# Identifying Maximal Non-Redundant Integer Cone Generators

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Abstract. A non-redundant integer cone generator (NICG) of dimension d is a set S of vectors from  $\{0,1\}^d$  whose vector sum cannot be generated as a positive integer linear combination of a proper subset of S. The largest possible cardinality of NICG of a dimension d, denoted by N(d), provides an upper bound on the sparsity of systems of integer equations with a large number of integer variables. A better estimate of N(d) means that we can consider smaller sub-systems of integer equations when solving systems with many integer variables. Consequently, applying better bounds on N(d) when deciding the logic of sets with cardinality constraints (BAPA) yields a more efficient decision procedure implementation, and more efficient software verification tools. Previous attempts to compute N(d) using SAT solvers have not succeeded even for d = 3. The only known values were computed manually: N(d) = d for d < 4 and N(4) > 4. We provide the first exact values for d > 3, namely, N(4) = 5, N(5) = 7, and N(6) = 9, which is a significant improvement of the known asymptotic bound (which would give only e.g.  $N(6) \leq 29$ , making a decision procedure impractical for d = 6). We also give lower bounds for N(7), N(8), N(9), and N(10), which are: 11, 13, 14, and 16, respectively. We describe increasingly sophisticated specialized search algorithms that we used to explore the space of non-redundant generators and obtain these results.

### 1 Introduction

The theory of sets and set operations plays an important role in software verification and data flow analysis [1]. Additionally, reasoning about sets is used for proving correctness of data structures, since a natural choice of an abstraction function is the abstraction function that maps the content of a data structure to a set. For full functional verification of complex data structures often it is important to maintain the number of elements stored in the data structure [8]. The logic in which one can express set relations, cardinality constraints and linear integer arithmetic is known under the name Boolean Algebra with Presburger Arithmetic (BAPA) [4]. The decidability of this logic was long known [3], but it was not until recently that [4] proved that BAPA admits quantifier-elimination and has asymptotically the same complexity as Presburger Arithmetic. The quantifier-elimination algorithm introduced in [4] reduces a given BAPA formula to a Presburger arithmetic formula using Venn regions. Many verification conditions expressing properties of complex data structures can be immediately formulated in quantifier-free fragment of BAPA [5], denoted QFBAPA. For these theoretical and practical reasons, we consider only the QFBAPA fragment in this paper.

Checking the satisfiability of a QFBAPA formula is an NP-complete problem, where the non-trivial aspect is showing the membership in NP [5]. The recent advances in SAT solvers made SAT instances coming from hardware and software verification more amenable to solution attempts than before. However, despite the existence of a polynomial encoding of QFBAPA into SAT, an efficient QFBAPA solver is still missing. The most recent QFBAPA implementation [7] uses the state-of-art efficient SMT solver Z3. This implementation relies on the DPLL(T) mechanism of Z3 to reason about the top-level propositional atoms of a QFBAPA formula. Although this implementation is based on an an algorithm that explores all Venn regions, it automatically decomposes problems into subcomponents when possible, and applies Venn region construction only within individual components. This approach is an important practical step forward, but there are still natural formulas that cannot be decomposed. For such cases, the running time of the procedure increases doubly-exponentially in the number of variables.

An alternative approach towards the efficient implementation is to explore the sparse model property of QFBAPA. In [5] was shown that, if a given QFBAPA formula is satisfiable, then there exists an equisatisfiable linear arithmetic formula that is polynomial in the size of the original formula. The decision procedure based on this theorem is described in detail in [5]. The procedure takes as an input a QFBAPA formula and converts it into an equisatisfiable Presburger arithmetic formula  $F_{PA}$ . Based on the newly derived  $F_{PA}$  and the theorem on a sparse solution for integer linear programming [2], the algorithm computes a positive integer N'(d). Number N'(d) denotes an upper bound of the size of a "small" model, of a dimension d, that we are searching for. N'(d) should be read as: if  $F_{PA}$  is satisfiable, then it is also satisfiable in a model with the size at most N'(d). The algorithm then runs in a loop and tries to incrementally construct a model of a size  $0, 1, \ldots$  up to size N'(d). As soon as the first model is found, the algorithm exits the loop and returns that the original QFBAPA formula is satisfiable. If no model is found after the loop execution is finished, then the input formula is unsatisfiable.

The number N'(d) is an upper bound and it can be easily computed from a dimension of a problem. However, this bound is not tight. Our goal is to establish the bound on N'(d) as tight as possible in order to make an efficient implementations of a QFBAPA solver more feasible. As an illustration of infeasibility, consider the fact that, if a solution has the size N, the values of the variables range up to  $2^N$ . Clearly, if N is too large, this decision procedure easily becomes impractical.

