Search Space Contraction in Canonical Labeling of Graphs

Adolfo Piperno

Dipartimento di Informatica, La Sapienza Università di Roma, Via Salaria 113, I-00198 Roma

Abstract

The individualization-refinement paradigm for computing a canonical labeling and the automorphism group of a graph is investigated. A new algorithmic design aimed at reducing the size of the associated search space is introduced, and a new tool, named *Traces*, is presented, together with experimental results and comparisons with existing software, such as McKay's *nauty*. It is shown that the approach presented here leads to a huge reduction in the search space, thereby making computation feasible for several classes of graphs which are hard for all the main canonical labeling tools in the literature.

Key words: (Practical) graph isomorphism, canonical labeling, partition refinement, automorphism group computation.

1. Introduction

A *canonical labeling* (or *canonical form*) of a graph G is a graph G' — isomorphic to G — representing the whole isomorphism class of G. In terms of computational complexity the theoretical status of canonical labeling (CL) is still unsettled, since an efficient algorithm for CL would imply an efficient algorithm for the graph isomorphism problem (GI). In practice, however, CL algorithms are widely used, as they enable (possibly large) sequences of graphs coming from both combinatorial problems and industrial applications to be checked for isomorphism by simply comparing their canonical forms.

The literature on methods for approaching GI and CL displays a peculiar "separation" between theoretical and practical studies. On the theoretical side, besides papers substantiating the thesis that GI is not NP-complete [28, 37] (a survey is in [1]), there are a large number of noteworthy pieces of mathematics showing the existence of polynomial solutions of GI for significant classes of graphs. While moderately exponential solutions have been provided for the general problem of graph isomorphism [3, 6], polynomial algorithms exist for planar graphs [18, 17], graphs of bounded genus [15], graphs with colored vertices and bounded

color-classes [2], graphs with bounded multiplicity of eigenvalues [5], graphs of bounded valence [26], and more (see [4]).

On the practical side, there are some noteworthy pieces of software which originate from the outstanding tool *nauty* [29]. *nauty* was introduced in the 1980s by McKay [31] and has become a standard in the area of canonical labeling and determination of the automorphism group of a graph. Moreover, it has been incorporated into more general mathematical software tools such as GAP [16] and MAGMA [27].

It is important to observe that, with the exception of planar graphs, none of the polynomial algorithms mentioned above has been implemented in software, as noted by Junttila and Kaski in [19]. A reasonable justification for this absence would seem to be that, given a class $\mathbb{C}$ of graphs for which an efficient algorithm for isomorphism testing exists, *nauty* is usually able to process almost all the graphs in $\mathbb{C}$ in a considerably smaller number of steps than that established by the theoretical bound (with respect to the number of vertices). However, there exist graphs in $\mathbb{C}$ for which *nauty* exhibits an exponential behavior, as shown by the series of graphs constructed by Miyazaki in [33]: all these graphs are 3-regular and have color-class size equal to 4, hence they intersect two classes of graphs for which polynomial solutions for GI exist. A further distinctive feature of Miyazaki's graphs is that the size of their automorphism group is quite large. This contrasts with the fact that graphs which are hard for *nauty* usually have a high degree of regularity but a small automorphism group.

In recent years the tools *saucy* [13, 12] and *bliss* [19, 20] have been introduced, aimed at handling large sparse graphs coming either from the satisfiability problem (SAT), or from industrial applications. Like *nauty* these are general purpose devices implementing backtrack algorithms based on the so called *individualization-refinement* technique, however they differ from *nauty* in respect of the data structures and heuristics used. We briefly recall here that the key of the individualization-refinement technique is the notion of *equitable partition*, a coloring of vertices of a graph such that any two vertices with the same color have the same number of neighbors in each color class. A vertex is *individualized* by assigning to it a fresh color, the coloring so obtained is *refined* when a new equitable partition (finer than the initial one) is produced. A backtrack search on the space of all possible individualizations, along with some initial assumptions that allow the associated tree to be pruned, produces the canonical form for the input graph. The complexity of a tool based on such a technique essentially derives from the size of the associated search space, and from the complexity of the refinement function (which is invoked once for every node of the search tree). On the other hand, the granularity of the refinement procedure (see *nauty*'s *vertex-invariants* [29]) may affect the size of the search tree.

In the present paper we start our investigation from an analysis of the main critical features of the individualization-refinement paradigm, namely (i) the visiting strategy of the search space, (ii) the manipulation of discovered automorphisms of the input graph, (iii) the refinement function, and (iv) the selection of the next individualization step. If we disregard implementation details, all four of these issues are treated in essentially the same way by each of the existing tools for canonical labeling of graphs, revealing that they are based on the same algorithmic conception — that introduced by *nauty* and described above. We will, instead, propose a new solution for each of the four issues, presenting a canonical labeling tool, named *Traces*, whose algorithmic structure differs from that of all previous tools. In fact, it is clear from the comparison between *nauty* and *bliss* that the adoption of suitable heuristics and data structures can produce a (sometimes significant) improvement in performance. But classes of graphs that are very hard for *nauty* are still very hard for *bliss*: this seems to be

due to the fact that these tools have the same conceptual bases. Therefore, it is our aim to experiment a tool with a different basic design.

Traces[1] computes a canonical form for a colored graph and/or a set of generators for its automorphism group. Its main innovations of can be summarized as follows: *Traces* does not use backtrack to traverse the search space: the case for adopting a kind of breadth-first strategy will be argued in this paper. Automorphisms which are detected are manipulated in *Traces* by means of the Schreier-Sims algorithm [39] (see also [38]); information about the group structure can be also used by the refinement procedure to eliminate redundant computations. In addition to the usual one, a refinement function producing finer partitions can be used for difficult graphs; such function also provides information for choosing the next individualization step. Partitions are compared (and possibly discarded) without computing them completely, using a linear representation which we call a *trace*.

We produce performance tables using the huge catalogue of benchmark graphs for canonical labeling and automorphism group computation compiled by Junttila and Kaski [19]. It turns out that, compared to other tools, *Traces* is able to significantly reduce the size of the search space in the case of hard graphs, often by several orders of magnitude. When the ratio between sizes of the search spaces is substantial, then *Traces* runs much faster than any other tool; otherwise, their timings are mostly comparable. Even better results are obtained in the case of automorphism group computation instead of canonical labeling. *Traces* may be slightly slower than some of the other tools when the associated search spaces are very small, usually when the input graph has a low degree of regularity or a high degree of symmetry. This is mainly due to the absence (in the current version) of a refinement procedure specific for sparse graphs.

All known classes of graphs which are intractable by the state-of-the-art tools are efficiently treated by *Traces*, though we need to point out that some of these classes were carefully tuned to cause those tools to behave exponentially. Particular attention will be given below to incidence graphs of projective planes, which are considered to be the hardest instances for canonical labeling (see discussions at *nauty* mailing list [2]). We will show that *Traces*, which is a general purpose device, treats these graphs within the best theoretically established bound, without the help of any additional procedure tailored to them.

1.1. *Structure of the paper*

In Section 2 some definitions and properties of graphs and partitions are introduced and the individualization-refinement technique is described. Section 3 presents an analysis of some fundamental issues in canonical labeling and argues the need for a new algorithmic design. Section 4 is dedicated to the new canonical labeling algorithm ant to its correctness proof. Experimental results are presented and commented upon in section 5.

2. Graphs and partitions

A (simple) *graph* is a pair (V, E), where V is a finite set of *vertices* and E is a set of unordered pairs of vertices called *edges*. If $(u, v) \in E$, we say that u and v are *adjacent* or *neighbors*. A (vertex) *colored graph* is a pair $G = (H, \chi)$, where H is a graph and χ is a function assigning colors to vertices of H.

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[1] *Traces* is available at `http://www.dsi.uniroma1.it/~piperno/pers/Traces.html`

[2] `http://dcsmail.anu.edu.au/cgi-bin/mailman/listinfo/nauty-list`

In this paper, $[n]$ will denote the set $\{1, \ldots, n\}$, while $\mathbb{G}_{[n]}$ will denote the set of colored graphs with vertex set $[n]$. The set of all colored graphs will be denoted by $\mathbb{G}$. Note that any graph is a colored graph in which all vertices have the same fixed color, and that it is not restrictive to assume that $\chi : [n] \to [n]$.

An *isomorphism* of graphs $G_1, G_2 \in \mathbb{G}_{[n]}$ is a permutation p of $[n]$ such that any two vertices u and v of G_1 are adjacent in G_1 if and only if $p(u)$ and $p(v)$ are adjacent in G_2. When considering graphs with colored vertices, isomorphisms must preserve colors, too. We will write $G_1 \simeq G_2$ when G_1 and G_2 are isomorphic. An *automorphism* is an isomorphism between a graph and itself. The *automorphism group* $\mathrm{Aut}(G)$ of a graph G is the set of all automorphisms of G with permutation composition as the group operation. If $\Gamma \subseteq \mathrm{Aut}(G)$ is a group of automorphisms of G, then Γ induces an equivalence relation on the vertices of G: two vertices v, w are equivalent if and only if there exists an automorphism in Γ which maps v to w; the resulting equivalence classes are called the *orbits* of the graph by Γ.

A function f from $\mathbb{G}$ to a set $\mathbb{D}$ is an *(isomorphism) invariant* on $\mathbb{G}$ iff $\forall G_1, G_2 \in \mathbb{G} : G_1 \simeq G_2 \Rightarrow f(G_1) = f(G_2)$. The image of a graph G under a function $\mathscr{C} : \mathbb{G} \to \mathbb{G}$ is a *canonical labeling* (or *canonical form*) of G iff (i) $\forall G \in \mathbb{G} : \mathscr{C}(G) \simeq G$, (ii) $\forall G_1, G_2 \in \mathbb{G} : G_1 \simeq G_2 \iff \mathscr{C}(G_1) = \mathscr{C}(G_2)$.

An *ordered partition* of $[n]$ is a sequence $\pi = (W_1, \ldots, W_r)$ of disjoint non-empty subsets of $[n]$, called *cells*, whose union is $[n]$. The set of ordered partitions of $[n]$ will be denoted by $\Pi_{[n]}$, while Π will denote the set of all ordered partitions. The *size* of a partition is the number of its cells

A cell of a partition $\pi \in \Pi_{[n]}$ is *trivial* when it contains only one element. The partition π is *discrete* if all its cells are trivial; π is the *unit partition* when it has only one cell, i.e. $\pi = ([n])$. For any $\pi \in \Pi_{[n]}$ and $v, w \in [n]$, we will write $v \sim_\pi w$ when v and w belong to the same cell of π. An *orbit partition* of a graph G with respect to a subgroup Γ of $\mathrm{Aut}(G)$ is any partition of vertices of G, whose cells are the orbits of G under Γ.

