DATA-DRIVEN VERIFICATION

A DISSERTATION
SUBMITTED TO THE DEPARTMENT OF COMPUTER SCIENCE
AND THE COMMITTEE ON GRADUATE STUDIES
OF STANFORD UNIVERSITY
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

Rahul Sharma
January 2016

I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(Alex Aiken) Principal Adviser

I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(David L. Dill)

I certify that I have read this dissertation and that, in my opinion, it is fully adequate in scope and quality as a dissertation for the degree of Doctor of Philosophy.

(John C. Mitchell)

Approved for the Stanford University Committee on Graduate Studies

Acknowledgments

Many people have assisted me in graduate school and what follows is an attempt to express my gratitude. My advisor, Alex Aiken, has been a constant source of inspiration. He has spent countless hours with me in discussions, writing papers, polishing talks, and providing an environment conducive to productive research. Any sanity I have left after the tumultuous years in grad school is all due to his support and fantastic advice. I thank John Mitchell for introducing me to computer security and helping me develop a positive (and relaxed) outlook during the initial years of my PhD. I thank David Dill, Noah Goodman, and Percy Liang for insightful discussions and serving on my defense committee.

A special thanks goes to Aditya Nori for collaborating with me when I was an undergraduate as well as a graduate student. He has always made himself available for timely advice, encouragement, and valuable feedback. I thank my office mate over the years, Eric Schkufza, for being both an excellent collaborator and a source of never-ending entertainment. I was fortunate to have had Mike Bauer and Sean Treichler as collaborators who have showed me the dark side of computer systems. I thank Ken McMillan for illuminating discussions during an internship at Microsoft. Several ideas in this thesis originated during discussions with Bharath and Saurabh, my friends at UC Berkeley. My colleagues, Adam, Ankur, Berkeley, Isil, Joe, Manolis, Osbert, Saswat, Stefan, Tom, and Wonyeol have patiently listened to my ideas and provided constructive feedback. Finally, I thank my Stanford friends Chinamy, Dinesh, Kartik, Navneet, and Raghu, for a memorable time and the lovely Divya Gupta for everything else.

This work would not have been possible without the unwavering love and support of my family. I dedicate this dissertation to Sushil Kumar Sharma, who sacrificed the most for these words.

Contents

List of Tables

List of Figures

Chapter 1

Introduction

Automatic software verification is an important but hard problem.Verifiers primarily rely on static analyses to reason about all possible program behaviors, where a purely static analysis makes inferences based solely on program text. However, since verification is so hard, to be successful it seems necessary to leverage all possible sources that can provide any useful information about the program. Hence, limiting a verifier to just the program text is unnecessarily restrictive. Programs are not just pages of text; they are meant to be executed. Our thesis is that verification can be aided and significantly improved by learning from data gathered from program executions.

In particular, we focus on the problem of *invariant inference* and its applications in verification. Invariant inference is a core problem that every software verifier must address. The traditional verifiers infer invariants by analyzing program text alone. The main contribution of this thesis is an effective technique to infer loop invariants by combining static analysis and machine learning applied to program executions.

A *loop invariant* is a predicate that holds for all possible executions of the loop. Loops are technically interesting because they can encode an infinite number of behaviors. The goal of an invariant inferencer is to find a loop invariant, a predicate that is valid for all behaviors that the loop can have. This inference problem is hard in general and tools apply a myriad of sophisticated techniques to this end. In contrast, an invariant checker proves whether a given predicate is an invariant or not, a substantially easier task. Unsurprisingly, existing static analyses for invariant checking are more mature than their inference counterparts.

We break down the problem of loop invariant inference into two phases. In the *guess* phase, the loop is executed on a few inputs and the observed program states are logged. These logs constitute our *data*. Subsequently, a *learner* guesses a *candidate* invariant from the data. This task is substantially easier than actual inference as the output of the learner is only a candidate invariant: there can be executions of the loop (that are absent in the data) for which the learned candidate does not hold. In the *check* phase, a static analysis proves whether the candidate invariant is an

actual invariant or not. In the former case, the inference succeeds. In the latter case, we repeat the process with additional data. We refer to this overall approach that alternates between guessing and checking as Guess-and-Check.

