BOOSTING ISOMORPHIC MODEL FILTERING WITH INVARIANTS

A PREPRINT

João Araújo

Universidade Nova de Lisboa, Lisbon, Portugal jj.araujo@fct.unl.pt

Choiwah Chow*

Universidade Aberta, Lisbon, Portugal 1702603@estudante.uab.pt

Mikoláš Janota

Czech Technical University in Prague, Czechia mikolas.janota@cvut.cz

January 26, 2022

ABSTRACT

The enumeration of finite models is very important to the working discrete mathematician (algebra, graph theory, etc) and hence the search for effective methods to do this task is a critical goal in discrete computational mathematics. However, it is hindered by the possible existence of many isomorphic models, which usually only add noise. Typically, they are filtered out *a posteriori*, a step that might take a long time just to discard redundant models. This paper proposes a novel approach to split the generated models into mutually non-isomorphic blocks. To do that we use well-designed hand-crafted invariants as well as randomly generated invariants. The blocks are then tackled separately and possibly in parallel. This approach is integrated into Mace4 (the most popular tool among mathematicians) where it shows tremendous speed-ups for a large variety of algebraic structures.

Keywords Computational algebra \cdot Finite model enumeration \cdot Isomorphism \cdot Invariant \cdot Random generation of invariants \cdot Mace4 \cdot Hashing

1 Introduction

To study and get intuition on different types of relational algebras (groups, semigroups, and their ordered versions, quasigroups, fields, rings, MV-algebras, lattices, etc.), mathematicians resort to libraries of all order n models (for small values of n) of the algebra they are interested in. These libraries allow experimentation such as forming and/or testing conjectures etc., to gain insights into the algebras in question. Indeed, GAP [14], the most popular computational algebra system, has many libraries of different algebras (semigroups, quasigroups, etc.), and more are needed. These libraries are so important that the search for them has a long history in mathematics predating for many years the use of computers. (See Appendix B of [12]; and for more recent results please see OEIS [28], where many of the sequences are the number of order n non-isomorphic models of a given class of algebras.)

Many of these algebras can be defined in first-order logic (FOL) and there are tools to allow mathematicians to encode their algebras and produce a meaningful library. The problem is that usually the tools, such as Mace4 [22], which can be easily learned and used by mathematicians and hence is very popular among them, generate too many isomorphic models (see Section 2 for the definition of isomorphism) that need to be eliminated [4]. For example, out of the 230,984 models for the implication algebras (see definition in [3]) of order 10 generated by Mace4, only $18 \approx 0.0078\%$) of them are pairwise non-isomorphic.

Redundant models may either be eliminated during the search phase or filtered out afterwards. Guaranteeing that search never produces isomorphic models is a hard problem and is rarely seen in modern solvers. This paper, therefore, tackles the second problem, i.e., the removal of redundant models from an already enumerated set.

^{*}Corresponding author

In the context of finite model enumeration, the complexity of checking whether two models are isomorphic is only part of the problem. Another source of complexity is the large number of models that need to be checked. If every model is checked against all others, then the performance degrades rapidly as the total number of models increases.

If we assign to each generated model a vector that is invariant under isomorphism and put all models having the same invariant vectors into separate blocks, then models across the blocks will not be isomorphic. This splits the problem into substantially smaller sub-problems. Moreover, processing of the blocks can easily be done in parallel as models across blocks cannot be isomorphic. Parallel processing is an important facet of our approach since modern-day computers are more often than not equipped with multiple cores.

Our contributions to the area of isomorphic model elimination are*:

- 1. Devise an invariant-based parallel algorithm that can be applied to algebras defined by first-order logic formulas and containing at least one binary operation or relation (see Section 5).
- 2. Design a small basic set of invariants that have high discriminating power, and yet are inexpensive to compute (see Section 3).
- 3. Add randomly generated invariants to the invariant-based algorithm to help discover invariants of high discriminating power (see Section 4).
- 4. Use a hash-map to store models partitioned by the invariant-based algorithm to allow fast storage and retrieval of models in the same block (see Section 5).

Our goal is to help mathematicians on two levels: first, provide them with a tool on their desktop that quickly produces a library for the algebra they are working on; second, run the tool on a cluster of computers to precompute libraries for the most famous classes of algebras, and add them to GAP [14] or a similar system.

2 Definitions and Preliminaries

We give a brief overview of the mathematics used in the subsequent sections; we draw mainly from Chapter 2 of [9].

A relational algebra is a triple (D, Σ_F, Σ_R) , where D is a set and Σ_F is a set of operations, that is, functions $f: D^n \to D$ and Σ_R is a set of relations, i.e., $R \in \Sigma_R$ is a subset of D^n . The *order* of a relational algebra is the size of its domain D. (Recall that examples of relational algebras are all imaginable algebras, (di)graphs, etc.; in the following, by algebra we mean relational algebra.)

While the concept of isomorphism is ubiquitous to scientific literature, its definition appears under slight variations. Throughout this paper, we rely on the following definition. Let A and B be structures defined on the same signature Σ_F, Σ_R . A function f from A to B is said to be an *isomorphism* if it is a bijection and preserves all operations and relations. This means that if $g \in \Sigma_F$, with the respective interpretations g^A and g^B in A and B, then $f(g^A(a_1,\ldots,a_n)) = g^B(f(a_1),\ldots,f(a_n))$, for all $a_1,\ldots,a_n \in A$. Analogously, f preserves $R \in \Sigma_R$ of arity n, with the respective interpretations R^A and R^B in A and B, if $(a_1,\ldots,a_n) \in R^A$ implies $(f(a_1),\ldots,f(a_n)) \in R^B$, for all $a_1,\ldots,a_n \in A$.