The *index* $ind(v, \pi)$ of a vertex $v \in [n]$ in an ordered partition $\pi \in \Pi_{[n]}$ is the index of the cell of π in which v appears, namely $ind(v, (W_1, \ldots, W_r)) = k$ when $v \in W_k$. The *position* of a vertex $v \in [n]$ in an ordered partition $\pi \in \Pi_{[n]}$ is defined by means of the function $pos : [n] \times \Pi_{[n]} \to [n]$ such that $ind(v, (W_1, \ldots, W_r)) = k \Rightarrow pos(v, (W_1, \ldots, W_r)) = 1 + \sum_{i=1}^{k-1} |W_i|$. The position of a cell W in an ordered partition π is defined as the position of an element of W in π (indeed, all the elements of W share the same position in π); with some overloading: $pos(W, \pi) = pos(v, \pi)$, for any $v \in W$.

For example, if $\pi = (\{2, 3\}, \{5\}, \{1, 4\}) \in \Pi_{[5]}$, then $pos(2, \pi) = pos(3, \pi) = 1 = pos(\{2, 3\}, \pi)$, while $pos(1, \pi) = pos(4, \pi) = 4 = pos(\{1, 4\}, \pi)$. In particular, $pos(v, ([n])) = 1$, for any $v \in [n]$.

If π_1 and π_2 are partitions, then π_1 is *finer* than π_2, and π_2 is *coarser* than π_1, if every cell of π_1 is a subset of some cell of π_2. (Note that partitions are both finer and coarser than themselves, and that π_1 is finer than π_2 iff $\forall v \in [n] : pos(v, \pi_1) \geqslant pos(v, \pi_2)$.)

Let $\pi \in \Pi_{[n]}$ and let $(\chi_1, \ldots, \chi_n)$ be a sequence of n colors. The graph $G = (H, \pi)$ is a colored graph if we interpret the partition π as a function assigning the $pos(v, \pi)$-th color in $(\chi_1, \ldots, \chi_n)$ to vertex v of G. We observe that the converse is also true: an ordered sequence of colors induces an ordered partition of vertices of a colored graph. Therefore in the rest of the paper we will denote a colored graph as a pair $G = (H, \pi)$, where π is an ordered partition of vertices of H, implicitly assuming the existence of an ordered sequence $(\chi_1, \ldots, \chi_n)$ of colors and a function χ such that, for any vertex v, $\chi(v) = \chi_{pos(v, \pi)}$.

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2.1. The individualization-refinement technique for canonical labeling

In this section the behavior of the individualization-refinement technique for canonical labeling is revisited. The method consists of a depth-first search of a space defined by classification and fixing of vertices. It is based on the fact that any permutation γ of vertices of a graph G can be viewed as a discrete partition whose cells appear in the order established by γ. Vertices of G are partitioned by a *refinement function*, which separates them in a way that no automorphism of G exists between different cells. The *individualization* of a vertex corresponds to select a subgroup of permutations fixing that vertex.

Let $\pi = (W_1,\ldots,W_r) \in \Pi_{[n]}$ be an ordered partition of $[n]$. For any $v \in [n]$, if v belongs to a non-trivial cell W_i, then we denote by $\pi{\downarrow}v$ the ordered partition obtained from π by splitting the cell W_i into the cells $\{v\}$ and $W_i - \{v\}$, namely $\pi{\downarrow}v = (W_1,\ldots,W_{i-1},\{v\},W_i - \{v\},W_{i+1},\ldots,W_r)$, if $v \in W_i$.

If $G = (H,\pi) \in \mathbb{G}_{[n]}$, then we say that $G' = (H,\pi{\downarrow}v)$ is obtained from G by *individualizing* vertex v. Note that $pos(w,\pi{\downarrow}v) = pos(w,\pi) + 1$ if $w \in W_i - \{v\}$.

Let $G = ((V,E),\pi) \in \mathbb{G}$ be a colored graph. We say that G is *equitable* when, for any pair of vertices $v,w \in V$, if $v \sim_\pi w$, then, for any cell W of π, v and w have the same number of neighbors in W. In this case, we say that π is a *stable* partition for (V,E).

Let $G = ((V,E),\pi) \in \mathbb{G}$ be an equitable graph. The *quotient graph* $Q(G) = (V',E')$ of G is a graph, with possible multiple edges and loops, having vertex set $V' = \{pos(v,\pi) \mid v \in V\}$ and edge multiset $E' = \{\!\{(pos(v,\pi),pos(w,\pi)) \mid (v,w) \in E\}\!\}$.
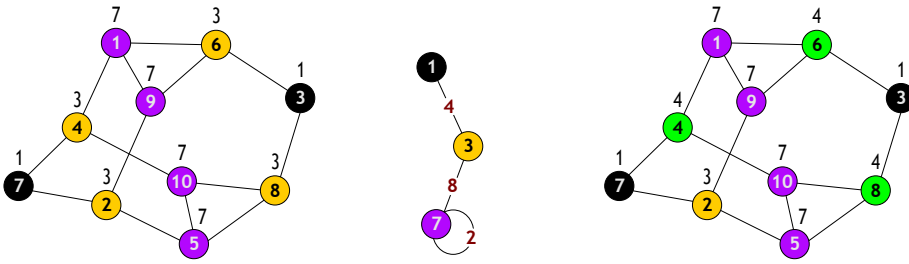

Figure 1. An equitable graph (left) and its quotient graph (center); individualization of vertex 2 (right). Numbers above vertices denote colors, which correspond to vertices of the quotient graph.

Figure 1 shows an equitable graph G (left) and its quotient graph (center). Figure 1 (right) displays the effect of individualizing vertex 2. The individualized vertex keeps its color (3), while other vertices in the original class take the next color (4). For every color appearing in G, there exists a corresponding vertex in $Q(G)$; an edge in $Q(G)$ has multiplicity k if G has k edges joining vertices with the corresponding colors.

Note that when the coloring partition of a graph G is discrete, then $Q(G)$ is isomorphic to G itself. Hence, if the quotients of two graphs with discrete color partitions are the same, then the two graphs are isomorphic.

Let $G = (H,\pi) \in \mathbb{G}$. A *refinement* of G is the image of G under a function $R : \mathbb{G} \to \mathbb{G}$ such that: (i) $R(H,\pi) = (H,\pi')$ is an equitable graph with π' finer than π; (ii) R preserves isomorphisms, i.e. $(H_1,\pi_1) \simeq (H_2,\pi_2) \Rightarrow R(H_1,\pi_1) \simeq R(H_2,\pi_2)$. To simplify the notation, when considering a function F on $\mathbb{G}$ we will write $F(H,\pi)$ instead of $F((H,\pi))$.

The refinement procedures implemented in canonical labeling tools (see also [22]) can be briefly described as follows. Using a specific scheduling, which is isomorphism invariant,

cells of π are visited. For each visited cell W, the multiplicities of adjacencies of elements of W are counted. The vertices in each cell Z are divided into subcells according to how many neighbors they have in W. This process is repeated until the graph is equitable.
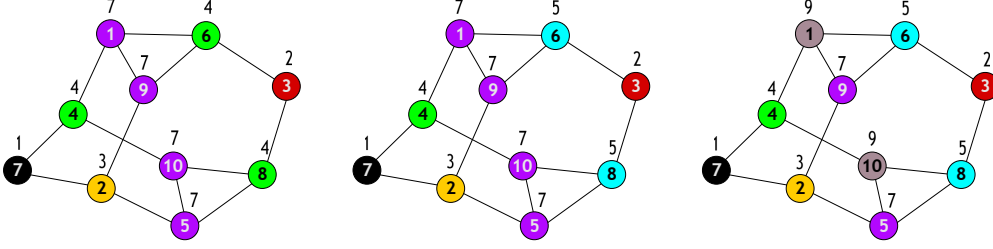

Figure 2. Refinement

In Figure 2, starting from the non-equitable colored graph in Figure 1 (right), the cell $\{3, 7\}$ is split (Figure 2 (left)), since vertex 7, but not 3, has one neighbor in the cell $\{2\}$. Similarly, the cell $\{4, 6, 8\}$ is split (Figure 2 (center)), since vertex 4, but not 6 and 8, has one neighbor in the cell $\{7\}$. Finally, the cell $\{1, 5, 9, 10\}$ is split (Figure 2 (right)) since vertices 5 and 9, but not 1 and 10, have one neighbor in the cell $\{2\}$. The graph in Figure 2 (right) is equitable.

The canonical labeling algorithm implemented by *nauty*, *saucy* and *bliss* is a depth-first search of a space defined by partition refinement and vertex individualization. Vertices are individualized according to a *target cell selector*. This is a function $T : \mathbb{G} \to [n]$ such that: (i) $T(H, \pi) = k$ is the position of a non-trivial cell of π; (ii) T is an isomorphism invariant, i.e. $(H_1, \pi_1) \simeq (H_2, \pi_2) \Rightarrow T(H_1, \pi_1) = T(H_2, \pi_2)$. The image of a graph G under T is the *target cell* of G.

The target cell selector used in *nauty*, *saucy* and *bliss* is defined in terms of adjacencies between cells, which are classified according to the presence of edges and non-edges with respect to other cells. The leftmost cell having the highest value in such classification is chosen as the target cell.

Given an equitable graph $G = (H, \pi)$, a refinement function R, and a non-empty sequence $v_1, \ldots, v_k$ of vertices of H, we will write $(H, \pi^{(v_1, \ldots, v_k)})$ to denote the graph obtained by individualization and refinement of $v_1, \ldots, v_k$, consecutively; more precisely

$$(H, \pi^{(v_1)}) = R(H, \pi \downarrow v_1) \text{ and } (H, \pi^{(v_1, \ldots, v_k)}) = R(H, \pi^{(v_1, \ldots, v_{k-1})} \downarrow v_k).$$

