else (: \mathfrak{G} a Cameron group of order $\geq m^{1+\log_2 m}$:) reduce \mathfrak{G} to Johnson group via weak Luks reduction (: Theorem 3.11, multiplicative cost $\leq m$:)
- 7. (: 𝔅 a Johnson group :)
 return Ω, G, 𝔅, 𝔅 (Johnson group), 𝔅, 𝔅

Our contribution is a ProcessJohnsonAction routine that takes the output of the last line as input. The paper is devoted to this algorithm; it is summarized in the Master Algorithm, starting with line 2 of that algorithm (Sec. 12).

3.4 Cost estimate

We describe the recurrent estimate of the cost.

By the cost of the algorithm we mean the number of group operations performed on the domain Ω .

For a real number $x \ge 1$, let T(x) denote the worst-case cost of solving String Isomorphism for strings of length $\le x$. Let $T_{\text{trans}}(x)$ denote the same quantity restricted to transitive groups and $T_{\text{Jh}}(x)$ the same quantity further restricted to the case when G acts on a minimal system of imprimitivity as a Johnson group of order $\geq m^{1+\log_2 m}$ where *m* is the number of blocks $(2 \leq m \leq x)$. We obtain the following recurrences. Here p(x) denotes a polynomial, representing the overhead incurred in the reductions. C_1 is an absolute constant. For x < 2 we set $T(x) = T_{\text{trans}}(x) = 1$. For $x \geq C_0$ (an absolute constant), Luks reductions yield the following recurrences:

- (i) $T(x) \leq \max \{\sum T_{\text{trans}}(n_i) + p(x)\}$, where the maximum is taken over all partitions of $\lfloor x \rfloor$ as $\lfloor x \rfloor = \sum_i n_i$ into positive integers n_i , including the trivial partition $n_1 = \lfloor x \rfloor$ (Chain Rule)
- (ii) $T_{\text{trans}}(x) \leq \max\{m^{2+\log_2 m}(T(x/m) + p(x)), m(T_{\text{Jh}}(x) + p(x))\}$, where the maximum is taken over all *m* where $2 \leq m \leq x$ (strong Luks reduction; $m = n \leq x$ covers the case when *G* is primitive)

Assume we are looking for an upper bound $T_1(x)$ on T(x) that satisfies $T_1(x) \ge x^{c \log_2 x}$ for some constant c > 1 and is a "nice" function in the sense that $\log \log T_1(x) / \log \log x$ is monotone nondecreasing for sufficiently large x. In this case we can replace item (i) by

(i')
$$T(x) \le 1.1T_{\text{trans}}(x)$$

(The factor 1.1 absorbs the additive polynomial term.) Moreover, we can ignore the first part of the right-hand side of Eq. (ii) since $T_1(x)$ automatically satisfies $T_1(x) \ge m^{2+\log_2 n}(T_1(x/m) + p(x))$ (for all $m, 2 \le m \le x$, assuming x is sufficiently large), so we only need to assume

(ii') $T_{\text{trans}}(x) \le 1.1 x T_{\text{Jh}}(x).$

(Again, the factor 1.1 absorbs the additive polynomial term.) Combining inequalities (i') and (ii') we obtain

(iii) $T(x) \leq 2xT_{\mathrm{Jh}}(x)$.

Our contribution is an inequality of the form

$$T_{\rm Jh}(x) \le q(x)T(3x/4),$$
 (20)

where q(x) is a quasipolynomial function. Combining with item (iii) we obtain

$$T(x) \le 2xq(x)T(3x/4) < q(x)^2T(3x/4)$$
(21)

which resolves to $T(x) = q(x)^{O(\log x)}$, yielding the desired quasipolynomial bound on T(x).

Definition 3.16. We refer to (G, \mathcal{B}) as the Johnson case if G is a transitive group with a system \mathcal{B} of imprimitivity such that G acts on \mathcal{B} as a Johnson group $\mathfrak{S}_k^{(t)}$ or $\mathfrak{A}_k^{(t)}$. We refer to k as the Johnson parameter.

To prove Eq. (20), we define a finer complexity estimate that involves the Johnson parameter.

For real numbers $x \ge y \ge 5$, let $T_{Jh}(x, y)$ denote the maximum cost of solving all Johnson cases with $n \le x$ and Johnson parameter $\ell(x) \le k \le y$ for some specific polylogarithmic function $\ell(x)$. For $y < \max\{5, \ell(x)\}$ we set T(x, y) = 0. We obtain recurrences of the form

(iv) $T_{\rm Jh}(x) = T_{\rm Jh}(x, x)$

(v)
$$T_{\rm Jh}(x,y) \le q_1(x) \left(T(3x/4) + T_{\rm Jh}(x,0.9y) \right)$$

where $q_1(x)$ is a quasipolynomial function. An upper bound of the form $T_{\text{Jh}}(x,y) \leq T(3x/4)q_1(x)^{O(\log y)}$ follows, hence Eq. (20) with $q(x) = q_1(x)^{O(\log x)}$ and therefore

$$T(x) = q_1(x)^{O(\log^2 x)}.$$
(22)

Explanation of item (v): we shall either reduce the domain (window) size n by a positive fraction, or reduce the Johnson parameter k by a positive fraction while not increasing n, at quasipolynomial multiplicative cost. These reductions are covered under our concept of "symmetry breaking."

4 Functors, canonical constructions

It is critical that all our constructions be *canonical*. We shall employ a considerable variety of constructions, so to define canonicity for all of them at once, we find the language of categories convenient. (No "category theory" will be required, only the concept of categories and functors.)

The only type of category we consider will be *Brandt groupoids*, i.e., categories in which every morphism is invertible. Our categories will be *concrete*, i.e., the objects X have an *underlying set* $\Box(X)$ and the morphisms are mappings between the objects (bijections in our case). (Strictly speaking, \Box is a functor from the given category to Sets.) We assume \Box is *faithful*, i.e., if objects X and Y have the same underlying set $\Box(X) = \Box(Y)$ and the identity map on this set is a morphism between X and Y then X = Y. We refer to the elements of $\Box(X)$ as the *points* or the *vertices* or the *elements* of X. When using the term "category," we shall tacitly assume it is a concrete, faithful Brandt groupoid. In fact, we can limit ourselves to categories where all objects have the same underlying set, so all morphisms are permutations.

We write Iso(X, Y) for the set of $X \to Y$ morphisms and Aut(X) = Iso(X, X). For a category we write $X \in \mathcal{C}$ if X is an object in \mathcal{C} .

We shall consider categories of various types of relational structures, including uniform hypergraphs, bipartite graphs with a declared partition into first and second parts, partitions (i. e., equivalence relations), any of these structures with colored vertices and/or edges, and special subcategories of these such as uniprimitive coherent configurations. Three categories to be referred to have self-explanatory names: Sets, ColoredSets, PartitionedSets. A group $G \leq \mathfrak{S}(\Omega)$ defines the category of G-isomorphisms of strings on the domain Ω ; the natural notation for this category, the central object of study in this paper, would seem to be "G-Strings."

Given two categories \mathcal{C} and \mathcal{D} , a mapping $F_o: \mathcal{C} \to \mathcal{D}$ is *canonical* if it is the mapping of objects from a functor $F: \mathcal{C} \to \mathcal{D}$. For an object $X \in \mathcal{C}$ we shall usually only describe the construction of the object F(X); the assignment of a morphism $F(f): F(X) \to F(Y)$ to a morphism $f: X \to Y$ will usually be evident. In such a case we refer to F_o as a canonical

assignment (or, most often, a canonical construction). Canonical color refinement procedures are examples of canonical constructions.

A canonical embedding of objects from category \mathcal{D} into objects from category \mathcal{C} is a functor $F : \mathcal{C} \to \mathcal{D}$ such that for every object $X \in \mathcal{C}$ we have $\Box(F(X)) \subseteq \Box(X)$ and for each morphism $f : X \to Y$ the mapping $F(f) : F(X) \to F(Y)$ is the restriction of f to $\Box(F(X))$.

Thus, a *canonical subset* of objects in C is a canonical embedding of objects from the category **Sets** into the objects of C. Note that the vertex set of a canonically embedded object is a canonical subset. If F is a canonical embedding then the restriction of Aut(X) to $\Box(F(X))$ is a subgroup of Aut(F(X)). In particular, a canonical subset of $\Box(X)$ is invariant under Aut(X).

We say that F is a canonical embedding of objects from \mathcal{D} onto objects from \mathcal{C} if $\Box(F(X)) = \Box(X)$ for all $X \in \mathcal{C}$.

A canonical vertex-coloring of objects in C is a canonical embedding of objects from ColoredSets onto the objects of C (all vertices receive a color). Similarly, a canonical partition of objects in C is a canonical embedding of objects from PartitionedSets onto the objects of C (all vertices belong to some block of the partition).

Finally, we would like to formalize the notion of *canonicity relative to an arbitrary choice*, such as individualization. In this case we consider a canonical set of objects; the objects individually are not canonical. Here is a possible definition.

Definition 4.1 (Category of tuples). Let \mathcal{D} be a category. Let \mathcal{E} be a class of non-empty sets of objects from \mathcal{D} with the following properties:

- (i) $X, X' \in \mathfrak{X} \in \mathcal{E}$ then $\Box(X) = \Box(X')$
- (ii) if $X, X' \in \mathfrak{X} \in \mathcal{E}$ and $Y \in \mathfrak{Y} \in \mathcal{E}$ and $f \in \mathrm{Iso}(X, Y)$ then there exists $Y' \in \mathfrak{Y}$ such that $f \in \mathrm{Iso}(X', Y')$.

Under these conditions we turn \mathcal{E} into a category as follows:

(a) for $\mathfrak{X} \in \mathcal{E}$ we set $\Box(\mathfrak{X}) = \Box(X)$ for any $X \in \mathfrak{X}$

(b) for $\mathfrak{X}, \mathfrak{Y} \in \mathcal{E}$, we set $\operatorname{Iso}(\mathfrak{X}, \mathfrak{Y}) = \bigcup \{ \operatorname{Iso}(X, Y) \mid X \in \mathfrak{X}, Y \in \mathfrak{Y} \}.$

Proposition 4.2. \mathcal{E} is a category.

Proof. We need to show that the morphisms in \mathcal{E} are closed under composition. Let $f \in$ Iso $(\mathfrak{X}, \mathfrak{Y})$ and $g \in$ Iso $(\mathfrak{Y}, \mathfrak{Z})$. We need to show that $fg \in$ Iso $(\mathfrak{X}, \mathfrak{Z})$. By definition, there exist objects $X \in \mathfrak{X}$ and $Y \in \mathfrak{Y}$ such that $f \in$ Iso(X, Y). Now $g \in$ Iso(Y', Z') for some objects $Y' \in \mathfrak{Y}$ and $Z' \in \mathfrak{Z}$. By assumption (ii) there exists $Z \in \mathfrak{Z}$ such that $g \in$ Iso(Y, Z). Therefore $fg \in$ Iso $(X, Z) \subseteq$ Iso $(\mathfrak{X}, \mathfrak{Z})$.

Definition 4.3 (Reduction at multiplicative cost). By a reduction of the isomorphism problem for objects $X, Y \in \mathcal{C}$ to objects in \mathcal{D} "at multiplicative cost s" we mean a functor $F: \mathcal{C} \to \mathcal{E}$ for some category \mathcal{E} of tuples of \mathcal{D} such that |F(Y)| = s. **Proposition 4.4.** If F is a reduction of Iso(X, Y) to \mathcal{D} as above then for any $X' \in F(X)$ we have

$$Iso(X,Y) = \bigcup \{ F^{-1}(Iso(X',Y')) \mid Y' \in F(Y) \}.$$
 (23)

Moreover, the terms in this union are disjoint, and all the nonempty terms have the same cardinality.

Note that X' is fixed in this union and is chosen arbitrarily from F(X).

Proof. Clear.

So if F and F^{-1} are efficiently computable per item then the cost of computing Iso(X, Y) is essentially the cost of computing s instances of computing Iso(X', Y') in \mathcal{D} , where X' is up to us to choose from F(X).

Definition 4.5. Let F be a reduction of the isomorphism problem in \mathcal{C} to \mathcal{D} at a multiplicative cost. Consider the category \mathcal{D}^F whose objects are the pairs (X, X') where $X \in \mathcal{C}$ and $X' \in F(X)$. We set $\Box(X, X') = \Box(X)$ and $\operatorname{Iso}((X, X'), (Y, Y')) = F^{-1} \operatorname{Iso}(X', Y')$.

Proposition 4.6. C^F is a category.

Definition 4.7. Let $H : \mathcal{C}^F \to \mathcal{H}$ be a functor and let $(X, X') \in \mathcal{C}^F$. We say that F(X, X') is canonically assigned to X relative to X'.

An example of this procedure is individualization. Let \mathcal{C} have two objects, each of them a hypergraph. Suppose we individualize an ordered set of t vertices of the hypergraph X; we do the same with Y. We consider the category \mathcal{D} of all individualized versions of X and Y. The category \mathcal{E} will have two objects, the set of individualized versions of X and the set of individualized versions of Y. Suppose after some choice $\vec{u} = (u_1, \ldots, u_t)$ of the ordered set of individualized vertices we find a canonically (in \mathcal{C}^F) embedded large UPCC U in X. We then say that U is canonical *relative to* \vec{u} . For those \vec{u} for which the procedure does not work, we embed the empty UPCC. The multiplicative cost will be $s = n(n-1) \dots (n-t+1) \leq n^t$ where n is the number of vertices of X.

But this type of argument will also occur when it cannot be phrased in terms of individualizing vertices of an object; for instance, we shall canonically construct other objects and individualize vertices of those with similar effect.

We illustrate the meaning of relative canonicity in Corollary 6.10 which we restate without reference to this concept as Corollary 6.11.

5 Breaking symmetry: colored partitions

5.1 Colored α -partitions

Definition 5.1. A colored partition of a set Ω is a coloring of the elements of Ω along with a partition of each color class. We say that this is a colored equipartition if all blocks within the same color class have equal size. Given a colored partition Π , let C_1, \ldots, C_r be the color classes and $\{B_{ij} \mid 1 \leq j \leq k_i\}$ be the blocks of C_i . We say that Π is admissible if for each color

class C_i of size $|C_i| \ge 2$, all the blocks of C_i have size $|B_{ij}| \ge 2$. $(B_{ij} = C_i$ is permitted.) Let $\rho(\Pi) = \max_{i,j} |B_{ij}|$. For $0 < \alpha \le 1$, a colored α -partition is an admissible colored partition Π such that $\rho(\Pi) \le \alpha n$ where $n = |\Omega|$.

The category **ColoredPartitions** has as its objects sets with a colored partition. The morphisms are the bijection that preserve color and preserve the given equivalence relation (partition) in each color class.

Definition 5.2. A canonical colored partition of objects of a category C is a canonical embedding of objects from the category ColoredPartitions onto the objects of C.

In other words this means assigning a colored partition of the vertex set of each object in C such that isomorphisms in C preserve colors and preserve the equivalence relation on each color class.

Proposition 5.3. Given a colored partition, one can canonically refine it to a colored equipartition. Here refinement means refining the colors; the blocks will not change, so if the partition was admissibe, it remains admissible.

Proof. Encode the size of each block in the color of its elements.

Finding canonical colored 3/4-partitions will be one of our key indicators of progress.

Observation 5.4. Let $\alpha \ge 1/2$. A colored equipartition is an α -partition if either each color class has size $\le \alpha n$, or the unique color-class of size > n/2 (the "dominant color class") is nontrivially partitioned (at least two blocks, the blocks have size ≥ 2).

5.2 Effect of coloring on *t*-tuples

Let Γ be a set and $\Phi = {\Gamma \choose t}$ the set of *t*-tuples of Γ . Let $|\Gamma| = m$; so $|\Phi| = {m \choose t}$. We shall need to examine the effect of a coloring of Γ on Φ . This will be used repeatedly in Section 11.

Lemma 5.5. Let Γ be the disjoint union of color classes $\Delta_1, \ldots, \Delta_k$. This induces a canonical coloring of $\Phi = {\Gamma \choose t}$ as follows: the color of $T \in {\Gamma \choose t}$ is the vector $(|T \cap \Delta_i| | 1 \le i \le k)$. Then

- (a) the size of each color class in Φ is $\leq (2/3)|\Phi|$ with the possible exception of one of the k sets $\binom{\Delta_i}{t}$.
- (b) $\left|\binom{\Delta_i}{t}\right| / |\Phi| \le \left(|\Delta_i|/m\right)^t$.

Proof. Item (b) is trivial. We prove item (a) by induction on k. The statement is vacuously true for k = 1. The case k = 2 is the content of Prop. 5.7 below with $m_i = |\Delta_i|$ and $t_i = |T \cap \Delta_i|$. Let $k \ge 3$ and let $\Gamma' = \Delta_{k-1} \cup \Delta_k$. Apply the inductive hypothesis to the coloring $(\Delta_1, \ldots, \Delta_{k-2}, \Gamma')$ of Γ . We are done except that we need to consider the color classes included in $\binom{\Gamma'}{t}$. But applying the case k = 2 we see that all of those color classes have size $\le (2/3)\binom{|\Gamma'|}{t} < (2/3)|\Phi|$ with the possible exception of the two sets $\binom{\Delta_i}{t}$ for i = k - 1, k. \Box

Corollary 5.6. We use the notation of Lemma 5.5. Let $\alpha < 1$ and $t \geq 2$. Then any α -coloring of Γ (every color class has size $\leq \alpha |\Gamma|$) induces a max $(2/3, \alpha)$ -coloring of $\binom{\Gamma}{t}$.

Proof. Combine the two conclusions in Lemma 5.5.

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5.2.1 A binomial inequality

Proposition 5.7. Let m_1, m_2, t_1, t_2 be integers; let $m = m_1 + m_2$ and $t = t_1 + t_2$. Assume $t \le m/2$ and $t_i \ge 1$ for i = 1, 2. Then

$$\binom{m_1}{t_1}\binom{m_2}{t_2} \le \frac{2}{3}\binom{m}{t}.$$
(24)

We first make the following observation.

Claim 5.8. *Let* $1 \le k \le n - 1$ *. Then*

$$\binom{n}{k}^2 \le 4\binom{n}{k-1}\binom{n}{k+1}.$$
(25)

Proof. Expanding and simplifying, the Claim reduces to the statement

$$\frac{k+1}{k} \le 4 \cdot \frac{n-k}{n-k+1}.$$
(26)

This is true because $(k+1)/k \le 2$ and $(n-k)/(n-k+1) \ge 1/2$.

Proof of Prop. 5.7. By Claim 5.8, if $1 \le t_i \le m_i - 1$ then we have

$$\binom{m_i}{t_i}^2 \le 4 \binom{m_i}{t_i - 1} \binom{m_i}{t_i + 1}.$$
(27)

Let $a_s = \binom{m_1}{s}\binom{m_2}{t-s}$. Then, if $1 \le s \le m_i - 1$ and $1 \le t - s \le m_2 - 1$, multiplying Eq. (27) for i = 1, 2 and substituting $t_1 = s$ and $t_2 = t - s$, we obtain

$$a_s^2 \le 16a_{s-1}a_{s+1} \le 4(a_{s-1} + a_{s+1})^2 \tag{28}$$

and therefore $a_s \leq 2(a_{s-1} + a_{s+1})$. Observe that $\sum_{s=0}^t a_s = \binom{m}{t}$. It follows that under the conditions $1 \leq s \leq m_i - 1$ and $1 \leq t - s \leq m_2 - 1$ we have $(3/2)a_s \leq a_{s-1} + a_s + a_{s+1} \leq \binom{m}{t}$, hence $a_s \leq (2/3)\binom{m}{t}$, as desired.

It remains to consider the cases when $t_i = m_i$ for i = 1 or 2. Let us say i = 1, so $t_1 = m_1$. So we have

$$\binom{m_1}{t_1}\binom{m_2}{t_2} = \binom{m_2}{t_2} \le \binom{m-1}{t_2} \le \binom{m-1}{t-1} = \frac{t}{m}\binom{m}{t} \le \frac{1}{2}\binom{m}{t}.$$
 (29)

This inequality will be used many times in the analysis of our algorithms; we shall refer to it each time we find a canonical coloring of our set Γ .

We highlight a corollary that will be used in Case 2 in Sec. 7.11.1.

Corollary 5.9. Let $r \ge 1$, $t \ge 1$ and $m \ge 2t$. Then $\binom{m}{t}^r \le \left(\frac{2}{3}\right)^{r-1} \binom{mr}{tr}$.

Proof. By induction on r, using Prop. 5.7.

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6 Breaking symmetry: the Design Lemma

In this section we describe the first of two combinatorial symmetry-breaking tools.

Given a relational structure $\mathfrak{X} = (\Omega, \mathcal{R})$ with non-negligible symmetry defect (see Def. 2.14), we wish to efficiently find a subgroup $G \leq \mathfrak{S}(\Omega)$ such that G is substantially smaller than $\mathfrak{S}(\Omega)$ such that $\operatorname{Aut}(\mathfrak{X}) \leq G$. We are not able to achieve this, but we do achieve it after individualizing a small number of vertices. We divide the task into two parts: first we reduce the general case of k-ary relational structures to UPCCs (uniprimitive coherent configurations – recall that these are binary relational structures (k = 2)) (the "Design Lemma," Section 6.1), and, second, we solve the problem for UPCCs (Section 7).

6.1 The Design Lemma: reducing *k*-ary relations to binary

In this section we prove one of the main technical results of the paper.

Theorem 6.1 (Design lemma). Let $1/2 \leq \alpha < 1$ be a threshold parameter. Let $\mathfrak{X} = (\Omega, \mathcal{R})$ be a k-ary relational structure with $n = |\Omega|$ vertices, $2 \leq k \leq n/4$, and relative strong symmetry defect $\geq 1 - \alpha$. Then in time $n^{O(k)}$ we can find a sequence S of at most k - 1 vertices such that by individualizing each element of S we can find either

- (a) a canonical (relative to S) colored α -partition of the vertex set, or
- (b) a canonically (relative to S) embedded uniprimitive coherent configuration \mathfrak{X}^* on some set $W \subseteq \Omega$ of vertices of size $|W| \ge \alpha n$.

Observation 6.2. Let $DL(\alpha)$ be the statement of the Design Lemma for a particular $\alpha \ge 1/2$. If $1 > \alpha' \ge \alpha \ge 1/2$ then $DL(\alpha')$ follows from $DL(\alpha)$.

Proof. Assume $DL(\alpha)$ holds. Let $U \subseteq \Omega$ be a largest strong symmetric subset of Ω ; let $\beta = |U|/n$. Assume $\beta \leq \alpha'$ so the assumption of $DL(\alpha')$ holds.

Case 1. $\beta \leq \alpha$.