This decomposition of inference into a guessing phase and a checking phase has several potential advantages. A static analysis that performs inference can easily get confused by program text. This situation is prevalent in the analysis of aggressively optimized code. Such programs can employ convoluted implementations for otherwise simple computations to maximize performance. In contrast to a static analysis, the learner infers candidate invariants solely from data and does not look at the program text at all. The program text needs to be analyzed only by the checker that solves the easier problem of invariant checking. Therefore, a Guess-and-Check based approach can succeed where a traditional static analysis can fail. Next, this separation allows us to leverage the significant advances achieved in statistical machine learning. Since machine learning techniques are very different from the techniques routinely used in verification, the Guess-and-Check based inference engines have different strengths and weaknesses compared to traditional static analysis based inference engines. Finally, the decomposition substantially simplifies the architecture of a verifier and leads to simpler implementations. The learners are just data crunching algorithms which are easy to implement. For checking, we use off-the-shelf SMT solvers and take advantage of recent advances in automatic theorem proving.

1.1 Contributions

To remain tractable, current static analysis tools infer very restricted classes of loop invariants. One class of invariants that is common, and for which existing tools are reasonably good, is conjunctions of linear integer inequalities. Using the Guess-and-Check approach, we can produce invariants for richer classes. This dissertation makes a number of contributions that are reflected in the structure of the remaining chapters.

A harder problem, which is addressed by only a few static analyses, is the inference of *algebraic* invariants (polynomial equalities). As a simplification, all existing tools for inferring algebraic invariants approximate integral program variables by real-valued variables. Although this approximation yields simpler inference tasks, it is unsound and such tools are known to generate incorrect invariants. Chapter 2 describes a sound and relatively complete algorithm for inference of algebraic invariants that uses as data *states* (valuation of program variables) gathered from running program tests, elementary linear algebra routines for learning, and SMT solvers for checking. Not only does this technique always find correct invariants (if the SMT solver can answer all queries correctly), the inferred invariant is the best possible in the given class.

Equality invariants are useful in compiler optimizations. The main challenge in optimizations is to ensure that the optimized program is equivalent to the original. While proving the correctness of

compiler optimizations has been a research goal for decades, it is only recently that the first verified compiler (CompCert, see below) was developed, and that was for a subset of C and the proof of correctness was extremely labor-intensive. Our goal in Chapter 3 is to automatically check the correctness of the code generated by existing production compilers.

Correctness of binaries can be ensured by sacrificing performance. CompCert [95] produces binaries that are provably equivalent to the source. This guarantee is feasible as CompCert has no loop optimizations and therefore the translation to binary is straightforward compared to a production compiler like `gcc` that performs aggressive optimizations. Chapter 3 presents the first sound equivalence checker that proves the equivalence of two x86 binaries. This checker proves the equivalence of `gcc` optimized code with CompCert generated code, thus providing a formal proof that the binary generated by `gcc` with optimizations enabled is equivalent to the original C source. The core problem in this equivalence checking is invariant inference and we extend the techniques described in Chapter 2 to infer equality invariants that relate the two binaries.

Another very difficult case for static analysis is the inference of disjunctive invariants that are sufficient to prove a given set of safety properties. Naive approaches tend to generate a very large or even an unbounded number of disjunctions, leading to non-terminating analyses. Therefore, to ensure tractability, all existing tools use a user-provided or an ad-hoc bound on the number of disjunctions. Developing on top of a probably approximately correct (PAC) learning algorithm, Chapter 4 present the first invariant inference technique that does not place any ad-hoc restriction on the number of disjunctions while also guaranteeing that the discovered invariants are of a bounded size. To achieve this goal, the Guess-and-Check approach requires two kinds of data: *reachable* program states obtained by running the program and *bad* states that can lead to the violation of the given safety properties. The learner is a *classification* engine that finds a predicate separating the reachable and the bad states. As before, the checker is an off-the-shelf SMT solver.