2.2. Backtrack construction of the search tree

Assuming a fixed refinement function R and a target cell selector T, the *search tree* $\mathcal{T}(H, \pi)$ of a graph $G = (H, \pi)$ is a tree in which each node represents an equitable graph $G' = (H, \pi')$ where π' is finer than π; in particular:
  - the root of $\mathcal{T}(H, \pi)$ represents the refinement of G;
  - if a node of $\mathcal{T}(H, \pi)$ represents (H, π') and π' is discrete, then that node is a leaf;
  - otherwise, let $\pi_v = (W_1, \ldots, W_i, \ldots, W_k)$ be the partition of the graph (H, π_v) at node v of $\mathcal{T}(H, \pi)$ and let $W_i = \{v_1, \ldots, v_h\}$ be the target cell of that graph, as determined by a fixed function. Then the tree rooted at v has the trees $\mathcal{T}(H, \pi_v \downarrow v_1), \ldots, \mathcal{T}(H, \pi_v \downarrow v_h)$ as children.
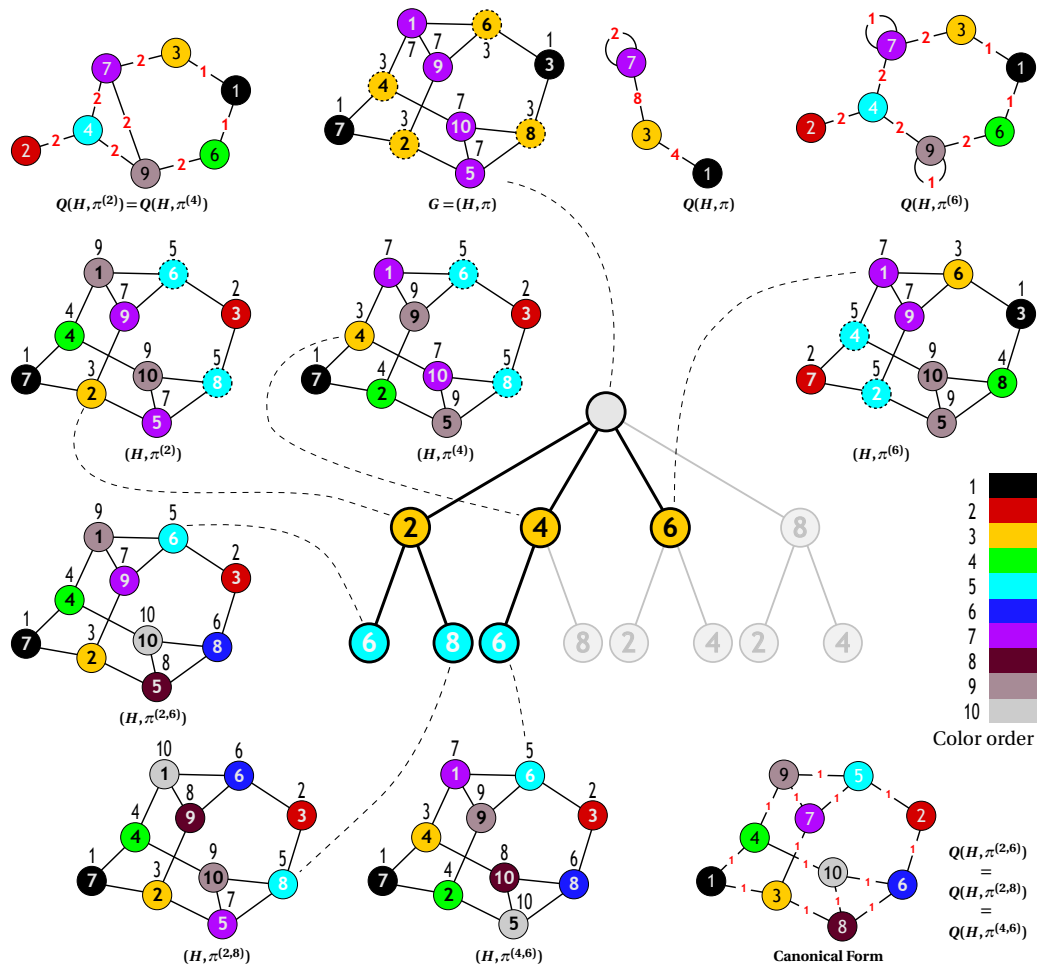
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Figure 3. Backtrack construction and pruning of the search tree

We observe that: (i) isomorphic graphs have isomorphic search trees, due to the fact that both the target cell selector and the refinement function are isomorphism invariant; (ii) isomorphic leaf nodes of $\mathcal{T}(G)$ allow to detect automorphisms of G (see e.g. [4, 22, 31]).

The typical behavior of algorithms based on the individualization-refinement mechanism is exemplified by the backtrack search in Figure 3, where each node of the tree is labeled by an individualized vertex, and is connected by a dashed line to the graph represented by that node. Only part of the whole backtrack tree is actually generated. The other parts of the tree are either shown to be equivalent to parts already generated, or are pruned by means of invariant information discovered while traversing the tree itself.

Once it has been computed, the leftmost leaf of the tree is stored for comparing it with subsequent leaves, in order to find automorphisms of the graph. Such an automorphism is found when two discrete partitions induce the same quotient. In this case the backtrack search restarts from the next individualized vertex of the least common ancestor of the two leaves which determine the automorphism. This mechanism guarantees, by the orbit-stabilizer the-

orem (see e.g. [8]), the correctness of the algorithm for computing generators and size of the automorphism group of the input graph.

In order to compute the canonical labeling a further leaf is stored, which is the best one according to some initially defined ordering, and is updated if necessary during the traversal of the tree.

For example, in Figure 3, $Q(H, \pi^{(4,6)})$ is equal to $Q(H, \pi^{(2,6)})$. The corresponding generator for the automorphism group of G is $\gamma = (1,9)(2,4)(5,10)$. It follows from the existence of an automorphism of G which maps vertex 2 onto vertex 4 that the whole tree rooted at 2 carries the same information as the one rooted at 4; therefore the computation of the latter can be cancelled without loss of information.

Instead, looking at the next backtrack step we observe that $Q(H, \pi^{(6)})$ is different from $Q(H, \pi^{(2)})$. This implies the non-existence of any automorphism mapping vertex 2 onto vertex 6. In the example of Figure 3 we have pruned the tree at the current node, since it has been assumed that it will not produce a "better" canonical form than the initially stored one (which in this case coincides with the leftmost one).

The algorithm terminates producing a set of generators for the automorphism group of the input graph G, and the canonical form of G.

3. Introducing *Traces*

The main tools existing in the literature for canonical labeling of graphs and/or automorphism group computation by means of the individualization-refinement technique are *nauty* [31, 29], *saucy* [13, 12] (recently improved in [14]) and *bliss* [19, 20]. Other tools, such as Kocay's *Groups&Graphs* [21], Leon's *partition backtrack* algorithms [24, 25] and Kreher and Stinson's [23] software, being of a more general nature, will not be considered for comparison here.

We mention some relevant differences among the three selected tools:
- *nauty* implements some invariants allowing finer partitions from the refinement process, in order to speed-up the computation for suitable classes of graphs;
- *saucy* is especially tailored for sparse graphs, and it computes the automorphism group for the input graph, only, without considering the canonical labeling problem;
- *bliss* uses efficient data structures and new heuristics for computing partitions and refinements, and for traversing the search space.

It is important to observe that, if we disregard implementation details, each of these tools is based on the same conception, the one described in the previous section. There are four main elements in this algorithmic structure:
- the strategy for building and pruning the search tree, which is the depth-first one;
- the absence of specific tools for manipulating information coming from the group of detected automorphisms;
- the refinement procedure, known as 1-dimensional Weisfeiler-Lehman algorithm [40] or *vertex classification*;
- the target cell selector, based on local properties of adjacencies of nodes.

The tool we are going to introduce in the present paper is named *Traces*: it is based on different designs for dealing with all four of the aforementioned issues.
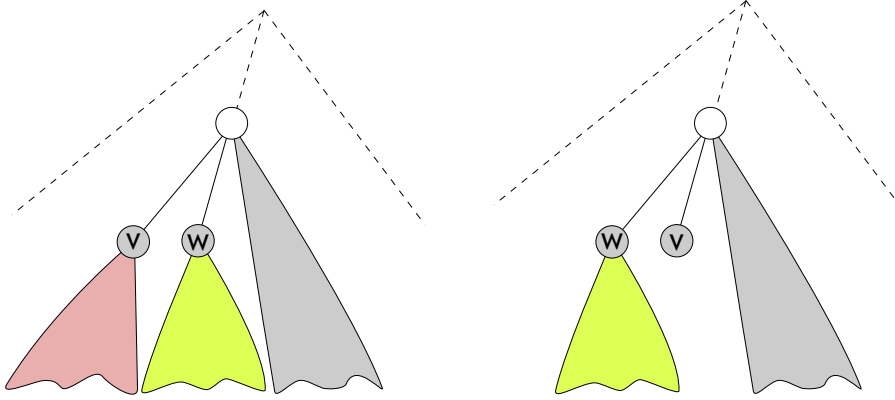
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Figure 4. Inefficiency of the backtrack strategy

3.1. *Search space construction.*

The central innovation of *Traces* over other canonical labeling algorithms concerns the search space construction strategy.

We observe that a backtrack search (i.e. a depth-first visit of the search space) may cause inefficiencies when, at some level, it is possible to *prune the tree by a node invariant*. This happens when two nodes appearing at the same level in $\mathscr{T}(H, \pi)$ are associated to partitions which induce different quotient graphs. Therefore, one of the subtrees rooted at those nodes could be pruned. In a case such as this, a depth-first strategy might force visiting a whole subtree which will later be discarded.

As an example, let us assume, as depicted in Figure 4, that the quotient graph associated to the node labeled by w, $Q(H, \pi^{(\vec{u}, w)})$ is "better", according to some predefined ordering, e.g. lexicographic, than $Q(H, \pi^{(\vec{u}, v)})$. In other words, we are assuming that the canonical form is not associated to a leaf of the tree rooted at v. If v comes before w during the construction of $\mathscr{T}(H, \pi)$, then the whole subtree rooted at v is visited before it is realized that its construction could have been avoided (Figure 4, left). Conversely, if w comes before v during the construction of $\mathscr{T}(H, \pi)$, then only the root of that subtree (which might, in fact, be huge) is visited (Figure 4, right). It turns out that the efficiency in pruning the search tree depends strictly on the order in which vertices are stored in the target cell, but this order is unpredictable, since cells are sets. Furthermore, the circumstances that have just been described are a cause of instability for the whole canonization process: completely different performances can be obtained from isomorphic instances of the same graph. In a certain sense we can say that a depth-first search is incapable of capturing the structure of a graph, since its efficiency depends on the graph's representation.

These considerations suggest it would be better to implement a breadth-first strategy for building the search space, thus enabling all the subtrees whose root does not produce the "best" partition to be pruned, for each level of $\mathscr{T}(H, \pi)$.

However, we must observe that a breadth-first strategy does not allow for pruning of the search tree by means of automorphism detection, because automorphisms are discovered by comparing the leaves of the tree. Therefore, a simple breadth-first strategy would only be able to detect automorphisms during its final iteration.

Our aim is to define a strategy which combines the advantages of a breadth-first traversal (early pruning of useless subtrees) with those of a depth-first search (automorphism detection). Consequently we propose to use the following variant of the breadth-first strategy for traversing the search space:

for any level ℓ of $\mathcal{T}(H, \pi)$ and for any node v appearing at ℓ, either v is discarded or one and only one path toward a leaf of $\mathcal{T}(H, \pi)$ is computed.

This path will be called an *experimental path.* In particular, we will have: (i) for any level ℓ, non-discarded nodes at ℓ share the same quotient graph; (ii) the computation of the experimental path is started only if v is not known to be equivalent (by automorphism) to some previously computed node at level ℓ.