In this case we can apply $DL(\alpha)$. If $DL(\alpha)$ returns case (a) (a colored α -partition, canonical with respect to a set $S \subseteq \Omega$ with $|S| \leq k - 2$), we are done (case (a) holds for $DL(\alpha')$) because an α -partition is also an α' -partition. If $DL(\alpha)$ returns case (b) (a certain set Wwith $|W| \geq \alpha n$, canonical with respect to S) then we are done (case (b)) if $|W| \geq \alpha' n$. If $\alpha n \leq |W| < \alpha' n$ then the coloring $(W, \Omega \setminus W)$ is an α -coloring (since $\alpha \geq 1/2$), and therefore an α' -coloring, so we return case (a) for $DL(\alpha')$.

Case 2. $\alpha < \beta \leq \alpha'$.

In this case the coloring $(U, \Omega \setminus U)$ is an α' -coloring, so we return case (a) for $DL(\alpha')$.

It follows that it would suffice to prove the Design Lemma for $\alpha = 1/2$.

Remark 6.3. If we can compute $\operatorname{Aut}(\mathfrak{X}^*)$ then we achieve a major reduction in $\operatorname{Aut}(\mathfrak{X})$ because $|\operatorname{Aut}(\mathfrak{X}^*)| \leq \exp(\widetilde{O}(\sqrt{n}))$ [Ba81].

There are two ways to compute $Aut(\mathfrak{X}^*)$: either directly or recursively.

Direct computation of Aut(\mathfrak{X}^*) can be done in $\exp(\widetilde{O}(n^{1/3}))$ (Sun–Wilmes [SuW]). Using this result would yield an overall $\exp(\widetilde{O}(n^{1/3}))$ GI test, sufficient to break the decades-old $\exp(\widetilde{O}(\sqrt{n}))$ barrier.

Notation 6.4. Let $\mathfrak{X}_{(S)}$ denote the *k*-ary coherent configuration obtained from the *k*-ary relational structure \mathfrak{X} by individualizing each element of *S* and applying *k*-dimensional WL refinement.

Procedure Split-or-UPCC

01 for $S \subset \Omega$, $|S| \leq k-1$

02if no vertex-color in $\mathfrak{X}_{(S)}$ has measure $> \alpha$ 03**return** the colored partition, **exit** (: goal (a) achieved :) else (: we have a vertex-color class C(S) of measure $> \alpha$:) 04let $\mathfrak{X}^*(S)$ denote the substructure of the 2-skeleton $\mathfrak{X}^{(2)}_{(S)}$ induced on C(S) (Defs. 2.5, 2.4) 05(: $\mathfrak{X}^*(S)$ is a homogeneous classical coherent configuration :) 0607if $\mathfrak{X}^*(S)$ is imprimitive 08split C(S) into the connected components of a disconnected off-diagonal constituent 09 **return** colored partition and blocks of C(S), exit (: goal (a) achieved :) 10else (: now $\mathfrak{X}^*(S)$ is primitive :) 11 return $\mathfrak{X}^*(S)$, exit (: goal (b) achieved; $\mathfrak{X}^*(S)$ is a UPCC :)

Theorem 6.5. Under the conditions of Theorem 6.1, Procedure Split-or-UPCC terminates, achieving goals (a) or (b).

We need to justify the comment on line 11: we need to show that the configuration $\mathfrak{X}^*(S)$ returned on line 11 is not a clique configuration. The proof relies on Fisher's inequality on block designs (see "Case 1" below).

Proof. Unless we succeed already for $S = \emptyset$ on line 02, we have a (unique) color-class $C := C(\emptyset)$ of size $> \alpha n$ in $\mathfrak{X}_{(\emptyset)}$. Let $\overline{C} = \Omega \setminus C$.

The classical coherent configuration $\mathfrak{X}^*(\emptyset)$ (induced by the 2-skeleton $\mathfrak{X}^{(2)}_{(\emptyset)}$ on the vertex set C) is homogeneous (all its vertices have the same color). If it is imprimitive then we are done on line 09. If it is uniprimitive, we are done on line 11.

Henceforth we assume $\mathfrak{X}^*(\emptyset)$ is primitive but not uniprimitive, i.e., it is the clique configuration. In other words, all ordered pairs of distinct elements in C have the same color in $\mathfrak{X}^*(\emptyset)$.

Claim 6.6. No transposition of the form $\tau = (x, y)$ $(x, y \in C)$ belongs to Aut (\mathfrak{X}) .

Proof. By coherence, the color of the pair (x, y) is "aware" of whether or not $\tau \in \operatorname{Aut}(\mathfrak{X})$ (Prop. 2.30). (Alternatively, we could explicitly include this information in the color of the pair before refinement – but this is not necessary.) But this means if one such transposition belongs to $\operatorname{Aut}(\mathfrak{X})$ then all do, so $\mathfrak{S}(C) \leq \operatorname{Aut}(\mathfrak{X})$, contradicting the assumption that the relative strong symmetry defect of \mathfrak{X} is $\geq 1 - \alpha$.
For $S \subseteq \Omega$, let D(S) denote the largest color-class of $\mathfrak{X}_{(S)}$ in $C \setminus S$.

Let S be a smallest subset of Ω such that $D(S) \neq C \setminus S$. Note that $S \neq \emptyset$; we need to prove that such a subset exists at all.

Claim 6.7. S exists and $|S| \leq k - 1$.

Proof. Let $x, y \in C$, $x \neq y$. Since the transposition $\tau = (x, y)$ does not belong to Aut (\mathfrak{X}) , there exist i and $\vec{z} \in R_i$ such that $\vec{z}^{\tau} \notin R_i$. Let $\vec{z} = (z_1, \ldots, z_k)$ and let $Z = \{z_1, \ldots, z_k\}$. Individualizing each vertex in $Z \setminus \{x, y\}$ splits x from y.

If $|D(S)| \leq \alpha n$, we succeed on line 02 since individualizing S splits C into relative canonical subsets of size $\leq \alpha n$ and \overline{C} is canonical and small $(|\overline{C}| \leq (1 - \alpha)n)$. Assume now that $|D(S)| > \alpha n$.

We break the situation into two cases according to whether or not $S \subseteq C$.

Case 1. $S \not\subseteq C$.

Let $x \in S \setminus C$ and $Q = S \setminus \{x\}$. So $C \setminus Q$ is a color class in $\mathfrak{X}_{(Q)}$ and therefore in $\mathfrak{X}^*_{(Q)}$. So the vertex set of $\mathfrak{X}^*(Q)$ is $C \setminus Q = C \setminus S$.

If $\mathfrak{X}^*(Q)$ is imprimitive, we succeed on lines 07–09.

If $\mathfrak{X}^*(Q)$ is a UPCC, we succeed on line 11.

In the remaining case, $\mathfrak{X}^*(Q)$ is a clique.

Let B denote the vertex-color class of x in $\mathfrak{X}_{(Q)}$. For $y \in B$, let $M(y) = D(Q \cup \{y\})$ and $\overline{M}(y) = C \setminus M(y) \setminus Q$. Consider the hypergraph $\mathcal{H} = (C \setminus Q; \{\overline{M}(y) : y \in B\})$. This hypergraph is uniform and regular because⁵ of the coherence of $\mathfrak{X}_{(Q)}$. Moreover, \mathcal{H} is a block design (BIBD), i.e., every pair $\{u, v\} \subset C \setminus Q$ belongs to the same number of sets $\overline{M}(y)$, because of coherence (see the previous footnote) and our current assumption that $\mathfrak{X}^*_{(Q)}$ is a clique (all pairs of vertices in $D(Q) = C \setminus Q$ have the same color in $\mathfrak{X}^*_{(Q)}$).

But Fisher's inequality asserts that a BIBD has at least as many blocks as it has vertices, hence $|B| \ge |C \setminus Q|$, a contradiction because $|B| < (1 - \alpha)n \le n/4$ $|C| \ge \alpha n \ge 3n/4$, and $|Q| \le k - 2 < n/4$. This shows that Case 1 cannot occur.

Case 2. $S \subset C$.

If $|C \setminus S| \leq \alpha n$ then we already succeeded on line 02. So assume $|C \setminus S| > \alpha n$.

Let $x \in S$ and $Q = S \setminus \{x\}$. For $y \in C \setminus Q$ let $M(y) = D(Q \cup \{y\})$ and

 $\overline{M}(y) = C \setminus (M(y) \cup Q \cup \{y\})$. The value of |M(y)| does not depend on y because of the homogeneity of $C \setminus Q$ in $\mathfrak{X}_{(Q)}$. So $|M(y)| = |M(x)| = |D(S)| > \alpha n$ for every $y \in C \setminus Q$ and therefore $d := |\overline{M}(y)| < (1 - \alpha)n$. (This quantity also does not depend on y.)

Consider the following digraph X(Q) on the vertex set $C \setminus Q$: introduce the edge $y \to z$ if $z \in \overline{M}(y)$. This is a *d*-regular digraph. (Both the in-degrees and the out-degrees are equal because of homogeneity.)

Compare X(Q) with the coherent configuration $\mathfrak{X}^*(Q)$. They have the same set of vertices, $C \setminus Q$. Note that $|C \setminus Q| > |C \setminus S| > \alpha n$. Moreover, k-dimensional WL is "aware" of X(Q)(because $|Q| \le k - 2$), so $\mathfrak{X}^*(Q)$ is a refinement of X(Q) and therefore $\mathfrak{X}^*(Q)$ has rank

⁵An alternative to proving this would be to explicitly include the size of $\overline{M}(x)$ in the color of $x \in B$ and the \mathcal{H} -degree of $y \in C \setminus Q$ in the color of y. But k-dim WL is automatically "aware" of these quantities.

 $\geq 3.$ (Again, if not convinced, see the previous footnote: we could explicitly include the "edge/non-edge of X(Q)" information in the color of the pairs in $C \setminus Q$.) So if $\mathfrak{X}^*(Q)$ is primitive, we succeed in line 11; if it is imprimitive, we succeed in line 09.

6.2 Local asymmetry to global irregularity: local guides

In this section we describe one of the ways the Design Lemma will be used multiple times.

Let $|\Omega_1| = |\Omega_2| = n$ and let $k \le n/6$. Typically, k will be polylogarithmic; k is our "locality parameter."

Recall that by "categories" we mean concrete (every object has an underlying set, morphisms are mappings) Brandt groupoids (every morphism is invertible – an isomorphism) (see Sec. 4).

Let \mathcal{L} be a category with $2\binom{n}{k}$ objects, namely, an objects $X_i(L)$ for every $L \in \binom{\Omega_i}{k}$; the underlying set of these objects is L, i.e., $\Box(X_i(L)) = L$.

Let \mathcal{C} be a category with two objects, \mathfrak{X}_1 and \mathfrak{X}_2 , each with underlying sets Ω_i ($\Box(\mathfrak{X}_i) = \Omega_i$).

Definition 6.8. We say that \mathcal{L} is an *k*-local guide for \mathcal{C} if for every morphism $f : \mathfrak{X}_i \to \mathfrak{X}_j$ $(i, j \in \{1, 2\})$, the restriction of f to any $L \in \binom{\Omega_i}{k}$ is a morphism $X_i(L) \to X_j(L^f)$.

Definition 6.9. Let us say that the set $L \in {\binom{\Omega_i}{k}}$ is *full* for index *i* if $\operatorname{Aut}(X_i(L)) \ge \mathfrak{A}(L)$.

Corollary 6.10 (Local guide). Let α be a threshold parameter, $3/4 \leq \alpha < 1$. Let C be a category with two objects, \mathfrak{X}_1 and \mathfrak{X}_2 , with underlying sets $\Box(\mathfrak{X}_i) = \Omega_i$ where $|\Omega_1| = |\Omega_2| = n$. Let $3 \leq k \leq n/4$. Let the category \mathcal{L} be a k-local guide to the category C. Assume further that none of the sets $L \in \binom{\Omega_1}{k}$ is full for i = 1. Then we can individualize a sequence $S \in \Omega_1^{k-2}$ of vertices of \mathfrak{X}_1 and find, in time $n^{O(k)}$, either a relatively canonical (for \mathfrak{X}_1) colored α -partition of Ω_1 or a relatively canonically (for \mathfrak{X}_1) embedded UPCC on some vertex set $W(S) \subseteq \Omega_1$ with $|W(S)| \geq \alpha n$.

To illustrate the meaning of individualization and relative canonicity, we restate this corollary without reference to those concepts.

Corollary 6.11 (Local guide, restated). Let α be a threshold parameter, $3/4 \leq \alpha < 1$. Let \mathcal{C} be a category with two objects, \mathfrak{X}_1 and \mathfrak{X}_2 , with underlying sets $\Box(\mathfrak{X}_i) = \Omega_i$ where $|\Omega_1| = |\Omega_2| = n$. Let the category \mathcal{L} be a k-local guide to the category \mathcal{C} . Assume $n \geq 4k$. Assume further that none of the sets $L \in \binom{\Omega_1}{k}$ is full for i = 1. Then, in time $n^{O(k)}$, we can either refute isomorphism of \mathfrak{X}_1 and \mathfrak{X}_2 , or, for i = 1, 2, find a set $\mathcal{S}_i \subseteq \Omega_i^{k-2}$ and for each $S \in \mathcal{S}_i$ find either a colored α -partition $\mathfrak{Y}_i(S)$ of Ω_i or a UPCC $\mathfrak{Y}_i(S)$ on some vertex set $W_i(S) \subseteq \Omega_i$, $|W_i(S)| \geq \alpha n$, such that for any $S_1 \in \mathcal{S}_1$ we have

$$\operatorname{Iso}(\mathfrak{X}_1, \mathfrak{X}_2) = \bigcup_{S_2 \in \mathcal{S}_2} \operatorname{Iso}(\mathfrak{X}_1(S_1), \mathfrak{X}_2(S_2))$$
(30)

where $f \in \operatorname{Iso}(\mathfrak{X}_1(S_1), \mathfrak{X}_2(S_2))$ if $f \in \operatorname{Iso}(\mathfrak{X}_1, \mathfrak{X}_2)$ and $S_1^f = S_2$ and $\mathfrak{Y}_1(S_1)^f = \mathfrak{Y}_2(S_2)$.

"Local asymmetry" in the title refers to the sets L not being full; global irregularity refers to the existence of a canonical structure (colored 3/4-partition or large UPCC) that drastically restricts potential isomorphisms.

Proof. We shall introduce invariants of \mathfrak{X}_i . If we find any invariant that differs for \mathfrak{X}_1 and \mathfrak{X}_2 , exit with rejection. We shall not mention this explicitly below but simply assume that the two invariants are the same for \mathfrak{X}_1 and \mathfrak{X}_2 .

In particular, we assume that none of the $L \in \binom{\Omega_2}{k}$ is full for i = 2.

For a set A, let $A^{\langle k \rangle}$ denote the set of odered k-tuples of distinct elements of A; so $A^{\langle k \rangle} \subseteq A^k$. Let $\mathcal{P}_i = \Omega_i^{\langle k \rangle}$ and $\mathcal{P} = (\mathcal{P}_1 \times \{1\}) \dot{\cup} (\mathcal{P}_2 \times \{2\})$. For $\vec{u} = (u_1, \dots, u_k) \in \mathcal{P}_i$ let $L(\vec{u}) = \{u_1, \dots, u_k\} \in {\Omega_i \choose k}$. For $i, j \in \{1, 2\}$ let $\vec{u} = (u_1, \dots, u_k) \in \mathcal{P}_i$ let $L(\vec{u}) = \{u_1, \dots, u_k\} \in {\Omega_i \choose k}$.

For $\vec{u} = (u_1, \ldots, u_k) \in \mathcal{P}_i$ let $L(\vec{u}) = \{u_1, \ldots, u_k\} \in \binom{\Omega_i}{k}$. For $i, j \in \{1, 2\}$ let $\vec{u} = (u_1, \ldots, u_k) \in \mathcal{P}_i$ and $\vec{v} = (v_1, \ldots, v_k) \in \mathcal{P}_j$. We say that the pairs (\vec{u}, i) and (\vec{v}, j) are equivalent, written as $(\vec{u}, i) \sim (\vec{v}, j)$, if there exists $\alpha \in \text{Iso}(X_i(L(\vec{u})), X_j(L(\vec{v})))$ such that $\vec{u}^{\alpha} = \vec{v}$. The ~ relation is an equivalence relation on $\mathcal{P} \times \{1, 2\}$ because \mathcal{L} is a category (closed under composition of morphisms).

Let Ξ denote the set of ~ equivalence classes. For $Q \in \Xi$, let $Q_i = \{\vec{u} \mid (\vec{u}, i) \in Q\}$. Since \mathcal{L} is a k-local guide for \mathcal{C} , it follows that the assignment $\mathfrak{X}_i \mapsto Q_i$ is canonical (for \mathcal{C}) for each Q. Let $\mathfrak{Z}_i = (\Omega_i; Q_i \mid Q \in \Xi)$. These are k-ary relational structures, canonically assigned to \mathfrak{X}_i .

Claim. The strong symmetry defect of \mathfrak{Z}_i is at least n - k + 1 > 3n/4.

Proof. Indeed, no subset $L \in {\Omega_i \choose k}$ can be strongly symmetrical in \mathfrak{Z}_i since $\operatorname{Aut}(X_i(L)) \neq \mathfrak{S}(L)$.

Now apply the Design Lemma to \mathfrak{Z}_i with $\alpha = 3/4$. If a canonical colored 3/4-partition is returned, return that coloreed partition, exit.

Else (: a UPCC \mathfrak{Y}_i on a set $W_i \subseteq \Omega_i$ is returned where $|W_i| \ge 3n/4$:) if $|W_i| \le \alpha n$ then return the coloring $(W_i, \Omega_i \setminus W_i)$; otherwise return \mathfrak{Y}_i .

7 Split-or-Johnson

In this section we provide our second main combinatorial symmetry-breaking tool. The output of the Design Lemma was either a canonical colored α -partition for, say, $\alpha = 3/4$, or a canonically embedded large UPCC. In this section our algorithm takes a UPCC as input and attempts to find a canonical colored α -partition for, say, $\alpha = 3/4$.

This is not always possible. Johnson schemes are barriers to good partitions; the Johnson scheme $\mathfrak{J}(m,t)$ requires a multiplicative cost of $\exp(\Omega(m/t))$ for a canonical α -partition with any constant $\alpha < 1$ to arise. This follows from Prop. 7.1 below.

Since $n = \binom{m}{t}$, this cost is prohibitive: for bounded t it results in an exponential, $\exp(\Omega(n^{1/t}))$, algorithm.

We shall demonstrate that in a well defined sense, *Johnson schemes are the only barriers*. Our algorithm takes a UPCC and returns a canonical colored 3/4-partition or a canonically embedded Johnson scheme that takes up a 3/4 fraction of the vertex set, at a quasipolynomial multiplicative cost.

This cost is equivalent to the cost of individualizing a polylogarithmic number of vertices, although this is not how it happens. Canonical auxiliary structres are constructed, and vertices of those are individualized – these could be called "ideal vertices" from the point of view of the input UPCC.

The bulk of the work is the same task – find a good partition or return a large Johnson scheme – where the input is an uneven bipartite graph with large symmetry defect. We want to partition the large part, or find an embedded Johnson scheme in it; so that part stays essentially constant, while we iteratively reduce the small part.

7.1 The resilience of Johnson schemes

Johnson schemes are highly resilient against partitioning. Here is a formal statement of this observation.

Proposition 7.1. Let $0 < \epsilon \leq 1/3$. The multiplicative cost of a (relative) canonical $1 - \epsilon$ -partition of the Johnson scheme $\mathfrak{J}(m,t)$ is $\geq (t/\epsilon)^{\epsilon m/t}$.

Proof. This is an immediate consequence of the following lemma.

Lemma 7.2. Let $G \leq \operatorname{Aut}(\mathfrak{J}(m,t))$ and $0 < \epsilon \leq 1/3$. If G is intransitive with no orbit of length $\geq (1-\epsilon)n$ (where $n = \binom{m}{t}$) is the number of vertices of $\mathfrak{J}(m,t)$) or G has an orbit of length $> (1-\epsilon)n$ on which the action of G is imprimitive then the index of G in $\operatorname{Aut}(\mathfrak{J}(m,t))$ is $m!/|G| \geq (t/\epsilon)^{\epsilon m/t}$.

Proof. Let us view G as a subgroup of \mathfrak{S}_m , so $G^{(t)} \leq \mathfrak{S}_m^{(t)}$ is the subgroup of $\operatorname{Aut}(\mathfrak{J}(m,t))$ in question. Assume $|\mathfrak{S}_m:G| < 1.9^m$ (otherwise the conclusion is amply satisfied). Let rbe the smallest value such that $|\mathfrak{S}_m:G| < \binom{m}{r}$. Then, by the Jordan–Liebeck Theorem (Thm. 8.16) we have that $G \geq (\mathfrak{A}_m)_{(T)}$ for some $T \subset [m]$, |T| < r. Let $\Gamma = [m] \setminus T$. This means that $G^{(t)} \geq \mathfrak{A}^{(t)}(\Gamma)$ so $G^{(t)}$ is primitive on a subset of size $> \binom{m-r}{t}$. But $\binom{m-r}{t}/\binom{m}{t} \geq (1-r/m)^t > 1-(rt/m)$. So we have $\epsilon \leq rt/m$ and therefore

$$|\mathfrak{S}_m:G| \ge \binom{m}{r} \ge (m/r)^r = \left((m/r)^{r/m}\right)^m \ge (t/\epsilon)^{\epsilon m/t}.$$
(31)

Remark 7.3. This result means that for fixed t (e. g., t = 2, the most severe bottleneck case for decades), the multiplicative cost of obtaining a constant-factor reduction in the domain size $n = \binom{m}{t}$ is exponential in m; and $m > n^{1/t}$.

7.2 Bipartite graphs: terminology, preliminary observations

We use the term "bipartite graph" in the sense of having a declared ordered bipartition of the vertex set. Let $X = (V_1, V_2; E)$ be a bipartite graph; here $E \subseteq V_1 \times V_2$. The vertex set

is $V_1 \cup V_2$; the V_i are its "parts." Isomorphisms of X and $X' = (V'_1, V'_2; E')$ are bijections $V_1 \cup V_2 \to V'_1 \cup V'_2$ that map V_i to V'_i and induce a bijection $E \to E'$.

We shall consider vertex-colored bipartite graphs $X = (V_1, V_2; E, f)$ where $f : V_1 \cup V_2 \rightarrow \{\text{colors}\}$; under this scenario, vertices in the two parts do not share colors. Isomorphisms preserve color by definition.

The neighborhood $N_X(v)$ (or N(v) if X is clear from the context) of vertex $v \in V_i$ is the set of vertices adjacent to v; so $N(v) \subseteq V_{3-i}$.

Recall the definition of strong and weak twins (Def. 2.11).