We are interested in deriving the smallest possible number N'(d), denoted by N(d), which still preserves the desired property: if formula has a solution, then it also has a solution of the size N(d). This paper will focus on computing the values of N(d) using various combinatorial algorithms and their optimizations.

The existence of N(d) is guaranteed by the main theorem on a sparse solution for integer linear programming [2], which states that if a vector is an element of an integer cone, then it is also an element of some smaller integer cone. The key observation in [5] was not to use any "small" integer cone, but the smallest one. For this purpose in [5] was introduced so called a *non-redundant integer cone*, representing an integer cone, which does not contain a smaller cone that could generate a given vector.

The key contribution of this paper is a computation of the exact tight values of N(d) for some d. We also improve previously known bounds for N'(d). A computation of N'(d) is an algorithmically challenging task. Earlier computations [5] found the exact values only for d = 1, 2, 3.

The following table outlines in comparison the information we knew about N(d) earlier and the new values derived in this paper:

	previou	s known	new results	
d	lower bound	upper bound	lower bound	upper bound
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	5	16	5	5
5	6	22	7	7
6	7	29	9	9
7	8	36	11	19
8	10	43	13	43
9	11	51	14	51
10	12	59	16	58

We obtained those results by applying the following techniques:

- 1. we reduced the search space by establishing the isomorphisms between solutions
- 2. we used the already known solution for N(d) to obtain better estimate on N'(d+1)
- 3. we applied Gaussian elimination method to check whether the returned set of vectors is indeed a non-redundant integer cone
- 4. we used randomized algorithms to obtain a better estimation for some N'(d) values, and for checking efficiency of our implementation

### 2 Preliminaries

This section summarizes the previously known results that are necessary for a better understanding of the rest of the paper. We recall the definitions and the theorems introduced in [5].

Quantifier-free Boolean Algebra with Presburger Arithmetic (QFBAPA) is a theory that includes reasoning about set relations and operations, and reasoning about integer linear arithmetic. Sets and integers are connected through the cardinality operator. A simple decision procedure for QFBAPA uses Venn regions and reduces checking satisfiability of a QFBAPA formula to checking satisfiability of a corresponding linear integer arithmetic formula. As an illustration consider the following QFBAPA formula:

$$|U| = 100 \land \bigwedge_{1 \le i < j \le 3} |x_i \cup x_j| = 30 \land \bigwedge_{1 \le i \le 3} |x_i| = 20 \land \bigwedge_{1 \le i \le 3} |x_i| \subseteq U.$$

With  $l_i$  we denote fresh integer variables. The above formula is equisatisfiable with the following formula written in a matrix form:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix} \begin{pmatrix} l_{000} \\ l_{011} \\ l_{100} \\ l_{101} \\ l_{110} \\ l_{111} \end{pmatrix} = \begin{pmatrix} 100 \\ 30 \\ 30 \\ 30 \\ 20 \\ 20 \\ 20 \end{pmatrix}$$
(1)

The details of the translation algorithm can be found in [5]. However, this newly derived formula might have an exponential size in the size of the original formula. In this example too, the number of variables is exponential in the number of sets in the original formula.

**Definition 1.** Let  $X \subseteq \mathbb{Z}^d$  be a set of integer vectors. An integer cone generated by X, denoted with int\_cone(X), is a linear additive closure of vectors of X:

 $int\_cone(X) = \{\lambda_1 x_1 + \ldots + \lambda_n x_n | n \ge 0, \ x_i \in X, \ \lambda_i \ge 0 \ , \ \lambda_i \in \mathbb{Z}\}.$ 

Note that checking satisfiability of (1) reduces to checking whether a vector belongs to an integer cone. The number of vectors in the integer cone can be infinite and we are interested in deriving the "small" subset of them that would still generate the same initially given vector. We apply the results obtained in the operational research community on sparse solutions of integer linear programming problems.

**Theorem 1 (Theorem 1 in [2]).** Let  $X \subseteq \mathbb{Z}^d$  be a finite set of integer vectors and  $M_X = \max\{n | n = |x_{ij}|, x_{ij} \text{ is an ordinate of vector } x_i, x_i \in X\}$ . Assume that  $b \in \operatorname{int\_cone}(X)$ . Then there exists a subset  $\tilde{X} \subseteq X$  such that  $b \in \operatorname{int\_cone}(\tilde{X})$ and  $|\tilde{X}| \leq 2d \log_2 (4dM_X)$ .