Figure 5 shows the behavior of the search strategy we have just defined. In order to focus on the traversal we have omitted the pruning operations, which will be introduced in the definition of the canonical labeling algorithm. In Figure 5.(a), after the individualization-refinement of the first vertex in the target cell, an experimental path is shown, ending with the discrete partition π_1. In (b), the same operation is illustrated for the second vertex in the target cell. The new experimental path leads to the partition π_2, which can now be compared with π_1, possibly deriving an automorphism of the input graph. In the affirmative case, the detected automorphism maps the vertices which have been fixed to produce π_1 onto those fixed to produce π_2. In (c), the computation of the first level is completed. Figure 5.(d,e) show the traversal of levels 2 and 3. Without entering into implementation details, we assume that an experimental path already computed at some level is not computed again at subsequent levels.
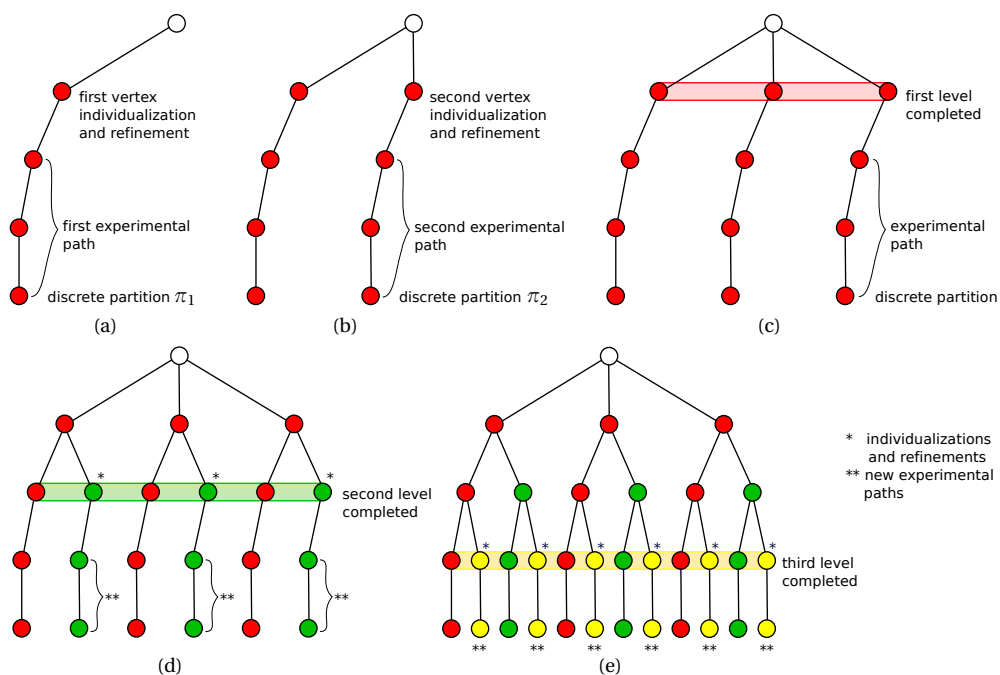

Figure 5. Traversing the search space with *Traces.*

3.2. The use of detected automorphisms.

When a generator γ of the automorphism group of the graph is found by comparing two leaves l_1 and l_2 of $\mathscr{T}(H, \pi)$, *nauty* prunes the search tree at the level where the deepest common ancestor of l_1 and l_2 appears. In addition, it stores some information about fixed points and cycles of γ to be used later for the so called *early pruning* of the search tree, namely the pruning by automorphism which can be obtained without detecting any further isomorphism. This happens in the example of Figure 3, where the rightmost subtree of the root (labeled by 8) is pruned because of the presence of a previously found generator which associates 8 to 6.
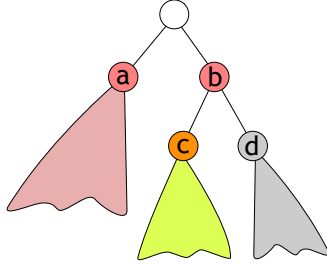

Figure 6. A subtree to be pruned by automorphism

Such a simple structure, though very powerful in most cases, cannot in general obtain the maximal pruning by automorphisms. For example, consider the tree in Figure 6, where it is assumed that the exploration of the subtree rooted at a has produced the generators $\gamma_1 = (\text{v c})(\text{w b})$ and $\gamma_2 = (\text{v d})(\text{w b})$ for some v, w. The permutation $\gamma = (\text{v c d})$ belongs to the group generated by γ_1 and γ_2. Such a permutation proves that the subtrees rooted at c and d are equivalent, since it fixes b and sends c to d. Therefore, one of the subtrees rooted at c or d should be pruned. However, it is impossible to establish the equivalence between c and d by looking at γ_1 and γ_2 separately, as *nauty* does.

In order to apply pruning by automorphism to its maximal extent, *Traces* uses the Schreier-Sims algorithm ([39], see also [38] for a description and an extensive bibliography on this subject) for manipulating the automorphism group of the considered graph. This algorithm is an efficient method for computing a *base* and a *strong generating set* of a permutation group. It is used in *Traces*: (i) for computing the orbits of point stabilizers which correspond to sequences of individualized vertices; (ii) for computing the size of the automorphism group; (iii) for testing whether an automorphism is already present in the group generated by the discovered automorphisms; (iv) for avoiding redundant computations during the refinement process. The Schreier-Sims algorithm is not used by *nauty*, *saucy* and *bliss*. In each of these tools only the orbits of stabilizers of vertices which are individualized along the leftmost path are computed and put to work for pruning the search tree. The Schreier-Sims algorithm is used by Kreher and Stinson in the canonical labeling algorithm described in [23].

3.3. Refinement procedure and target cell selector.

A relevant feature of *nauty* is that it gives the user the opportunity of using some sort of invariant to assist the built-in refinement procedure. The use of invariants enables additional information to be collected during the refinement process, in order to obtain finer partitions, therefore reducing the size of the search tree.

Algorithm 1 2-dimensional refinement

Input: A colored graph $G = (H, \pi)$

1: **repeat**
2:     Apply 1-dimensional refinement to (H, π), thus updating π
3:     **for each** vertex v in any non-singleton cell of π **do**
4:         Classify v according to the isomorphism type of the quotient of $R(H, \pi{\downarrow}v)$
5:     **end for**
6:     Update π according to the new classification
7: **until** no refinement occurred at step 4

Some invariants are very useful for several families of difficult graphs. However, their selection is left by *nauty* to the user, as the use of a vertex invariant requires the identification of the input graph, thus contradicting the assumption of a general purpose algorithm.

In the present paper, we experiment the option for the user to adopt the 2-dimensional Weisfeiler-Lehman refinement procedure [40, 4] as an *universal* invariant, to be applied to any hard graph without consideration of its family.

In the 2-dimensional Weisfeiler-Lehman refinement, ordered pairs of vertices of a graph $G = (([n], E), \pi)$ are colored, initially using three colors: edges, non-edges, and the diagonal; in particular, the diagonal coloring reflects π. The coloring is iteratively refined by classifying edges according to the number of colored triangles they participate in. The algorithm stops when no further refinement is possible: the final coloring of diagonal elements is called a 2-*stable* partition of vertices of G. The refinement process is usually represented (see e.g. [7, 11]) by a $n \times n$ matrix $\mathbf{W}$ whose entry w_{ij} is the color of the edge or non-edge (i, j), if $i \neq j$, the color of vertex i otherwise ($1 \leq i, j \leq n$). We observe that, if $\mathbf{W}$ represents a 2-stable partition, then for $1 \leq i \leq n$ the i-th row of $\mathbf{W}$ identifies a stable partition π_i of vertices of G with singleton vertex i. In addition, if $w_{ii} \neq w_{jj}$ for some i, j, then the isomorphism class of the quotient graph of $G_i = (([n], E), \pi_i)$ is different from that of $G_j = (([n], E), \pi_j)$. This suggests the definition of Algorithm 1 for computing 2-dimensional refinement.

Let R be the 1-dimensional Weisfeiler-Lehman refinement function (namely, *nauty*'s refinement). In Algorithm 1, every vertex v of the graph $G = (H, \pi)$ is classified according to the isomorphism type of $Q(R(H, \pi{\downarrow}v))$, the quotient of the graph obtained by R after individualizing v. The resulting ranking yields a new partition of vertices. The classification is repeated until a stable partition is reached.

It must be observed that the 2-dimensional Weisfeiler-Lehman refinement is computationally much heavier than the 1-dimensional one — as well as for *nauty*'s invariants, computation is added to the refinement process. In the worst case we could be losing a factor of n (the number of vertices of the considered graph) in time ([4]), since the refinements of all vertex individualizations are needed to stabilize the partition. In the next two sections, we introduce some techniques which are implemented in *Traces* in order to simplify the 2-dimensional Weisfeiler-Lehman refinement and to obtain some additional information from it.

In fact, a motivation for using the 2-dimensional algorithm is to collect information from it in order to select the target cell to be considered at the next individualization step. In particular, during the classification of a vertex v (step 3 of the algorithm), the number of cells of $R(H, \pi{\downarrow}v)$ is computed. The target cell associated to the whole refinement process is chosen as the leftmost one whose vertices produce the maximum of such values. Experiments reveal that this kind of *look-ahead* technique is useful for decreasing both the size and the the depth of the search tree.

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Remark 3.1. Two negative results must be mentioned while considering *nauty's* refinement procedure and target cell selector: (i) Miyazaki's sequence of graphs ([33]) showing the exponential behavior of *nauty*; (ii) Cai, Fürer and Immerman's construction ([10]) about (non) identification of graphs via the generalized k-dimensional Weisfeiler-Lehman refinement. Miyazaki proved that the choice of the target cell can be responsible for the existence of intractable graphs for *nauty*. On the other hand, in [10] the authors show that there does not exist k such that the k-dimensional refinement is able to capture the orbit partition of any graph.

As a matter of fact, while Miyazaki's result has a negative impact on *nauty* and other practical isomorphism tools, Cai, Fürer and Immerman's construction provides a theoretical justification for the individualization-refinement technique, since it proves that, (at least) in the presence of Weisfeiler-Lehman refinement, it is impossible to detect the orbit partition of the automorphism group of a graph directly, without the help of a search space construction.

3.4. Comparing partition refinements

It is crucial for every tool based on the individualization-refinement technique to have an efficient procedure for computing refinements and for comparing them.

Refinements are compared in our tool without computing them completely. This possibility has already been observed by Junttila and Kaski in [19] in the case of singleton cells emerging during the refinement process (the consequent invariant is called *partial leaf certificate*, and is adopted in *Traces*, too).

In addition to this, we implement an invariant, which we call *refinement trace*, based on the following observation: the whole refinement process, namely the sequence of cell splitting, is an (isomorphism) invariant, not only its final result. Assume that the cell W of the partition π is split during the refinement process into W' and W''. This splitting gives the partition π' such that: $pos(W', \pi') = pos(W, \pi)$ and $k = pos(W'', \pi') = pos(W, \pi) + |W'|$. The new position k created by splitting the cell W is a *trace element* of the refinement process. The refinement trace is the sequence of trace elements successively introduced during refinement; it is isomorphism invariant and can be stored into an array. Moreover, let us consider the alternation of individualization and refinement steps which is needed to compute a discrete partition; the whole process has its own trace, since the individualization operation consists of a cell splitting, too. The trace has a length of at most n, and each of its elements appears exactly once in it. Note that, since they are sequences of integers, traces can be ordered, e.g. component-wise.