An important property of isomorphisms is that they preserve sets defined by some fixed formula. More precisely, suppose we have two finite relational algebras A and B, on a signature Σ , isomorphic under $f:A\to B$. In addition, suppose we have a set S contained in A^k and definable by a FOL formula Φ in the language of Σ . Then f(S) is precisely the subset of B^k that satisfies Φ (cf. Theorem 1.1.10 in [21]).

For example, suppose we have two isomorphic finite algebras: (A,*) and (B,*), with $f:A\to B$ an isomorphism. Suppose also that S is the set $\{(x,y)\in A\mid (\exists z\in A)\ (x*^Az)*^Ay=x*^A(z*^Ay)\}$. As S is the set of all elements in A^2 that satisfy a FOL in a language with the function symbol *, then $f(S):=\{(f(x),f(y))\mid (x,y)\in S\}$ is precisely the set of all pairs $(x,y)\in B^2$ such that $(\exists z\in B)\ (x*^Bz)*^By=x*^B(z*^By)$.

This idea is usually expressed by saying that sets definable by FOL formulas are invariant (or preserved) under isomorphism. This guarantees that when we split the list of algebras using invariants based on defining formulas, algebras in different blocks are non-isomorphic; algebras inside the same block might be isomorphic or non-isomorphic. Therefore, to discard the redundant algebras we only have to check within each block. This is the ground for our invariants-based algorithm. For future reference, we state these considerations as a proposition.

^{*}Some preliminary ideas and results have been presented in [2]. This paper adds more invariants including randomly generated invariants and proves their validity. It also reports substantially more experimental results and drills deeper into related work.

Proposition 1. Let A and B be algebras of a signature Σ and $f:A\to B$ be their isomorphism. Then any vector $(a_1,a_2,\ldots,a_m)\in A^m$ satisfies a first-order formula in the common language Σ if and only if the vector $(f(a_1),f(a_2),\ldots,f(a_m))\in B^m$ satisfies the same first-order formula in B.

3 Basic Invariants

The goal of this section is to introduce our list of basic invariants.

We start by observing that the axioms satisfied by an algebra might render some invariants useless. For example, if the algebra is a group, then the invariant that counts the number of idempotents would be useless (there is exactly one idempotent in each group). Thus, we need multiple invariants with inner algebraic meaning and large discriminating power in order to target as many different algebraic properties/classes as possible. On the other hand, we should choose properties that are inexpensive to compute and not very many as that could slow down the computation.

Our choices of invariants are based on concepts ubiquitous in various kinds of algebras. For example, one of our invariants (**B5**) is based on the fact that idempotents appear in many algebras; in particular, it is well-known that every finite semigroup has at least one idempotent and hence this invariant is useful for a wide range of algebras, especially those that have a semigroup reduct.

As observed above, the overwhelming majority of the most popular algebras are defined using operations of arity at most 2 (see page 26 of [9]), so we design most of our invariants around binary operations. We have 10 invariants from binary operations, 4 from binary relations, 4 from unary operations, and 1 from ternary operations to target different common algebraic structures. Together they have high discriminating powers, and yet are easy and inexpensive to compute.

In the following discussions on invariants, the domain of the algebra is denoted by $D = \{1, 2, \dots, n\}$.

3.1 Invariants from Unary Operations

For each unary operation g in the algebra, we compute the invariants for each element $x \in D$:

- **U1** 1 if q(x) = x, 0 otherwise (fixed point);
- **U2** 1 if $g(x) \neq x$ and g(g(x)) = x, 0 otherwise (transposition);
- **U3** The number of $y \in D$ such that g(y) = x (size of the inverse image);
- **U4** The number of $y \in D$ such that g(g(y)) = x (size of the inverse image under g^2).

The correctness of these invariants follows readily from Proposition 1. Of course, the correctness of these invariants can also be proved directly (without using Proposition 1); as a sample illustration, we provide the details for invariant **U3** in the next result.

Proposition 2. Let f be an isomorphism of algebras A and B and v_A, v_B be invariant vectors calculated according to U3 for A and B, respectively. Then $v_A = v_B$.

Proof. For $C \in \{A, B\}$, $x \in C$, and g^C an interpretation of g in C, define $K_x^C := \{y \in C \mid g^C(y) = x\}$. We claim that $K_{f(x)}^B = f(K_x^A)$, i.e. x and f(x) will be represented by the same number $|K_{f(x)}^B| = |f(K_x^A)|$, in the (sorted) vectors v_A and v_B , respectively.

If $y \in K_x^A$, then $g^A(y) = x$ so that $f(g^A(y)) = f(x)$ and hence $g^B(f(y)) = f(x)$, that is, $f(K_x^A) \subseteq K_{f(x)}^B$. It follows that

$$|K_x^A| = |f(K_x^A)| \le |K_{f(x)}^B|.$$

As $f^{-1}: B \to A$ is an isomorphism too, the foregoing argument shows that

$$|K_u^B| = |f^{-1}(K_u^B)| \le |K_{f^{-1}(u)}^A|.$$

Taking in the previous formula u = f(x) we get

$$|K^B_{f(x)}| = |f^{-1}(K^B_{f(x)})| \leq |K^A_{f^{-1}(f(x))}| = |K^A_x|.$$

Now $|K_x^A| = |f(K_x^A)| \le |K_{f(x)}^B| \le |K_x^A|$ implies $|K_x^A| = |f(K_x^A)| = |K_{f(x)}^B|$. As $f(K_x^A) \subseteq K_{f(x)}^B$ it follows that $f(K_x^A) = K_{f(x)}^B$ (as we are dealing with finite structures).