This theorem establishes the bound on the number of vectors of the cone needed to generate a given vector. Because  $M_X = 1$ , the number of vectors in the "smaller" cone is bounded by  $2d \log_2 d + 4d$ . In [5] it was observed that this bound can be reduced to  $2d \log_2 d$  by taking into account that the vectors are non-negative. **Definition 2.** Let  $X \subseteq \mathbb{Z}^d$  and let b be an integer vector. Set X is called a non-redundant integer cone generator for b, denoted by NICG(X, b), if:

- $-b \in int\_cone(X)$
- for every  $x \in X$  holds:  $b \notin \text{int\_cone}(X \setminus \{x\})$ .

Nevertheless, we want to avoid computing a non-redundant integer cone generator for every given vector. The following theorem proved in [5], shows that it is enough to consider only one particular vector, namely  $\Sigma X = \sum_{x \in X} x$ . We define NICG(X) as NICG(X,  $\Sigma X$ ).

**Lemma 1** Let  $X \subseteq \mathbb{Z}_{\geq 0}^d$  be a set of non-negative integer vectors. The following two statements are equivalent:

- there exists a non-negative integer vector b such that NICG(X, b) holds
- NICG(X) holds

Our original motivation was to check satisfiability of QFBAPA formulas. The decision procedure can be outlined as follows: we reduce satisfiability of the initial QFBAPA formula to check the membership in an integer cone, where the generating vectors are bit vectors. Applying Theorem 1 results in the small model property. Therefore, our new goal becomes to compute the number N(d) for a given dimension d. The number N(d) sets an upper bound on the cone size: if a vector is a member of an integer cone, then it is a member of a cone generated with at most N(d) vectors. To translate it back to the QFBAPA satisfiability problem: if a QFBAPA formula is satisfiable, then it also has a model where at most polynomially many Venn regions are non-empty. The number of non-empty Venn regions is determined using N(d). The decision procedures runs in the loop from 0 to N(d) and tries to incrementally construct a model of a size  $0, 1, \ldots, N(d)$ .

Lemma 1 justifies the following definition:

**Definition 3.** Let d be a non-negative integer. With N(d) we denote the cardinality of a set X such that NICG(X) holds and for any set Y of a greater size does not hold NICG(Y)

$$N(d) = \max\{|X| \mid X \subseteq \{0, 1\}^d, \text{ NICG}(X)\}$$

Lastly we provide is the summary on known lower and upper bounds on the value of N(d), as well as the computed values for N(d) for some d:

**Theorem 2.** For a positive integer  $d \ge 1$  and N(d) the following holds:

- 1.  $d \leq N(d)$
- 2.  $N(d) \leq (1 + \varepsilon(d))(d \log_2 d)$ , where  $\varepsilon(d) \leq 1$  and  $\lim_{d \to \infty} \varepsilon(d) = 0$
- 3.  $N(d) + 1 \le N(d+1)$
- 4. N(d) = d, for d = 1, 2, 3
- 5. N(d) > d for  $d \ge 4$

In the rest of the paper we will describe the algorithms and optimizations we used to compute N(4), N(5) and N(6). We will also provide improved lower bounds on N(7) and N(8).

## 3 Core Techniques: N(4)=5, N(5)=7

In this section we present methods that we initially used to compute values of N(4) and N(5). Figure 1 describes a simple algorithm that checks whether a set of vectors  $X \subseteq \{0, 1\}^d$  is a non-redundant integer cone.

```
\operatorname{NICG}(X)
   // Global variable that stores NICG property of X.
   found = FALSE
   for each vector x \in X
        ININTCONETEST(X \setminus \{x\}, \sum X)
        if found == TRUE
             return FALSE
   return TRUE
ININTCONETEST(X, b)
   if b == 0
        found = \text{TRUE}
        return
   if X == \emptyset
        return
   newB = b
   x = take any element from X
   while TRUE
        ININTCONETEST(X \setminus \{x\}, newB)
        newB = newB - x
        if found == \text{TRUE} or newB contains negative component
             return
```

Fig. 1: Program NICG: checks whether for a set of integer vector X holds NICG(X)

A simple incremental algorithm for computing the value N(d) works as follows: the algorithm starts with n and constructs a set X of the cardinality n, which has the property NICG(X). In the next iteration n gets increased and the algorithm repeats the same steps. As soon as the algorithm encounters the first n for which it cannot construct a NICG(X) of the cardinality n, it stops and returns N(d) = n - 1. The correctness of this algorithm is guaranteed by the following theorem, originally proved in [5]:

**Lemma 2** If NICG(X) and  $Y \subseteq X$ , then NICG(Y).

Using this approach we computed N(5) = 7 after approximately 3 hours.