Assume now that the refinement of $G_1 = (H_1, \pi_1)$ has been computed and $\tau = (\tau_1, \ldots, \tau_m)$ is its trace. Assume also that, while computing the refinement of $G_2 = (H_2, \pi_2)$, there exists a trace element τ'_i which is different from the corresponding τ_i. This is sufficient to establish that the refinements of G_1 and G_2 will be different. Obviously, if we choose an ordering on traces and τ'_i is "better" than τ_i, then the refinement of G_2 will be completed and its trace will be stored for later comparisons.

A similar mechanism is implemented in *saucy* [14] for comparing refinements. The main difference is that *saucy* considers the trace of the leftmost backtrack path, only. All subsequent refinements are compared against this trace. In our algorithm the trace is updated as soon as a better one is found. At the end of the computation the best trace will be obtained, namely the one which is associated to the canonical form of the input graph.

3.5.   2-dimensional Weisfeiler-Lehman refinement and automorphisms

The 2-dimensional refinement procedure (Algorithm 1) is used in *Traces* in conjunction with the Schreier-Sims algorithm, in two different ways.

Given a graph $G = (H, \pi)$, let Γ be a subgroup of its automorphism group. Let us assume that, for some $k \geq 0$ and for some vertices $v_1, \ldots, v_k$, the graph $G' = (H, \pi^{(v_1, \ldots, v_k)})$ appears at a node of $\mathcal{T}(G)$. Let w be a vertex in the target cell associated to G', so that the refinement of $(H, \pi^{(v_1, \ldots, v_k)} \downarrow w)$ must be computed. Using the Schreier-Sims algorithm, the orbits of the stabilizer of Γ with respect to $v_1, \ldots, v_k, w$ can be computed. This enables the classification step of Algorithm 1 to be simplified: for each cell of $\pi^{(v_1, \ldots, v_k)} \downarrow w$, only one vertex for each orbit is classified, all the other ones being equivalent to it.

On the other hand, when the classification of vertices from a cell produces discrete partitions, the corresponding colored graphs are compared for checking whether they induce an automorphism of the graph. Therefore, automorphism can be detected during the refinement process, too.

Furthermore, while refining $(H, \pi^{(v_1, \ldots, v_k)} \downarrow w)$, let W be the leftmost cell such that the classification of its vertices produces discrete partitions, and let us assume that W is not a singleton cell. All vertices in W give the same quotient graph, otherwise Algorithm 1 would split it. Therefore, for any $u, v \in W$ there is an automorphism of G which maps u onto v. Moreover, as defined in Section 3.3, W is the target cell returned by the refinement procedure. As a consequence, we infer that the current node of the search tree will have one leaf as its unique child. *Traces*' refinement will therefore return this leaf as the result of the current refinement.
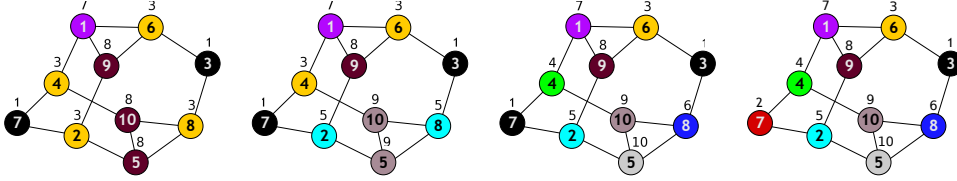
Figure 7. (a) Individualization of vertex 1 and refinement.

As an example, still considering the graph $G = (H, (\{3, 7\}, \{2, 4, 6, 8\}, \{1, 5, 9, 10\}))$ of Figure 2 (left), note that G is equitable and hence not refinable by the 1-dimensional Weisfeiler-Lehman algorithm. While applying the 2-dimensional algorithm, all vertices are classified by individualizing them and comparing the quotients of the resulting refinements. It turns out that the third cell produces equivalent discrete partitions, thus allowing for the detection of some automorphisms of the graph. In particular Figure 7 shows that the refinement starting from the individualization of 1 yields the partition $(\{3\}, \{7\}, \{6\}, \{4\}, \{2\}, \{8\}, \{1\}, \{9\}, \{10\}, \{5\})$. Similarly, the refinement starting from the individualization of 5 yields the partition $(\{3\}, \{7\}, \{8\}, \{2\}, \{4\}, \{6\}, \{5\}, \{10\}, \{9\}, \{1\})$. Comparison of the partitions thus obtained enables the automorphism $(1\ 5)(2\ 4)(6\ 8)(9\ 10)$ to be found.

4.   The Canonical labeling Algorithm

We introduce two orderings on graphs to be used in the description of the canonical labeling algorithm and in the proof of its correctness.

Definition 4.1. Let π_1 and π_2 be two stable partitions of vertices of the graph H.

(i) We say that the colored graph $G_1 = (H, \pi_1)$ is 1-*dim better* than $G_2 = (H, \pi_2)$ when either π_1 has more cells than π_2, or π_1 and π_2 have the same number of cells and $Q(G_1)$ is lexicographically smaller than (or equal to) $Q(G_2)$.

(ii) We say that G_1 is 2-*dim better* than G_2 when either G_1 is 1-dim better than G_2 or $Q(G_1) = Q(G_2)$ and $Q(H, \pi_1^{(v_1)})$ is 1-dim better than $Q(H, \pi_2^{(v_2)})$, where v_1 and v_2 are elements of the target cell of G_1 and G_2, respectively.

(iii) For $k = 1, 2$, we say that G_1 is k-*dim equal* to G_2 if G_1 is k-dim better than G_2 and G_2 is k-dim better than G_1.

Two versions of *Traces*' canonical labeling algorithm are defined in Algorithm 2, depending on the use of 1-dimensional or 2-dimensional Weisfeiler-Lehman refinement; each version exhibits its own target cell selector:

- in the case of 1-dimensional refinement, the target cell will be chosen according to the following rule: at the initial level it is the largest one; at level $\ell > 0$, the largest cell which is contained in the target cell at level $\ell - 1$ (or at level $\ell - 2$ if the target cell at level $\ell - 1$ has been transformed into singletons, and so on backwards).
- in the case of 2-dimensional refinement, the target cell will be selected as described in Section 3.3.

Remark 4.2. Note that: (i) the outermost **while**-loop is executed until a discrete partition is found. (ii) For each level, the list of graphs to be considered at the next level is built. (iii) New generators of the automorphism group of the input graph can be found either during the refinement process (but only with 2-dimensional refinement, see Section 3.5), or comparing graphs coming from experimental paths. (iv) In the latter case, the current graph is not added to the list of graphs to be considered at the next level (see the **if**-statement at line 17), since it is equivalent to a previously computed graph. (v) Pruning by automorphism is allowed by the **if**-statement at line 9, where the orbits of the stabilizer of the group (with respect to the vertices which are fixed along the path from the root of the search tree to the current node) are computed by the Schreier-Sims algorithm. For each orbit, only one vertex (a representative) is individualized. More precisely, for each orbit *Traces* chooses as representative its smallest vertex.

The following hold with $k = 1, 2$.

Proposition 4.3. *For each ℓ, all the graphs computed by Algorithm 2 at level ℓ are k-dim equal.*

Proof. Induction on ℓ. Easy when $\ell = 0$, since there is only one graph at the initial level. During the construction of the list of graphs at the next level, if a better graph is obtained, then the whole list is re-initialized (line 13) and all the previously computed graphs are discarded; if a worse graph is obtained, it is not added to the list (see the **if**-statements at lines 11-12). □

Lemma 4.4. *For any colored graph G, the final level of $\mathcal{T}(G)$ produced by Algorithm 2 consists of only one node.*

Proof. Follows from Proposition 4.3, using the argument of Remark 4.2.(iv). □

Lemma 4.5. *Let $k \in \{1, 2\}$. The k-dimensional refinement function and the corresponding target cell selector used by Algorithm 2 are invariant under isomorphism.*

Algorithm 2 Canonical Labeling with k-dimensional refinement ($k \in \{1, 2\}$)

Remark: throughout the algorithm "the group" refers to the group generated by the successively detected automorphisms;
$^{(\star)}$ use the k-dimensional algorithm; $^{(\star\star)}$ in the 2-dim case, only.

Input: A colored graph G

  1: Initialize the automorphism group of G
  2: Refine$^{(\star)}$ G to (H, π), possibly$^{(\star\star)}$ adding new generators to the group
  3: $\ell = 0$ {initial level}
  4: Build the list of graphs at level 0, whose element is (H, π), only
  5: **while** the number of cells of partitions at the current level ℓ is less than n **do**
  6:     **while** the list of graphs at the current level is not empty **do**
  7:        Consider the head of the list, which, for some $v_{h_1}, \ldots, v_{h_\ell}$, contains the graph
           $(H, \pi^{(v_{h_1}, \ldots, v_{h_\ell})})$, and remove it from the structure   {the current graph}
  8:        **for each** vertex $v_{h_{\ell+1}}$ in the target cell of the current graph **do**
  9:           **if** for $i = 0, \ldots, \ell$: $v_{h_{i+1}}$ is an orbit representative of the stabilizer of the group with
             respect to $v_{h_1}, \ldots, v_{h_i}$ **then**
10:              Produce $(H, \pi^{(v_{h_1}, \ldots, v_{h_\ell}, v_{h_{\ell+1}})})$ after individualization of $v_{h_{\ell+1}}$ and refinement$^{(\star)}$, possibly $^{(\star\star)}$ adding new generators to the group
11:              **if** the obtained graph is k-dim better or equal than the best one computed **then**
12:                 **if** it is k-dim better **then**
13:                    Initialize (as empty) the list of graphs at the next level
14:                 **end if**
15:                 Compute an experimental path {trivial when the current partition is discrete}
16:                 Check for automorphisms and possibly add new generators to the group
17:                 **if** the next level list is empty **or** no automorphism is found **then**
18:                    Append the current graph to the next level list
19:                 **end if**
20:              **end if**
21:           **end if**
22:        **end for**   {end of vertex individualizations for the current graph}
23:     **end while**   {end of graphs at the current level}
24:     $\ell = \ell + 1$
25:     Let the list of graphs at the next level become the list at the current level
26: **end while**

Proof. It is well known that 1- and 2-dimensional Weisfeiler-Lehman refinements are isomorphism invariant [40, 4]. When $k = 2$, *Traces* uses the 2-dimensional refinement at every level of the search tree except at the final one, where (see Section 3.5) a further 1-dimensional refinement step is executed. Therefore, the adopted refinement is isomorphism invariant.

    Let us first consider Algorithm 2 in the case $k = 1$. Let $G = (H, \pi)$ and let $S = (a_0 = 0, b_0 = n), (a_1, b_1), \ldots, (a_h, b_h)$ be a sequence of pairs on integers such that: $\forall i \in \{1, \ldots, h\}$: (i) $a_i < b_i$; (ii) a_i is the position of a cell of π; (iii) either $b_i = n$ or b_i is the position of a cell of π. Let $\tilde{h}$ be the largest index in $\{1, \ldots, h\}$ such that there exists a non-trivial cell of π whose position p is such that $p \geq a_{\tilde{h}}$ and $p < b_{\tilde{h}}$. The target cell of G is the leftmost cell with maximal size whose position lies within the interval $[a_{\tilde{h}}, a_{\tilde{h}}]$. If $G_1 = (H, \pi_1)$ and $G_2 = (H, \pi_2)$ are isomorphic and we choose their target cell according to the same sequence S, then the same target cell will be selected for G_1 and G_2, since the sequences of sizes of cells in π_1 and π_2 are equal. It follows

by induction on the depth of the search tree, using Proposition 4.3, that the sequences

$$S_0 = (0, n); S_{\ell+1} = S_\ell, (a, b)$$

where a is the position of the target cell W_a at level ℓ according to S_ℓ and $b = a + |W_a|$, are isomorphism invariant, as well as the target cell selector.