Definition 7.4. Let $X = (V_1, V_2; E, f)$ be a colored bipartite graph. We say that vertices $x, y \in V_i, x \neq y$ are *twins* if they have the same color (in particular, they belong to the same part) and they have the same neighborhood: N(x) = N(y). For a subset $T \subseteq V_i$ we use the phrase "all vertices in T are twins" to mean that all pairs of distinct vertices in T are twins.

It is clear that the "twin-or-equal" realtion is an equivalence relation.

Observation 7.5. In a bipartite graph the following are equivalent for vertices $x, y \ (x \neq y)$:

(a) x and y are twins;

- (b) x and y are strong twins;
- (c) x and y are weak twins.

Proof. Obvious.

As a consequence, we don't need to make a distinction between weak and strong "symmetrical sets:" a subset of V_i is symmetrical if all vertices in V_i are of the same color and all of them have the same neighborhood. The maximal symmetrical sets are the twin equivalence classes.

Definition 7.6. Let $X = (V_1, V_2; E, f)$ be a vertex-colored bipartite graph. We call a subset $T \subseteq V_i$ a symmetrical subset of V_i if $|T| \ge 2$ and all vertices in T are twins.

Definition 7.7. For $0 \le \alpha \le 1$ we say that X is α -symmetrical in part i if there is a symmetrical subset $T \subseteq V_i$ of size $|T| \ge \alpha |V_i|$.

Definition 7.8 (Biregular). We say that the bipartite graph $X = (V_1, V_2; E)$ is *biregular* if for i = 1, 2, each vertex in V_i has the same degree.

Recall that Prop. 2.24 asserts that each bipartite edge-color class in a coherent configuration is biregular. This is especially useful for us in combination with the following fact that is used to justify a subroutine in the main algorithm in this section (Sec. 7), see Lemma 7.17.

Proposition 7.9 (Biregular defect). Let $X = (V_1, V_2; E)$ be a nontrivial (not empty and not complete) biregular bipartite graph. Then the symmetry defect of V_1 in X is $\geq 1/2$.

Proof. By taking the complement if eccessary, we may assume the density of Y is $|E|/(|V_1||V_2|) \le 1/2$; so every vertex in V_i has degree $\le |V_{3-i}|/2$. Assume $S \subseteq V_i$ is symmetrical. Let $x \in V_i$ be adjacent to $y \in V_{3-i}$. But then y is adjacent to all vertices if S, so $|S| \le \deg(y) \le |V_i|/2$. \Box

7.3 Split-or-Johnson: the Extended Design Lemma

In each result in this section, canonicity involves a combination of the following categories (cf. Section 4): binary relational structures (Theorem 7.10), vertex-colored bipartite graphs (Theorem 7.11), k-ary relational structures (Theorem 7.12), and the category of colored partitions in each result.

Recall the definitions of canonical colored partition and an α -partition (Defs. 5.2 and 5.1). Recall that "UPCC" means uniprimitive coherent configuration (Def. 2.32). We can now state the two main results of Section 7.

Theorem 7.10 (UPCC Split-or-Johnson). Let $\mathfrak{X} = (V; R_1, \ldots, R_r)$ be a UPCC with n vertices and let $2/3 \leq \beta < 1$ be a threshold parameter. Then at quasipolynomial multiplicative cost we can find either

(a) a canonical colored β -partition of V, or

(b) a canonically embedded nontrivial Johnson scheme on a subset of V of size $\geq \beta n$.

(The time bounds do not depend on β .)

Theorem 7.11 (Bipartite Split-or-Johnson). Let $X = (V_1, V_2; E, f)$ be a vertex-colored bipartite graph with $|V_1| \ge 2$ and let $2/3 \le \alpha < 1$ be a threshold parameter. Assume $|V_2| < \alpha |V_1|$. Assume moreover that the symmetry defect of X on V_1 is at least $1 - \alpha$. Then at quasipolynomial multiplicative cost we can find either

(a) a canonical colored α -partition of V_1 , or

(b) a canonically embedded nontrivial Johnson scheme on a subset of V_1 of size $\geq \alpha |V_1|$.

(The time bounds do not depend on α .)

These results will be proved recursively by mutual reduction to each other.

Combining the Design Lemma and Theorem 7.10 we obtain our overall combinatorial partitioning tool, the main result of the combination of Sections 6 and 7.

Theorem 7.12 (Extended Design Lemma). Let $3/4 \leq \alpha < 1$ be a threshold parameter. Let $\mathfrak{X} = (\Omega, \mathcal{R})$ be a k-ary relational structure with n vertices, $2 \leq k \leq n/4$, and relative strong symmetry defect $> 1 - \alpha$. Then at a multiplicative cost of $q(n)n^{O(k)}$, where q(n) is a quasipolynomial function, we can find either

(a) a canonical colored α -partition of the vertex set, or

(b) a canonically embedded nontrivial Johnson scheme on a subset $W \subseteq \Omega$ of size $|W| \ge \alpha n$.

(The time bounds do not depend on α .)

7.4 Minor subroutines

First we describe a reduction of Theorem 7.10 to Theorem 7.11. The procedure will also serve as a subroutine to the algorithm for Theorem 7.11.

Lemma 7.13 (UPCC-to-bipartite). Let $\mathfrak{X} = (V; \mathcal{R})$ be a UPCC with n vertices and let $2/3 \leq \beta \leq 1$ be a threshold parameter. Then at a multiplicative cost of $\leq n$ and polynomial additive cost one can either

- (i) achieve objective (a) of Theorem 7.10, or
- (ii) reduce the given instance of Theorem 7.10 to Theorem 7.11 by computing a threshold parameter $\alpha \geq 2/3$ and a (relative) canonically embedded biregular bipartite graph $X = (V_1, V_2; E)$ with $V_1 \cup V_2 \subseteq V$, and $|V_1| \geq \beta n$ such that a solution to each part of Theorem 7.11 for X is also a solution to the corresponding part of Theorem 7.10 for \mathfrak{X} .

Proof. Let $\mathfrak{X} = (V; R_1, \ldots, R_r)$ where $R_1 = \operatorname{diag}(V)$ is the diagonal. Let d_i be the out-degree of the vertices in R_i ; so $d_1 = 1$. Pick a vertex $x \in V$. Let $C_i = \{y \in V \mid (x, y) \in R_i\}$; so $|C_i| = d_i$. Individualize x; this splits V into the (relative) canonical subsets C_i . (See the definition of relative canonicity in Sec. 4.) If $d_i \leq \beta n$ for all i, we are done (objective (a) has been achieved).

Assume now that (say) $d_2 > \beta n$; so (V, R_2) is an undirected graph (since $d_2 \ge n/2$) and its complement has diameter 2 ([Ba81, Prop. 4.10]). Let $(x, z) \in R_2$ and let $y \in V$ be such that $(x, y) \in R_i$ and $(z, y) \in R_j$ where $i, j \ge 3$. Consider the bipartite graph $X = (C_2, C_i; E)$ where $E = (C_2 \times C_i) \cap R_j$.

X is a biregular (Prop. 2.24) bipartite graph with $|C_2| > \beta n \ge 2n/3$ and therefore $|C_i| < n/3 < |C_2|/2$. We have $E \neq \emptyset$ since $(z, y) \in E$. The degree of $y \in C_i$ is $d_j < n/3 < 2n/3 \le d_2$ and therefore E is not complete, i.e., $E \neq C_2 \times C_i$. It follows that in each part, the relative symmetry defect of X is $\ge 1/2$ (Prop. 7.9).

Let now $\alpha = \beta n/d_2$. So $\alpha > \beta \ge 2/3$.

If the relative symmetry defect of X in C_2 is between 1/2 and and α then we have a canonical colored β -partition of V_1 (the nontrivial twin equivalence classes of X, one block for the vertices in C_2 without twins, and one block $V_1 \setminus C_2$).

Else, apply Theorem 7.11 to X to obtain either obtain a canonical colored α -partition of C_2 (and thereby a canonical colored β -partition of V_1 as above) or the embedded nontrivial Johnson scheme of the required size.

Our next routine takes a colored bipartite graph $X = (V_1, V_2; E)$ and helps make V_2 homogeneous. Recall that we say that $x, y \in V_1$ are *twins* if the transposition $\tau = (x, y)$ is an automorphism of X, i.e., if x and y have the same neighborhood.

Procedure Reduce-Part2-by-Color

Input: A threshold parameter α , $2/3 \le \alpha < 1$

- a colored bipartite graph $X = (V_1, V_2; E, f)$ where $|V_1| \ge 3$ and $|V_2| < \alpha |V_1|$ such that there are no twins in V_1 ;
 - a partition $V_2 = C_1 \cup C_2$ where each C_j is a union of color classes.

Output: $j \in \{1,2\}$ such that in the induced colored bipartite subgraph $X_j = X[V_1, C_j]$ the symmetry defect of V_1 is $\geq 1 - \alpha$

The procedure computes the symmetry defect of V_1 in each X_j .

Lemma 7.14. In at least one of X_1 and X_2 , the symmetry defect of V_1 is at least $1 - \alpha$.

Proof. Let $n_1 = |V_1|$. Assume for a contradiction that for j = 1, 2 there exists a subset $D_j \subseteq V_1$ of size $|D_j| > \alpha n_1$ that is symmetrical in X_j . This means all vertices in D_j are twins with respect to C_j ; therefore all vertices in $D_1 \cap D_2$ are twins in X. Since X has no twins, we infer $|D_1 \cap D_2| \le 1$. But $|D_1 \cap D_2| > (2\alpha - 1)n_1 \ge n_1/3$, so $n_1 \le 2$, a contradiction. \Box

7.5 Bipartite Split-or-Johnson

In this section and the two subsequent sections we prove Theorem 7.11.

Proof. We use the notation of Theorem 7.11. Let $n_i = |V_i|$. We view X as a vertex-colored graph where the vertex-colors discriminate between V_1 and V_2 . We may assume at all times that $|E| \leq |V_1||V_2|/2$ (otherwise take the bipartite complement). E is not empty because of the positive symmetry defect assumption.

In this proof we say that $x, y \in V_1$ are *twins* if the transposition $\tau = (x, y)$ belongs to Aut(X), i.e., x and y have the same neighborhood in X. This is the same as being *strong twins* according to definition 2.11. We note that in a bipartite graph, weak twins are automatically strong twins (Prop. 2.38), so there is no need for this distinction.

Here is the algorithm.

Procedure Bipartite Split-or-Johnson

- Input: a threshold parameter $3/4 \le \alpha < 1$ a vertex-colored bipartite graph $X = (V_1, V_2; E, f)$ such that $|V_2| < \alpha |V_1|$ and the symmetry defect of X on V_1 is at least $1 - \alpha$
- Output: Output: item (a) or (b) of Theorem 7.11.
 - 1. If $n_1 \leq C_0$ for some absolute constant C_0 , individualize $(1 \alpha)n_1$ vertices of V_1 , exit (: objective (a) achieved :)
 - 2. If $n_2 \leq q(n_1)$ for some specific quasipolynomial function q then individualize all vertices of V_2 , apply naive vertex refinement, return colored partition of V_1 , exit Claim. This is a colored α -partition.

Proof. All vertices of the same color in V_1 are twins.

3. Apply WL refinement to X. Let $\mathfrak{X} = (V; R_1, \ldots, R_r)$ denote the resulting CC and let \mathfrak{X}_i be the subconfiguration induced by V_i . Let $\mathfrak{X}_3 = (V_1, V_2; R_i \mid R_i \subseteq V_1 \times V_2)$. (: \mathfrak{X}_1 and \mathfrak{X}_2 are coherent; \mathfrak{X}_3 is a refinement of E:) (: $\operatorname{Aut}(X) = \operatorname{Aut}(\mathfrak{X}_3)$ because $\operatorname{Aut}(X) \leq \operatorname{Aut}(\mathfrak{X}_3)$ by the canonicity of \mathfrak{X}_3 ; and $\operatorname{Aut}(\mathfrak{X}_3) \leq \operatorname{Aut}(X)$ because \mathfrak{X}_3 is a refinement of E:)

- 4. If all color classes in V_1 have size $\leq \alpha n_1$ then return the colored partition of V_1 , exit (: objective (a) achieved :)
- 5. Let $W_1 \subseteq V_1$ be a color class such that $|W_1| > \alpha n_1$. Update $\alpha \leftarrow \alpha |V_1|/|W_1|, V_1 \leftarrow W_1$, X and \mathfrak{X}_i : the induced substructures on $W_1 \cup V_2$ (: \mathfrak{X}_1 is homogeneous :)
- 6. If there are twins in V₁, let {C₁,...,C_k} be the twin-equivalence classes.
 (: This is an equipartition because of the homogeneity of X₁; and each class has ≥ 2 elements by definition. :)
 Return this partition, exit. (: canonical colored 1/2-partition found :)
 (: To verify this, we need k ≥ 2. Indeed if k = 1, all elements of V₁ (previously W₁) are twins now, but then they were twins before the update, contradicting the assumption on symmetry defect. :)
- 7. (: There are no twins in V₁ :)
 If X₂ is not homogeneous, partition V₂ as V₂ = C₁ ∪C₂ where the C_i are nonempty unions of color classes. Apply procedure Reduce-Part2-by-Color (Sec. 7.4). The procedure selects j ∈ {1,2}. Update X and X_i to their induced subconfigurations on V₁ ∪ C_i (: The symmetry defect of X on V₁ is ≥ 1/3 > 1 − α :)
- 8. (: Both \mathfrak{X}_1 and \mathfrak{X}_2 are homogeneous and there are no twins in V_1 :) We need to consider the following cases:
 - (i) \mathfrak{X}_2 is imprimitive: Section 7.7
 - (ii) \mathfrak{X}_2 is primitive but not uniprimitive, i. e., \mathfrak{X} is the clique configuration (has rank 2): "block design case," Section 7.8
 - (iii) \mathfrak{X}_2 is uniprimitive but not known to be a Johnson scheme: Section 7.9
 - (iv) \mathfrak{X}_2 is a Johnson scheme: Section 7.11

Remark 7.15. An explanation to subitem (iii) of item (8). When a UPCC is received, we could determine in polynomial time whether or not it is a Johnson scheme, and if so, find an isomorphism to a Johnson scheme. But we don't investigate; the information that a given UPCC is *not* a Johnson scheme seems useless at this point (although conjecturally it could be helpful⁶.). We only land in case (iv) when the algorithm receives a UPCC explicitly labeled as a Johnson scheme. This happens in Case 1 of the "Block design case," Sec. 7.8. In this case the embedded Johnson scheme will be received along with an explicit isomorphism with some Johnson scheme $\mathfrak{J}(m, t)$.

⁶See the last question in Sec. 13.3

7.6 Measures of progress

Throughout the process, $n_1 = |V_1|$ will not increase. We say that a parameter *m* is significantly reduced if $m_{\text{new}} \leq 0.9m_{\text{old}}$. We deem to have made major progress if any of the following occurs:

- n_2 is significantly reduced
- \mathfrak{X}_2 moves from clique to UPCC while n_2 does not increase
- \mathfrak{X}_2 moves from UPCC to Johnson scheme while n_2 does not increase

7.7 Imprimitive case

Case: \mathfrak{X}_2 is a homogeneous, imprimitive coherent configuration; \mathfrak{X}_1 is homogeneous, and there are no twins in V_1 .

Lemma 7.16. Under the assumptions of item 8 in Procedure Bipartite Split-or-Johnson we can either return a canonical colored 1/2-partition of V_1 at a multiplicative cost of $< n_2$, or return, at only additive polynomial cost (no multiplicative cost) a canonical bipartite graph $Y = (V_1, W_2; F)$ such that $|W_2| \leq |V_2|/2$ such that the symmetry defect of V_1 in Y is $\geq 1/2$.

Let B_1, \ldots, B_m be the connected components of a disconnected non-diagonal color, say R_2 . The idea is either to replace V_2 by one of the blocks (reducing n_2 to $n_2/m \le n_2/2$) or to contract each block (reducing n_2 to $m \le n_2/2$), significant progress in each case. We shall see that one of these is always possible without reducing the symmetry defect on V_1 below 1/2.

Let $J = \{c(x, y) \mid x \in V_1, y \in V_2\}$. Let d_j be the degree of $y \in V_2$ in color R_j^{-1} . $(d_j$ does not depend on y because of the homogeneity of \mathfrak{X}_2 .) Note that $|J| \ge 2$ because the coloring of $V_1 \times V_2$ is a refinement of E; so $d_j < n_1$ for all $j \in J$.

Procedure ImprimitiveCase

- If (∀j ∈ J)(d_j ≤ n₁/2) then individualize some x ∈ V₂. This splits V₁ into color classes of size d_j. Return this partition of V₁, exit.
 (: canonical colored 1/2-partition of V₁ found :)
- 2. else (: for some $j \in J$ we have $d_j > n_1/2$:) For i = 1, ..., m let $Z_i = X(V_1, B_i; R_j)$.
 - (i) if (∃i)(the symmetry defect of V₁ in Z_i is ≥ 1/2) then Y ← Z_i
 (: This involves choosing i at a multiplicative cost of m. The gain is a reduction n₂ ← n₂/m :)
 - (ii) (: the symmetry defect of V_1 in each Z_i is less than 1/2:) Let $h \in J$, $h \neq j$. Let $Y = (V_1, [m]; \overline{R}_h)$ where $(x, i) \in \overline{R}_h$ if $(\exists y \in B_i)((x, y) \in R_h)$ (: contracting each block, $n_2 \leftarrow m$:)

return Y

Lemma 7.17. In subcase (ii) of item 2 (contracting the blocks), V_1 has symmetry defect $\geq 1/2$ in the contracted bipartite graph Y.

Proof. Y is biregular by Cor. 2.29. Moreover \overline{R}_h is not empty because R_h is not empty. Claim. Y is not complete.

Proof. For each $i \leq m$ there is a (unique) Z_i -twin equivalence class $C_i \subseteq V_1$ such that $|C_i| > n_1/2$.

Subclaim. $C_i \times B_i \subseteq R_j$.

Proof. The vertices of C_i are twins in Z_i . In other words, for each $x \in B_i$ the set $C_i \times \{x\}$ is monochromatic (has a single color), i. e., $C_i \times \{x\} \subseteq R_\ell$ for some $\ell \in J$. It follows that $d_\ell > n_1/2$. Therefore $\ell = j$, proving the Subclaim.

Now Y is not complete because it has no edge from i to C_i .

Since Y is biregular, nonempty and not complete, we infer by Prop. 7.9 that Y has symmetry defect $\geq 1/2$, as claimed.

This also completes the proof of Lemma 7.16.

7.8 Block design case

Assumptions: no twins in V_1 , \mathfrak{X}_2 is the clique configuration (rank-2).

Let $\mathcal{H} = (V_2, \mathcal{E})$ be the hypergraph of neighborhoods of vertices in V_1 . This hypergraph has no multiple edges because there are no twins in V_1 .

Case 1. \mathcal{H} is the complete d_1 -uniform hypergraph.

In this case V_1 can be indentified with $V_1 = \binom{V_2}{d_1}$, the vertex set of a canonically embedded Johnson scheme, achieving goal (b) of Theorem 7.11. Note that the vertices of this Johnson scheme (elements of V_1) come labeled by the d_1 -subsets of V_2 . With this we not only exit this routine but exit the main algorithm.

Case 2. There is an \mathcal{H} -twin equivalence class $C \subseteq V_2$ of size $|C| \ge n_2/2$. (Note that the vertices of C are not necessarily twins in X.)

Apply procedure Reduce-Part2-by-Color to the coloring $(C, V_2 \setminus C)$. If $V_2 \setminus C$ is selected, we have made significant progress (reduced $|V_2|$ by half). If C is selected, the vertices of C continue to be twins in the reduced \mathcal{H} which brings us to Case 1, terminating the main algorithm.

Case 3. The relative symmetry defect of \mathcal{H} is $\geq 1/2$. (Note that for hypergraphs we don't need to make the distinction between strong and weak symmetry defect, Prop. 2.38.)

Case 3a. $d_1 \leq (7/3) \log_2 n_1$.

Apply the Design lemma to \mathcal{H} , viewed as a d_1 -ary relational structure. (Multiplicative cost $n_2^{d_1} < n_2^{(7/3)\log_2 n_1}$).

Case 3a1. The Design lemma returns a canonical colored 3/4-partition of V_2 .

Recompute \mathfrak{X} and thereby \mathfrak{X}_2 . Colored (3/4)-partition on V_2 persists (colors can only get refined). Apply Reduce-Part2-by-Color to the coloring. If color class selected is greater than $3n_2/4$, this color class is equipartitioned; apply Procedure ImprimitiveCase (Sec. 7.7). In either case, significant progress: n_2 reduced to $\leq 3n_2/4$.

Case 3a2. The Design lemma returns a UPCC \mathfrak{Y} canonically embedded on a subset $W \subseteq V_2$ with $|W| \ge (3/4)n_2$.

Apply Reduce-Part2-by-Color to the partition $(W, V_2 \setminus W)$. If the procedure selects $V_2 \setminus W$, significant progress $(n_2 \text{ reduced to } \le n_2/4)$. If it selects W, go to Sec. 7.9.

Let $U \subseteq V_2$ be the part selected, and $(\mathfrak{X}_2)_{\text{new}}$ the homogeneous coherent configuration obtained on U. If $(\mathfrak{X}_2)_{\text{new}}$ is a UPCC, exit, significant progress.

If $(\mathfrak{X}_2)_{\text{new}}$ is not a UPCC, i.e., it has rank 2, then U was a clique in \mathfrak{Y} and therefore $|U| \leq |W|/2 \leq n_2/2$ by Prop. 2.19, a significant reduction of $|V_2|$.

Case 3b. $d_1 > 7/3 \log_2 n_1$.

Let $t = \lceil (7/4) \log_2 n_1 \rceil$. So $t \leq (3/4)d_1$. By Lemma 2.42, the symmetry defect of the *t*-skeleton $\mathcal{H}^{(t)}$ of \mathcal{H} is greater than 1/4. Let us apply the Design lemma to $\mathcal{H}^{(t)}$. The result is either a 3/4-partition of V_2 (done, exit),

or a UPCC on a subset of V_2 of size $\geq (3/4)n_2$ (significant progress, exit).

7.9 UPCC

Situation: \mathfrak{X}_2 is uniprimitive, not known to be a Johnson scheme, there are no twins in V_1 Apply the procedure of Lemma 7.13 ("UPCC-to-Bipartite") to \mathfrak{X}_2 with $\alpha := 2/3$.

- (I) If the algorithm of Lemma 7.13 returns a canonical colored 2/3-partition of V_2 , apply procedure Reduce-Part2-by-Color (Sec. 7.4) to reduce V_2 to one of its color classes (: significant progress :)
- (II) else (: the algorithm of Lemma 7.13 returns a canonically embedded nontrivial biregular bipartite graph $X'' = (V'_1, V'_2; E')$ with $W := V'_1 \cup V'_2 \subseteq V_2$ and $|V'_1| \ge 2/3|V_2|$. :) (: Note that $|V'_1| < |V_1|$ and $|V'_2| \le |V_2|/3$, a significantly smaller instance :)

Recursively apply Theorem 7.11 to X' with threshold parameter $\alpha = 2/3$.