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**Optimization: Binary Search.** Instead of incrementally constructing all the sets, we can apply Lemma 2 together with Theorem 2 to devise an algorithm that computes the value of N(d) in the binary search manner. The algorithm makes a guess n on the value N(d) and tries to construct a set X such that |X| = n and NICG(X). If no such set exists, then N(d) < n, otherwise  $n \le N(d)$ .

As an illustration, consider d = 5. Applying Theorem 2 to compute the bounds on the value of N(5), the algorithm derives the interval in which N(5) occurs:  $6 \le N(5) \le 11$ . The first guess is N(5) = 8. Then the algorithm tries to construct a set X such that |X| = 8 and NICG(X). Because such a set does not exist, the algorithm will not construct it implying  $6 \le N(5) \le 7$ . The next guess is N(5) = 7. Since there exists a set X such that |X| = 7 and NICG(X), the algorithm will construct such a set and output N(5) = 7.

**Incremental Construction vs Binary Search.** We have implemented both, the incremental construction and the binary search approach, to derive N(5). The binary search approach found N(5) faster than the incremental construction approach. However, our experimental results show that the binary search approach is slower than the incremental construction approach in computing N(d) for d > 5. The difference in the experimental results is caused by the fact that testing the existence of a set X such that NICG(X) is computationally more expensive than testing the existence of a set Y such that NICG(Y) when |X| > |Y|. Another issue with the binary search approach is that if the initial interval is not tight enough, the algorithm might make a guess on N(d) that is significantly larger than the value N(d) itself.

As an example consider d = 5. In the incremental approach the algorithm must examine at most  $\binom{31}{6} + \binom{31}{7} + \binom{31}{8} = 11254581$  sets of vectors. In the binary search approach the algorithm must examine  $\binom{31}{7} + \binom{31}{8} = 2921750$  sets of vectors, where the value 31 represents cardinality of the set  $\{0,1\}^5 \setminus \{0,0,0,0,0\}$ .

**Optimization: Preserving Sums.** In order to obtain a more efficient computation of N(d) we tried an approach based on preserving sums of vectors, which can be later reused in the computation. The idea on preserving sums was motivated by the following observation: if  $Y \subset X$  and NICG(X), then  $\Sigma X \notin \text{int_cone}(Y)$ . To benefit from the observation, for every examined Y for which NICG(Y) holds the algorithm must keep track of the sum  $\Sigma Y$ . We have tried this heuristic, but did not obtain any significant improvement. The advantage of such an approach is that the algorithm can compute new sums quickly, and detect not NCIG faster. The disadvantage is the process of maintaining sums. The search algorithm must be aware which sums should be stored and which removed. In certain cases the search algorithm must copy the whole data structure that keeps the sums. Our experiments have shown that maintaining so much information is more costly than the calculation.

### 3.1 Isomorphic sets

So far the algorithms searched for the solution over **all** sets of vectors of given cardinality. We applied optimizations to early detect if set does not improve the solution. Also, we introduced approaches which improved maintaining information about the sets. But common to all those cases was that almost all the sets were examined. This was a big drawback: we will demonstrate that one does not need to examine all the sets. To motivate our observations, consider the following two sets:  $X_1 = \{(1, 1, 0), (0, 1, 0)\}$  and  $X_2 = \{(0, 1, 1), (0, 1, 0)\}$ . Performing a permutation  $\begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$  on indices of components of the vectors in  $X_1$  we obtain  $X_2$ . Permuting components of the vectors does not affect the solution. Therefore, if set  $X_1$  does not lead to the solution, then  $X_2$  does not lead, too. Similarly, if  $X_1$  leads to the solution,  $X_2$  leads as well. The observation allow us to consider only vectors that are not isomorphic, where isomorphism between two sets of vectors is defined as follows:

**Definition 4.** We say that two sets of vectors  $X, Y \subseteq \{0, 1\}^d$  are isomorphic if there exists a permutation P over the set  $\{1, \ldots, d\}$  and a bijective function  $f_P: X \to Y$  defined as

$$f_P(x) = y \Leftrightarrow x_i = y_{P(i)}, i = 1, \dots, d.$$

Basically, there are two ways to check, call it check functions, whether we already considered an isomorphic set:

- 1. For each considered set X so far, mark all isomorphic sets to X, i.e. mark all d! sets (note that some of them might repeat) storing them in a structure *marked*. Before a new set is processed check whether it is in *marked*.
- 2. Store each considered set in a structure *done*. When there is a new set X to be examined, run all d! permutations on X. For each permutation p check if p(X) is in *done*.