In the 2-dimensional case the adopted target cell selector is trivially isomorphism invariant by construction. $\square$

Proposition 4.6 (Correctness). *Given two colored graphs G_1 and G_2, let Q_1 and Q_2 be the quotient graphs associated to the graphs produced by Algorithm 2 at its final iteration, respectively. If G_1 and G_2 are isomorphic, then $Q_1 = Q_2$.*

Proof. From Proposition 4.3 and from Lemma 4.5, we have that for any $\ell \geq 0$ and for any graph appearing at level ℓ in $\mathscr{T}(G_1)$ there exists one graph isomorphic to it at level ℓ in $\mathscr{T}(G_2)$. The correctness of Algorithm 2 follows from Lemma 4.4. $\square$

5. Experimental results

The algorithm presented in the paper is now compared with *nauty* and *bliss*. A comparison with *saucy* can be obtained from our performance tables and those presented in [19]. We observe that *saucy* is extremely efficient on some families of graphs which mainly come from encodings of the satisfiability problem, while it is usually slower than all the other tools outside those classes. Moreover, *saucy* does not compute a canonical labeling.

5.1. Methodological statement

Traces implements a general purpose algorithm aimed at reducing the search space associated to canonical labeling and/or to the computation of the automorphism group of a graph. The algorithm which only computes a set of generators for the automorphism group of the input graph - fully described in [35] - is obtained by means of a slight modification of the canonical labeling algorithm.

Every canonical labeling tool based on the individualization-refinement technique spends most of its execution time in refining partitions. We take 1-dimensional refinement as the unit of measurement of the size of the search tree, since one refinement is completed for each node of the tree by all canonical labeling tools. In the case of experiments with 2-dimensional refinement, the number of 1-dimensional steps needed during the refinement process will be counted and reported in tables.

The selected benchmarks are divided in two parts: (i) those displaying a large search space (hard graphs), and (ii) those with a small search space (easy graphs). The use of 2-dimensional refinement is not considered for easy graphs.

In our experiments, whenever possible, we have chosen the appropriate invariant to establish the best performance for *nauty*. It has to be noted that the choice of a correct invariant is a subtle operation; as an example, the invariant *cellfano2* is useful to break the regularity of incidence graphs of projective planes, as it looks for occurrences of Fano subplanes into the considered graph. But it reveals itself to be extremely inefficient in the case of projective planes with very large automorphism group (e.g. pp16-1).

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							nauty 2.4		bliss 0.50		Traces	
Graph	Ref	V	E	$|Aut|$	Orbs	Inv	Time	Size	Time	Size	Time	Size
pp16-1	[20]	546	4641	$> 3.42 \cdot 10^{10}$	1	–	0.05	127	0.01	100	0.07	841
pp16-2	[20]	546	4641	$2^8 \cdot 3 \cdot 5$	10	CF	62.90	10	671.53	46,005,059	35.28	110,215
pp16-4	[20]	546	4641	$2^{12} \cdot 3$	6	CF	74.22	23,986	104.33	8,164,407	12.53	38,054
pp16-6	[20]	546	4641	$2^{11} \cdot 3^2$	5	CF	61.78	12	3,152.94	539,781,990	15.53	55,631
pp16-7	[20]	546	4641	$2^{14} \cdot 3^2$	3	CF	61.61	4979	576.89	81,992,440	1.22	6,323
pp16-8	[20]	546	4641	$2^{15} \cdot 3^3$	3	CF	62.55	727	1.88	199,505	0.36	4,561
pp16-9	[20]	546	4641	$2^{12} \cdot 3^2 \cdot 5^2$	6	CF	60.96	39	200.69	18,774,117	0.36	7,288
pp16-11	[20]	546	4641	$2^{12} \cdot 3^2 \cdot 7$	6	CF	60.27	88	301.97	45,204,426	0.89	16,971
pp16-15	[20]	546	4641	$2^{11} \cdot 3^3$	8	CF	60.34	42	1,712.23	230,978,343	3.47	29,545
pp16-17	[20]	546	4641	$2^{11} \cdot 3^2 \cdot 5$	8	CF	60.29	151	66.03	5,025,112	1.89	31,465
pp16-19	[20]	546	4641	$2^8 \cdot 3^2$	14	CF	59.20	10	839.73	63,454,501	61.68	183,989
pp16-21	[20]	546	4641	$2^7 \cdot 3^3$	12	CF	59.14	7	4,991.69	518,875,221	43.11	127,208
pp25	[34]	1302	16926	$2^7 \cdot 3 \cdot 5^3 \cdot 31$	2	CF	**5,000**	20	2,456.04	118,865,645	13.59	6,836
pp27	[34]	1514	21196	$2^3 \cdot 3^7 \cdot 7$	4	CF	**5,000**	3	1,704.90	116,513,018	431.23	109,978
mz-aug2-18	[20]	432	684	2^{38}	252	–	66.00	5,374,331	7.39	1,406,880	1.04	73,415
mz-aug2-20	[20]	480	760	2^{42}	280	–	337.76	23,573,421	30.11	5,639,006	1.25	77,379
mz-aug2-22	[20]	528	836	2^{46}	308	–	1,616.68	102,760,999	123.07	22,587,583	1.54	94,211
mz-aug2-30	[20]	720	1140	2^{62}	420	–	**5,000**	225,143,802	**5,000**	797,139,792	3.42	178,099
mz-aug2-50	[20]	1200	1900	2^{102}	700	–	**5,000**	140,555,243	**5,000**	832,923,145	17.57	597,191
had-52	[20]	208	5512	$2^4 \cdot 13$	2	CQ	0.09	13	0.29	13,082	0.20	2,678
had-100	[20]	400	20200	$2^4 \cdot 5^2$	2	CQ	1.62	13	2.62	53,932	2.69	6,503
had-184	[20]	736	68080	$2^6 \cdot 23$	2	CQ	33.40	107	22.39	115,937	9.86	16,633
had-232	[20]	928	108112	$2^6 \cdot 29$	2	CQ	102.14	128	50.81	181,668	25.33	19,307
had-sw-32-1	[20]	128	2112	2^2	42	CQ	0.06	66	2.49	124,818	0.55	18,584
had-sw-88	[20]	352	15664	2^2	132	CQ	20.32	140	204.90	3,147,799	35.47	160,480
had-sw-112	[20]	448	25312	2^2	224	CQ	99.63	223	560.90	10,990,338	198.76	402,977
sts-67	[20]	737	35376	3	253	AT	0.12	3	8.31	157,566	1.63	510
sts-sw-21-10	[20]	70	945	1	70	AT	0.01	1	0.02	3,011	0.01	142
sts-sw-55-1	[20]	495	19305	1	495	AT	0.04	1	7.58	206,416	1.19	992
sts-sw-79-11	[20]	1027	58539	1	1027	AT	0.24	1	69.79	937,652	14.36	2056
GenQuad-1	[36]	2752	481600	$2^8 \cdot 3^2 \cdot 7^5$	2	–	**5,000**	3,802,052	981.98	1,291,025	2.60	17857
Hypercube	[30]	3161	18780	$2^5 \cdot 3^2$	42	–	1,215.88	186,798	32.45	146,987	2.59	49961

Table 1. Graphs with large search tree: Canonical Form (*nauty* invariants [29]: CF = cellfano2, CQ = cellquads, AT = adjtriang)

Remark 5.1. At present, *Traces* is implemented as an additional command of *nauty*: it uses the data structures of *nauty 2.4*, with the exception of the graph representation (adjacency matrix in *nauty*, adjacency list in *Traces*). Indeed, the current version of *Traces* is a prototype which has been implemented with the intention of substantiating from the experimental standpoint the algorithmic design described in this paper, with a particular attention to the new search strategy and the use of the Schreier-Sims algorithm. In particular, *Traces* does not implement any special data structure or procedure to handle large sparse graphs.

Leon's implementation of the Schreier-Sims algorithm is used in the present version of *Traces* for automorphism group computations. This code is part of a more general package ([24]) and we expect a substantial improvement from a new implementation of the Schreier-Sims algorithm, specialized for our purposes, which is currently under development.

5.2. Experiments and comments

Experiments were carried out on a Apple MacBook Pro with Intel Core i7 processor at 2.66 GHz and 4 GB RAM, under gcc 4.0.