Similar arguments can easily be used to directly prove the correctness of the other invariants.

3.2 Invariants from Binary Operations

For each domain element $x \in D$, we compute the following invariants for each binary operation in the algebra:

- **B1** The smallest integer n such that $x^n = x^k, n > k > 1$ where we define x^n to be $(\dots (x*x)*x)*x$... for n x's (periodicity).
- **B2** The number of $y \in D$ such that x = (xy)x (number of inverses).
- **B3** The number of distinct xy for all $y \in D$ (size of right ideal).
- **B4** The number of distinct yx for all $y \in D$ (size of left ideal).
- **B5** 1 if xx = x, 0 otherwise (*idempotency*).
- **B6** The number of $y \in D$ such that x(yy) = (yy)x (number of commuting squares).
- **B7** The number of $y \in D$ such that x = yy (number of square roots).
- **B8** The number of $y \in D$ such that x(xy) = (xx)y (number of square associatizers).
- **B9** The number of pairs of $y, z \in D$ such that zy = yz = x (number of commuting pairs).
- **B10** The number of $y \in D$ such that there exist pairs of $s, t \in D$ where x = st and y = ts (number of conjugates).

3.3 Invariants from Binary Relations

For each domain element $x \in D$, the following invariants are calculated for each binary relation R:

- **R1** The number of distinct y such that R(x, y).
- **R2** The number of distinct y such that R(y, x).
- **R3** 1 if R(x, x), 0 otherwise. (reflexivity)
- **R4** The number of y such that R(x, y) & R(y, x).

3.4 Invariants from Ternary Operations

Ternary operations are very rare. Indeed, no ternary operation exists in the definition in any of the 158 algebras listed in the ALF database [3], although a few of them come from the Skolemization of binary operations. Moreover, calculations involving ternary operations are often very expensive as deeply nested loops are involved. Thus, only one simple invariant would be included in the algorithm. For each domain element $x \in D$, we compute one invariant for each ternary operation:

T1 The number of times x appears in the ternary operation table. (frequency)

We call the hand-crafted invariants listed above the *basic invariants* to differentiate them from the randomly generated invariants which will be discussed in Section 4. It should be simple to see that the validity of these basic invariants follows from Proposition 3.

4 Random Invariants

As discussed in Section 3, we need different invariants to target different algebraic structures. The basic invariants are inspired by our knowledge of the most popular algebras, however, there are many other (less common) algebraic structures and new ones are permanently appearing.

Therefore, we need a general way (adaptable to each class of algebras) of generating invariants with good discriminating power. A practical solution to this problem is to generate a large set of invariants with a random number of operations and a random number of variables, and then automatically discover the best subset to use.

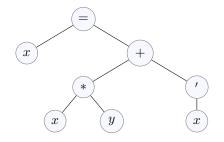


Figure 1: Expression tree for x = (x * y) + x'.

4.1 Generation of Random Invariants

A first-order formula can be represented by an expression tree with operations in the internal nodes and variables in the leaves. For example, Fig. 4.1 shows the tree representation of the first-order formula

$$x = (x * y) + x' \tag{1}$$

It is simple to randomly generate such an expression tree, as shown in Algorithm 1. For simplicity, the root is set to be an operation that evaluates to true or false, and it always has two children. It is the only node that can be assigned the equality relation. It may also be a binary relation if there is one in the algebra.

```
Algorithm 1: Generation of Random First-order Formula
```

```
input: A list of binary/unary operations/relations, max depth of tree, list of variables
   output: An expression tree representing a first-order formula
2 Function BuildNode (level) begin
       /*recursively build a node
       /*maxLevel is maximum depth of tree allowed
      if level = maxLevel then
3
          nodeType \leftarrow leaf
4
       else
5
         nodeType ← random pick a leaf, unary, or binary operation
 6
       create newNode
       if nodeType = leaf then
8
           newNode.value ← randomly pick a variable
          return newNode
10
       newNode.op ← randomly pick a unary or binary operation
11
       newNode.left \leftarrow buildNode (level +1)
12
       if newNode.op is a binary operation then
13
          newNode.right ← buildNode (level +1)
14
15
       return newNode
16 begin
17
       create root node R
       R.\mathsf{op} \leftarrow \mathsf{randomly} pick the equality operation, or one of the binary relations (if exists)
18
       R.\mathsf{left} \leftarrow \mathsf{BuildNode}(1)
19
       R.\mathsf{right} \leftarrow \mathsf{BuildNode}(1)
20
       return R
21
```

Proposition 3. If we fix a variable in the first-order formula generated by Algorithm 1 as the base variable, then the number of solutions will be an invariant.

Proof. Correctness is shown as in Proposition 2.

We may choose any of the variables in the randomly generated first-order formula as the base variable for the invariant. For example, if we choose x as the base variable for the first-order formula (1), then the invariant would read: The number of $y \in D$ such that x = (x * y) + x', which is a valid invariant by the foregoing argument.

4.2 Quality Measure of Random Invariants

After a large set of invariants is generated, a small subset will be selected based on its ability to reduce the work of the next step in filtering out isomorphic models. For a block with m models, the worst-case scenario requires comparing every pair of models for isomorphism. There would be m(m-1)/2 comparisons in total. Based on this observation, we measure the quality of invariants by a score as follows: For a collection of invariants that induces a set of blocks of models $\{S_i \mid 1 \le i \le n\}$, its score is computed as

$$\sum_{i \in \{1..n\}} |S_j|(|S_j| - 1) \tag{2}$$

The goal is to find the set of invariants having the minimum score over all possible combinations of randomly generated invariants in conjunction with the basic invariants.