We used this approach for  $d \leq 7$ . There are  $2^{64}$  different sets in case d = 6. A particular set can be isomorphic to at most 6! other sets. Because this is an equivalence relation, at least  $\frac{2^{64}}{6!}$  non-isomorphic sets should be stored somehow. This is far away too much. To avoid this problem, we can use a bit different method. Let us define

 $X^{(k)} = \{x | x \in X \text{ and } x \text{ contains exactly } k \text{ non-zero components} \}.$ 

Then we say X and Y are isomorphic if  $(X^{(1)}, X^{(2)})$  is isomorphic to  $(Y^{(1)}, Y^{(2)})$ . With such a method, sets  $X = \{(1,0,0,0), (1,1,1,0)\}$  and  $Y = \{(1,0,0,0), (1,1,0,1)\}$  will not be considered as isomorphic, although they are isomorphic by a permutation  $\begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 4 \\ 1 & 2 & 4 \\ 3 \end{pmatrix}$ . Thus, it does not cover all isomorphic pairs, but allow us to shrink the usage of memory.

Finally, the required memory is sufficiently small that we can store sets in the both cases in an array. As a result, the check function can be executed in a constant time. The first approach uses  $O(d! \cdot T)$  time (T is number of non-isomorphic sets) for marking, and  $O(d! \cdot M)$  memory. Once we do that, the check function is performed in a constant time.

The second approach uses O(1) time to store an examined set, and it uses O(M) memory. For each stored set X there are multiple isomorphic sets. Note that some of those sets do not always have d! isomorphic sets, like for example  $\{(1, 0, 0, 0)\}$ . Actually, most of the time they have less than d!. Before storing a set X we have to generate d! other sets and check whether they are in *done* or not. There are T' isomorphic sets, where for d = 6 the value T' is a few hundred times bigger than T. This approach gives the time complexity  $O((T + T') \cdot d!)$ , and the memory complexity O(M).

In our case, we have already shrank memory, thus the memory is not an issue, but time efficiency. Therefore we choose the first approach.

Using this optimization we obtained a method that in a few minutes calculates N(5) = 7.

### 4 Gaussian Elimination: N(6)=9

In Section 3 we described a different approaches towards a construction of NICG sets. Most of the approaches consider NICG property only of currently calculated set. We also argued why the approach in which we try to maintain as many information as possible is not very efficient. Knowing that, we decided to merge ideas from the both approaches and come with a more efficient algorithm.

The idea about maintaining too much information is not good, as we have explained. However, maintaining some amount of "not NICG(Y)" information might reduce the search space, and thus improve the running time. The property "not NICG(Y)" allow us to avoid computing over every set X such that  $Y \subset X$ . For instance, consider an example where  $Y = \{(1, 0, 0, 0, 0), (0, 1, 0, 0, 0), (1, 1, 0, 0, 0)\}$ . Y is not NICG because  $\sum Y = 2(1, 1, 0, 0, 0)$ . There are  $\binom{28}{4} + \binom{28}{5} + \binom{28}{6} + \binom{28}{7} + \binom{28}{8} = 4787640$  sets X, such that  $|X| \leq 8, Y \subset X$ . Most of those sets would be considered if we do not shrink them using the fact not NICG(Y). Quite a lot of sets is affected by only one set, thus we decided to use information about not NICG sets.

On the other side, we decided not to use information about NICG sets, but for a given set X to test NICG(X) on fly. In Section 1 we saw that answering NICG(X) is the same as answering is there a solution to the corresponding system of equations. Instead of using the procedure ININTCONETEST to answer that, we try to solve system using Gaussian elimination.

Answering whether a given set X has the NICG(X) property by solving the corresponding system with Gaussian elimination might look like an inefficient approach. To understand such a view, consider a system of five equations and eight variables (what could be the case for d = 5) such that its solution contains three parameter-variables. Each component of a vector sum of the eight binary vectors is a non-negative integer value not greater than 8. Therefore there are  $9^3$  possibilities to assign values to the three parameters.

A system that represents a set for  $d \ge 6$  might contain even more parametervariables resulting in even more possible assignments to the parameter-variables. However, it turned out that, for the systems our search algorithms constructed, Gaussian method works very good since most of the parameter-variable assignments are not valid.