| | | | | | | | nauty 2.4 | | bliss 0.50 | | Traces | |
Graph	Ref	V	E	|Aut|	Orbs	Inv	Time	Size	Time	Size	Time	Size
pp16-1	[20]	546	4641	$>3.42\cdot10^{10}$	1	–	0.05	144	0.01	144	0.08	841
pp16-2	[20]	546	4641	$2^8\cdot3\cdot5$	10	CF	60.37	10	976.65	80,597,650	2.15	22,194
pp16-4	[20]	546	4641	$2^{12}\cdot3$	6	CF	70.89	27857	115.02	10,311,534	2.23	8,569
pp16-6	[20]	546	4641	$2^{11}\cdot3^2$	5	CF	61.97	12	5,386.10	968,486,421	0.83	28,561
pp16-7	[20]	546	4641	$2^{14}\cdot3^2$	3	CF	66.30	17859	1,445.07	210,159,039	0.35	3,256
pp16-8	[20]	546	4641	$2^{15}\cdot3^3$	3	CF	62.18	857	10.80	1,170,686	0.20	5,126
pp16-9	[20]	546	4641	$2^{12}\cdot3^2\cdot5^2$	6	CF	62.47	183	353.70	35,107,649	0.23	9,290
pp16-11	[20]	546	4641	$2^{12}\cdot3^2\cdot7$	6	CF	61.79	56	1,388.90	219,395,299	0.27	25,514
pp16-15	[20]	546	4641	$2^{11}\cdot3^3$	8	CF	61.75	135	2,003.88	278,419,116	0.56	29,566
pp16-17	[20]	546	4641	$2^{11}\cdot3^2\cdot5$	8	CF	61.62	750	134.46	14,074,851	0.40	43,636
pp16-19	[20]	546	4641	$2^8\cdot3^2$	14	CF	60.62	10	1,189.43	130,609,514	3.14	33,119
pp16-21	[20]	546	4641	$2^7\cdot3^3$	12	CF	61.79	7	**10,000**	1,682,088,433	2.83	29,732
pp25	[34]	1302	16926	$2^7\cdot3\cdot5^3\cdot31$	2	–	**10,000**	5,052,799	2,546.45	118,865,645	17.01	9,214
pp27	[34]	1514	21196	$2^3\cdot3^7\cdot7$	4	–	**10,000**	4,435,071	**10,000**	818,906,445	52.82	30,004
pp64	[36]	8322	270465	$2^{15}\cdot3^3\cdot7^2$	8	–	**10,000**	197,575	**10,000**	319,961,863	416.82	80,479
mz-aug2-18	[20]	432	684	2^{38}	252	–	62.04	5,374,331	3.51	1,048,954	0.92	73,415
mz-aug2-20	[20]	480	760	2^{42}	280	–	297.56	23,593,421	14.80	4,194,764	1.10	77,379
mz-aug2-22	[20]	528	836	2^{46}	308	–	1,407.27	102,760,999	64.64	16,777,766	1.50	94,211
mz-aug2-30	[20]	720	1140	2^{62}	420	–	**10,000**	429,873,822	**10,000**	1,801,193,025	3.63	178,099
mz-aug2-50	[20]	1200	1900	2^{102}	700	–	**10,000**	275,778,055	**10,000**	1,283,172,635	19.69	597,191
had-52	[20]	208	5512	$2^4\cdot13$	2	CQ	0.08	13	0.33	15,533	0.12	1,553
had-100	[20]	400	20200	$2^4\cdot5^2$	2	CQ	1.47	13	2.62	58,613	1.63	3,679
had-184	[20]	736	68080	$2^6\cdot23$	2	CQ	30.69	107	23.34	125,285	6.29	28,652
had-232	[20]	928	108112	$2^6\cdot29$	2	CQ	92.56	128	56.51	199,679	14.93	32,066
had-sw-32-1	[20]	128	2112	2^2	42	CQ	0.05	66	2.79	141,932	0.07	3,095
had-sw-88	[20]	352	15664	2^2	132	CQ	18.75	140	214.73	3,645,512	2.34	12907
had-sw-112	[20]	448	25312	2^2	224	CQ	90.63	226	555.42	1,090,338	6.22	10,230
had-236	[20]	944	111864	2	472	CQ	3,054.55	9	**10,000**	98,665,940	99.63	22,014
GenQuad-1	[36]	2752	481600	$2^8\cdot3^2\cdot7^5$	2	–	**10,000**	5,989,083	997.82	1,291,833	3.14	30,339
GenQuad-2	[36]	7300	2693700	$2^7\cdot3^{10}\cdot5^2$	2	–	**10,000**	1,502,419	**10,000**	50,993,419	3.91	2,071★
Hypercube	[30]	3161	18780	$2^5\cdot3^2$	42	–	1,545.82	186,798	47.74	186,796	9.69	1,484★

Table 2. Graphs with large search tree: Automorphism Group (*nauty* invariants [29]: CF = cellfano2, CQ = cellquads; ★: run with 1-dimensional refinement)

Graphs are selected from the library of benchmarks which is attached to the *bliss* distribution ([20]), with the addition of some very hard graphs; these are available in DIMACS format at the *Traces* web page. Concerning the benchmark families of graphs which are not presented here, either they display trivial results (small differences among all of the tools), or they reveal results similar to some of the presented classes.

With reference to the classification in the *bliss* library we have selected graphs from the following families:

- affine and projective geometries: graphs ag2-x, pg2-32;
- Cai-Fürer-Immerman construction: graphs cfi-x;
- constraint satisfaction problems: graphs difp-20-0, fpga-x-y, s3-3-3-3, urq8-5;
- Hadamard matrices: graphs had-x, had-sw-x (with some switching operations);
- Miyazaki constructions: graphs mz-x, mz-aug-x, mz-aug2-x;
- projective planes: graphs ppx: some of them are from [34] or from Gordon Royle [36];
- other graphs of combinatorial origin: graphs GenQuad-x and Hypercube are from Gordon Royle [36] and Brendan McKay [30];
- random regular graphs: graphs rnd-3-reg-x-y;
- strongly regular graphs: graphs latin-x, latin-sw-x-y, lattice-30, sts-x, sts-sw-x-y;
- complete graphs: graphs k-x;
- grid graphs: graphs grid-x-y, grid-w-x-y.

Graph	Ref	V	E	$|Aut|$	Orbs	nauty 2.4			bliss 0.50		Traces		
						Inv	Time	Size	Time	Size	Time	Grp	Size
ag2-16	[20]	528	4352	$2^{14}\cdot3^2\cdot5^2\cdot17$	2	–	0.02	155	0.01	102	0.03	0.03	208
ag2-49	[20]	4851	120050	$2^{10}\cdot3^2\cdot5^2\cdot7^6$	2	–	0.87	51	0.25	51	0.36	0.12	71
cfi-20	[20]	200	300	2^{11}	80	–	0.02	146	0.02	259	0.01	0.01	186
cfi-80	[20]	800	1200	2^{41}	320	–	2.79	1,125	0.07	1,999	2.73	0.67	1,049
difp-20-0	[20]	8965	23082	1	8965	–	1.89	1	0.01	1	0.16	0.00	1
fpga-10-8	[20]	688	1320	$2^{23}\cdot3$	519	–	0.01	300	0.01	300	0.18	0.14	242
fpga-13-11	[20]	1500	3125	$2^{32}\cdot3^7$	1116	–	0.21	780	0.01	780	0.97	0.76	560
grid-3-20	[20]	8000	22800	$2^4\cdot3$	220	–	1.33	5	0.03	5	1.40	0.09	4
grid-w-2-100	[20]	10000	20000	$2^7\cdot5^4$	1	–	12.43	7	0.04	7	1.99	0.28	11
grid-w-3-20	[20]	8000	24000	$2^{10}\cdot3\cdot5^3$	1	–	3.36	8	0.04	8	1.98	0.26	14
k-70	[20]	70	2415	$>1.97\cdot10^{100}$	1	–	0.01	2,485	0.01	2,485	0.88	0.85	689
k-100	[20]	100	4950	$>9.33\cdot10^{157}$	1	–	0.01	5,050	0.02	5,050	7.24	7.18	890
latin-30	[20]	900	39150	$2^6\cdot3^3\cdot5^2$	1	–	0.10	21	0.07	51	0.07	0.03	233
lattice-30	[20]	900	26100	$>1.40\cdot10^{65}$	1	–	0.16	930	0.13	901	0.74	0.70	149
mz-18	[20]	360	540	2^{39}	90	–	0.06	593	0.01	593	0.14	0.13	500
mz-50	[20]	1000	1500	2^{103}	250	–	**600**	–	0.03	3,249	4.91	4.73	2,283
mz-aug-22	[20]	440	1012	2^{47}	110	–	0.10	730	0.01	826	0.26	0.25	466
paley-461	[20]	461	53015	$2\cdot5\cdot23\cdot461$	1	–	0.01	6	0.04	6	0.01	0.00	8
pg2-32	[20]	2114	34881	$>1.09\cdot10^{13}$	1	–	2.71	1,040	0.16	753	0.21	0.06	513
rnd-3-reg-3000-1	[20]	3000	4500	1	3000	DI	0.69	1	0.23	3,001	0.67	0	1
rnd-3-reg-10000-1	[20]	10000	15000	1	10000	DI	39.36	1	2.86	10,001	6.89	0	1
s3-3-3-3	[20]	11076	20218	2^{12}	7836	–	1.07	91	0.03	91	0.92	0.61	272
urq8-5	[20]	3906	20331	1	3906	–	0.12	1	0.01	1	0.06	0	1

Table 3. Graphs with small search tree: Canonical Form (*nauty* invariants [29]: DI = distances)

For each experiment the following information is reported in Tables 1 (canonical labeling of graphs with large search tree), 2 (automorphism group computation for graphs with large search tree) and 3 (canonical labeling of graphs with small search tree): the name of the graph and a reference to it, the number of its vertices and edges; the size of the automorphism group of the graph and the number of its orbits; for *nauty*, the vertex-invariant used; for all the tools considered, the execution time (in seconds) and the size of the associated search space. When an experiment is interrupted (after a reported number of seconds shown in bold face), the size of the already computed portion of the search space is displayed.

2-dimensional refinement is used for the graphs reported in Tables 1,2, while 1-dimensional refinement is used for the graphs in Table 3. Diagrams in Figures 10 and 9 present comparison among the considered tools for some classes of graphs.

5.2.1. Tables 1,2: graphs with large search space

For all the graphs considered, *Traces* exhibits a drastic decrease of the size of their search space, with clear consequences for computation time. The gain in performance of *Traces* with respect to *nauty* and *bliss* is considerable for all graphs of combinatorial origin. Several classes of graphs which cannot be efficiently treated by *nauty* and *bliss* are handled by *Traces* in a few seconds.

It turns out that the hardest instances are graphs with small automorphism group, such as some Hadamard graphs. In particular, critical examples for *Traces* with 1-dimensional refinement are from the had-sw family. The contrast with the efficiency of the 2-dimensional refinement suggests that the comparison between refinement traces has to be improved in the case of 1-dimensional refinement.

The reader can verify (see also Figure 9 (bottom)) an exponential contraction of the search space of *Traces* with respect to those of *nauty* and *bliss* in the case of Miyazaki's sequence mz-aug2-x. Now, Miyazaki's graphs are carefully tuned (their labeling, too) to cause *nauty* (and
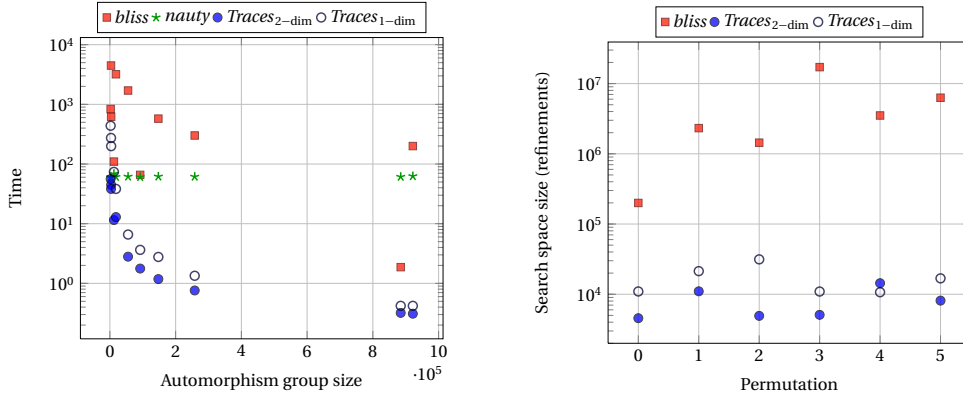
Figure 8. Non-Desarguesian projective planes of order 16 (left); relabelings of PP16-8 (right)

therefore *bliss*) as much trouble as possible, but other more "natural" classes of graphs which are intractable for *nauty* and *bliss*, such as unions of non isomorphic strongly regular graphs with the same parameters, are efficiently treated by *Traces*. At present, we do not know of any class of graphs forcing *Traces* to exhibit a proven exponential behavior.

Finally, we observe (see Table 2) that *Traces*' performance is almost always better in the automorphism group computation mode compared to the canonical labeling mode.