If a canonical colored 2/3-partition of V'_1 is returned, add V'_2 and $V_2 \setminus W$, separately colored, to it, to obtain a canonical colored 2/3-partition of V_2 . Apply Reduce-Part2-by-Color to make significant progress (reducing n_2 by a factor of 2/3).

Else (: the algorithm returns a nontrivial Johnson scheme on a subset W of V_2 of size $\geq 2n_2/3$:)

apply procedure Reduce-Part2-by-Color to the canonical 2-coloring $(W_2, V_2 \setminus W_2)$ of V_2 if procedure Reduce-Part2-by-Color selects $V_2 \setminus W_2$, update $V_2 \leftarrow V_2 \setminus W_2$, recurse

(: significant progress: n_2 reduced by a factor of 3 :)

else (: procedure Reduce-Part2-by-Color selects W :)

enter subcase (iv) of item 8.

7.10 Local to global symmetry

In this section we make preparations to handle the case when \mathfrak{X}_2 is a Johnson scheme.

Notation 7.18. Let $\mathcal{H} = (V, \mathcal{E})$ be a hypergraph and $x \in V$. We denote the induced subhypergraph $\mathcal{H}[V \setminus \{x\}]$ by $\mathcal{H} - x$.

Lemma 7.19 (Exchange/augment). Let $\mathcal{H} = (V, \mathcal{E})$ be a t-uniform hypergraph. Let $V = A \dot{\cup} B$ where $|B| \geq 1$ and |A| > (t+1)|B|. Assume $\mathfrak{S}(A) \leq \operatorname{Aut}(\mathcal{H})$. Assume moreover that $(\forall x \in A)(\exists u \in B)$ such that $\mathfrak{S}(A \cup \{u\} \setminus \{x\}) \leq \operatorname{Aut}(\mathcal{H} - x)$. Then $(\exists v \in B)(\mathfrak{S}(A \cup \{v\}) \leq \operatorname{Aut}(\mathcal{H}))$.

Proof. For $x \in A$ let f(x) denote an element $u \in B$ such that $\mathfrak{S}(A \cup \{u\} \setminus \{x\}) \leq \operatorname{Aut}(\mathcal{H} - x)$. By the pigeon-hole principle there exists $u \in B$ such that $|f^{-1}(u)| \geq t + 2$. We claim that v := u satisfies the conclusion of the lemma.

Let $\tau = (x, u)$ denote the transposition that swaps x and u. We need to show that $\tau \in \operatorname{Aut}(\mathcal{H})$. I. e., we need to show that for all $E \in \mathcal{E}$ we have $E^{\tau} \in \mathcal{E}$.

Let $y \in f^{-1}(u) \setminus (E \cup \{x\})$. So $\mathfrak{S}(A \cup \{u\} \setminus \{y\}) \leq \operatorname{Aut}(\mathcal{H}-y)$. In particular, $\tau \in \operatorname{Aut}(\mathcal{H}-y)$ and therefore $E^{\tau} \in \mathcal{E}$.

Remark 7.20. It is easy to see that |A| > |B|t would suffice in place of |A| > |B|(t+1).

The next lemma asserts that if every small induced subhypergraph of a uniform hypergraph has high symmetry then the hypergraph has extremely high symmetry.

Lemma 7.21 (Local to global symmetry). Let $s \ge 0$, $t \ge 2$, and

 $\ell = \max\{t+3, (t+2)(t+3)s\}$. Let $\mathcal{H} = (V, \mathcal{E})$ be a t-uniform hypergraph with $m \geq \ell$ vertices. Assume that for every subset $L \subseteq V$ of size $|L| = \ell$ the symmetry defect of the induced subhypergraph $\mathcal{H}[L]$ is at most s. Then the symmetry defect of \mathcal{H} is at most s.

Note that this lemma talks about the *absolute* (as opposed to relative) symmetry defect.

Proof. Let k be the largest value such that the following holds:

 (C_k) For every subset $K \subseteq V$ of size |K| = k the symmetry defect of the induced subhypergraph $\mathcal{H}[K]$ is at most s.

The assumption is (C_{ℓ}) . We need to show (C_m) . We prove (C_k) for $k = \ell, \ell + 1, \ldots, m$ by induction.

Assume (C_{k-1}) for some $k > \ell$. Let |K| = k. For $x \in K$ set $K_x = K \setminus \{x\}$. Let $S_x \subset K_x$ denote a subset of size $|S_x| = s$ such that $\mathfrak{S}(K_x \setminus S_x) \leq \operatorname{Aut}(\mathcal{H}[K_x])$.

Let x_1, \ldots, x_{t+3} be t+3 distinct elements of K. (These exist because $\ell \ge t+3$.) Let $U = \bigcup_{i=1}^{t+3} S_{x_i}$; so $|U| \le (t+3)s < |K|$.

Claim 1. $\mathfrak{S}(K \setminus U) \leq \operatorname{Aut}(\mathcal{H}[K]).$

Proof. Let $\tau = (u, v)$ be a transposition in $K \setminus U$ $(u, v \in K \setminus U)$. We need to show that $\tau \in \operatorname{Aut}(\mathcal{H}[K])$, i.e., for all $E \in \mathcal{E}[K]$ we need to show $E^{\tau} \in \mathcal{E}[K]$.

Pick an *i* such that $x_i \notin E \cup \{u, v\}$. So $E \subset K_{x_i}$ and τ fixes S_{x_i} pointwise (because $S_{x_i} \subseteq U$). It follows that $\tau \in \operatorname{Aut}(\mathcal{H}[K_x])$ and therefore $E^{\tau} \in \mathcal{E}[K]$, completing the proof of Claim 1.

Let now B be a minimal subset of U such that $\mathfrak{S}(K \setminus B) \leq \operatorname{Aut}(\mathcal{H}[K])$.

Claim 2. $|B| \leq s$.

Proof. Assume for a contradiction that $|B| \ge s + 1$. Let $A = K \setminus B$.

Claim 3. The assumptions of Lemma 7.19 hold with $\mathcal{H}[K]$ in the place of \mathcal{H} .

Proof. We have |A| > (t+1)|B| because $|B| \le |U| \le s(t+3)$ and $|K| > \ell \ge (t+2)(t+3)s \ge (t+2)|B|$.

We have $\mathfrak{S}(A) \leq \operatorname{Aut}(\mathcal{H}[K])$ by the definition of B. Let now $x \in A$. We need to find $u \in B$ such that $\mathfrak{S}(A \cup \{u\} \setminus \{x\}) \leq \operatorname{Aut}(\mathcal{H}[K_x])$. We claim that any $u \in B \setminus S_x$ will do.

By assumption, $\mathfrak{S}(K_x \setminus S_x) \leq \operatorname{Aut}(\mathcal{H}[K_x])$. Moreover, $\mathfrak{S}(K_x \setminus B) \leq \operatorname{Aut}(\mathcal{H}[K_x])$ because $\mathfrak{S}(K \setminus B) \leq \operatorname{Aut}(\mathcal{H}[K])$. Now $\mathfrak{S}(K_x \setminus S_x)$ and $\mathfrak{S}(K_x \setminus B)$ generate $\mathfrak{S}(K_x \setminus (B \cap S_x))$ because $K_x \setminus (B \cap S_x)$ is the union of $K_x \setminus S_x$ and $K_x \setminus B$ and the intersection of these two sets is nonempty (because $|S_x \cup B| \leq (t+4)s < \ell \leq k-1 = |K_x|)$.

Finally we observe that $\mathfrak{S}(K_x \setminus (B \cap S_x)) \ge \mathfrak{S}(A \cup \{u\} \setminus \{x\})$ (because $u \notin S_x$). This completes the proof of Claim 3.

Now by Lemma 7.19 we infer that for some $v \in B$ we have $\mathfrak{S}(A \cup \{v\}) \leq \operatorname{Aut}(\mathcal{H}[K])$, contradicting the minimality of B, completing the proof of Claim 2.

This completes the proof of (C_k) , the inductive step in the proof of Lemma 7.21.

7.11 Bipartite graph with Johnson scheme on small part

Situation: $X = (V_1, V_2; E)$ is a biregular bipartite graph with $|V_2| < |V_1|$, there are no twins in V_1 , and \mathfrak{X}_2 is a Johnson scheme $\mathfrak{J}(\Gamma, t)$ with $t \ge 2$ (so $V_2 = {\Gamma \choose t}$).

We write $|\Gamma| = m$, $n_i = |V_i|$, and $n = n_1 + n_2$. So $n_2 = \binom{m}{t}$ and therefore $t < 2 \log n_2 / \log m$.

Let d_i be the degree of the vertices in V_i in X (so $d_i|V_i| = |E|$).

The goal is a canonical colored α -partition of V_1 .

We may assume the density of X is $|E|/|V_1||V_2| \leq 1/2$ (otherwise take the bipartite complement).

For $v \in V_1$ let $\mathcal{E}(v)$ denote the set of neighbors of v in X viewed as a set of t-subsets of Γ . We call the t-uniform hypergraph $\mathcal{H}(v) = (\Gamma, \mathcal{E}(v))$ the neighborhood hypergraph of v.

Color $v \in V_1$ by $|\mathcal{E}(v)|$. If no color-class is greater than αn_1 , return this coloring, exit. Otherwise let C be the largest color class (so $|C| > \alpha n_1$). Let $\alpha' = \alpha |V_1|/|C|$. Let X' be the subgraph of X induced by (C, V_2) . Update $X \leftarrow X'$ (in particular $V_1 \leftarrow C$) and $\alpha \leftarrow \alpha'$. Do not update \mathfrak{X}_2 . Note that there will still be no twins in V_1 , and $|V_2|$ continues to be less than $\alpha |V_1|$ (because the value $\alpha |V_1|$ has not changed).

Set $\ell = \max\{(\log_2 n_1)^2, (\log_2 n_2)^3 / \log_2 \log_2 n_2\}.$

Our algorithm will be recursive on $m = |\Gamma|$, so a significant reduction of m will count as significant progress.

If $m \leq 2\ell$, individualize each element of Γ . This immediately individualizes each vertex in V_2 (each *t*-subset of Γ has a distinct set of colors), and thereby each vertex in V_1 (since there are no twins in V_1). Return the resulting canonical coloring of V_1 , exit.

Assume now $m > 2\ell$.

7.11.1 Subroutines

The algorithm will try to find canonical structures on Γ (coloring, equipartition, ℓ -ary relation, UPCC, Johnson scheme). First we describe subroutines how to proceed if such a structure is found.

Case 1: A canonical coloring of Γ is found.

Let Γ_i denote the *i*-th color class, so $\Gamma = \Gamma_1 \cup ... \cup \Gamma_r$ $(2 \leq r \leq m)$. This results in a canonical coloring of V_2 as follows. Let $t = t_1 + \cdots + t_r$ $(t_i \geq 0)$ be an ordered *r*-partition of the integer *t*. Associate with this partition the set $V_2(t_1, ..., t_r) = \{T \in \binom{\Gamma}{t} \mid (\forall i)(|T \cap \Gamma_i| = t_i)\}$. These sets will be the color classes of V_2 . Apply Reduce-Part2-by-Color to this coloring. Let $V_2(t_1, ..., t_r)$ be the color class selected by Reduce-Part2-by-Color. If more than one of the t_i satisfy $0 < t_i < |\Gamma_i|$ then we have a nontrivial canonical partition of $V_2(t_1, ..., t_r)$ into $\binom{|\Gamma_i|}{t_i}$ blocks for one of these values *i* (each block being defined by the set $T \cap \Gamma_i$). Apply Procedure ImprimitiveCase to this partition.

In the remaining case, all but one of the t_j are either 0 or $|\Gamma_j|$. Let *i* denote the one exception, so the vertices of V_2 can now be labeled by $\binom{\Gamma_i}{t_i}$. We are back to the Johnson case, having reduced Γ to one of the Γ_i . This is significant progress if the partition of Γ we started from was good, say all $|\Gamma_i| \leq 3m/4$.

Case 2. A nontrivial canonical equipartition of Γ is found.

Let Γ_i denote the *i*-th block of the partition, so $\Gamma = \Gamma_1 \dot{\cup} \dots \dot{\cup} \Gamma_r$ $(2 \leq r \leq m/2)$. This results in a canonical coloring of V_2 as follows: Let $t = t_1 + \dots + t_r$ $(t_i \geq 0)$ be an unordered *r*-partition of t $(t_1 \geq t_2 \geq \dots \geq t_r)$. Such an unordered partition will correspond to those $T \in {\Gamma \choose t}$ for which the multiset $\{|T \cap \Gamma_i| \mid 1 \leq i \leq r\}$ is the same as the multiset $\{t_1, \dots, t_r\}$. Each of these color classes is further canonically partitioned into blocks corresponding to the ordered partitions (now the t_i are not necessarily nonincreasing); the blocks will be of the form $V_2(t_1, \dots, t_r)$ as defined above. We first apply Reduce-Part2-by-Color to the coloring of V_2 , and then apply Procedure ImprimitiveCase to this partition.

The case remaining is when the color class selected is not partitioned into blocks. This occurs if all the t_i are equal: $t_i = t/r$. The size of this color class is $\binom{m/r}{t/r}^r$ which is at most 2/3 of $\binom{m}{t}$, the original size of V_2 , according to the Cor. 5.9 (setting $t \leftarrow t/r$ and $m \leftarrow m/r$). Return the reduced V_2 , exit (significant progress).

This completes the subroutine for Case 2.

Case 3. A canonical ℓ -ary relational structure on Γ with $\ell \geq 3$ and relative strong symmetry defect $\geq 1/4$ found.

In this case, apply the Design Lemma (multiplicative cost $m^{O(\ell)}$). If a canonical colored 3/4-partition is returned, apply Cases 1 and 2 for significant progress in either reducing $|V_2|$ or reducing to the Johnson case with significantly reduced $|\Gamma|$.

If the Design Lemma returns a UPCC canonically embedded in Γ on a set $W \subseteq \Gamma$ with $|W| \geq 3m/4$ vertices, apply Case 1 to the coloring $(W, \Gamma \setminus W)$. We make significant progress unless Case 1 returns the update $\Gamma \leftarrow W$. In this case, go to Case 4.

Case 4. Γ is the set of vertices of a canonically embedded UPCC.

In this case we recursively apply Theorem 7.10 ("UPCC Split-or-Johnson") through Lemma 7.13 ("UPCC to bipartite") with parameter $\beta = 3/4$. Note that $|\Gamma| < 1 + \sqrt{2n_2}$, a dramatic reduction of the size of the problem.

If Theorem 7.10 returns a canonical colored 3/4-partition of Γ , apply Cases 1 and 2 to make significant progress.

If Theorem 7.10 returns a Johnson scheme on a subset $W \subseteq \Gamma$ of size $|W| \ge 3m/4$ then apply Case 1 to the coloring $(W, \Gamma \setminus W)$. We make significant progress unless Case 1 returns the update $\Gamma \leftarrow W$. So in this case we have a Johnson scheme on Γ and move to Case 5.

Case 5. $\Gamma = \binom{\Gamma'}{t'}$ is the vertex set of a canonically embedded Johnson scheme $\mathfrak{J}(\Gamma', t')$ $(t' \ge 2)$. In this case V_2 is identified with the set

$$V_2 \leftarrow \binom{\binom{\Gamma'}{t'}}{t}.$$
(32)

This is a highly structured set with ample imprimitivity of which we take advantage. Each vertex $x \in V_2$ can now be viewed as a t'-uniform hypergraph $\mathcal{H}(x)$ with t edges on the vertex set Γ' .

If $m' \leq \ell = (\log_2 n)^3 / \log_2 \log_2 n$, we individualize each element of Γ' . This in turn individualizes each element of Γ , then each element of V_2 , and finally each element of V_1 , at a multiplicative cost of $|\Gamma'|! < \ell^\ell < \exp_2(3(\log_2 n_2)^3)$.

Now assume $m' > \ell$.

Lemma 7.22. V_2 is canonically 1/6-color-partitioned by classical WL applied to the tripartite graph on (V_2, Γ, Γ') where each $v \in V_2$ is adjacent to the corresponding t-tuple in Γ and each $w \in \Gamma$ is adjacent to the corresponding t'-tuple in Γ' .

Proof. Let $U(x) \subseteq \Gamma'$ denote the union of the edges of $\mathcal{H}(x)$. So $|U(x)| \leq tt'$.

Claim. If $m' > \ell$ then $tt' < 2\log_2 n_2 / \log_2 \log_2 n_2$.

Proof. First note that if $1 \le b \le a/2$ then $\binom{a}{b} \ge (a/b)^b \ge 2^b$, so $b \le \log_2\binom{a}{b}$. Applying this twice we see that $t \le \log_2\binom{m}{t} = \log_2 n_2$ and $t' \le \log_2\binom{m'}{t'} = \log_2 n_2 \cdot \operatorname{So} t' < \sqrt{m'}$.

and $t < \sqrt{m'} < \sqrt{\binom{m'}{t'}}$. Now if $b \leq \sqrt{a}$ then $\binom{a}{b} > (a/b)^b \geq a^{b/2}$, so, bootstrapping, we obtain

$$n_2 = \binom{\binom{m'}{t'}}{t} > \binom{m'}{t'}^{t/2} > (m')^{tt'/4}$$

$$(33)$$

and therefore $tt' < 2 \log n_2 / \log_2 \log_2 n_2$.

Let us color V_2 as $V_2 = Q \cup R$ where $x \in Q$ exactly if |U(x)| = tt' (all edges of $\mathcal{H}(x)$ are disjoint). (WL is "aware" of this coloring, so the WL coloring is a refinement of this.) By Prop. 2.37 ("Random hypergraphs") we have $|R|/|V_2| \leq (tt')^2/m'$. The right-hand side goes to zero, so for sufficiently large n we have $|R|/|V_2| \leq 1/6$, say.

For $x, y \in Q$ let us now say that $x \sim y$ if U(x) = U(y). This equivalence relation gives a canonical equipartition on Q. (Again, WL is "aware" of this relation.) The size of each equivalence class is $(tt')!/(t!(t'!)^t) \geq 3$ (because $t, t' \geq 2$; the smallest case occurs when t = t' = 2). The number of equivalence classes is $\binom{m'}{tt'} \geq \binom{m'}{4}$ which goes to infinity, so for sufficiently large n it will be at least 6, say.

In summary, the (Q, R) canonical coloring together with the \sim canonical equivalence relation on Q provides a canonical colored 1/6-partition of V_2 . (In fact, it is a o(1)-partition.) WL gives a refinement of these.

Now apply Reduce-Part2-by-Color to the color-partition obtained. If a color class of size $\leq n_2/6$ is returned, we reduced n_2 by a factor of 6, significant progress. If a larger color class is returned, it is nontrivially equipartitioned. Apply Procedure ImprimitiveCase, significant progress.

This completes Case 5.

7.11.2 Local guides for the Johnson case

After these subroutines, we now turn to the main algorithm for the case when $V_2 = \begin{pmatrix} 1 \\ t \end{pmatrix}$ is the vertex set of the canonically embedded Johnson scheme $\mathfrak{J}(\Gamma, t)$.

For $L \subseteq \Gamma$ let X[L] denote the subgraph of X induced by $\left(V_1, {L \choose t}\right)$. Our "test sets" will be the ℓ -subsets $L \subset \Gamma$ (i. e., $L \in {\Gamma \choose \ell}$). Determine the isomorphisms among all the X(L) for all the test sets L (by brute force over all bijections between each pair L_1, L_2) at an additive cost of $m^{O(\ell)} n^{O(1)}$.

Case A: Not all the X[L] are isomorphic.

This gives us a canonical coloring of $\binom{\Gamma}{\ell}$ at additive quasipolynomial cost. (The color of L is the isomorphism type of X(L). This does not require canonical forms, only a comparison of all graphs of the form X(L) arising from X and its counterpart airising from the other input string (with which we are testing isomorphism). But in this quasipolynomial-size category, even lex-first labeling would be feasible in quasipolynomial time.)

We consider the symmetry defect of the resulting edge-colored ℓ -uniform hypergraph \mathcal{K} on vertex set Γ . Recall that we do not need to distinguish weak and strong defect in case of hypergraphs (see Prop. 2.38).

Case A1. \mathcal{K} has symmetry defect < m/4.

Let $S \subset \Gamma$ be the unique largest symmetrical set for \mathcal{K} ; so |S| > 3m/4. Apply Case 1 to the coloring $(S, \Gamma \setminus S)$. We make significant progress except when Case 1 returns the update $\Gamma \leftarrow S$. If this is the case, we enter Case B below.

Case A2. \mathcal{K} has symmetry defect $\geq m/4$.

In this case we view \mathcal{K} as an ℓ -ary relational structure and move to Case 3.

Case B. All the X[L] are isomorphic.

Let $G(L) \leq \mathfrak{S}(L)$ denote the image of the action of $\operatorname{Aut}(X(L))$ on L.

Case B1. $G(L) \neq \mathfrak{S}(L)$.

We should always have discussed the progress of the two input strings \mathfrak{x}_1 and \mathfrak{x}_2 (of which we wish to decide *G*-isomorphism) in combination. The general argument is that either the progress of the parameters is not identical, in which case we reject isomorphism and exit, or it is identical, so it suffices to follow one of them as long as canonicity with respect to the pair of objects is observed.

Due to the delicate nature of the argument involved in the prerequisite for the present case, Corollary 6.10 ("Local guide"), we make an exception at this time. This will also illustrate the general principle tacitly present in all combinatorial partitioning arguments.

We shall apply Corollary 6.10 with the following assignment of the variables: $\alpha \leftarrow 3/4$, $\Omega_1 \leftarrow \Gamma$, $n \leftarrow m$, $k \leftarrow \ell$. Rename X as X_1 . The graph X_1 derives from an input string \mathfrak{x}_1 . Let \mathfrak{x}_2 be the other input string and let X_2 be the graph X derived by the same procedure from \mathfrak{x}_2 . This defines Ω_2 . The objects of the category \mathcal{L} correspond to the pairs (L,i)where $L \in \binom{\Omega_i}{\ell}$. The morphisms $(L,i) \to (L',j)$ are the bijections $L \to L'$ induced by the $X_i(L) \to X_j(L')$ isomorphisms. The two abstract objects of category \mathcal{C} are denoted \mathfrak{X}_1 and \mathfrak{X}_2 . The underlying set of \mathfrak{X}_i is $\Box(\mathfrak{X}_i) = \Omega_i$. The morphisms are the bijections $\Omega_1 \to \Omega_2$ induced by the isomorphisms $X_1 \to X_2$.