Another issue with classical approaches to invariant inference is that they are closely tied to particular decidable logics, resulting in a plethora of highly specialized invariant inference algorithms each handling its own restricted class of programs. Chapter 5 presents an approach to infer arbitrary invariants. Given an arbitrary invariant class, a Markov Chain Monte Carlo (MCMC) sampler is used to generate candidate invariants from that class; the sampler is guided by a cost function based on data. The sampler can consume data in the form of reachable states, bad states, and inductive *pairs* (a two-tuple (s, t) of program states with the property that if s is reachable then t is reachable). Since SMT solvers are available for many theories, instantiating the Guess-and-Check approach with MCMC samplers as learners and suitable SMT solvers yields inference engines for many classes, including those for which invariant inference techniques were previously unknown. For invariant classes for which inference techniques are known, this framework yields inference engines that have competitive performance with the specialized approaches. We use this framework

to generate inference procedures that prove safety properties of numerical programs, prove non-termination of numerical programs, prove functional specifications of array manipulating programs, prove safety properties of string manipulating programs, and prove functional specifications of heap manipulating programs that use linked list data structures. Finally, Chapter 6 concludes with a discussion of future work.

1.2 Collaborators and Publications

The work for this dissertation was in collaboration with Alex Aiken, Berkeley Churchill, Saurabh Gupta, Bharath Hariharan, Aditya Nori, and Eric Schkufza. The ideas discussed here appear in the following conference papers [127, 129, 130, 133].

Chapter 2

Algebraic Invariants

The task of generating loop invariants lies at the heart of any program verification technique. A wide variety of techniques have been developed for generating linear invariants, including methods based on abstract interpretation [40, 85] and constraint solving [35, 71], among others. The topic has progressed to the point that techniques for discovering linear loop invariants are included in industrial strength tools for software reliability [12, 39, 109].

Recently, researchers have also applied these techniques to the generation of non-linear loop invariants [41, 103, 107, 120, 121, 125]. These techniques discover *algebraic invariants* of the form

$$\wedge_i f_i(x_1, \ldots, x_n) = 0$$

where each f_i is a polynomial in the variables $x_1, \ldots, x_n$ of the program. Note that algebraic invariants implicitly handle disjunctions: if $f_1 = 0 \vee f_2 = 0$ is an invariant then $f_1 = 0 \vee f_2 = 0 \Leftrightarrow f_1 f_2 = 0$. Thus, algebraic invariants are as expressive as arbitrary boolean combinations of algebraic equations.

Most previous techniques for algebraic loop invariants are based on Gröbner bases computations, which cause a considerable slowdown [25]. Therefore, there has been recent interest in techniques for generating algebraic invariants that do not use Gröbner bases [25, 107] (see Section 2.7). In this chapter, we address the problem of invariant generation from a data-driven perspective. In particular, we use techniques from linear algebra to analyze data generated from executions of a program in order to efficiently "guess" a candidate invariant. This phase can leverage test suites of programs for data generation. This guessed invariant is subsequently checked for validity via a decision procedure. Our algorithm Guess-and-Check for generating algebraic invariants calls these guess and check phases iteratively until it finds the desired invariant – the guess phase is used to compute a candidate invariant I and the check phase is used to validate that I is indeed an invariant. Failure to prove that I is an invariant results in counterexamples or more data which are

used to refine the guess in the next iteration. Furthermore, we are also able to prove a bound on the number of iterations of Guess-and-Check.

Our guess and check data-driven approach for computing invariants has a number of advantages:

- Checking whether the candidate invariant is an invariant is done via a decision procedure. Our thesis is that using a decision procedure to check the validity of a candidate invariant can be much more efficient than using it to infer an actual invariant.
- Since the guess phase operates over data, its complexity is largely independent of the complexity or size of the program (the amount of data depends on the number of variables in scope though). This is in contrast to approaches based on static analysis, and therefore it is at least plausible that a data-driven approach may work well even in situations that are difficult for static analysis. Moreover, the guess step just involves basic matrix manipulations, for which very efficient implementations exist.

There are major drawbacks, both theoretical and practical, with most previous techniques for algebraic invariants. First, these techniques either restrict predicates on branches to either equalities or dis-equalities [34, 103], or cannot handle nested loops [89, 121], or interpret program variables as real numbers [25, 120, 125]. It is well known that the semantics of a program assuming integer variables, in the presence of division and modulo operators, is not over-approximated by the semantics of the program assuming real variables. Therefore, these approaches may not produce correct invariants in cases where the program variables are actually integers. Our technique does not suffer from these drawbacks: our check phase can consume a rich syntax and answer queries over both integers and reals (see Section 2.3.2). Moreover, since these techniques can find algebraic invariants, they can find non-linear invariants representing boolean combinations of linear equalities. If a loop has the invariant $y = x \vee y = -x$ then these techniques can find the invariant $x^2 = y^2$ that is semantically equivalent to the linear invariant:

$$x = y \vee x = -y \Leftrightarrow (x + y)(x - y) = 0 \Leftrightarrow x^2 = y^2$$

But if the invariant is to be consumed by a verification tool that works over linear arithmetic (as most tools do), then $x^2 = y^2$ is not useful. A simple extension to our technique allows us to extract an equivalent (disjunctive) linear invariant from an algebraic invariant when such a linear invariant exists. This extension is possible as our technique is data-driven (see Section 2.5).