5.2.2. Table 3: graphs with small search space.

Graphs exhibiting a small search space (with respect to the size of their vertex set) turn out to have either a large automorphism group or a trivial one. In the first case, the search space is massively pruned by automorphisms, in the second case just a few individualization steps are needed to obtain discrete partitions. These are the most favorable situations for the individualization-refinement technique.

Still, *Traces* is able to reduce both the depth and size of the search space, and it almost always displays better performances than *nauty*. If we disregard the cases where *nauty* uses vertex invariants, the sizes of search trees of *nauty* and *bliss* are always similar, often exactly the same. Therefore, it is reasonable to assume that the difference between their performances is due to the efficiency of *bliss* in handling sparse graphs, and to expect an improvement in *Traces*' performances when suitable data structures are adopted.

The time spent by *Traces* via the Schreier-Sims algorithm in group computation (reported in Table 3) becomes significant when dealing with very large automorphism groups: this is evident in the case of complete graphs.

5.2.3. Remarks about some particular experiments

Traces seems to have a stable behavior on different instances of graphs in the same family and also on different representations of the same graph, as shown in Figure 8. In particular, Figure 8 (left) compares the execution time of *Traces* and *bliss* with respect to the size of the automorphism groups of graphs in the family pp-16 (projective planes of order 16), clearly showing that graphs with larger group are more efficiently treated by *Traces*. This is what we expect from tools based on pruning by automorphism.
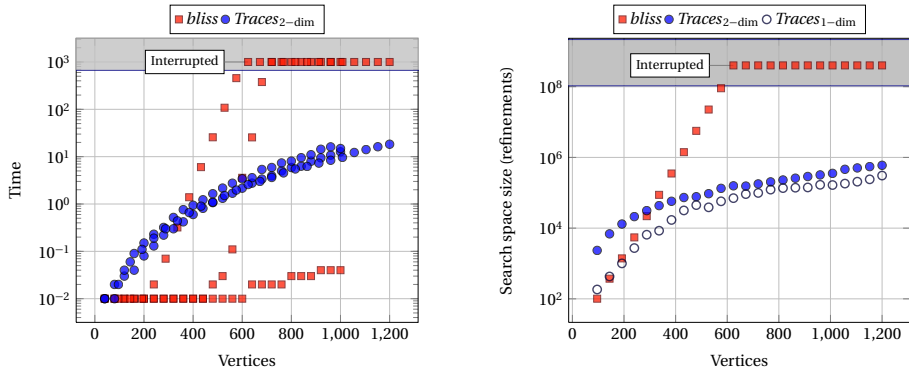
Figure 8 (right) compares the sizes of search spaces coming from random permutations of vertices of pp-16-8. It comes out that *Traces* has a stronger ability of capturing the structure of the graph, thus abstracting from its representation. A further evidence of such claim can
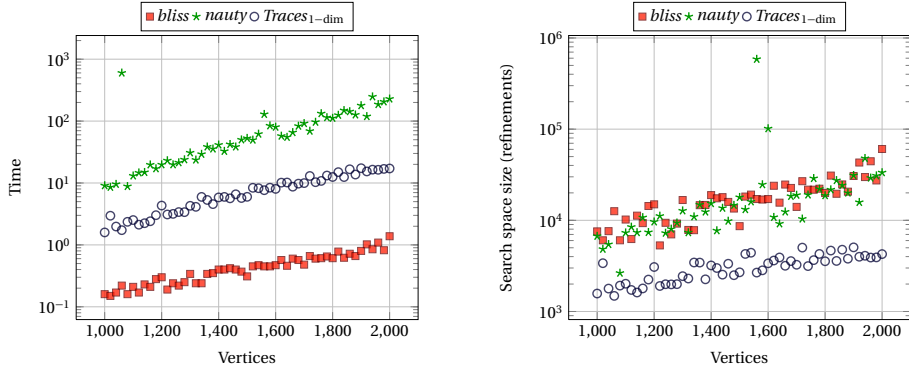
Cai, Fürer and Immerman's graphs [10]
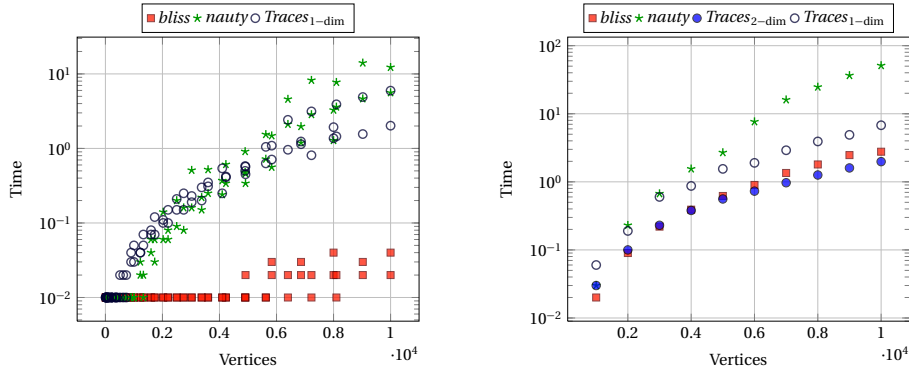
Grid graphs (left); Random 3-regular graphs (right)

Miyazaki's graphs [33]

Figure 9.

be also deduced from the series cfi-x, where, though not reported into the tables, the depth of *Traces*' search space is equal to the main parameter introduced by Cai, Fürer and Immerman in their construction [10].

Incidence graphs of projective planes are considered among the hardest examples for prac-

tical graph isomorphism testing, since they exhibit a high degree of regularity, whilst they can have a rather small automorphism group. The best known algorithm for such graphs is due to Miller [32] and is based on a theorem by Bruck [9] about the order of subplanes into projective planes. It is interesting to mention that *Traces* exactly mimics the behavior of Miller's algorithm, thanks to the correct response of the target cell selector, without the need of any ad hoc modification. In fact, at every iteration an individualization selects a vertex corresponding to a point of the plane which is not collinear with the previously selected ones. The refinement (either 1-, or 2-dimensional) yields a partition whose singleton vertices constitute a subplane of the input plane. This seems to be a further evidence of the fact that *Traces* captures relevant structural properties of such graphs. In addition, Miller's construction does not consider, as *Traces* does, the presence of automorphisms; therefore *Traces* always runs below the theoretical bound established in [32]. We are currently investigating whether automorphism detection may turn Miller's algorithm, which has a subexponential time complexity, into a polynomial one.

Finally, we have experimented with the possibility of running *Traces* when the automorphism group of the input graph is known in advance. The group can be computed more efficiently than canonical labeling in *Traces*, as shown comparing Tables 1 and 2. Interesting results can be obtained for large and highly symmetric graphs. For instance, the graph GenQuad-2, which is the collinearity graph of a generalized quadrangle of order $(9, 81)$, can be canonized in 7 seconds (instead of more than 5000!) when its automorphism group, which can be computed in 4 seconds with simple refinement, is known. This huge difference is due to the use of information coming from the group structure during the refinement process.

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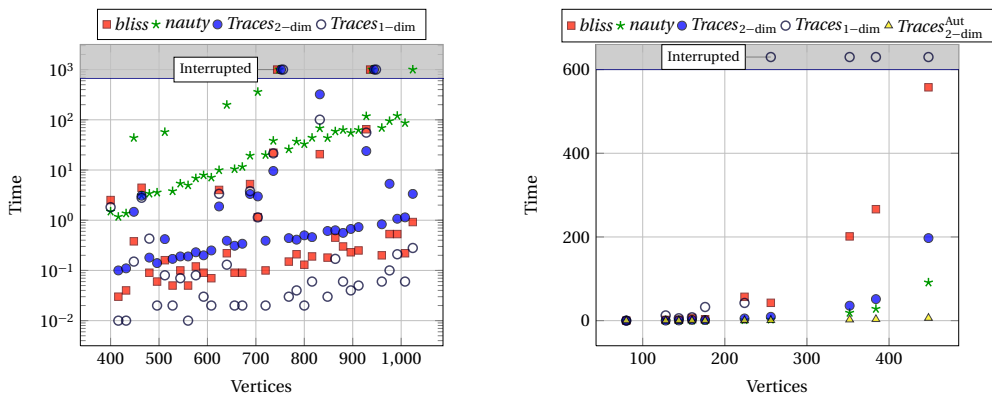
Hadamard graphs: had (left); had-sw (right)
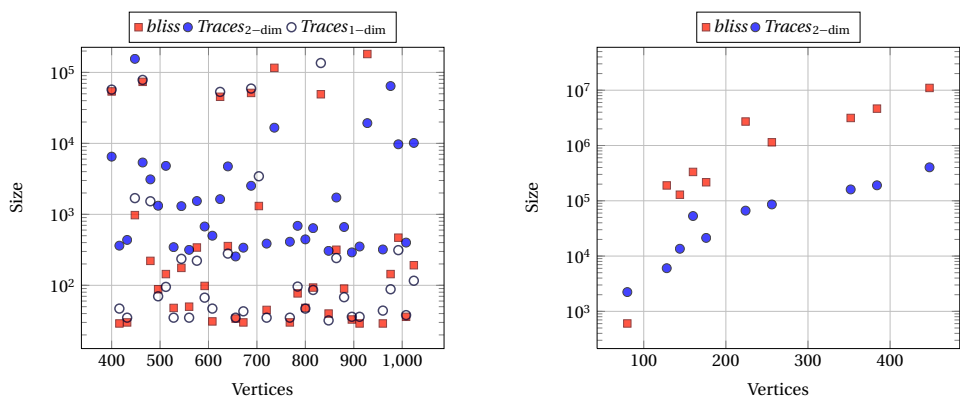
Search space size (refinements) of Hadamard graphs: had (left); had-sw (right)
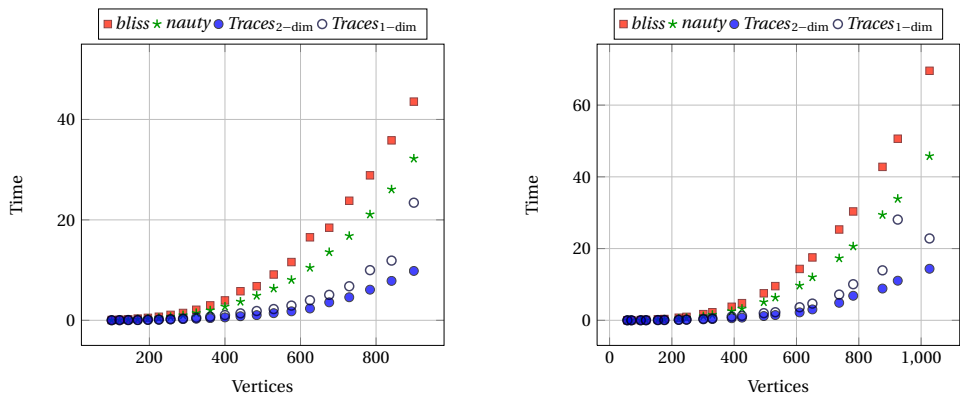
Some strongly regular graphs: latin-sw (left); sts-sw (right)

Figure 10.

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