This approach verified result for  $d \leq 5$  and gave N(6) = 9 in around a thirty minutes.

Below are given examples of sets of vectors that represent solutions for  $d = 1 \dots 6$ . Those sets are obtained by applying the described approaches.

d	1	2	3	4	5	6
N(d)	1	2	3	5	7	9
a solution	(1)	$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 \ 1 \ 1 \ 1 \ 0 \\ 1 \ 1 \ 0 \ 1 \\ 0 \ 1 \ 0 \ 1 \\ 0 \ 0 \ 1 \ 1 \\ \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix}$

Table 1: Solutions for different d values, an example solution per a value. Full set of solutions is available at [6].

### 5 Speeding up Search using Weak Isomorphisms

In Subsection 3.1 we have seen two approaches that might be used to eliminate isomorphic states. One of the approaches is time inefficient, and another one is memory costly. Both, time and memory inefficiency, grows exponentially, which suggests that any of those approaches can be used only for small d values. On the other side, both of these methods are very strict in sense that for a given type of isomorphism, the methods eliminate all isomorphic states (i.e. detect all isomorphic  $(X^{(1)}, X^{(2)})$  states, as has been already explained).

Every approach to the problem we have used so far can be described by the following algorithm:

SOLVE(currSolution, nonUsedVectors)

SOLVE(currSolution, nonUsedVectors)

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The algorithm above generates a search tree. The method we use to eliminate isomorphic states in the search tree directly affects both, the running time and the memory usage.

As we can see, on one side are the introduced methods that eliminate a lot of states, but they use too much time, or too much memory. On the other side, if we do not use any method for elimination we have to search over a huge tree, but then we do not use any extra time or memory for elimination. Instead of devising a method that rely on benefits only of one or the another side, we have tried to "meet in the middle".

A method that we describe is not so strict in elimination, as the previous methods were, but it is very efficient as we are going to show by the results.

Suppose the algorithm is in a state (currSolution = X, nonUsedVectors = A), and it chooses to examine vector = x. In this state the algorithm must decide which states  $(X \cup y, A \setminus x)$  it is **not** going to visit, knowing that it is going to visit  $(X \cup x, A \setminus x)$ . Note that even if NICG $(X \cup x)$  returns FALSE, the state  $(X \cup x, A \setminus x)$  can be considered as a visited one, but such that it does not lead to the solution. Obviously, if  $X \cup x$  is isomorphic to  $X \cup y$ , there is no point to search over subtree represented by  $X \cup y$ . By isomorphism between sets X and Y we denoted existence of a permutation that maps X to Y. Additionally, we observe that if there exists a permutation P such that P(X) = X and P(x) = y, then there exists a permutation P' such that  $P'(X \cup x) = X \cup y$ . The opposite does not stand always.

Consider even more specific type of permutations that make two states being isomorphic. We say that a permutation P 'preserves order of ones' of a collection of vectors X, if the following holds:

$$(\forall x \in X)(\forall i \in \{1, \dots, d\})x_i = 1 \Rightarrow P(i) = i,$$

where by  $x_i$  is denoted vector-component of x at the position i. In other words, when P is applied on X it does not change order of ones in that collection of binary vectors. Of course, it immediately leads to the conclusion P(X) = X. This type of permutations we call "1-order preserving" permutations.

In our algorithm we describe 1-order preserving permutations by using a single boolean array fixedPerms of the size d. If fixedPerms[i] = TRUE it means that the array represents a collection of permutation such that for every permutation P from the collection it stands P(i) = i. The array fixedPerms is updated in the following way:

- Initially,  $fixedPerms = \{FALSE\}^d$ .

- When a new vector x is added to the current state X, array *fixedPerms* is updated as follows:

for 
$$i = 1 \dots d$$
  
if the *i*-th component of  $x == 1$   
 $fixedPerms'[i] = TRUE$ 

Therefore, for each newly added vector the algorithm updates fixedPerms in O(d) time. For each state the algorithm needs additional d bits to represent the

corresponding array. Testing whether two vectors x and y are isomorphic with respect to 1-order preserving collection given by *fixedPerms* can be done as follows:

ISOMORPHICVECTORS(x, y, fixedPerms)if number of ones in  $x \neq$  number of ones in yreturn FALSE for  $i = 1 \dots d$ if fixedPerms[i] == TRUE if the *i*-th components of x and y differ return FALSE return TRUE

The method ISOMORPHICVECTORS for particular input executes in O(d) time.