Our assumption is that all objects of the form (L, 1) are isomorphic. If this is not true for the objects (L, 2), reject isomorphism, exit. Let now $L_i \in \binom{\Omega_i}{\ell}$. If the objects $(L_1, 1)$ and $(L_2, 2)$ are not isomorphic, reject isomorphism, exit.

So now all objects in the category \mathcal{L} are isomorphic.

For $L \in {\Omega_i \choose \ell}$, let $G_i(L)$ denote the restriction of $\operatorname{Aut}(X_i(L))$ to L. We say that $L \in {\Omega_i \choose \ell}$ is *full* for i if $G_i(L) = \mathfrak{S}(L)$. Our current assumption is that $G_i(L)$ is not full (for at least one pair (L, i), and therefore for all pairs (L, i)).

Thus the assumptions of Corollary 6.10 are satisfied. If the algorithm of Corollary 6.10 returns a colored 3/4-partition of Ω_i , return that partition and move to Cases 1 and 2 to make significant progress.

If Corollary 6.10 returns a UPCC canonically embedded on at least 3m/4 elements of $\Omega_1 = \Gamma$, move to Case 4. Note that $m \leq 1 + \sqrt{2n_2}$, a drastic reduction in the domain size.

Now we return to discussing only one of the input strings.

Case B2. $G(L) = \mathfrak{S}(L)$.

Since all the X(L) are isomorphic, this is now true for all $L \in {\Gamma \choose \ell}$. For $v \in V_1$ let $\mathcal{H}(v, L) = (L, \mathcal{E}(v, L))$ be the induced subhypergraph of $\mathcal{H}(v)$ on L. Then, for each $v \in V$ and $\sigma \in G(L)$ there is at least one vertex $v(\sigma)$ such that $\mathcal{H}(v, L)^{\sigma} = \mathcal{H}(v(\sigma), L)$. So the number of vertices is $n_1 \geq |\mathfrak{S}(L) : \operatorname{Aut}(\mathcal{H}(v, L))|$. Let s be the largest value such that $n_1 \geq {\ell \choose s}$. Since $n_1 < \exp(\sqrt{\ell})$, it follows from Theorem 8.16 that $\operatorname{Aut}(\mathcal{H}(v)) \geq \mathfrak{A}(L \setminus S)$ for some set $S \subset L$, |S| = s. Since ${\ell \choose s} > (\ell/s)^s$, we see that $s \leq 2 \log_2 n_1 / \log_2 \log_2 n_1$.

Now it follows from Lemma 7.21 ("Local to global symmetry lemma") that for every v there is a set $S(v) \subset \Gamma$ with |S(v)| = s such that $\operatorname{Aut}(\mathcal{H}(v)) \geq \mathfrak{A}(\Gamma \setminus S(v))$. (By Prop. 2.38 it follows in fact that $\operatorname{Aut}(\mathcal{H}(v)) \geq \mathfrak{S}(\Gamma \setminus S(v))$.) Let S(v) denote the smallest such subset for $\mathcal{H}(v)$. This subset is easy to find in polynomial time. (To apply Lemma 7.21 we need to verify that $\ell > (t+2)(t+3)s$ which is true because both t and s are $O(\log n/\log \log n)$.)

Now consider the bipartite graph $Y = (V_1, \Gamma; F)$ where $g \in \Gamma$ is adjacent to $v \in V_1$ if $g \in S(v)$. The map $X \mapsto Y$ is a canonical transformation (object map of a functor) to an instance with V_2 greatly reduced $(|\Gamma| < 1 + \sqrt{2|V_2|})$.

If none of the twin-equivalence classes of Y in V_1 are greater than $2n_1/3$, return Y, exit. Else, let $S \subset \Gamma$ be the set that is equal to S(v) for at least a 2/3 fraction of the elements of V_1 . Individualize each point in S. In the next round of refinement of the graph Y this will individualize each vertex v with S(v) = S. We justify this last statement in Cor. 7.24 below.

Observation 7.23. The X-neighborhood of each $v \in V_1$ is determined by the trace $\mathcal{H}(v)_{S(v)}$ of the neighborhood hypergraph $\mathcal{H}(v)$ in S(v).

Proof. The X-neighborhood of each $v \in V_1$ is determined by its neighborhood hypergraph $\mathcal{H}(v)$. A subset $E \subset \Gamma$ belongs to $\mathcal{H}(v)$ if and only if $E \cap S(v) \in \mathcal{H}(v)_{S(v)}$.

Corollary 7.24. If, for some $v \in V_1$, we individualize each element of the set S(v) then, after a refinement step in the graph Y, the vertex v is individualized.

Proof. This follows from Obs. 7.23 in view of the assumption that there are no X-twins in V_1 .

This completes Case B2 and thereby the subroutine for the Johnson case. This in turn completes the Bipartite Split-or-Johnson and UPCC Split-or-Johnson algorithms.

8 Alternating quotients of a permutation group

To understand the structure of the groups where Luks reduction stops, we need some group theory.

In Luks's barrier situation we have a giant representation $\varphi : G \to \mathfrak{S}(\Gamma)$, meaning the image of G is a giant, i.e., $G^{\varphi} \geq \mathfrak{A}(\Gamma)$. We shall assume that $k = |\Gamma| > \max\{8, 2 + \log_2 n_i\}$ where n_0 is the length (size) of the largest orbit of G. We say that $x \in \Omega$ is affected by φ if $G_x^{\varphi} \not\geq \mathfrak{A}(\Gamma)$. The key result is that the pointwise stabilizer of all unaffected points is still mapped onto $\mathfrak{S}(\Gamma)$ or $\mathfrak{A}(\Gamma)$ by φ (Unaffected Stabilizer Theorem, Thm. 8.11). This result will be responsible for the key algorithm of the paper (Procedure LocalCertificates in Sec. 10).

Finally we show that if a permutation group $G \leq \mathfrak{S}_n$ has an alternating quotient of degree $k \geq \max\{9, 2\log_2 n\}$ then for sufficiently large n this can only happen in the trivial way, namely, that for some $t \geq 1$, G has a system of imprimitivity with $\binom{k}{t}$ blocks on which G acts as the Johnson group $\mathfrak{A}_k^{(t)}$. Moreover, in every orbit there is a canonical choice of the blocks corresponding to φ which is unique; we refer to these as the *standard blocks*. These are some of the items in our "Main Structure Theorem" (Theorem 8.19).

8.1 Simple quotient of subdirect product

First we state a lemma that is surely well known but I could not find a convenient reference.

Lemma 8.1 (Simple quotient of subdirect product). Let $G \leq K_1 \times \cdots \times K_m$ be a subdirect product; let M_i be the kernel of the $G \to K_i$ epimorphism. Assume there is an epimorphism $\varphi : G \to S$ where S is a nonabelian simple group. Then $(\exists i)(M_i \leq \ker \varphi)$. In particular, one of the K_i admits an epimorphism on S.

Simplified proof by P. P. Pálfy. Let $N = \ker \varphi$. Assume for a contradiction that $N \ngeq M_i$ for all *i*. Then $M_i N = G$ (because N is a maximal normal subgroup). It follows that $[G, \ldots, G] = [M_1 N, \ldots, M_m N] \le N[M_1, \ldots, M_m] \le N(\bigcap_{i=1}^m M_i) = N$, so $[G/N, \ldots, G/N] = 1$, a contradiction because $G/N \cong S$ is nonabelian simple.

In our applications, S will be \mathfrak{A}_k and the K_i the restrictions of the permutation group G to its orbits.

8.2 Large alternating quotient of a primitive group

The result of this section is Lemma 8.5.

First we need to state a corollary to the basic structure theorem of primitive groups, the O'Nan–Scott Theorem, [DiM, Thm. 4.1A]. The proof of this theorem is elementary.

Definition 8.2. The *socle* Soc(G) of a group G is the product of its minimal normal subgroups.

Fact 8.3. (i) The socle is a direct product of simple groups.

(ii) The socle of a primitive permutation group is a direct product of isomorphic simple groups.

The following is an easy corollary to the O'Nan–Scott Theorem.

Corollary 8.4 (O'Nan–Scott). Let $G \leq \mathfrak{S}_n$ be a primitive group with a nonabelian socle $\operatorname{Soc}(G) \equiv R^s$ where R is a nonabelian simple group. Then $n \geq 5^s$.

Now we state our result.

Lemma 8.5. Let $G \leq \mathfrak{S}(\Omega)$ be primitive. Assume $\varphi : G \to \mathfrak{A}_k$ is an epimorphism where $k > \max\{8, 2 + \log_2 n\}$. Then φ is an isomorphism; hence $G \cong \mathfrak{A}_k$.

Proof. Let N = Soc(G). By Fact 8.3 N can be written as $N = R_1 \times \cdots \times R_s$ where the R_i are isomorphic simple groups.

Case 1. N is abelian (the "affine case") and therefore regular, i. e., n = |N|. In this case $N \cong \mathbb{Z}_p^s$ and $G/N \leq \operatorname{GL}(s,p)$ for some prime p, so $n = p^s$. Moreover \mathfrak{A}_k is involved in $\operatorname{GL}(s,p)$. It is shown in [BaPS, Prop. 1.22] that if \mathfrak{A}_k is involved in $\operatorname{GL}(s,p)$ then, combining a result of Feit and Tits [FeT] with [KlL, Prop. 5.3.7], for $k \geq 9$ it follows that $k \leq s + 2$. But we have $s + 2 \leq 2 + \log_p n < k$, a contradiction, so this case cannot occur.

Case 2. N is nonabelian. By Cor. 8.4 we have $s \leq \log_5 n$. In particular, k > s.

Following $[BaB]^7$, let Pker(G) ("permutation kernel") denote the kernel of the induced permutation action $G \to \mathfrak{S}_s$ (permuting the copies of R by conjugation by elements of G). Then $Pker(G) \leq Aut(R_1) \times \cdots \times Aut(R_s)$. It follows that $Pker(G)/N \leq Out(R_1) \times \cdots \times Out(R_s)$ is solvable by Schreier's Hypothesis (a known consequence of the CFSG).

Now $G/\operatorname{Pker} G \leq \mathfrak{S}_s$ and s < k so $G/\operatorname{Pker} G$ cannot involve \mathfrak{A}_k . The solvable group $\operatorname{Pker}(G)/N$ also does not involve \mathfrak{A}_k . It follows that G/N does not involve \mathfrak{A}_k and therefore $\operatorname{ker} \varphi \not\geq N$.

Let M be a minimal normal subgroup of G.

Case 2a. $M \neq N$. Then there is a unique other minimal normal subgroup, M^* , the centralizer of M, which is isomorphic to M. It follows that M is regular, so n = |M|. Moreover, s is even and $|M| = |\mathfrak{A}_k|^{s/2}$. Hence, $n \geq |\mathfrak{A}_k| > 2^k > n$, a contradiction. So this case cannot occur.

Case 2b. M = N is the unique minimal normal subgroup of G. Since $N \nleq \ker \varphi$, it follows that $\ker \varphi = 1$.

Remark 8.6. The assumption $k > 2 + \log_2 n$ is tight infinitely often, as shown by the affine case of even dimension in characteristic 2. In this case $G = \mathbb{Z}_2^{k-2} \rtimes \mathfrak{A}_k$ acts primitively on $n = 2^{k-2}$ elements as follows: \mathfrak{A}_k acts on \mathbb{Z}_2^k by permuting the coordinates; restrict this action to the zero-weight subspace $\sum x_i = 0$, and then to the quotient space by the one-dimensional subspace $x_1 = \cdots = x_k = 1$ (this is contained in the zero-weight subspace when the dimension is even). In this case, $k = 2 + \log_2 n$, and \mathfrak{A}_k is a proper quotient of G.

8.3 Alternating quotients versus stabilizers

Lemma 8.7. Let $G \leq \mathfrak{S}(\Omega)$ be a transitive permutation group and $\varphi : G \to \mathfrak{A}_k$ an epimorphism where $k > \max\{8, 2 + \log_2 n\}$. Then $G_x^{\varphi} \neq \mathfrak{A}_k$ for any $x \in \Omega$.

Proof. We proceed by induction on the order of G. Let $N = \ker \varphi$. Assume for a contradiction that $G_x^{\varphi} = \mathfrak{A}_k$, i.e., $NG_x = G$.

Let B be a maximal block of imprimitivity containing x (so $|B| < |\Omega|$). (If G is primitive then $B = \{x\}$.) So $G_B \ge G_x$ and therefore $NG_B = G$.

Let Ω' be the set of *G*-images of *B*. This is a system of imprimitivity on which *G* acts as a primitive group; let *K* be the kernel of this action.

 $^{^{7} \}rm{Introduced}$ in [BaB] (1999), this notation was subsequently adopted in computational group theory (see. e. g., [HoS]).

Since N is a maximal normal subgroup of G, we have $K \leq N$ or KN = G.

If $K \leq N$ then φ maps the primitive group G/K onto \mathfrak{A}_k and therefore by Lemma 8.5, $G/K \cong \mathfrak{A}_k$, hence K = N and therefore $KG_B = G$. But obviously $G_B \geq K$, so $G = KG_B = G_B$ and therefore $|\Omega'| = 1$, i.e., $B = \Omega$, a contradiction.

So we have KN = G, i. e., $K^{\varphi} = \mathfrak{A}_k$. Let $\Omega_1, \ldots, \Omega_m$ denote the orbits of $K \ (m \ge 1)$. Let K_i denote the restriction of K to Ω_i and $M_i \triangleleft K$ the kernel of the $K \to K_i$ epimorphism. By Lemma 8.1, $(\exists i)(M_i \le N)$. The set $(\Omega_1, \ldots, \Omega_m)$ is a system of imprimitivity for G on which G acts transitively, so the M_i are conjugate subgroups in G and therefore $M_i \le N$ for all i. Let $x \in \Omega_i$. It follows from $M_i \le N$ that the epimorphism $K \to \mathfrak{A}_k$ (restriction of φ to K) factors across K_i as $K \to K_i \xrightarrow{\psi} \mathfrak{A}_k$, so $K_i^{\psi} = \mathfrak{A}_k$. By the inductive hypothesis, applied to K_i , we infer that $(K_i)_x^{\psi} \neq \mathfrak{A}_k$. On the other hand, $(K_i)_x^{\psi} = K_x^{\varphi} \triangleleft G_x^{\varphi} = \mathfrak{A}_k$. We conclude that $|(K_i)_x^{\psi}| = 1$ and therefore $n \ge |x^{K_i}| = |K_i : (K_i)_x| \ge |K_i^{\psi} : (K_i)_x^{\psi}| = |K_i^{\psi}| = k!/2 > 2^k > n$, a contradiction.

Remark 8.8. Again, the assumption $k > 2 + \log_2 n$ is tight; the Lemma fails infinitely often if $k = 2 + \log_2 n$ is permitted. This is shown by the same examples as in Remark 8.6.

Next we extend Lemma 8.7 to not necessarily transitive groups.

Lemma 8.9. Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and $\varphi : G \to \mathfrak{A}_k$ an epimorphism. Assume $k > \max\{8, 2 + \log_2 n_0\}$ where $n_0 = n_0(G)$ denotes the length of the largest orbit of G. Then $G_x^{\varphi} \neq \mathfrak{A}_k$ for some $x \in \Omega$.

Proof. Let $\Omega_1, \ldots, \Omega_m$ be the orbits of G and let G_i be the restriction of G to Ω_i . So G is a subdirect product of the G_i . Let M_i denote the kernel of the $G \to G_i$ epimorphism. By Lemma 8.1, $(\exists i)(M_i \leq \ker \varphi)$, so φ factors across the restriction $G \to G_i$ as $G \to G_i \xrightarrow{\psi} \mathfrak{A}_k$. So $G_i^{\psi} = \mathfrak{A}_k$.

Let $x \in \Omega_i$. We apply Lemma 8.7 to G_i and notice that $G_x^{\varphi} = (G_i)_x^{\psi} \neq \mathfrak{A}_k$.

The following result, Theorem 8.11, along with a companion observation, Cor. 8.13, will be the principal tools for our central algorithm, the LocalCerticates procedure. Recall that $G_{(D)}$ denotes the pointwise stabilizer of D in G ($D \subseteq \Omega$).

Definition 8.10 (Affected). We say that the homomorphism $\varphi : G \to \mathfrak{S}_k$ is a giant representation if $G^{\varphi} \geq \mathfrak{A}_k$. We say that $x \in \Omega$ is affected by φ if $G_x^{\varphi} \not\geq \mathfrak{A}_k$.

Theorem 8.11 (Unaffected Stabilizer Theorem). Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and $\varphi: G \to \mathfrak{S}_k$ a giant representation. Assume $k > \max\{8, 2 + \log_2 n_0\}$ where $n_0 = n_0(G)$ denotes the length of the largest orbit of G. Let D be the set of elements of Ω not affected by φ . Then $G_{(D)}^{\varphi} \geq \mathfrak{A}_k$.

Proof. First assume $G^{\varphi} = \mathfrak{A}_k$. The set D is G-invariant and $G_{(D)}$ is the kernel of the restriction map $G \to \mathfrak{S}(D)$. Let $P \leq \mathfrak{S}(D)$ be the image of this map (restriction of G to D), so $P \cong G/G_{(D)}$. Since $G_{(D)} \triangleleft G$, we have $G_{(D)}^{\varphi} \triangleleft G^{\varphi} = \mathfrak{A}_k$. Assume for a contradiction that $G_{(D)}^{\varphi} \neq \mathfrak{A}_k$; it follows that $|G_{(D)}^{\varphi}| = 1$, i.e., $G_{(D)} \leq \ker(\varphi)$. Hence φ factors across P as

 $G \to P \xrightarrow{\psi} \mathfrak{A}_k$. It follows that $P^{\psi} = G^{\varphi} = \mathfrak{A}_k$ so ψ is an epimorphism. By Lemma 8.9 we have $P_x^{\psi} \neq \mathfrak{A}_k$ for some $x \in D$. But $P_x^{\psi} = G_x^{\varphi} = \mathfrak{A}_k$ (because $x \in D$ is not affected by φ), a contradiction.

Now if $G^{\varphi} = \mathfrak{S}_k$ then let $G_1 = \varphi^{-1}(\mathfrak{A}_k)$. Let φ_1 be the restriction of φ to G_1 , so $\varphi_1 : G_1 \to \mathfrak{A}_k$ is an epimorphism. Moreover, $x \in \Omega$ is affected by φ if and only if x is affected by φ_1 (because \mathfrak{A}_k has no subgroup of index 2). An application of previous case to (G_1, φ_1) completes the proof.

Proposition 8.12. Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and $\varphi : G \to H$ an epimorphism. Let $\Delta \subseteq \Omega$ be an orbit of G and $x \in \Delta$. Let $L = G_x^{\varphi}$; assume $L \neq H$. Then ker (φ) is not transitive on Δ ; in fact, each orbit of ker (φ) in Δ has length $\leq |\Delta|/k$ where k = |H : L|.

Proof. Let $N = \ker(\varphi)$ and $|\Delta| = d$. So $d = |G : G_x|$. The length of the N-orbit x^N is $|N:N_x|$. We have $|G:NG_x| = |G^{\varphi}:G_x^{\varphi}| = |H:L| = k$. Therefore $|NG_x:G_x| = d/k$. But $|N:N_x| = |(N \cap NG_x):(N \cap G_x)| \le |NG_x:G_x| \le d/k$.

Corollary 8.13 (Affected Orbit Lemma). Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and φ : $G \to \mathfrak{S}_k$ a giant representation. Assume $k \geq 5$. Then, if Δ is an affected G-orbit, i.e., $\Delta \cap D = \emptyset$, then ker(φ) is not transitive on Δ ; in fact, each orbit of ker(φ) in Δ has length $\leq |\Delta|/k$.

Proof. For $k \geq 5$, the largest proper subgroup of \mathfrak{A}_k has index k, and the largest subgroup of \mathfrak{S}_k not containing \mathfrak{A}_k also has index k. So the statement follows from Prop. 8.12.

Remark 8.14. If $k \ge \max\{9, 2\log_2 n_0\}$ then we can use Theorem 8.19 to make a more detailed statement. We observe that ker(φ) fixes each standard block (setwise), so the length of each orbit of ker(φ) contained in Δ is $\le |\Delta|/{\binom{k}{t_{\Delta}}}$.

8.4 Subgroups of small index in \mathfrak{S}_n

Observation 8.15. Let $T, U \subset \Omega$, |T|, |U| < n/2, where $n = |\Omega| \ge 5$. Assume $\mathfrak{A}(\Omega)_{(T)} \le \mathfrak{S}(\Omega)_U$. Then $U \subseteq T$.

Proof. By assumption, $|\Omega \setminus T| \ge 3$ and therefore $\Omega \setminus T$ is an orbit of $\mathfrak{A}(\Omega)_{(T)}$ so it must be part of an orbit of $\mathfrak{S}(\Omega)_U$. Since $|\Omega \setminus T| > n/2 > |U|$, we must have $\Omega \setminus T \subseteq \Omega \setminus U$, as claimed.

According to Dixon and Mortimer [DiM, p. 176], the following result goes back to Jordan (1870) [Jor, pp. 68–75]; a modern treatment was given by Liebeck [Lie83, Lemma 1.1]. We cite from the version given in [DiM, Thm. 5.2A,B]. Uniqueness follows from Observation 8.15.

Theorem 8.16 (Jordan–Liebeck). Let $\mathfrak{A}(\Omega) \leq K \leq \mathfrak{S}(\Omega)$. Let $H \leq K$ and $1 \leq r < n/2$ where $n = |\Omega| \geq 9$. Assume $|K:H| < \binom{n}{r}$. Then there exists a unique $T \subset \Omega$ with |T| < n/2such that $\mathfrak{A}(\Omega)_{(T)} \leq H \leq \mathfrak{S}(\Omega)_T$. This unique T satisfies |T| < r. **Notation 8.17.** Under the assumptions of Theorem 8.16 we write T(H) for the unique subset $T \subset \Omega$ guaranteed by the Theorem. So we have

$$\mathfrak{A}(\Omega)_{(T(H))} \le H \le \mathfrak{S}(\Omega)_{T(H)}.$$
(34)

Remark 8.18. $T(H) = \emptyset$ if and only if $\mathfrak{A}(\Omega) \leq H \leq \mathfrak{S}(\Omega)$.

8.5 Large alternating quotient acts as a Johnson group on blocks

Recall that the homomorphism $\varphi: G \to \mathfrak{S}_k$ is a giant representation if $G^{\varphi} \geq \mathfrak{A}_k$.

Theorem 8.19 (Main structure theorem). Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and $\varphi: G \to \mathfrak{S}_k$ a giant representation. Assume $k \geq \max\{9, 2\log_2 n_0\}$ where $n_0 = n_0(G)$ denotes the length of the largest orbit of G.