4.3 Selecting Random Invariants

We are not aware of any tractable algorithm for finding the optimal subset from a large set of random invariants according to the quality measure stated above. A feasible solution is to apply a greedy algorithm (see page 282 of [26] for the general discussions) to a small sample of the models to find an approximate optimal subset. In practice, it is sufficient to use a sample size of 0.1–0.2%, or a thousand, whichever is larger, of the original set of models (see Section 6 for discussions). The algorithm is detailed in Algorithm 2. The idea of the algorithm is to start with the basic invariants, then add the random invariants and calculate the scores one-by-one, keeping the random invariant only if it gives a better score. Then repeat the process of adding random invariants, calculating the scores, and picking the best random invariant that minimizes the score until it cannot be further improved, or a preset maximum number of trials is reached. This subset of random invariants, which may or may not be truly optimal, will then be used together with the basic invariants for the next step.

Algorithm 2: Selecting Random Invariants with Greedy Algorithm

```
input: A set of random invariants R, a set of models M, and maximum trials T
   output: A set K \subseteq R of random invariants with |K| < T
   K \leftarrow \emptyset
 2 bestScore \leftarrow \infty
 3 \text{ done} \leftarrow \text{false}
   while \negdone \wedge |K| < T do
 5
        done ← true
        a \leftarrow \emptyset
 6
 7
        foreach r \in R \setminus K do
             trialScore \leftarrow score of K \cup \{r\} on M according to equation (2)
 8
 9
             if trialScore < bestScore then
10
                  bestScore ← trialScore
11
                 a \leftarrow r
        if a \neq \emptyset then
12
             done ← false
13
             K \leftarrow K \cup \{a\}
14
15 return K
```

Note that the main purpose of adding randomly generated invariants is not to divide the models into more blocks in all cases, but to increase the robustness of the algorithm by the automatic discovery of important invariants in some cases.

[†]We conjecture that the problem is NP-hard; it resembles K-means clustering, which is NP-hard [1].

5 The Invariant Algorithm

First, we describe the algorithm without the randomly generated invariants. For each domain element of a model, we calculate the basic invariants and put them into an ordered list, which is called the invariant vector of that element. If the model has multiple unary, binary, or ternary operations, then invariant vectors are calculated for each of them for all elements, and all the invariant vectors of the same domain element are concatenated to form a combined invariant vector for that domain element. It follows that each model with n domain elements will be associated with n combined invariant vectors. Isomorphic models must have the same set of invariant vectors.

To facilitate comparisons of invariant vectors, we sort the elements by their invariant vectors lexicographically. It follows that models isomorphic to each other must have the same sorted invariant vectors.

Our goal is not only to compare two models for isomorphism but to extract all non-isomorphic models from a list of models. In that case, we set up a hash map to store blocks of the models where models in different blocks are guaranteed to be non-isomorphic. We use the invariant vectors for each model to send the model efficiently to the block (in the hash map) to which it belongs. That is, the keys in this hash map are the invariant vectors, and the values are the blocks of the models. After all models are hashed into the hash map, the blocks stored in the hash map can be processed separately, and possibly in parallel, to extract one representative model from each isomorphism class. An example of construction and use of invariants can be found in [2].

To add random invariants to the algorithm, a preprocessing step is added to select an optimal subset of random invariants before the normal process. As described in Section 4.3, we construct a list of random invariants, calculate basic invariants and the random invariants on a small sample of the input models. Then apply the greedy algorithm to find an optimal subset of random invariants for further processing (see Section 4.3). Finally, proceed to normal processing with the basic invariants and the optimal random invariants together.

Note that our invariant-based algorithm does not compare models for isomorphism. It only cuts down the size of the problem to improve the performance of existing isomorphism filters such as Mace4's *isofilter*.

Invariants have the potential to cope with the increasing size of the order of the algebra very well as illustrated in the following example. Suppose an invariant with extremely low discriminating power gives only 2 values, 0 and 1. However, when applied to the models of an algebra of order 2, it could actually give 4 possible invariant vectors: [0,0], [0,1], [1,0], [1,1]. It is easy to generalize this observation: applying an invariant that gives at most m values to the models of an algebra of order n could result in a maximum of n distinct invariant vectors. Furthermore, if n invariants give n0 and n1 values, then the maximum number of invariant vectors would be

$$\prod_{i=1}^{k} m_i^{\ n} \tag{3}$$

From the above analysis on the intricate interactions between invariants, we can make two more important observations:

- 1. Combining invariants of low discriminating powers could give an invariant vector of surprisingly high discriminating power if they are targeting different areas of the algebraic structures.
- 2. In general, the number of non-isomorphic models increases rapidly as the order of the algebra increases, but so does the maximum number of possible invariant vectors. This helps invariants to retain their discriminating powers to some extent as the order of the algebra increases. This explains why the invariant-based algorithm is very scalable.

6 Experimental Results

We have implemented an invariant-based preprocessor to Mace4's isomorphic models filters. We run experiments on a 6-core Intel® Core[™] i7-9850H CPU computer, with 32 Gb RAM installed.

The ALF database [3] contains a collection of 158 algebras of high interest to the research community of algebra. Their definitions are conveniently given in first-order formulas that Mace4 can directly process. We use Mace4 to generate models for each algebra of the highest possible order that it can complete within 2 minutes. Mace4 is not able to generate models for 5 of them within that time limit, and they are excluded from the tests. The excluded algebras are: #112 Kleene algebra, #113 Concurrent Kleene algebra, #114 Omega algebra, #137 Steiner quasigroup, and #138 Steiner loop. In addition, Mace4's *isofilter* is not able to handle two of the largest algebras (#8 BL-algebras and #56 Linear Heyting algebras), each has between 1 to 3 million models. These two algebras are also excluded from most of the statistics of the experimental results. So, we end up with 151 algebras in many of our analyses.