As we have seen, eliminating states according to 1-order preserving collection is both time and memory efficient. However, such approach is a bit weak, and it does not eliminate all isomorphic states. This can be illustrated with the following example. Suppose *currSolution* =  $\{(1,1)\}$  and *nonUsedVectors* =  $\{(1,0), (0,1)\}$ . The only permutation that does not change order of ones in *currSolution* is  $\begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}$ , therefore *fixedPerms* = {TRUE, TRUE}. Thus, call of ISOMORPHICVECTORS((1,0), (0,1), {TRUE, TRUE}) will return FALSE. However, there exists a permutation  $\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$  that maps  $\{(1,1), (1,0)\}$  onto  $\{(1,1), (0,1)\}$ , what means that these two states should be considered as isomorphic.

Although the last approach is based on weak isomorphism it runs faster then the previously described approaches for  $d = 1 \dots 6$ . For d = 6 there exist 254 non-isomorphic solutions. The algorithm that uses Gaussian elimination finds 80000 solutions, with many of them being isomorphic. The search lasts for about 45 minutes. The algorithm that implements the weak isomorphism finds nearly 5000 solutions in about 5 minutes.

## 6 Randomizing Search Order; New Lower Bounds

The algorithms we have presented so far deterministically choose the next state from the current state. We developed a randomized algorithm that chooses a next state randomly in such a way that all states reachable from the current state have the same probability to be chosen. The uniform probability distribution on choice over the states is achieved by shuffling list of states reachable from the current state, and then picking the first state from the shuffled list as the next state. Although the implementation difference is minor, results are significantly better than using deterministic algorithm, as can be seen in the following paragraph.

We did not succeed to get exact values for N(7), N(8), N(9) or N(10). Instead, we got better lower estimate of these values. Those estimates are:  $N(7) \ge 11$ ;  $N(8) \ge 13$ ;  $N(9) \ge 14$ ;  $N(10) \ge 16$ . It is interesting that in less than a second we got result  $N(6) \ge 9$ . In a few minutes we got  $N(7) \ge 11$ , and in an hour we got  $N(8) \ge 13$ ,  $N(9) \ge 14$  and  $N(10) \ge 16$ . On the other hand, deterministic algorithm uses the following amount of time:  $N(6) \ge 9$  in a minute;  $N(7) \ge 11$  after a few hours;  $N(8) \ge 13$  we did not get even after a day of running the algorithm.

#### Better estimate of N'(7) using Decomposition: from 36 7 to 19

The best known estimate so far for N'(7) is 36. We successfully improved this upper bound to 19 as follows:

Let X be a solution for d = 7, i.e.  $X \subseteq \{0,1\}^7$  and |X| = N(7). Then set X can be decomposed into two subsets  $X_0$  and  $X_1$  such that

- $-X_0 \cap X_1 = \emptyset,$  $-X_0 \cup X_1 = X,$
- $-X_0$  contains only vectors which first component is 0,
- $-X_1$  contains only vectors which first component is 1.

From Lemma 2 it follows that  $X_0$  and  $X_1$  are NICG sets. Since the first component of each vector in  $X_0$  is 0,  $X_0$  can be considered as a set of 6-dimensional vectors. Therefore,  $|X_0| \leq N(6)$ . In order to estimate an upper bound on  $|X_1|$ , we use the same algorithm as we use to obtain N(6), with the input defined as set  $\{x \mid x \in \{0,1\}^7 \land x_1 = 1\}$ . Running the algorithm on such a set we get the final result, a set Y, after 30 minutes with |Y| = 10. Therefore,  $|X_1| \le 10$ . Since every solution for d = 7 can be decomposed into  $X_0$  and  $X_1$ , with upper bounds 9 and 10, respectively, it implies that solution for d = 7 is of cardinality of at most 9 + 10 = 19.

#### Improvement of N'(d) for Arbitrary d 8

#### 8.1 Isomorphism on row additions

Each NICG set of vectors X can be described as a matrix of dimension  $d \times |X|$ , where each column of the matrix represents a single vector from X, and no two different columns represent the same vector. In this section we introduce an isomorphism of NICG solutions that involves additions and substructions on rows of matrices.

Consider an NICG set of vectors X, and the corresponding matrix M. We will say that two rows,  $i_1$  and  $i_2$ , do not share variable if there does not exists jsuch that  $M_{i_1,j} = 1$  and  $M_{i_2,j} = 1$ . We can state the following lemma.