(a) For every $x \in \Omega$ there exists a unique subset $T(x) \subset [k]$ such that |T(x)| < k/4 and

$$(\mathfrak{A}_k)_{(T(x))} \le G_x^{\varphi} \le (\mathfrak{S}_k)_{T(x)}.$$
(35)

- (b) The element $x \in \Omega$ is affected by φ if and only if $|T(x)| \ge 1$.
- (c) For each orbit Δ there is an integer $t_{\Delta} \ge 0$ such that $|T(x)| = t_{\Delta}$ for every $x \in \Delta$. We say that Δ is affected by φ if $t_{\Delta} \ge 1$, i. e., the elements of Δ are affected.
- (d) At least one orbit is affected. In fact, if D is the union of the unaffected blocks then $G_{(D)}^{\varphi} \geq \mathfrak{A}_k$.
- (e) (Johnson group action on blocks) For every orbit Δ the equivalence relation T(x) = T(y) $(x, y \in \Delta)$ splits Δ into $\binom{k}{t_{\Delta}}$ blocks of imprimitivity, labeled by the t_{Δ} -subsets of [k]. We refer to these blocks as the standard blocks for φ . The action of G on the set of standard blocks in Δ is $\mathfrak{A}_k^{(t_{\Delta})}$. If $t_{\Delta} \geq 1$ then this is a Johnson group and the kernel of this action is ker φ ; if $t_{\Delta} = 0$ then the action is trivial (its kernel is G, there is just one block, namely Δ).
- (f) If $B \subseteq \Delta$ is a standard block and $x \in B$ then $G_B^{\varphi} = (G^{\varphi})_{T(x)}$ (so it is either $(\mathfrak{S}_k)_{T(x)}$ or $(\mathfrak{A}_k)_{T(x)}$).
- (g) If $\Psi = \{C_1, \ldots, C_r\}$ is another system of imprimitivity on the orbit Δ such that the kernel of the action $G \to \mathfrak{S}(\Psi)$ is $\ker(\varphi)$ then $r = \binom{k}{t'}$ for some $t' < t_{\Delta}$ and the G-action on Ψ is $\mathfrak{S}_k^{(t')}$ or $\mathfrak{A}_k^{(t')}$. In particular, the standard blocks form the unique largest system of imprimitivity on which the kernel of G-action is $\ker(\varphi)$. Moreover, if $x \in C_i$ then $|T(G_{C_i})| = t'$ and $T(G_{C_i}) \subset T(x)$.

Proof. Item (a) follows from the Jordan–Liebeck theorem (Thm. 8.16), setting $K = G^{\varphi}$ and $H = G_x^{\varphi}$ (so $T(x) = T(G_x^{\varphi})$) and noting that

$$\binom{k}{\lfloor k/4 \rfloor} > 2^{k/2} \ge n_0 \ge |x^G| = |G:G_x| \ge |G^{\varphi}:G_x^{\varphi}|.$$
(36)

Item (b) is immediate from Eq. (35) and the definition of being "affected."

Item (c) follows from the observation that for $x \in \Omega$ and $\sigma \in G$ we have

$$G_{x^{\sigma}} = G_x^{\sigma}$$
 and therefore $T(x^{\sigma}) = T(x)^{\sigma^{\varphi}}$. (37)

Item (d) is of greatest importance; it is the content of the "Unaffected Stabilizer Theorem" (Thm. 8.11).

To see Item (e), let Δ be an orbit and let [x] denote the equivalence class (block) of $x \in \Delta$ under the equivalence relation stated. By Eq. (37), this equivalence relation is *G*-invariant and *G* acts transitively on the blocks. We also infer from Eq. (37) that the blocks in Δ are in 1-to-1 correspondence with the t_{Δ} -subsets of [k] (noting that \mathfrak{A}_k acts transitively on $\binom{[k]}{t_{\Delta}}$). Moreover, through this bijection, the *G*-action on the blocks in Δ is equivalent to the action of \mathfrak{A}_k on $\binom{[k]}{t_{\Delta}}$. This bijection also proves item (f).

To see item (g), first we note that $r \geq 3$ (in fact, $r \geq k$) because the kernel of the action on Ψ has index $\geq k!/2$ and therefore $r! \geq k!/2$. Let $x \in C_i$ and $H = G_{C_i}$. So $G_x \leq H$ and H is a maximal subgroup of G of index ≥ 3 . Let $N = \ker(\varphi)$; so $N \leq H$ and $3 \geq |G:H| = |G^{\varphi}: H^{\varphi}|$. Moreover, H^{φ} is a maximal subgroup of \mathfrak{S}_k or \mathfrak{A}_k containing $G_x^{\varphi} \geq (\mathfrak{A}_k)_{(T(x))}$. For $T \subset [k]$ with |T| < k/2, the only maximal subgroups of \mathfrak{S}_k containing $(\mathfrak{A}_k)_{(T)}$ are of the form $(\mathfrak{S}_k)_U$ for $U \subseteq T$. Intersecting these with \mathfrak{A}_k we obtain the maximal subgroups of \mathfrak{A}_k containing $(\mathfrak{A}_k)_{(T)}$. This proves that $T(G_{C_i}) \subset T(x)$. Setting $t' = |T(G_{C_i})|$, the corresponding Johnson group action on Ψ follows the lines of the proof of item (e).

Remark 8.20 (Tight bound for k). The actual condition on k, sufficient for most conclusions of the theorem, is that $k > \max\{8, 2 + \log_2 n_0\}$ and $\frac{1}{2} \binom{k}{\lfloor k/2 \rfloor} > n_0$. The latter translates to $k > \log_2 n_0 + (1/2 + o(1)) \log_2 \log_2 n_0$. The only difference would be that instead of |T(x)| < k/4 we would only get |T(x)| < k/2, sufficient for our goals.

Our assumption $k \ge \max\{9, 2\log_2 n_0\}$ is generously sufficient for both conditions above. Under this condition we shall not only have |T(x)| < k/4 but $|T(x)| < H^{-1}(1/2)(1+o(1))k < k/9$ (for large k). Here H(x) is the binary entropy function, so $H^{-1}(1/2) \approx 0.11003 < 1/9$. — We note that any bound of the form $k > c \log n_0$ would work for the purposes of this paper; the actual value of c will not affect our complexity estimate.

Remark 8.21 (Multiple systems of imprimitivity). The presence of multiple systems of imprimitivity with the same kernel as discussed in Item (g) is a real possibility. Consider for instance the action $\mathfrak{S}_k \to \mathfrak{S}_{k(k-1)}$ defined by the action of \mathfrak{S}_k on the k(k-1) ordered pairs; let $G \leq \mathfrak{S}_{k(k-1)}$ be the image of this action. Then G has two systems of imprimitivity on which \mathfrak{S}_k acts in its natural action (there are k blocks in each system), and there is a unique system of imprimitivity with $\binom{k}{2}$ blocks on which the action is $\mathfrak{S}_k^{(2)}$. The latter are the standard blocks; in this case each standard block has 2 elements. Each of the three actions is faithful, so their kernel is the same, namely, the idenity.

Finally, and algorithmic observation.

Proposition 8.22. Given a giant representation $\varphi : G \to \mathfrak{S}_k$, we can find the standard blocks in each G-orbit in polynomial time.

Proof. Standard.

9 Verification of top action

In this section we show that if $\varphi : G \to \mathfrak{S}(\Gamma)$ is a giant representation then we can recognize whether or not φ maps $\operatorname{Aut}_G(\mathfrak{x})$ onto a giant and if so can find $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$, all this at the cost of O(m) calls to String Isomorphism on windows of size $\leq n/m$, where $m = |\Gamma|$. Note that the solution to the recurrence f(n) = O(mf(n/m)) is subquadratic.

Proposition 9.1 (Lifting). Let $G \leq \mathfrak{S}(\Omega)$ and $H \leq \mathfrak{S}(\Gamma)$ be permutation groups, $\varphi : G \to H$ a homomorphism, and $N = \ker(\varphi)$. Given these data, the strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$ and $\overline{\sigma} \in H$, one can reduce, in polynomial time, the computation of the set $\varphi^{-1}(\overline{\sigma}) \cap \operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ (set of liftings of $\overline{\sigma}$ to isomorphisms) to a single call to $\operatorname{Iso}_N(\mathfrak{x}', \mathfrak{y})$ for some string \mathfrak{x}' .

Proof. If $\overline{\sigma} \notin G^{\varphi}$ then return "empty." Otherwise let $\sigma \in \varphi^{-1}(\overline{\sigma})$ and $\mathfrak{x}' = \mathfrak{x}^{\sigma}$. Then $\varphi^{-1}(\overline{\sigma}) \cap \operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y}) = \sigma \operatorname{Iso}_N(\mathfrak{x}^{\sigma}, \mathfrak{y})$.

Remark 9.2. *H* does not need to be a permutation group. What we need is that *H* permit constructive membership testing, i. e., for any list of elements $\tau_1, \ldots, \tau_k, \rho \in H$ we should be able to efficiently decide whether or not $\rho \in K$ where *K* is the subgroup generated by the τ_i , and if the answer is affirmative, to produce a straight-line program that constructs ρ from the τ_i (see Def. 3.9). Constructive membership testing can be done, for instance, for matrix groups over finite fields of odd characteristic in quantum polynomial time [BaBS].

Definition 9.3. A subcoset of a group G is a coset of a subgroup. Let $H \leq G$ be groups and $\tau \in G$. We say that the subset $S \subseteq H\tau$ is a set of *coset generators* of $H\tau$ if $H\tau$ is the smallest subcoset of G containing S. (Note that ay intersection of subcosets of G is either empty or a subcoset; so every subset of G generates a subcoset of G.)

Observation 9.4. Let S be a set of generators of the group G. Then $S \cup \{1\}$ is a set of coset generators of G, i.e., no proper subcoset of G contains $S \cup \{1\}$.

Proposition 9.5 (TopAction1). Let $G \leq \mathfrak{S}(\Omega)$ and $H \leq \mathfrak{S}(\Gamma)$ be permutation groups, $\varphi: G \to H$ a homomorphism, and $N = \ker(\varphi)$. Let S be the given set of generators of H. Given these data and the strings $\mathfrak{x}, \mathfrak{y}: \Omega \to \Sigma$, we can achieve the following by recursively calling |S| + 1 instances of String Isomorphism with respect to N, at polynomial cost per instance:

- (i) decide whether or not φ maps $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ onto H;
- (ii) if the answer is affirmative, find $\text{Iso}_G(\mathfrak{x}, \mathfrak{y})$.

Proof. Let $S' = S \cup \{1\}$; so S' is a set of coset generators of H. Apply Prop. 9.1 to each $\overline{\sigma} \in S'$. If there is a $\overline{\sigma} \in S'$ for which the algorithm returns the empty set ($\overline{\sigma}$ does not lift to an isomorphism), return the answer "no" to item (i). Else, return the answer "yes" to item (i) and observe that $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ is the right subcoset of G generated by the subcosets $\varphi^{-1}(\overline{\sigma}) \cap \operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ ($\overline{\sigma} \in S'$) found by Prop. 9.1.

Corollary 9.6 (TopAction2). Let $G \leq \mathfrak{S}(\Omega)$ be a transitive permutation group and $\varphi : G \rightarrow \mathfrak{S}(\Gamma)$ a giant representation, where $|\Gamma| = m > \max\{8, 2 + \log_2 n\}$. Given these data and the strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$, we can achieve the following by recursively calling $\leq 4k$ instances of String Isomorphism with window size $\leq n/k$ for some $m \leq k \leq n$, at polynomial cost per instance:

- (i) decide whether or not φ maps $\operatorname{Iso}_G(\mathfrak{x},\mathfrak{y})$ onto a giant coset, i. e., $\operatorname{Iso}_G(\mathfrak{x},\mathfrak{y})^{\varphi} \geq \mathfrak{A}(\Gamma)\tau$ for some $\tau \in \mathfrak{S}(\Gamma)$;
- (ii) if the answer is affirmative, find $Iso_G(\mathfrak{x}, \mathfrak{y})$.

Proof. First assume $G^{\varphi} = \mathfrak{A}(\Gamma)$. Apply Prop. 9.5 to $H := \mathfrak{A}(\Gamma)$ with S a pair of generators of H. This reduces our questions to three instances of N-isomorphism where $N = \ker(\varphi)$. Now N is intransitive with k orbits for some $k \leq n$. Each orbit has equal length (because $N \triangleleft G$) so Luks's Chain Rule performs the desired reduction, calling 3k instances of window size n/k. We need to justify the inequality $k \geq m$. Lemma 8.7 (our first lemma toward the Unaffected Stabilizer Theorem, Theorem 8.11) says that Ω is affected. Then the Affected Orbit Lemma (Cor. 8.13) asserts that each orbit of N has length $\leq n/m$.

Now if $G^{\varphi} = \mathfrak{S}(\Gamma)$ then apply weak Luks reduction, reducing *G*-isomorphism to two instances of G_1 -isomorphism where $G_1 = \varphi^{-1}(\mathfrak{A}(\Gamma))$.

Remark 9.7. If $m \ge \max\{9, 2\log_2 n\}$ then $n/k = \binom{m}{t}$ for some $1 \le t < m/4$ by item (e) of the Main Structure Theorem (Theorem 8.19).

Corollary 9.8 (TopAction3). Let $G \leq \mathfrak{S}(\Omega)$ be a transitive permutation group and $\varphi : G \rightarrow \mathfrak{S}(\Gamma)$ a giant representation, where $|\Gamma| = m > \max\{8, 2 + \log_2 n\}$. Given these data and the strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$, we can achieve the following by recursively calling $\leq 6k$ instances of String Isomorphism with window size $\leq n/k$ for some $m \leq k \leq n$, at polynomial cost per instance:

- (i) decide whether or not φ maps $\operatorname{Aut}_G(\mathfrak{x})$ onto a giant, i. e., $\operatorname{Aut}_G(\mathfrak{x})^{\varphi} \geq \mathfrak{A}(\Gamma)$;
- (ii) if the answer is affirmative, find $Iso_G(\mathfrak{x}, \mathfrak{y})$.

Proof. If $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})^{\varphi}$ is a giant coset, we are done by Cor. 9.6. We claim that if If $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})^{\varphi}$ is not a giant coset then \mathfrak{x} and \mathfrak{y} are not *G*-isomorphic. Indeed, if $\mathfrak{x} \cong_G y$ then $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y}) = \operatorname{Aut}_G(\mathfrak{x})\sigma$ where σ is any element of $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$. It follows that $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})^{\varphi} = \operatorname{Aut}_G(\mathfrak{x})^{\varphi}\overline{\sigma}$ is a giant coset (where $\overline{\sigma} = \sigma^{\varphi}$).

Corollary 9.9 (TopAction4). Let $G \leq \mathfrak{S}(\Omega)$ be a transitive permutation group and $\varphi: G \to \mathfrak{S}(\Gamma)$ a giant representation. where $|\Gamma| = m \geq \max\{16, 4 + 2\log_2 n\}$. Let $\mathfrak{x}, \mathfrak{y}: \Omega \to \Sigma$ be strings. Assume Γ has a canonical coloring with respect to \mathfrak{x} with a color class C of size |C| > m/2 such that the restriction of $\operatorname{Aut}_G(\mathfrak{x})^{\varphi}$ to C is a giant (includes $\mathfrak{A}(C)$). Then we can find $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ by recursively calling $\leq 6k$ instances of String Isomorphism with window size $\leq n/k$ for some $|C| \leq k \leq n$, plus a number of instances of total size $\leq n$ and maximum size $\leq 2n/3$.

Proof. Since $m \ge \max\{9, 2\log_2 n\}$, by the Main Structure Theorem (Theorem 8.19) Ω can be divided into standard blocks on which G acts as a Johnson group. The standard blocks are labeled by $\binom{\Gamma}{t}$ for some $t \ge 1$; and $\Omega(C)$ denotes the unon of the standard blocks labeled by the elements of the set $\binom{C}{t}$.

Let $C_{\mathfrak{x}} = C$. By canonicity, there is a corresponding color class $C_{\mathfrak{y}} \subseteq \Gamma$ (which may be empty). Apply items 1 to 6 of Procedure Align (Sec. 11.1) with $\mathfrak{X}(\mathfrak{x}) := C_{\mathfrak{x}}$ and $\mathfrak{X}(\mathfrak{y}) := C_{\mathfrak{y}}$. The result is that

- if $|C_{\mathfrak{x}}| \neq |C_{\mathfrak{y}}|$ then isomorphism is rejected
- else \mathfrak{y} is updated so now $C_{\mathfrak{x}} = C_{\mathfrak{y}} = C$
- from the coloring $(C, \Gamma \setminus C)$ of Γ we infer a canonical coloring of Ω ; one of the color classes is $\Omega(C)$; and we begin the application of the Chain Rule with this color class.

Now we process $\Omega(C)$ via Cor. 9.8. This can be done because $|C| > m/2 \ge \max\{8, 2 + \log_2 n\}$. Then proceed to the remaining color classes in accordance with the Chain Rule.

The bound 2n/3 on the length of the remaining color classes comes from Lemma 5.5.

Remark 9.10. The cost of this procedure can generously be overestimated by 6T(2n/3) where T(n) is the maximum cost of instances of size $\leq n$.

10 The method of local certificates

10.1 Local certificates for giant action: the core algorithm

In this section we consider the case of an imprimitive G and present the group-theoretic Divide-and-Conquer method. This is the core algorithm of the entire paper.

The situation we consider is as follows.

The input is a transitive permutation group $G \leq \mathfrak{S}(\Omega)$, a giant representation $\varphi: G \to \mathfrak{A}(\Gamma)$ (i.e., a homomorphism such that $G^{\varphi} \geq \mathfrak{A}(\Gamma)$), and two strings $\mathfrak{x}, \mathfrak{y}: \Omega \to \Sigma$

 $\varphi: G \to \mathfrak{A}(\Gamma)$ (i.e., a homomorphism such that $G^{+} \geq \mathfrak{A}(\Gamma)$), and two strings $\mathfrak{x}, \mathfrak{y}: \Omega \to \Sigma$ (Σ is a finite alphabet).

Notation: $n = |\Omega|, m = |\Gamma|$. We shall assume $m \ge 10 \log_2 n$.

Notation 10.1. Recall that for a subgroup $L \leq G$ and a subset $A \subseteq \Gamma$ we write L_A to denote the setwise stabilizer of A in L with respect to the representation $\varphi : L \to \mathfrak{S}(\Gamma)$. We say that A is L-invariant if $L_A = L$. We write $\psi_A : G_A \to \mathfrak{S}(A)$ for the map that restricts the G^{φ} -action to A. If A is L-invariant then $L^A := L^{\psi_A}$ is the restriction of L^{φ} to A. In particular, $\psi_{\Gamma} = \varphi$ and $L^{\Gamma} = L^{\varphi}$.

We note that the group G_A can be computed trivially in polynomial time as $G_A = \varphi^{-1}(\mathfrak{S}(\Gamma)_A).$

Definition 10.2 (Full set). Let $A \subseteq \Gamma$. We say that A is *full* with respect to \mathfrak{x} if $\operatorname{Aut}_G(\mathfrak{x})_A^A \geq \mathfrak{A}(A)$, i. e., the *G*-automorphisms of \mathfrak{x} induce a giant on A. Notation: $\mathcal{F}(\mathfrak{x}) = \{A \in \binom{\Gamma}{k} \mid A \text{ is full }\}$ and $\overline{\mathcal{F}}(\mathfrak{x}) = \binom{\Gamma}{k} \setminus \mathcal{F}(\mathfrak{x})$.

We consider the problem of deciding whether or not a given small "test set" $A \subset \Gamma$ is full and compute useful certificates of either outcome. We show that this question can efficiently (in time $k! \operatorname{poly}(n)$) be reduced to the String Isomorphism problem on inputs of size $\leq n/k$ where k = |A| is the size of our test set; we shall choose $k = O(\log n)$.

Certificate of non-fullness. We certify non-fullness of the test set $A \subset \Gamma$ by computing a permutation group $M(A) \leq \mathfrak{S}(A)$ such that (i) $M(A) \not\geq \mathfrak{A}(A)$ and (ii) $M(A) \geq \operatorname{Aut}_G(\mathfrak{x})^A_A$ (M(A) is guaranteed to contain the projection of the *G*-automorphism group of \mathfrak{x}).

Such a group M(A) can be thought of as a constructive refutation of fullness.

Certificate of fullness. We certify fullness of the test set $A \subset \Gamma$ by computing a permutation group $K(A) \leq \mathfrak{S}(\Omega)$ such that (i) $K(A) \leq \operatorname{Aut}_G(\mathfrak{x})$ and (ii) A is K(A)-invariant and $K(A)^A \geq \mathfrak{A}(A)$.

Note that K(A) represents an easily (poly-time) verifiable proof of fullness of A.

Our ability to find K(A), the certificate of fullness, may be surprising because it means that from a local start (that may take only a small segment of \mathfrak{x} into account), we have to build up global automorphisms (automorphisms of the full string \mathfrak{x}). Our ability to do so critically depends on the "Unaffected Stabilizer Theorem" (Thm. 8.11).

Theorem 10.3 (Local certificates). Let $A \subseteq \Gamma$ where |A| = k. We refer to A as our "test set." Assume $\max\{8, 2 + \log_2 n\} < k \leq m/10$. By making $\leq k!n^2$ calls to String Isomorphism problems on domains of size $\leq n/k$ and performing $k! \operatorname{poly}(n)$ computation we can decide whether or not A is full and

(a) if A is full, find a certificate $K(A) \leq \operatorname{Aut}_G(\mathfrak{x})$ of fullness of A

(b) if A is not full, find a certificate $M(A) \leq \mathfrak{S}(A)$ of non-fullness.

The families $\{(A, K(A)) : A \in \mathcal{F}(\mathfrak{x})\}$ and $\{(A, M(A)) : A \in \overline{\mathcal{F}}(\mathfrak{x})\}$ are canonical.

Definition 10.4 (Affected). Let $G \leq \mathfrak{S}(\Omega)$ be a permutation group and and $\varphi : G \to \mathfrak{S}(\Gamma)$ a homomorphism. Consistently with previous usage, for a subgroup $H \leq G$ we say that $x \in \Omega$ is affected by (H, φ) if $H_x^{\varphi} \not\geq \mathfrak{A}(\Gamma)$. Let $\operatorname{Aff}(H, \varphi)$ denote the set of elements affected by (H, φ) , i. e.,

$$\operatorname{Aff}(H,\varphi) = \{ x \in \Omega \mid H_x^{\varphi} \geq \mathfrak{A}(\Gamma) \}.$$
(38)

Note that if φ restricted to H is not a giant representation then all of Ω is affected by (H, φ) .

If $x \in \Omega$ is affected by (H, φ) then all elements of the orbit x^H are affected by (H, φ) . In other words, $Aff(H, \varphi)$ is an *H*-invariant set. So we can speak of *affected orbits* of *H* (of which all elements are affected).

We observe the dual monotonicity of the Aff operator.