It is also interesting to note that our algorithm is an iterative refinement procedure similar to the counterexample-guided abstraction refinement (CEGAR) [32] technique used in software model checking. In CEGAR, we start with an over-approximation of program behaviors and perform iterative refinement until we have either found a proof of correctness or a bug. Guess-and-Check technique is dual to CEGAR—we start with an under-approximation of program behaviors and add more behaviors until we are done. Most techniques for invariant discovery using CEGAR like

techniques have no termination guarantees. Since we focus on the language of polynomial equalities for invariants, we are able to give a termination guarantee for our technique. If a loop has no non-trivial polynomial equation of a given degree as an invariant then our procedure will return the trivial invariant *true*.

Our main contribution is a new sound data-driven algorithm for computing algebraic invariants. In particular, our technical contributions are:

- We provide a data-driven algorithm for generation of invariants restricted to conjunctions of algebraic equations. We observe that a known algorithm [107] is a suitable fit for our guessing step. We formally prove that this algorithm computes a sound under-approximation of the algebraic loop invariant. That is, if G is the guess or candidate invariant, and I is an invariant then $G \Rightarrow I$. This guess contains all algebraic equations constituting the invariants and possibly more spurious equations.

- We augment our guessing procedure with a decision procedure to obtain a sound and (relatively) complete algorithm: if the decision procedure successfully answers the queries made, then the output is an invariant and we do generate all valid invariants up to a given degree d. Moreover we are able to prove a bound on the number of decision procedure queries.

- Using the observation that a boolean combination of linear equalities with d disjunctions (in DNF form) is equivalent to an algebraic invariant of degree d [103, 147], we describe an algorithm to generate an equivalent linear invariant from an algebraic invariant.

- We evaluate our technique on benchmark programs from various papers on generation of algebraic loop invariants and our results are encouraging—starting with a small amount of data, Guess-and-Check terminates on all benchmarks in one iteration, that is, our first guess is an actual invariant.

The remainder of this chapter is organized as follows. Section 2.1 motivates and informally illustrates the Guess-and-Check algorithm for algebraic invariants over two example programs. Section 2.2 introduces the background for this algorithm. Section 2.3 presents the Guess-and-Check algorithm and also proves its correctness and termination. Section 2.4 discusses the theory of arrays and Section 2.5 describes our technique for obtaining disjunctive linear invariants from algebraic invariants. Section 2.6 evaluates our implementation of the Guess-and-Check algorithm on several benchmarks for algebraic loop invariants. Finally, Section 2.7 surveys related work.

2.1 Overview of the Technique

Assume we are given a loop $L = \texttt{while}\ B\ \texttt{do}\ S$ with variables $\vec{x} = x_1, \ldots, x_n$. The initial values of $\vec{x}$, that is, the possible values which $x_1, \ldots, x_n$ can take before the loop starts executing are given by

```
1:  assume(x=0 && y=0);
2:  while (*) do
3:    writelog(x, y);
4:    y := y+1;
5:    x := x+y;
6:  done
```

Figure 2.1: Example program 1 for algebraic invariants.

```
1:  assume(s=0 && j=k);
2:  while (j>0) do
3:    writelog(s, i, j, k);
4:    (s,j) := (s+i,j-1)
5:  done
```

Figure 2.2: Example program 2 for algebraic invariants.

a predicate $\varphi(\vec{x})$. Our goal is to find the strongest $I \equiv \wedge_i f_i(\vec{x}) = 0$, where each f_i is a polynomial defined over the variables $x_1, \ldots, x_n$ of the program such that $\varphi \Rightarrow I$ and $\{I \wedge B\}S\{I\}$. Any I satisfying these two conditions is an invariant for L. If we do not impose the condition that we need the strongest invariant, then the trivial invariant $I = \mathit{true}$ is a valid solution.