Lemma 3 Consider a matrix M, and assume that M contains at least two rows that do not share variable. Let two of these rows be  $i_1$  and  $i_2$ . Let a matrix M'be obtained from the matrix M by replacing the row  $i_2$  by the row-sum  $i_1+i_2$ . M represents NICG set of vectors if and only if M' represents NICG set of vectors.

**Corollary 1.** For NICG set X, and its corresponding matrix M, such that M contains two rows  $i_1$  and  $i_2$  such that every variable presented in  $i_1$  is presented in  $i_2$  as well, there exists an NICG set X' which can be obtained from X by replacing the row  $i_2$  by the row-subtruction  $i_2 - i_1$ .

Lemma 3 gives a new insight about isomorphic NICG sets. Using the lemma, we give a better estimate of N'(d), as presented in Section 8.2.

### 8.2 Upper Bound Improvement for large d

In this section we give a better estimate of N'(d). The improvement rely on result presented in Section 8.1. State the following lemma:

**Lemma 4** For each NICG set X, and its corresponding matrix M, there exists an NICG set X', along with its corresponding matrix M', such that

(1) |X| = |X'|, and (2) anothing at least on

(2) every row in M' contains at least one value 0.

*Proof.* If M satisfies the condition (2), then let X' = X and the proof is done. Therefore, assume that M contains a row i such that all its values are 1. It means that variables of every row j are contained in row i as well. By Corollary 1, there exists  $X_1$  that is obtained from X by replacing the row i by the row i - j. If  $X_1$  contains a row with 1s only, then we are going to apply Corollary 1 on  $X_1$ getting  $X_2$ . We continue this process until we get  $X_r$  that does not contain row with all 1s. Because there is finite number of rows,  $X_r$  will be obtained in a finite number of steps. Once we obtain  $X_r$ , let  $X' = X_r$ . By the construction and the corollary,  $X_r$  satisfies both (1) and (2), implying  $X_r$  is NCIG.

This completes the proof.

According to Lemma 4, there exists a solution X to the problem such that the corresponding matrix does not contain a row with all values being 1. Thus we have that every component of the sum of vectors of X never exceed N - 1. If we recall proof of Theorem 2 in [5], we obtain an upper bound on N to be the maximal value such that

$$2^N < N^d.$$

The last inequality gives a slight improvement on an upper bound of N(d).

The upper bound can be even more improved by using result N(d) > d + 1, for d > 4, given in [5]. Consider a solution X and its corresponding matrix M for d > 4. By Lemma 4 there exists a solution such that each row contains at least one 0 value. Assume each of the rows contains a single 0 value. Therefore, at least N(d) - d columns would contain 1s only. Since  $N(d) - d \ge 2$  for d > 4, the system is not NICG. Therefore, the assumption is wrong and there exist at least one row that contains 2 zeros. The last gives a new improvement on upper bound on N that can be described by the following inequality:

$$2^N \le N^{d-1} \cdot (N-1).$$

### 9 Different Approaches

In order to compute N(d) we used general solvers for solving systems of equations with non-negative integer variables. The solvers were used to give an answer whether a particular set of vectors X has the NICG property. If M is the matrix that represents X, then existance of the NICG property can be answered as follows:

- Let  $M^k$  be defined as a matrix which k-th column contains only 0s, and every other column is a copy of the corresponding column in M.
- If for every matrix  $M^k$ , for  $1 \le k \le \#$  of columns in M, there does not exist a non-negative integer solution, then X has the NICG property, otherwise it does not have.

We tried this approach using standard solvers GLPK and jOpt. None of them was even nearly efficient as our implementation of NICG property, the one implemented using Gaussian elimination. Probably, reason behind this is a fact that in our case we were mainly working with systems of small number of equations. For such systems our optimized implementation of Gaussian method has very good performance. On the other side, GLPK and jOpt probably implement efficient solutions but with high constant w.r.t to O-notation, what as the result gives that Gaussian elimination overperform those libraries.

### 10 Conclusions

QFBAPA has the small model property. An upper bound on the size of a small model is provided by the number N(d), where d is the dimension of the corresponding QFBAPA model. In this paper we computed the exact values for N(4), N(5) and N(6). We also significantly improved the known bounds for N(7), N(8), N(9) and N(10). Those numbers are used to determine the size of small models for QFBAPA formulas.

However, our motivation was twofold: first, we obtained the bounds that dramatically improve constant factors in the theoretically optimal algorithm for QFBAPA. Second, we provided another case study in developing domain-specific algorithms for combinatorial search. Although we found a domain-specific search algorithm to be the most effective, the problem may prove to be fruitful ground for future general-purpose constraint-solving techniques.

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