When random invariants are used in the experiment, the number of randomly generated invariants is 50, but at most 20 of the best of them will be used. The maximum depth of the expression tree (see Section 4.1) is 4, and the maximum number of variables in it is 3. In this section, random invariants are used unless otherwise specified.

Since we run a large comprehensive set of test cases for comparison, the size of each test case is necessarily limited (uniformly and systematically to make comparisons of results meaningful) by the computing resources available. However, even for the small model sizes used in our experiments, the addition of the invariant-based algorithm improves the overall speed by an order of magnitude, without using parallel processing (see Table 1).

The overheads of calculating invariants are observed to be on average about 20 to 30% of the total run time in our experimental setting (see the third column in 1). However, invariants improve the speed by orders of magnitudes for big algebras. For example, for the longest (in terms of runtime) 10 algebras in our experiment, the invariant-based algorithm improves the overall speed by over 50 times (see Table 1). In fact, a very desirable feature of the invariant-based algorithm is that the improvement increases dramatically as the size of the set of models grows. Granted, for algebras with short runtime, the use of invariants may not pay off. But for those cases, the degradation is really insignificant (see Fig. 2). Thus, in general, there is no need to have special logic to decide when not to use invariants.

Furthermore, Mace4's *isofilter* is not able to handle two of the largest data sets, but our invariant-based algorithm can partition these models into smaller blocks to fit in Mace4's limits (see Table 1).

			Total Runtime (s)	
	#Mace4 Outputs	Invariant Calc. Time (s)	With Invariants	Without Invariants
Shortest 10 Algebras	600	0.2	0.5	0.1
Longest 10 Algebras	9,239,818	430	1,982	87,591
All 151 Algebras	33,643,548	1,500	5,030	95,952
2 Isofilter Failed Algebras	4,075,054	208	727.3	N/A

Table 1: Isomorphism Filtering, w/ vs. w/o Invariants

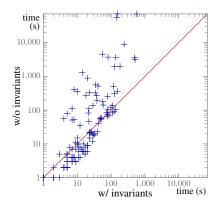


Figure 2: Runtimes: w/ vs. w/o Invariants (151 ALF Algebras)

The performance of the invariant-based algorithm relies heavily on the discriminating power of its invariants. The best possible case is that only 1 non-isomorphic model is in every block, in which case, only m-1 comparisons of models are needed to eliminate all isomorphic models from a block of m models. Our invariants are quite powerful as evidenced by the fact that the average number of non-isomorphic models per block is very close to 1 for the 151 algebras in the experiment (see Table 2).

6.1 Basic Invariants vs. Basic Invariants + Random Invariants

As shown in Table 2, the hand-crafted basic invariants have very good discriminating power (see the last column in the table). Nevertheless, the addition of random invariants improves the discriminating powers (see the middle column of the table). This increase in discriminating power comes with a small overhead in processing time as the number of random invariants is quite small, usually just a few. For example, 6 or fewer random invariants are used in about 90%

Table 2: Discriminating Power (153 ALF Algebras)

	Avg #Non-isomorphic Models per Block				
Percentile	w/ Random Invariants	w/o Random Invariants			
95th	1.346	2.677			
80th	1.036	1.179			
60th	1.003	1.018			
40th	1.000	1.005			

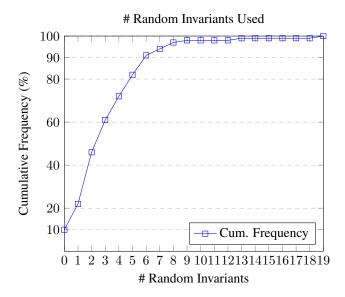


Figure 3: # of Random Invariants (153 ALF Algebras)

of the algebras (see Figure 3). For the case when the basic invariants are already doing a very good job, the addition of random invariants may not pay off. But the degradation is minimal because the job would finish fast when the discriminating powers of the invariants are high (See the scatter plot Fig. 4). Therefore, there is no need for special logic to decide when not to use random invariants. In our experiment, the overall run time for all 151 algebras is reduced when random invariants are added, with most of the improvements coming from the top 3 algebras, which are among the algebras that take the longest to finish (see Table 3 and Fig. 4).

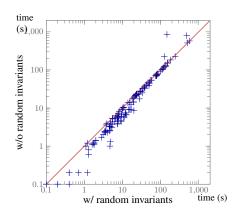


Figure 4: Runtimes: w/ vs. w/o Random Invariants

Table 3: Isomorphism Filtering Time, w/ and w/o Random Invariants

	Total Time (s)			
	With Random Invariants	Without Random Invariants		
Top 3 Improved Algebras	760	1,882		
All 151 Algebras	5,758	6,525		

6.2 Larger Data Sets

As remarked earlier, to cover a large variety of algebras, we have to limit the order of each algebra in the experiments. Small datasets do not adequately show the true advantage of the invariant-based algorithm. Here we present three examples in which we go two orders higher in each of the algebras, giving us test datasets of over a hundred million models. The first algebra (#88 Quasi-MV-algebra) is defined by one binary operation and 1 relation, the second one (#15 Brouwerian semilattices) by two binary operations, and the third one (#4 BCK-join-semilattice) by two binary operations and 1 relation. As shown in Table 4, at the baseline when the order of the algebra is small, the invariant algorithm slows down the process very slightly. However, as the order of the algebra goes higher, the invariant-based algorithm improves the speed by orders of magnitudes. In some cases, Mace4 is not able to handle a large number of models. In all the tests, we also observe that the discriminatory powers of the invariants hold up quite well in large datasets (see Table 5).