Observation 10.5. If $H_1 \leq H_2 \leq G$ then $\operatorname{Aff}(H_1, \varphi) \supseteq \operatorname{Aff}(H_2, \varphi)$.

The algorithm will consider the input in an increasing sequence of "windows" $W \subseteq \Omega$; in each round, the part of the input outside the window will be ignored. The group H(W) will be the subgroup of G_A that respects the string \mathfrak{x}^W , the restriction of \mathfrak{x} to W. The initial window is the empty set (the input is wholly ignored), so the initial group is G_A . Then in each round we add to W the set of elements of Ω affected by the current group H(W). I like to visualize this process as "growing the beard" (W being the beard). By the second round $W \neq \emptyset$ because $\operatorname{Aff}(G_A, \psi_A)$ cannot be empty (by the Unaffected Stabilizer Theorem).

As an increasing segment of \mathfrak{x} is taken into account, the group H(W) (the automorphism group of this segment) decreases, and thereby the set of elements affected by H(W) increases. (Previous windows will always be invariant under H(W).)

We stop when one of two things happens: either ψ_A restricted to H(W) is no longer a giant homomorphism, or the beard stops growing: no element outside W is affected by H(W).

In the former case we declare that our test set A is not full (witnessed by a non-giant group $M(A) := H(W)^A \leq \mathfrak{S}(A)$). Note that the reason M(A) is not a giant is still "local," it only depends on the restriction of \mathfrak{x} to the current window.

In the latter case we declare that A is *full*, and bring as witness the group $K(A) = H(W)_{(\overline{W})}$, the pointwise stabilizer of $\overline{W} = \Omega \setminus W$ in H(W). We claim two things about K(A). First, $K(A)^{\varphi} \geq \mathfrak{A}(\Gamma)$. This follows from the Unaffected Stabilizer Theorem (Thm. 8.11) since none of the elements of \overline{W} is affected. (This is why the beard stopped growing.) Second, we observe that $K(A) \leq \operatorname{Aut}_G(\mathfrak{g})$. Indeed, K(A) respects the letters of the string \mathfrak{g} on W (this is an invariant of the algorithm); and it fixes all elements outside W, so the letters of the string restricted to \overline{W} are automatically respected. (This observation was the "eureka moment" of this seven-year project. It occurred on September 14, 2015.)

Here is the algorithm in pseudocode, with a more formal proof.

Proof of Theorem 10.3. For $W \subseteq \Omega$ let $H(W) = \operatorname{Aut}_{G_A}^W(\mathfrak{x})$.

All sets denoted A, A', and A_i below will be subsets of Γ of size k (the "test sets"). An invariant of the **while** loop will be that A is invariant under the action of the group H(W), i.e., $H(W) \leq G_A$.

Procedure LocalCertificates

Input: $A \subset \Gamma$, |A| = kOutput: decision: "A full/not full," group K(A) (if full) or M(A) (if not full), set $W(A) \subseteq \Omega$

We need to show how to recompute H(W) on line 4. We write W_{old} for the value of W before the execution of line 03 and W_{new} after.

Procedure Recompute H(W)

04a $N \leftarrow H(W_{\text{old}})^A_{(A)}$ (: kernel of $H(W_{old}) \to \mathfrak{S}(A)$ map :) 04b $L \leftarrow \emptyset$ (: L will collect elements of $H(W_{\text{new}})$:) (: $H(W_{\text{old}})^A = \mathfrak{A}(A) \text{ or } \mathfrak{S}(A)$:) 04c for $\overline{\sigma} \in H(W_{\text{old}})^A$ select $\sigma \in H(W_{\text{old}})$ such that $\sigma^A = \overline{\sigma}$ (: lifting $\overline{\sigma}$ to Ω :) 04d $L(\overline{\sigma}) \leftarrow \operatorname{Aut}_{N\sigma}^{W_{\operatorname{new}}}(\mathfrak{x})$ (: performing strong Luks-reduction to N :) 04e $L \leftarrow L \cup L(\overline{\sigma})$ 04f 04g end(for) 04h return $H(W_{\text{new}}) \leftarrow L$

Justification. First we observe that on each iteration of the **while** loop on lines 02–05, $H(W_{\text{new}}) \leq H(W_{\text{old}})$ and $W_{\text{new}} \supseteq W_{\text{old}}$. In fact, these inclusions are proper or else we exit on line 02. In particular, A is invariant under H(W) throughout the process because it is invariant in line 01. It also follows that on line 07 we actually have $\text{Aff}(H(W), \psi_A) = W$. We also note that the **while** loop will be executed at least once (by the comment on line 01).

Claim 10.6. On line 08, $K(A)^A \ge \mathfrak{A}(A)$ and $K(A) \le \operatorname{Aut}_G(\mathfrak{x})$. In particular, A is full.

Proof. $K(A) \ge \mathfrak{A}(A)$ is the crucial consequence of Theorem 8.11, applied to the giant representation $\overline{\psi}_A : H(W_{\text{old}}) \to \mathfrak{S}(A)$. ($\overline{\psi}_A$ denotes the restriction of ψ_A to $H(W_{\text{old}})$.)

To show that $K(A) \leq \operatorname{Aut}_G(\mathfrak{x})$ let $\sigma \in K(A)$ and $u \in \Omega$. We need to show that $\mathfrak{x}(u^{\sigma}) = \mathfrak{x}(u)$. If $u \in W$ then this follows because $\sigma \in H(W) = \operatorname{Aut}_G^W(\mathfrak{x})$. If $u \in \overline{W}$ then $u^{\sigma} = u$. \Box

Claim 10.7. If A is not full then we reach line 10 with $M(A) \not\geq \mathfrak{A}(A)$ and $\operatorname{Aut}_G(\mathfrak{x})_A^A \leq M(A)$.

Proof. We reach line 10 by Claim 10.6. We then have $\operatorname{Aut}_G(\mathfrak{x})^A_A \leq M(A)$ because the relation $\operatorname{Aut}_G(\mathfrak{x})^A_A \leq H(W)$ is an invariant of the process.

Next we justify procedure Recompute H(W). This is immediate from the observation

$$H(W_{\text{old}}) = \bigcup_{\overline{\sigma}} N\overline{\sigma}$$
(39)

where the union extends over $\overline{\sigma} \in H(W_{\text{old}})$. So we can use strong Luks-reduction (over the orbits of N in W_{new}) to compute $\operatorname{Aut}_{H(W_{\text{old}})}^{W_{\text{new}}}(\mathfrak{x})$. But this group is $H(W_{\text{new}})$ because $W_{\text{new}} \supseteq W_{\text{old}}$.

Finally we need to justify the complexity assertion. This is where Cor. 8.13 ("Affected Orbits Lemma") plays a critical role.

The while loop is executed at most n times (because W strictly increases in each round; we exit on line 02 when the "beard" stops growing), so the dominant component of the

complexity is in recomputing H(W). We have reduced this to $\leq k!$ instances of string N-isomorphism on the window W_{new} .

By Cor. 8.13 ("Affected Orbits Lemma"), each orbit of N in W_{new} has length $\leq n/k$.

We conclude that strong Luks reduction reduces the recomputation of H(W) to $\leq n \cdot k!$ instances of String Isomorphism on windows of size $\leq n/k$, justifying the stated complexity estimate.

Our procedure does more than stated in Theorem 10.3. It also returns the set W(A). We summarize key properties of this assignment.

Proposition 10.8. As in Theorem 10.3, let a "test set" be a subset $A \subseteq \Gamma$ with |A| = k elements where $\max\{8, 2 + \log_2 n\} < k \le m/10$. For all test sets A we have

- (i) $\Omega(A) \subseteq W(A) \subseteq \Omega$
- (ii) W(A) is invariant under $\operatorname{Aut}_{G_A}(\mathfrak{x})$
- (iii) if A is full then $W(A) = \operatorname{Aff}(\operatorname{Aut}_{G_A}^{W(A)}(\mathfrak{x}))$
- (iv) if A is full then $K(A)^A$ fixes all elements of $\Omega \setminus W(A)$
- (v) the assignment $A \mapsto W(A)$ is canonical.

Proof. Evident from the algorithm.

We need to highlight one more fact about the structures we obtained.

Notation 10.9 (Truncation of strings). Let * be a special symbol not in the alphabet Σ . For the string $\mathfrak{x} : \Omega \to \Sigma$ and "window" $W \subseteq \Omega$ we define the string $\mathfrak{x}^W : |omgea \to (\Sigma \cup \{*\})$ by setting $\mathfrak{x}^W(u) = \mathfrak{x}(u)$ for $u \in W$ and $\mathfrak{x}^W(u) = *$ for $u \in \Omega \setminus W$.

Notation 10.10 (Coloring of strings). For the string $\mathfrak{x} : \Omega \to \Sigma$ and the "test set" $A \subseteq \Gamma$ we define the string $\mathfrak{x}_A : \Omega \to (\Sigma \times \{0,1\})$ by setting $\mathfrak{x}_A(u) = (\mathfrak{x}(u), 1)$ if $u \in \Omega(A)$ and $\mathfrak{x}_A(u) = (\mathfrak{x}(u), 0)$ if $u \notin \Omega(A)$.

Proposition 10.11 (Comparing local certificates). For all test sets $A, A' \subseteq \Gamma$ with |A| = |A'| = k and all strings $\mathfrak{x}, \mathfrak{x}' : \Omega \to \Sigma$ we can compute $\operatorname{Iso}_G\left(\mathfrak{x}_A^{W(A)}, (\mathfrak{x}')_{A'}^{W(A')}\right)$ by making $\leq k!n^2$ calls to String Isomorphism problems on domains of size $\leq n/k$ and performing $k! \operatorname{poly}(n)$ computation.

Proof. Run procedure LocalCertificates simultaneously on (\mathfrak{x}, A) and on (\mathfrak{x}', A') , maintaining the variable W for (x, A) and the variable W' for (\mathfrak{x}', A') . Further maintain the set $Q = \text{Iso}_G(\mathfrak{x}^W_A, (\mathfrak{x}')^{W'}_{A'})$. On line 01 we shall have $Q = G_A \sigma$ for any $\sigma \in G$ that takes A to A'.

Change line 04 to "recompute H(W) and Q."

Here is the modified "Recompute" code.

Procedure Recompute H(W) and Q

 $N \leftarrow H(W_{\text{old}})^A_{(A)}$ 04a (: kernel of $H(W_{old}) \to \mathfrak{S}(A)$ map :) (: L will collect elements of $H(W_{\text{new}})$:) 04b1 $L \leftarrow \emptyset$ $R \leftarrow \emptyset$ (: R will collect elements of Q_{new} :) 04b2 fix $\pi_0 \in Q_{\text{old}}$ 04c0(: $H(W_{\text{old}})^A = \mathfrak{A}(A) \text{ or } \mathfrak{S}(A)$:) for $\overline{\sigma} \in H(W_{\text{old}})^A$ 04c1select $\sigma \in H(W_{\text{old}})$ such that $\sigma^A = \overline{\sigma}$ 04d1 (: lifting $\overline{\sigma}$ to Ω :) $(: \pi \in Q_{\text{old}} :)$ 04d2 $\pi \leftarrow \sigma \pi_0$ $L(\overline{\sigma}) \leftarrow \operatorname{Aut}_{N\sigma}^{W_{\operatorname{new}}}(\mathfrak{x})$ 04e1 $R(\overline{\sigma}) \leftarrow \operatorname{Iso}_{N\pi}(\mathfrak{x}_{A}^{W_{\text{new}}}, (\mathfrak{x}')_{A'}^{W'_{\text{new}}})$ (: performing strong Luks-reduction to N :) 04e2(: collecting automorphisms :) 04f1 $L \leftarrow L \cup L(\overline{\sigma})$ 04f2 $R \leftarrow R \cup R(\overline{\pi})$ (: collecting isomorphisms :) end(for) 04g if $R = \emptyset$ then reject isomorphism, exit 04x else return $H(W_{\text{new}}) \leftarrow L$ and $Q \leftarrow R$ 04h

The analysis is analogous with the analysis of the Recompute H(W) routine.

Notation 10.12 (Sideburn). Assume A is full. Let W(A) (the "sideburn") denote the set of those elements of Γ that are affected by $K(A)^{\Gamma}$:

$$\widetilde{W}(A) = \operatorname{Aff}(K(A)^{\Gamma}) \tag{40}$$

Clearly $A \subseteq \widetilde{W}(A)$.

Growing the "sideburn" is analogous to growing the "beard" except we do not iterate (K(A) already consists of "global" automorphisms).

Recall the definition of the *minial degree* of a permutation group (Def. 2.2).

Proposition 10.13. Let $A \subseteq \Gamma$ be a full test set (subset with |A| = k where $k > \max\{8, 2 + \log_2 m\}$). Then the minimal degree of $K(A)^{\Gamma}$ is at most $|\widetilde{W}(A)|$.

Proof. Let $L(A) \leq \mathfrak{S}(\Gamma)$ denote the pointwise stabilizer of $\Gamma \setminus \widetilde{W}(A)$ in $K(A)^{\Gamma}$. Then, by the "Unaffected Stabilizer Theorem," (Thm. 8.11), $L(A)^A \geq \mathfrak{A}(A)$.

10.2 Aggregating the local certificates

We continue the notation of the previous section.

Theorem 10.14 (AggregateCertificates). Let $\varphi : G \to \mathfrak{S}(\Gamma)$ be a giant representation, where $G \leq \mathfrak{S}(\Omega)$, $|\Omega| = n$, and $|\Gamma| = m$. Let $\max\{8, 2 + \log_2 n\} < k < m/10$. Then, at a multiplicative cost of $m^{O(k)}$, we can either find a canonical colored 4/5-partition of Γ or find a canonically embedded k-ary relational structure with relative symmetry defect $\geq 1/2$ on Γ , or reduce the determination of $\operatorname{Iso}_G(\mathfrak{x}, \mathfrak{y})$ to $n^{O(1)}$ instances of size $\leq 2n/3$. *Proof.* We describe the procedure, interspersed with the justification.

Run the LocalCertificates routine for both inputs $\mathfrak{x}, \mathfrak{y}$ and all test sets $A \in \binom{1}{k}$.

Run the CompareLocalCertificates routine for all pairs $((\mathfrak{x}, A), (\mathfrak{x}', A'))$ where \mathfrak{x} is fixed, $\mathfrak{x}' \in {\mathfrak{x}, \mathfrak{y}}$, and $A, A' \in {\Gamma \choose k}$ are test sets (a total of $2{\binom{m}{k}}^2$ runs).

Let $F(\mathfrak{x})$ be the subgroup generated by the groups K(A) for all full subsets $A \in {\Gamma \choose k}$ with reference to input string \mathfrak{x} . So $F(\mathfrak{x})$, and with it $F(\mathfrak{x})^{\Gamma}$, are canonically associated with \mathfrak{x} . In particular, if $F(\mathfrak{y})$ is analogously defined for \mathfrak{y} , then $F(\mathfrak{x})^{\Gamma}$ is permutationally isomorphic to $F(\mathfrak{y})^{\Gamma}$, i.e., there exists a permutation $\alpha \in \mathfrak{S}(\Gamma)$ such that $F(\mathfrak{y})^{\Gamma} = \alpha^{-1}F(\mathfrak{x})^{\Gamma}\alpha$.

Below we ignore \mathfrak{y} and focus on \mathfrak{x} , omitting it from the notation, so we write $F = F(\mathfrak{x})$. But our guide is the above consequence of canonicity.

- 1 If there exists a full subset $A \in {\Gamma \choose k}$ such that $|\widetilde{W}(A)| \ge m/5$ then by individualizing each element of A we reduce the question to N-isomorphism at a multiplicative cost of $m^{O(k)}$. The N-orbits on $\widetilde{W}(A)$ have length $\le m/k$, so the N-orbits on Γ form a 4/5-partition. It follows by Cor. 5.6 that each N-orbit on Ω has size $\le 4n/5$. Process via Chain Rule, **exit**
- 2 (: Now $(\forall A)(|\widetilde{W}(A)| < m/4)$:)
- 2a If the nontrivial orbits (orbits of length ≥ 2) of F^{Γ} cover at least m/5 elements of Γ and no orbit of F^{Γ} has length > 4m/5 we found a colored 4/5-partition of Γ , exit
- 2b (: F^{Γ} has an orbit $C \subseteq \Gamma$ of length |C| > 4m/5. Note that since |C| > m/2, this orbit is canonical. :)
- 2b1 Assume F^C is doubly transitive. **Claim:** If F^C is doubly transitive then it is a giant, i.e., $F^C \ge \mathfrak{A}(C)$.

Proof of Claim. Assume F^C is doubly transitive. If F^C is not a giant, it follows that its minimal degree is $\geq |C|/4 > m/5$ assuming $|C| \geq 217$ (Bochert's theorem, Thm. 2.3) for which $m \geq 272$ is sufficient. But the minimal degree of F^C is at most the minimal degree of $K(A)^{\Gamma}$ which is at most $|\widetilde{W}(A)|$ by Prop. 10.13, a contradiction with the assumption that $|\widetilde{W}(A)| < m/5$.

(: So $F^C \ge \mathfrak{A}(C)$:) Now apply Cor. 9.9

2b2 (: F^{Γ} is transitive but not doubly transitive :) Let $\mathfrak{X} = (C; R_1, \ldots, R_r)$ be the orbital configuration of F^C (the R_i are the orbits of F^C on $C \times C$). This is a non-clique homogeneous coherent configuration, so $3 \leq r \leq m$. (: Warning: the numbering of the R_i is not canonical; isomorphisms may permute the R_i . :)

Let $R_1 = \text{diag}(C)$ be the diagonal

(: so for $i \ge 2$ the constituents $X_i = (C, R_i)$ are nontrivial biregular digraphs :) Individualize one of the X_i $(i \ge 2)$ (: multiplicative cost $r - 1 \le m - 1$:)

return X_i , exit

(: Note: X_i has relative symmetry defect $\geq 1/2$ by Cor. 2.20 because X_i is an irreflexive, biregular, nontrivial digraph. :)

2c Let $D \subseteq \Gamma$ be the set of fixed points of F^{Γ} . So in the remaining case we have $|D| \ge 3m/4$. Note that in this case, if $A \subset D$ then A is not full. (In fact even if $A \cap D \neq \emptyset$ then A is not full.)

Claim (Turning local asymmetry into global irregularity)

We can construct a canonical k-ary relational structure on D with symmetry defect (much) greater than 1/2.

Proof. Let \mathcal{P} denote set of ordered k-tuples of elements of Γ . Let us say that $\vec{u} = (u_1, \ldots, u_k) \in \mathcal{P}$ and $\vec{v} = (v_1, \ldots, v_k) \in \mathcal{P}$ are equivalent if there exists $\alpha \in \operatorname{Iso}_G\left(\mathfrak{x}_A^{W(A)}, (\mathfrak{x}_{A'})\right)$ such that $u_i^{\alpha} = v_i$ for all i where $A = \{u_1, \ldots, u_k\}$ and $A' = \{v_1, \ldots, v_k\}$. This is an equivalence relation on \mathcal{P} . It has at least k equivalence classes since in a single $A \subseteq D$ we have $|\mathfrak{A}(A) : M(A)| \geq k$ equivalence classes of the orderings of A. Each equivalence class is invariant under $\operatorname{Aut}_G(\mathfrak{x})^{\Gamma}$. So this is a k-ary relational structure. We claim that its symmetry defect is very large: greater than |D| - k > m/2. Indeed, no subset A of D of size k can be symmetrical since M(A) is a proper subgroup of $\mathfrak{A}(A)$.

Let $\mathfrak{X} = (C; R_1, \ldots, R_s)$ denote the resulting k-ary relational structure based on input \mathfrak{x} , and let $\mathfrak{X}' = (C'; R'_1, \ldots, R'_{s'})$ be the corresponding relational structure based on input \mathfrak{y} . If $s \neq s'$, reject isomorphism, exit.

To establish canonicity, we need to canonically number the relations in our category of 2 objects, one corresonding to \mathfrak{x} and the other to \mathfrak{y} . In other words, we need to find a permutation $\pi \in \mathfrak{S}_s$ such that every *G*-isomorphism $\mathfrak{x} \to \mathfrak{y}$ induces an isomorphism of \mathfrak{X} to $\mathfrak{Y} = (C'; S_1, \ldots, S_s)$ where $S_i = R'_{i\pi}$.

To this end we also compute all sets of isomorphisms $\operatorname{Iso}_G\left(\mathfrak{x}_A^{W(A)},(\mathfrak{y})_{A'}^{W'(A')}\right)$ for all $A, A' \in \binom{\Gamma}{k}$, where W' coreesponds to W under input \mathfrak{y} . If for some A' this set is empty for every A then reject isomorphism, exit. Otherwise if $\vec{v} = (v_1, \ldots, v_k) \in S_j$ where $\{v_1, \ldots, v_k\} = A'$ and the inverse of some isomorphism from $\operatorname{Iso}_G\left(\mathfrak{x}_A^{W(A)},(\mathfrak{y})_{A'}^{W'(A')}\right)$ takes \vec{v} to some $\vec{u} \in R_i$ then we set $j^{\pi} = i$. If the resulting relation π is not a permutation, reject isomorphism, exit. Otherwise we have the desired matching between the relations in \mathfrak{X} and the relations in \mathfrak{X}' .

Now **return** this canonical k-ary relational structure, **exit**

This completes the procedure and the proof.

11 Effect of discovery of canonical structures

Situation: We have a transitive group $G \leq \mathfrak{S}(\Omega)$ of degree $n = |\Omega|$ and a giant representation $\varphi: G \to \mathfrak{S}(\Gamma)$ (i. e., $G^{\varphi} \geq \mathfrak{A}(\Gamma)$). Assume $m := |\Gamma| \geq 10 \log_2 n$. Let Φ be the set of standard blocks for φ (see the Main Structure Theorem, Thm. 8.19, so $\Phi = \{B_T : T \in {\Gamma \choose t}\}$. The B_T partition Ω and form a system of imprimitivity for G.

In this section we study the effect of canonical structures embedded in Γ .

Both our group-theoretic partitioning algorithm (AggregateCertificates, Theorem 10.14) and our combinatorial partitioning algorithm (the Extended Design Lemma, Theorem 7.12) produce a canonical coloring of Γ with an additional canonical structure on some of the color classes. The additional structure can be an equipartition or a Johnson scheme. (We note that canonicity in each case is relative to arbitrary choices previously made and correspondigly came at a multiplicative cost.)

11.1 Alignment of input strings, reduction of group

A common features of the categories of these types of structures is that their G^{φ} -isomorphisms are easy to find $(G^{\varphi}$ is either $\mathfrak{S}(\Gamma)$ or $\mathfrak{A}(\Gamma)$). (This is trivial in linear time for colored equipartitions, and polynomial time for Johnson schemes).

We use these structures to align the input strings \mathfrak{x} and \mathfrak{y} and reduce the group G.