Our algorithm has two main phases, the guess phase and the check phase. The guess phase operates over data generated by testing the input program in order to guess a candidate invariant. This candidate invariant is subsequently checked for validity by the check phase which is just a black box call to an off-the-shelf decision procedure.

We will illustrate our technique over two example programs shown in Figures 2.1 and 2.2 respectively. Our objective is to compute loop invariants at the loop head of both these programs. Informally, a loop invariant over-approximates the set of all possible program states that are possible at a loop head.

First, let us consider the program shown in Figure 2.1. This program has a loop (lines 2–6) that is non-deterministic. In line 3, we have instrumentation code that writes the program state (in this case, the values of the variables x and y) to a log file. Equivalently, we could have added multiple instrumentations: after line 1 and before line 6. The loop invariant for this program is $I \equiv y + y^2 = 2x$. Since our approach is data driven, the starting point is to run the program with test inputs and accumulate the resulting data in the log. Assume that we run the program with an input that exercises the loop exactly once. On such an execution, we obtain a single program state $x = 0$, $y = 0$ at line 3. It turns out that for our technique to work, we need to assume an upper bound d on the degree of the polynomials that constitute the invariant. Note that this assumption can be removed by starting with $d = 0$, and iteratively incrementing d [120]. This assumption also avoids rediscovery of *implied* higher degree invariants. In particular, if $f(\vec{x}) = 0$ is an invariant, then so is the higher degree polynomial $(f(\vec{x}))^2 = 0$. As a consequence, if d is an upper bound on the degree of the polynomial, then we might potentially discover both $f(\vec{x}) = 0$ and $(f(\vec{x}))^2 = 0$ as invariants. For

this example, we assume that $d = 2$, which allows us to exhaustively enumerate all the monomials over the program variables up to the chosen degree. For our example, $\vec{\alpha} = \{1, x, y, y^2, x^2, xy\}$ is the set of all monomials over the variables x and y with degree less than or equal to 2. The number of monomials of degree d in n variables is large: $\binom{n+d-1}{d}$. Heuristics exist to discard the monomials that are unlikely to be a part of an invariant (Section 2.3.4).

Using $\vec{\alpha}$ and the program state $x = 0$, $y = 0$, we construct a *data matrix* A which is a 1×6 matrix with one row corresponding to the program state and six columns, one for each monomial in $\vec{\alpha}$. Every entry $(1, j)$ in A represents the value of the j^{th} monomial over the program. Therefore,

$$A = \begin{array}{|c|c|c|c|c|c|} \hline 1 & x & y & y^2 & x^2 & xy \\ \hline 1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \tag{2.1}$$

As we will see in Section 2.3.1, we can employ the null space of A to compute a candidate invariant I as follows. If $\{b_1, b_2, \ldots, b_k\}$ is a basis for the null space of the data matrix A, then

$$I \equiv \bigwedge_{i=1}^{k} (b_i^T \begin{bmatrix} 1 \\ x \\ y \\ y^2 \\ x^2 \\ xy \end{bmatrix} = 0) \tag{2.2}$$

is a candidate invariant that under-approximates the actual invariant. The null space of A is defined by the set of basis vectors

$$\left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{2.3}$$

Therefore, from Equation 2.2, we have the candidate invariant

$$I \equiv x = 0 \wedge y = 0 \wedge x^2 = 0 \wedge y^2 = 0 \wedge xy = 0 \tag{2.4}$$

Next, in the check phase, we check whether I as specified by Equation 2.3 is actually an invariant.

Abstractly, if $L \equiv \texttt{while}\ B\ \texttt{do}\ S$ is a loop, then to check if I is a loop invariant, we need to establish the following conditions:

1. If φ is a precondition at the beginning of L, then $\varphi \Rightarrow I$.
2. Furthermore, executing the loop body S with a state satisfying $I \wedge B$, always results in a state satisfying the invariant I.