Table 4: Isomorphism Filtering, w/ vs. w/o Invariants for Higher Orders

			Total Runtime (s)		
	Order	#Mace4 Outputs	With Invariants	Without Invariants	
#88 Quasi-MV-algebra	7	10,902	1.6	0.7	
	8	4,793,924	558	30,701	
	9	29,799,618	3,666	N/A^1	
#15 Brouwerian semilattices	6	47,349	12	4	
	7	2,247,564	440	1,964	
	8	146,875,177	40,017	N/A	
#4 BCK-join-semilattice	9	122,754	23	15	
	10	1,175,784	305	532	
	11	12,307,002	1,213	54,524	

¹ Isofilter fails after processing 4.5 million (15% of all) models in 11.5 hours.

Table 5: Discriminating Power of Invariants for Higher Orders

			Non-isomorphic Model		
	Order	#Blocks	Total	Avg per Block	
#88 Quasi-MV-algebra	7	567	477	1.19	
	8	153,163	55,544	2.76	
	9	264,972	141,750	1.87	
#15 Brouwerian semilattices	6	745	745	1.00	
	7	8,272	8,272	1.00	
	8	115,801	114,943	1.01	
#4 BCK-join-semilattice	9	26	26	1.00	
	10	47	47	1.00	
	11	82	82	1.00	

6.3 Parallel Processing

The invariant-based algorithm is very scalable since the data are divided into blocks that can be processed independently as long as resources are available. In this experiment, we apply parallel processing to the top 3 algebras with

the longest runtimes (close to 500s or more). We run each of them with 5 parallel threads and see about a 50 - 60% reduction in run times (see Table 6). The results would be even better if more resources are available as a large number of blocks are available in these cases.

Table 6: Isomorphism Filtering, Serial vs. Parallel

			Runtime (s)	
	Order	#Blocks	Serial	Parallel
#8 BL-algebras	5	735,820	574	254
#20 Commutative lattice-ordered monoids	7	15,499	510	240
#145 Digroup	12	17	488	177

7 Related Work

Classes of algebras can often be defined in first-order formulas. For these algebras, a finite model finder, such as Mace4 [22], SEM [30], and FALCON [29], FMSET [7], etc., can work on finding all their models. A well-known issue with this approach is that first-order formulas introduce symmetries into the problem, which leads to the generation of a huge number of isomorphic models in the outputs [27]. These isomorphic models can either be suppressed in the search phase or be removed in a postprocessing step after the models are generated.

Past work in enumerating non-isomorphic finite models has focused on not generating isomorphic models in the search phase. Symmetry breaking is thus a central focus of their research [10, 11, 27]. An excellent example of a simple, powerful, and general algorithm to break symmetry *dynamically* is the least number heuristic (LNH) [4, 29], which picks the smallest one not used so far when a new domain element is to be selected during the search. This is implemented in many solvers such as Mace4, SEM, FMSET, and FALCON. Another symmetry breaker, the eXtended least number heuristic (XLNH) [4,5], is based on similar ideas as the LNH, but could give better performance if there is at least one unary operation in the FOL clauses that define the model. It is also implemented in many finite model enumerators such as SEM.

The underlying idea of LNH can also be applied to break symmetries *statically*. This is necessary for approaches where we do not wish to modify the underlying solver. This is the case for finite model finders based on SAT solvers [10, 17, 27]. The issue is the overhead of encoding LNH in conjunctive normal form (CNF) as well as its complex interaction with the SAT solver. Originally, LNH was only encoded for constants [10]. Later, with additional effort, it was shown that other terms can also be considered [27].

The addition of symmetry-breaking input clauses could be useful in steering the searcher away from the needless exploration of sub-search space [11]. For example, it is well-known that a finite semigroup has at least one idempotent element, so we may add the clause 0 * 0 = 0 to the list of input clauses to cut off the search of the branch 0 * 0 = 1, etc. However, this kind of symmetry breaking often requires deep knowledge of the algebra in question, which may not be available when the algebra is first studied.

Most importantly, these symmetry-breaking techniques do not guarantee isomorph-freeness. While not generating isomorphic models would be ideal, but to guarantee that isomorphic models are not produced in the search phase is a hard problem that few modern-day solvers attempt to do. Systems that do try to do so, such as SEMK [8, 23] and SEMD [18], are either yet-to-be-completed or are better off allowing some isomorphic models in the outputs for some cases for better efficiency.

When isomorphic models are not totally suppressed in the search phase, they would need to be removed in the post-processing steps. Many of them use a limited number of invariants to help speed up the process. Mace4, for example, has a program, *isofilter*, to filter out isomorphic models that it generates in the search phase. It calculates one invariant, frequency of occurrence of domain element, that is, the number of times a domain element appears in the operation tables. It uses this invariant to help separate non-isomorphic models and to help guide the construction of isomorphic functions between potentially isomorphic models. Needless to say, the discriminating power of one single invariant is limited. Indeed, it fails miserably when the operation table is a Latin square, which is the case for quasigroups. To alleviate this issue, Mace4 has another program, *isofilter2*, which does not try to construct isomorphic functions between models, but to convert models to their canonical forms based on the same algorithm [23] used by SEMK. *Isofilter2* works very well with quasigroups, but the overhead in computing the canonical forms of the models is so high that it becomes slower than *isofilter* for many algebraic structures such as semigroups.