Let $\mathfrak{X}(\mathfrak{z})$ be the canonical structure associated with the input string $\mathfrak{z} \in {\mathfrak{x}, \mathfrak{y}}$. Alignment means that $\mathfrak{X}(\mathfrak{x}) = \mathfrak{X}(\mathfrak{y}')$ for a *G*-shifted copy \mathfrak{y}' of \mathfrak{y} .

Procedure Align

Input: canonical structures $\mathfrak{X}(\mathfrak{p})$, $\mathfrak{X}(\mathfrak{y})$ on Γ Output: string \mathfrak{y}' , permutation $\sigma \in G$, and group $G_1 \leq G$ such that

$$\operatorname{Iso}_{G}(\mathfrak{x},\mathfrak{y}) = \operatorname{Iso}_{G_{1}}(\mathfrak{x},\mathfrak{y}')\sigma \quad \text{and} \quad G_{1}^{\varphi} = \operatorname{Aut}(\mathfrak{X}(\mathfrak{x}))$$

$$\tag{41}$$

(: Note that it follows that $\mathfrak{X}(\mathfrak{x}) = \mathfrak{X}(\mathfrak{y}')$:)

Additional output if \mathfrak{X} has a dominant color class $\Delta \subseteq \Gamma$ ($|\Delta| > m/2$) and \mathfrak{X} involves an equipartition of Δ or a Johnson scheme on Δ : reduced set Γ' and giant representation $G \to \mathfrak{S}(\Gamma')$ for recursive processing of the corresponding window $\Omega(\Delta)$.

1. If $\mathfrak{X}(\mathfrak{x})$ and $\mathfrak{X}(\mathfrak{y})$ are not G^{φ} -isomorphic then reject isomorphism, exit

- 2. Else, let
 - (i) $\overline{\sigma} \in \operatorname{Iso}_{G^{\varphi}}(\mathfrak{X}(\mathfrak{x}), \mathfrak{X}(\mathfrak{y}))$ (: aligning in Γ :) (ii) $\sigma \in \varphi^{-1}(\overline{\sigma})$ (: lifting :) (iii) $\mathfrak{y}' = \mathfrak{y}^{\sigma^{-1}}$ (: aligning the inputs :) (iv) $G_1 = \varphi^{-1}(\operatorname{Aut}(\mathfrak{X}(\mathfrak{x})))$ (: reducing the group :)

(: Alignment as stated in Eq. (41) achieved :)

3. Update: $\mathfrak{y} \leftarrow \mathfrak{y}', G \leftarrow G_1$.
4. (: Each of our structures has an underlying coloring – possibly trivial :)

Let $(\Delta_1, \ldots, \Delta_k)$ be the coloring of $\mathfrak{X}(\mathfrak{x})$ (the Δ_j are the color classes); so Γ is the disjoin union of the Δ_j .

This coloring induces a canonical coloring of $\Phi = {\Gamma \choose t}$ as described in Lemma 5.5; let Φ_1, \ldots, Φ_s be the color classes. This coloring in turn lifts to a canonical coloring of Ω with corresponding color classes $\Omega_1, \ldots, \Omega_s$ where $\Omega_i = \bigcup_{T \in \Phi_i} B_T$. For $A \subseteq \Gamma$ recall the notation $\Phi(A) = {A \choose t}$ and $\Omega(A) = \bigcup_{T \in \Phi(A)} B_T$.

- 5. Apply the Chain Rule to the color classes Ω_i .
- 6. If $(\exists j)(|\Delta_j| > m/2)$ ("dominant color") then start the application of the Chain Rule with the window $\Omega(\Delta_j) = \bigcup_{T \in (\Delta_j)} B_T$.
- 7. While processing window $\Omega(\Delta_j)$
 - (A) if \mathfrak{X} gives a nontrivial equipartition of Δ_j then let Γ' be the set of blocks
 - (B) if Δ_j is the vertex set of a Johnson scheme $\mathfrak{J}(m', t')$ $(t' \ge 2)$ then identify Δ_j with $\Delta_j = \binom{\Gamma'}{t'}$ where $|\Gamma'| = m'$.
- 8. let $\varphi': G \to \mathfrak{S}(\Gamma')$ be the induced *G*-action on Γ' (: this is a giant representation :)

9. update:
$$\varphi \leftarrow \varphi', \Gamma \leftarrow \Gamma'$$

end(procedure)

11.2 Cost analysis

We are assuming that isomorphism of our canonical structures \mathfrak{X} is testable in polynomial time (which is certainly true for the types of structures considered), so Line 2 is executed in polynomial (in m) time.

We need to examine the efficiency of the application of the Chain rule in Lines (5), (6).

We measure complexity in terms of the number of group operations. We assume G and a giant representation $\varphi: G \to \mathfrak{S}(\Gamma)$ are given where $G \leq \mathfrak{S}(\Omega)$ with $|\Omega| = n$ and $|\Gamma| = m$. Let $T(G, \varphi)$ be the maximum cost over all input strings for the pair (G, φ) .

We use the notation of Section 3.4. So $T_{\rm Jh}(x, y)$ is the maximum of $T(G, \varphi)$ over all G and φ with the parameters $n \leq x$ and $m \leq y$. Moreover, $T_{\rm Jh}(x)$ is defined as $T_{\rm Jh}(x) = T_{\rm Jh}(x, x)$. T(x) is the upper bound for all groups G of degree $n \leq x$. (Note that n is the "window size.")

We are looking a function T(x) that is "nice" in the sense that $\log \log T(x)/\log \log x$ is monotone nondecreasing for sufficiently large x. (For the function $\exp((\log x)^c)$, this quantity is constant.)

In analyzing the complexity, we need to take into account the potentially quasipolynomial (in terms of m), say q(m), multiplicative cost of reaching our canonical structures \mathfrak{X} : we need

to compare not one but q(m) instances of $\mathfrak{X}(\mathfrak{y})$ with $\mathfrak{X}(\mathfrak{x})$). So the overall cost, including the application of the Chain rule, will be

$$T(G,\varphi) \le q(m) \sum_{i} T(|\Omega_i|)$$
(42)

If $(\forall i)(|\Omega_i| \leq 2n/3)$ then this yields (generously) the inequality

$$T(G,\varphi) \le m \cdot q(m)T(2n/3),\tag{43}$$

justifying Inequality (20). (In fact, for "nice" functions as postulated, we obtain $T(G, \varphi) \leq q(m)(T(n/3) + T(2n/3))$. But this gain of a factor of m will make no difference.)

If $(\exists i)(|\Omega_i| > 2n/3)$ then by Lemma 5.5, for this $i = i_0$ we must have $\Omega_{i_0} = \Omega(\Delta_j)$ where $|\Delta_j| > 2m/3$. The total contribution of all other Ω_i to the right-hand side of Eq. (42) is at most q(m)T(n/3).

Our progress on $\Omega(\Delta_j)$ is measured in terms of the reduced Γ . In the case of an equipartition, Γ' is the set of blocks of the partition, so $|\Gamma'| \leq m/2$. In case of a Johnson scheme $\mathfrak{J}(m',t')$ $(t' \geq 2)$ with vertex set $\Delta_j = \binom{\Gamma'}{t'}$, we have $m \geq |\Delta_j| = \binom{m'}{t'} \geq \binom{m'}{2} > (m'-1)^2/2$, so $m' < 1 + \sqrt{2m} < m/2$ (for $m \geq 12$). So in each case we obtain the inequality

$$T(G,\varphi) \le q(m)(T(n/3) + T_{\rm Jh}(n,m/2))$$
 (44)

justifying Eq. (v) in Sec. 3.4 and yielding the conclusion

$$T(n) \le q(n)^{O(\log^2 n)} \tag{45}$$

as in Eq. (22).

12 The Master Algorithm

The algorithm will refer to a polylogarithmic function $\ell(x)$ to be specified later.

Whenever a subroutine in the algorithm exits and returns a good color-partition of Ω , the algorithm starts over (recursively). If it returns a structure such as a UPCC, we move to the next line. If the subroutine returns isomorphism rejection, that branch of the recursion terminates and the algorithm backtracks.

Procedure String-Isomorphism

Input: group $G \leq \mathfrak{S}(\Omega)$, strings $\mathfrak{x}, \mathfrak{y} : \Omega \to \Sigma$

Output: $\operatorname{Iso}_G(\mathfrak{x},\mathfrak{y})$

- 1. Apply Procedure Reduce-to-Johnson (Luks reductions, Sec. 3.3)
 - (: The rest of this algorithm constitutes the ProcessJohnsonAction routine announced in Sec. 3.3)

- 2. (: G is transitive, G-action 𝔅 on blocks is Johnson group isomorphic to 𝔅_m or 𝔄_m :) set ℓ = (log n)³
 if m ≤ ℓ then apply strong Luks reduction to reduce to kernel of the G-action on the blocks (brute force on small primitive group 𝔅, multiplicative cost ℓ! :)
- 3. (: G-action on blocks is isomorphic to $\mathfrak{S}(\Gamma)$ or $\mathfrak{A}(\Gamma)$, $|\Gamma| = m > \ell$:) Let $\varphi : G \to \mathfrak{S}(\Gamma)$ be a giant representation (inferred from \mathfrak{G}) Let $N = \ker(\varphi)$ and let $\Phi = \{B_T \mid T \in {\Gamma \choose t}\}$ be the set of standard blocks (Thm. 8.19) (: the B_T partition Ω and G acts on Φ as $\mathfrak{S}^{(t)}(\Gamma)$ or $\mathfrak{A}^{(t)}(\Gamma)$:)
- 4. if G primitive (: i. e., Ω = Φ :)
 if t = 1 then find Iso_G(𝔅, 𝔅), exit (: trivial case: Ω = Γ, G = 𝔅(Ω); isomorphism only depends on the multiplicity of each letter in the strings 𝔅, 𝔅 :)
- 5. else (: t ≥ 2 :) view 𝔅, 𝔅 as edge-colored t-uniform hypergraphs ℋ(𝔅) and ℋ(𝔅) on vertex set Γ
 if relative symmetry defect of ℋ(𝔅) is < 1/2 then apply Cor. 9.9
- 6. else (: now their relative symmetry defect is $\geq 1/2$:) (: view these hypergraphs as *t*-ary relational structures :) apply Extended Design Lemma (Theorem 7.12)
- 7. (: canonical structure \mathfrak{X} on Γ found: colored equipartition or Johnson scheme :) apply Procedure Align to \mathfrak{X} (Sec. 11.1)
- 8. else (: G imprimitive, i. e., $|\Phi| \le (1/2)|\Omega|$:) apply AggregateCertificates (Theorem 10.14)
 - (: Note: this is where our main group-theoretic Divide-and-Conquer algorithm, Procedure LocalCertificates (Theorem 10.3) is used :)
- 9. if AggregateCertificates returns canonically embedded k-ary relational structure on Γ with relative symmetry defect $\geq 1/2$ then
- 11. else (: AggregateCertificates returns canonical colored equipartition on Γ :) $\mathfrak{X} \leftarrow$ colored equipartition returned
- 12. apply Procedure Align to \mathfrak{X} (Sec. 11.1)

The essence of the analysis is in the analysis of Procedure Align given in Section 11.1.

13 Concluding remarks

13.1 Dependence on the Classification of Finite Simple Groups

As mentioned in the Introduction, the algorithm, as stated, depends on the Classification of Finite Simple Groups (CFSG) via Cameron's classification of large primitive permutation groups. There is one other instance in which we rely on CFSG; we employ "Schreier's Hypothesis" in the proof of Lemma 8.5.

We are, however, able to considerably reduce the dependence of the proof on CFSG; we are able to *dispense with Cameron's result* by an application of the Extended Design Lemma (Theorem 7.12).

Cameron's result guaranteed that if we encountered a large primitive group acting on the set of blocks, the action was a Cameron group, which in turn had a subgroup of small index that was a Johnson group. This is done in Procedure Reduce-to-Johnson (Sec. 3.3).

We are able to replace this procedure by one that does not rely on Cameron's result; we locate this Johnson group combinatorially. Here is an outline.

Let \mathfrak{G} be the action of G on a minimal system of k blocks (the blocks are maximal), so $\mathfrak{G} \leq \mathfrak{S}_k$ is a primitive group.

If \mathfrak{G} is small (of order $\leq q(k)$ where q is a quasipolynomial function), we do strong Luks reduction to the kernel of the $G \to \mathfrak{G}$ epimorphism (brute force on \mathfrak{G}). This includes the case when \mathfrak{G} is doubly transitive but not a giant; then the order of \mathfrak{G} is quasipolynomially bounded, by an elementary result by Pyber [Py].

Giants are the t = 1 case of Johnson groups, so if \mathfrak{G} is a giant, we are done.

In the remaining cases, \mathfrak{G} is uniprimitive; let \mathfrak{X} be the orbital configuration of \mathfrak{G} . This is a uniprimitive coherent configuration. Apply Procedure UPCC Split-or-Johnson (Theorem 7.10) to \mathfrak{X} . The procedure either returns a canonical colored 3/4-partition of [k] (the domain on which \mathfrak{G} acts), representing significant progress, or returns a canonically embedded Johnson scheme $\mathfrak{J}(m,t)$ on a subset J of [k] of size $|J| = \binom{m}{t} \ge 3k/4$. After breaking up [k] via the Chain rule, we shall be left with J (Lemma 5.5). The G-action on $\mathfrak{J}(m,t)$ is a subgroup of $\mathfrak{S}_m^{(t)}$ and can be represented on the much smaller set [m]. If this is a giant action (the image contains \mathfrak{A}_m), we are in the same situation as if we had used Cameron's theorem. If the action is not giant, we recurse (find orbits and minimal block system for the action on [m], etc.).

13.2 How easy is Graph Isomorphism?

The first theoretical evidence against the possibility of NP-completeness of GI was the equivalence of existence and counting [Ba77, Mat], not observed in any NP-complete problem. The second, stronger evidence came from the early theory of interactive proofs: graph isomorphism is in coAM, and therefore if GI is NP-complete then the polynomial-time hierarchy collapses to the second level (Goldreich–Micali–Wigderson 1987 [GoMW]). Our result provides a third piece of evidence: GI is not NP-complete unless all of NP can be solved in quasipolynomial time.

A number of questions remain. The first one is of course whether GI is in P. Such

expectations should be tempered by the status of the *Group Isomorphism* problem⁸: given two groups by their Cayley tables, are they isomorphic? It is easy to reduce this problem to GI. In fact, Group Isomorphism seems much easier than GI; it can trivially be solved in time $n^{O(\log n)}$ where *n* is the order of the group. But in spite of considerable effort and the availability of powerful algebraic machinery, Group Isomorphism is still not known to be in P. We are not even able to decide Group Isomorphism⁹ in time $n^{O(\log n)}$.

A closely related challenge that deserves attention is the String Isomorphism problem on $n = p^k$ points, with respect to the linear group $\operatorname{GL}(k, p)$. The order of this group is about $p^{k^2} = n^{\log_p n}$; the question is, can this problem be solved in time $p^{o(k^2)}$ (or perhaps even in $\operatorname{poly}(n)$ time). I note that this problem can be encoded as a GI problem for graphs with $\operatorname{poly}(n)$ vertices so if $\operatorname{GI} \in P$ then this problem is in P as well.

The result of the present paper amplifies the significance of the Group Isomorphism problem (and the challenge problem stated) as a barrier to placing GI in P. It is quite possible that the intermediate status of GI (neither NP-complete, nor polynomial time) will persist.

In fact, even putting GI in coNP faces the same obstacle: Group Isomorphism is not known to be in coNP.

13.3 How hard is Graph Isomorphism?

Paradoxically, from a structural complexity point of view, GI (still) seems harder than factoring integers. The decision version of Factoring (given positive integers x, y, does x have divisor d in the interval $2 \le d \le y$?) is in NP \cap coNP while the best we can say about GI is NP \cap coAM. Factoring can be solved in polynomial time on a quantum computer, but no quantum advantage has yet been found for GI. On the other hand, apparently hard instances of factoring abound, whereas we don't know how to construct hard instances of GI. Could this be an indication that in structural complexity maybe we are not asking the right questions?

Even more baffling is another complexity arena, where GI is provably hard, on par with many NP-hard problems: relaxation hierarchies in proof complexity theory (Lovász–Schrijver, Sherali–Adams, Sum-of-Squares hierarchies). Building on the seminal paper by Cai, Furer, and Immerman [CaiFI], increasingly powerful hierarchies have recently been shown to be unable to refute isomorphism of graphs on sublinear levels [AM, OWWZ, SnSC], showing that

⁸In complexity theory, the "Group Isomorphism Problem" refers to groups given by Cayley tables; in other words, complexity is compared to the order of the group. From the point of view of applications, this complexity measure is of little use; in computational group theory, groups are usually given in compact representations (permutation groups, matrix groups given by lists of generators, *p*-groups given by power commutator presentation, etc.). But the fact remains that even in the unreasonably redundant representation by Cayley tables, we are unable to solve the problem is polynomial time.

⁹A simple algorithm, proposed by Tim Gowers on Dick Lipton's blog in November 2011, has a chance of running in $n^{O(\sqrt{\log n})}$. Let the *k*-profile of a finite group *G* be the function *f* on isomorphism types of *k*-generated groups where f(H) counts those *k*-tuples of elements of *G* that generate a subgroup isomorphic to *H*. For what *k* do *k*-profiles discriminate between nonisomorphic groups of order *n*? It is known that $k < (1/2)\sqrt{\log_2 n}$ is insufficient for infinitely many values of *n* (Glauberman, Grabowski [GlG]). Whether some *k* that is not much greater than $\sqrt{\log n}$ suffices is an open question that I think would deserve attention. The test case is *p*-groups of class 2; the Glauberman–Grabowski examples belong to this class.

GI tests based on these hierarchies necessarily have exponential (even factorial) complexity. However, hard-to-distinguish CFI pairs of graphs and the related pairs of which isomorphism is hard to refute in these hierarchies are vertex-colored graphs with bounded color classes. Testing isomorphism of such pairs of graphs was shown to be in polynomial time via the first application of group theory (1979/80) that used hardly more than Lagrange's Theorem from group theory [Ba79a, FuHL]. One lesson is that these hierarchies have difficulty capturing the power of even the most naive applications of group theory. Given that hardness with respect to these hierarchies can now be proved by reduction from GI, this raises the question, in what sense these hierarchies indicate hardness.

13.4 Outlook

On the bright side, a number of GI-related questions may look a bit more hopeful now. While GI is complete over the isomorphism problems of *explicit structures*, there are interesting classes of non-explicit structures where progress may be possible. Two important examples are *equivalence of linear codes* and *conjugacy (permutational equivalence) of permutation groups*. The former easily reduces to the latter. Both of these problems belong¹⁰ to NP \cap coAM and therefore they are not NP-complete unless the polynomial-time hierarchy collapses. In spite of this complexity status, no moderately exponential (exp(n^{1-c})) algorithm is known for either problem. GI reduces to each of these problems [Lu93]¹¹. Regarding both problems, see also [BaCGQ, BaCQ].

The present paper does not address the question of *canonical forms*. Do graphs permit quasipolynomial-time computable canonical forms?

It would be of great interest to find stronger structural results to better correspond to the "local \rightarrow global symmetry" philosophy. This raises difficult mathematical questions that our algorithmic divide-and-conquer techniques bypass, but results of this flavor could make the algorithm more elegant and more efficient.

Finally a more concrete question. Let $\mathfrak{X} = (V; \mathcal{R})$ be a homogeneous coherent configuration with *n* vertices. Let $W \subseteq V$, $|V| \ge \alpha n$. Suppose that the induced configuration $\mathfrak{X}[W]$ is a Johnson scheme. Is there a constant $\alpha < 1$ such that this implies that \mathfrak{X} itself is a Johnson scheme?

A result in this direction could be a step toward an elementary characterization of Cameron groups as the only primitive groups of large order. Steps toward this goal have previously been made in [Ba81] for the case $|G| > \exp(n^{1/2+\epsilon})$ and in a remarkable recent paper by Sun and Wilmes [SuW] for the case $|G| > \exp(n^{1/3+\epsilon})$.

13.5 Analyze this!

The purpose of the present paper is to give a guaranteed upper bound (worst-case analysis); it does not contribute to practical solutions. It seems, for all practical purposes, the Graph Isomorphism problem is solved; a suite of remarkably efficient programs is available (nauty,

¹⁰To see that these problems belong to coAM, one can adapt the GMW protocol [GoMW] by conjugating the group by a random permutation and choosing a uniform random set of O(n) generators.

¹¹Luks's reduction is explained by Miyazaki in a post on The Math Forum, Sep. 29, 1996.

saucy, Bliss, conauto, Traces). The article by McKay and Piperno [McP] gives a detailed comparison of methods and performance. Piperno's article [Pi] gives a detailed description of *Traces*, possibly the most successful program for large, difficult graphs.

These algorithms provide ingenious shortcuts in backtrack search. One of the most important questions facing the theorist in this area is to analyze these algorithms. While Miyazaki's graphs provide hard cases for the early version of *nauty*, the recent update overcomes that difficulty.

The question is, does there exist an infinite family of pairs of graphs on which these heuristic algorithms fail to perform efficiently? The search for such pairs might turn up interesting families of graphs.

Alternatively, can one prove strong worst-case upper bounds on the performance of any of these algorithms?

The comparison charts in [McP] seem to suggest that we lack true benchmarks – difficult classes of graphs on which to compare the algorithms. Encoding class-2 p-groups as graphs could provide quasipolynomially difficult examples, but right now we have no guarantee that the heuristics could not be tricked into much worse, (moderately?) exponential behavior.

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The most direct forerunner of this paper was my joint work with Paolo Codenotti on hypergraph isomorphism [BaCo]; that paper combined the group theory method with a web of combinatorial partitioning techniques. In particular, I found an early version of the Design Lemma in the wake of that work. (A much simpler observation is called "Design Lemma" in that paper.)

Some of the group theory used in the present paper was inspired by my joint work with Péter Pál Pálfy and Jan Saxl [BaPS]; in particular, the rendering of a result of Feit and Tits [FeT] in that paper turned out to be particularly handy in the proof of the main group theoretic lemma of this paper ("Unaffected Stabilizer Theorem," Theorem 8.11).

I am grateful to three long-time friends who helped me verify critical parts of this paper: Péter Pál Pálfy and László Pyber the proof of various versions of the group-theoretic "Main structure theorem" (Theorem 8.19) that includes the crucial "Unaffected Stabilizer Theorem," and Gene Luks the LocalCertificates procedure (Sec. 10), the core algorithm of the paper. Their comments helped improve the presentation, and, more significantly, raised my confidence that these items actually work. All other parts of the paper seem quite "faulttolerant," with multiple solutions, and a bag of tricks to rely on, should any gaps be found. Naturally, any errors that may remain in these items (or any other part of the paper) are my sole responsibility.

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