The loops package [25] in GAP [14] is not a finite model enumerator but provides a stand-alone function to extract non-isomorphic models from a list of quasigroups. It uses 9 invariants, some of which are expensive to calculate, to help separate non-isomorphic models, and to guide the construction of isomorphic functions between models having the same invariant vectors. These 9 invariants exploit the specific properties of the quasigroup, and may not be effective for other algebraic structures. On the other hand, our invariants target many different areas in the common algebraic structures. Furthermore, their invariant vectors are limited to one binary operation table. Our invariant vectors can be constructed from multiple unary, binary, and ternary operation tables.

Invariants are sometimes incorporated into the finite-model enumerating algorithm for specific algebras. These invariants are sometimes very simple and easy to compute, such as those in the algorithm for enumerating quandles [13]. But others may be very complicated, not easy to implement, and not cheap to compute as in the case of the algorithm for enumerating inverse semigroups [20] using the constraint solver, Minion [15]. Furthermore, the number of invariants used in these cases is usually very small, often two or fewer. Recall expression 3 on page 7 which shows that the number of invariants could increase the discriminating power drastically. Our invariants are cheap to calculate, are applicable to more algebraic structures, and are high in number to provide more opportunities for separating non-isomorphic models. Moreover, they can easily be incorporated into any finite model enumerator.

Neither Mace4's nor loops' isomorphic model filters make use of the hash table to store the models so that non-isomorphic models will never be compared once they are separated by their invariant vectors. This introduces some inefficiencies in their algorithms. Thus, both could benefit immensely from the reduced number of models in the blocks created by our invariant-based algorithm as a preprocessing step.

Another important feature in the invariant-based algorithm is randomization. Using randomization in the search phase in Boolean Satisfiability (SAT) and Constrained Programming (CSP) algorithms is a tried and tested technique [6, 16, 19]. This strategy is built into many SAT solvers such as Chaff [24]. However, using randomly generated invariants to help separate non-isomorphic models in the finite model enumeration is a novel idea. It helps solve the hardest problems in filtering isomorphic models as shown in our experiments, and consequently, increases the robustness of the invariant-based algorithm.

8 Future Work and Conclusions

As pointed out in section 6, the efficiency of the invariant-based algorithm relies heavily on the discriminating powers of both the hand-crafted and the randomly generated invariants. Future work will therefore concentrate on finding powerful invariants to target common algebraic structures, and to find the best parameters to generate optimal random invariants. For example, what depth and breadth of the expression tree would be most cost-effective in generating random invariants? What is the best range of ratios of binary operations to unary operations in a random invariant? What is the best size of the sample to use in finding the optimal set of random invariants?

In summary, we present in this paper an algorithm that uses invariants both as discriminators and as hash keys to partition a set of models into blocks, in which no models across blocks are isomorphic. The blocks are hashed into a hasp map so that they will not be processed together. Included in the algorithm is the novel idea of using randomly generated invariants to supplement hand-crafted invariants to make the algorithm more robust. We show that the invariant-based algorithm is simple, efficient, scalable, and parallelizable. It is also compatible with most, if not all, existing finite model enumerators. It can be used as a stand-alone preprocessor to split models into blocks to feed into isomorphic model filters, or it can be directly incorporated into them. Future research will concentrate on finding powerful invariants in different areas of algebraic structures, and on the automatic discovery of optimal random invariants.

Acknowledgments

The results were supported by the Ministry of Education, Youth and Sports within the dedicated program ERC CZ under the project POSTMAN no. LL1902 and Fundação para a Ciência e a Tecnologia, through the projects UIDB/00297-/2020 (CMA), PTDC/MAT-PUR/31174/2017, UIDB/04621/2020 and UIDP/04621/2020. This scientific article is part of the RICAIP project that has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 857306.

References

- [1] Daniel Aloise, Amit Deshpande, Pierre Hansen, and Preyas Popat. Np-hardness of euclidean sum-of-squares clustering. *Mach. Learn.*, 75(2):245–248, 2009.
- [2] João Araújo, Choiwah Chow, and Mikoláš Janota. Filtering isomorphic models by invariants. In Laurent D. Michel, editor, 27th International Conference on Principles and Practice of Constraint Programming (CP 2021), volume 210 of Leibniz International Proceedings in Informatics (LIPIcs), pages 4:1–4:9, Dagstuhl, Germany, 2021. Schloss Dagstuhl Leibniz-Zentrum für Informatik.
- [3] João Araújo, David Matos, and João Ramires. Axiomatic library finder (database). https://axiomaticlibraryfinder.pythonanywhere.com.
- [4] Gilles Audemard, Belaid Benhamou, and Laurent Henocque. Predicting and detecting symmetries in FOL finite model search. *J. Autom. Reason.*, 36(3):177–212, 2006.
- [5] Gilles Audemard and Laurent Henocque. The eXtended least number heuristic. In Rajeev Goré, Alexander Leitsch, and Tobias Nipkow, editors, *Automated Reasoning, First International Joint Conference, IJCAR 2001, Siena, Italy, June 18-23, 2001, Proceedings*, volume 2083 of *Lecture Notes in Computer Science*, pages 427–442, Berlin, Heidelberg, 2001. Springer.
- [6] Luís Baptista and João P. Marques Silva. Using randomization and learning to solve hard real-world instances of satisfiability. In Rina Dechter, editor, *Principles and Practice of Constraint Programming CP 2000, 6th International Conference, Singapore, September 18-21, 2000, Proceedings*, volume 1894 of *Lecture Notes in Computer Science*, pages 489–494, Berlin, Heidelberg, 2000. Springer.
- [7] Belaid Benhamou and Laurent Henocque. A hybrid method for finite model search in equational theories. *Fundam. Informaticae*, 39(1-2):21–38, 1999.
- [8] Thierry Boy de la Tour and Prakash Countcham. An isomorph-free SEM-like enumeration of models. *Electronic Notes in Theoretical Computer Science*, 125(2):91–113, 2005. Proceedings of the 5th International Workshop on Strategies in Automated Deduction (Strategies 2004).
- [9] Stanley Burris and Hanamantagouda P. Sankappanavar. *A course in universal algebra*, volume 78 of *Graduate texts in mathematics*. Springer, New York, NY, 1981.
- [10] Koen Claessen and Niklas Sörensson. New techniques that improve MACE-style finite model finding. In *Proceedings of the CADE-19 Workshop: Model Computation Principles, Algorithms, Applications*, 2003.
- [11] James M. Crawford, Matthew L. Ginsberg, Eugene M. Luks, and Amitabha Roy. Symmetry-breaking predicates for search problems. In Luigia Carlucci Aiello, Jon Doyle, and Stuart C. Shapiro, editors, *Proceedings of the Fifth International Conference on Principles of Knowledge Representation and Reasoning (KR)*, pages 148–159, San Francisco, CA, 1996. Morgan Kaufmann.
- [12] John D. Dixon and Brian Mortimer. Permutation Groups. Springer, New York, NY, 1996.
- [13] Mohamed Elhamdadi, Jennifer Macquarrie, and Ricardo Restrepo. Automorphism groups of quandles. *J. Algebra Appl.*, 11(1), 2012.
- [14] The GAP Group. GAP Groups, Algorithms, and Programming, Version 4.11.1, 2021.
- [15] Ian P. Gent, Christopher Jefferson, and Ian Miguel. Minion: A fast scalable constraint solver. In Gerhard Brewka, Silvia Coradeschi, Anna Perini, and Paolo Traverso, editors, ECAI 2006, 17th European Conference on Artificial Intelligence, August 29 September 1, 2006, Riva del Garda, Italy, Including Prestigious Applications of Intelligent Systems (PAIS 2006), Proceedings, volume 141 of Frontiers in Artificial Intelligence and Applications, pages 98–102, Amsterdam, Netherlands, 2006. IOS Press.
- [16] Carla P. Gomes, Bart Selman, and Henry A. Kautz. Boosting combinatorial search through randomization. In Jack Mostow and Chuck Rich, editors, Proceedings of the Fifteenth National Conference on Artificial Intelligence and Tenth Innovative Applications of Artificial Intelligence Conference, AAAI 98, IAAI 98, July 26-30, 1998, Madison, Wisconsin, USA, pages 431–437, Menlo Park, CA / Cambridge, MA, 1998. AAAI Press / The MIT Press.
- [17] Mikoláš Janota and Martin Suda. Towards smarter MACE-style model finders. In Gilles Barthe, Geoff Sutcliffe, and Margus Veanes, editors, *LPAR-22*. 22nd International Conference on Logic for Programming, Artificial Intelligence and Reasoning, volume 57 of EPiC Series in Computing, pages 454–470, Manchester, UK, 2018. EasyChair.
- [18] Xiangxue Jia and Jian Zhang. A powerful technique to eliminate isomorphism in finite model search. In Ulrich Furbach and Natarajan Shankar, editors, *Automated Reasoning*, pages 318–331, Berlin, Heidelberg, 2006. Springer Berlin Heidelberg.

- [19] I. Lynce, L. Baptista, and J. Marques-Silva. Complete unrestricted backtracking algorithms for satisfiability. In *In Proceedings of the International Symposium on Theory and Applications of Satisfiability Testing*, pages 214–221, 2002.
- [20] Martin E. Malandro. Enumeration of finite inverse semigroups. Semigroup Forum, 99:679–723, 2019.
- [21] David Marker. Model Theory: An Introduction. Springer, New York, NY, 2002.
- [22] William McCune. Mace4 reference manual and guide. (Technical Memorandum No. 264):20, August 2003.
- [23] Brendan D McKay. Isomorph-free exhaustive generation. Journal of Algorithms, 26(2):306–324, 1998.
- [24] Matthew W. Moskewicz, Conor F. Madigan, Ying Zhao, Lintao Zhang, and Sharad Malik. Chaff: Engineering an efficient SAT solver. In *Proceedings of the 38th Design Automation Conference, DAC 2001, Las Vegas, NV, USA, June 18-22, 2001*, pages 530–535, New York, NY, 2001. ACM.
- [25] Gábor Nagy and Petr Vojtěchovský. LOOPS, computing with quasigroups and loops in GAP, Version 3.4.1. https://gap-packages.github.io/loops/, Nov 2018. Refereed GAP package.
- [26] Christos H. Papadimitriou and Kenneth Steiglitz. *Combinatorial Optimization: Algorithms and Complexity*. Prentice-Hall, Upper Saddle River, NY, 1982.
- [27] Giles Reger, Martin Riener, and Martin Suda. Symmetry avoidance in MACE-style finite model finding. In Andreas Herzig and Andrei Popescu, editors, *Frontiers of Combining Systems 12th International Symposium, FroCoS 2019, London, UK, September 4-6, 2019, Proceedings*, volume 11715 of *Lecture Notes in Computer Science*, pages 3–21, Switzerland AG, 2019. Springer.
- [28] Neil J. A. Sloane and The OEIS Foundation Inc. The on-line encyclopedia of integer sequences, 2020.
- [29] Jian Zhang. Constructing finite algebras with FALCON. Journal of Automated Reasoning, 17:1–22, 08 1996.
- [30] Jian Zhang and Hantao Zhang. SEM: a system for enumerating models. In *IJCAI*, pages 298–303, 1995.