The above checks for validating I are performed by an off-the-shelf decision procedure [43]. For our example, we first check whether the precondition at the beginning of the loop implies I:

$$(x = 0 \wedge y = 0) \Rightarrow (x = 0 \wedge y = 0 \wedge x^2 = 0 \wedge y^2 = 0 \wedge xy = 0)$$

This condition is indeed valid, and therefore we check whether the following condition on the loop body (lines 4–5) also holds (we can obtain the predicate representing the loop body via symbolic execution [86]):

$$\begin{aligned}(x = 0 \wedge y = 0 \wedge x^2 = 0 \wedge y^2 = 0 \wedge xy = 0 \wedge y' = y + 1 \wedge x' = x + y') \Rightarrow \\ (x' = 0 \wedge y' = 0 \wedge x'^2 = 0 \wedge y'^2 = 0 \wedge x'y' = 0)\end{aligned}$$

This predicate is not valid, and we obtain a counterexample $x' = 1$, $y' = 1$ at line 3 of the program. Let us assume that we generate more program states at line 3 by executing the loop for 4 iterations. As a result, we get a data matrix that also includes the row from the previous data matrix as shown below.

$$A = \begin{array}{|c|c|c|c|c|c|} \hline 1 & x & y & y^2 & x^2 & xy \\ \hline 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 2 & 4 & 9 & 36 \\ 1 & 6 & 3 & 9 & 36 & 18 \\ 1 & 10 & 4 & 16 & 100 & 40 \\ \hline \end{array} \tag{2.5}$$

It is important to observe from A that the monomials x^2 and xy are "quickly growing" monomials. In other words, the values of these monomials increase rapidly with the number of iterations of the loop (heuristically, from our experiments, we find that these rapidly increasing monomials are unlikely to play a part in the invariant). Therefore, we remove them and we show how this is done formally in Section 2.3.4. After removing rapidly increasing monomials, we obtain the following data

matrix.

$$A = \begin{array}{|c|c|c|c|} \hline 1 & x & y & y^2 \\ \hline 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 3 & 2 & 4 \\ 1 & 6 & 3 & 9 \\ 1 & 10 & 4 & 16 \\ \hline \end{array} \tag{2.6}$$

As with the earlier iteration, we require the basis of the null space of A and this is defined by the singleton set:

$$\left\{ \begin{bmatrix} 0 \\ 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix} \right\} \tag{2.7}$$

Therefore, from Equation 2.2 and Equation 2.7, it follows that the candidate invariant is:

$$I \equiv 2x - y - y^2 = 0 \tag{2.8}$$

Now, the conditions that must hold for I to be a loop invariant are:

1. $(x = 0 \wedge y = 0) \Rightarrow y + y^2 = 2x$, and
2. $(y + y^2 = 2x \wedge y' = y + 1 \wedge x' = x + y') \Rightarrow (y' + y'^2 = 2x')$

both of which are deemed to be valid by the check phase, and therefore $I \equiv y + y^2 = 2x$ is the desired loop invariant.

Next, consider the program shown in Figure 2.2, adapted from [125]. For this program, we want to find the loop invariant $I \equiv s = i(k - j)$. Let us assume that the upper bound on the degree of the desired invariant is $d = 2$. Let $\vec{\alpha}$ be the set of all candidate monomials with degree less than or equal to 2. Therefore,

$$\vec{\alpha} = \{1, s, i, j, k, si, sj, sk, ij, ik, jk, s^2, i^2, j^2, k^2\} \tag{2.9}$$

The number of candidate monomials can be large when compared to the number of monomials which actually occur in the invariant. For instance, if the number of variables is 25, and the upper bound on the degree is 3, then the number of candidate monomials is around 3300. Note that the algorithms for computing null space of a matrix are quite efficient and null space of a matrix with

3300 columns can be computed in seconds. Hence we believe that the guess phase will scale well with the number of variables.

Line 3 appends the program state (in this case, the values of the variables s, i, j and k) to a log file. Running the program with a test input $i = 0$, $j = 1$, $s = 0$ and $k = 1$ results in the following data matrix A.

$$A = \begin{array}{|c|c|c|c|c|c|} \hline 1 & s & i & j & k & \dots \\ \hline 1 & 0 & 0 & 1 & 1 & \dots \\ \hline \end{array} \tag{2.10}$$

The basis for the null space of this matrix is given by the following set of vectors:

$$\left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \\ 1 \\ \vdots \end{bmatrix}, \dots \right\} \tag{2.11}$$

This results in the candidate invariant $I \equiv s = 0 \wedge i = 0 \wedge j = 1 \wedge k = 1$. However, the check $(s = 0 \wedge j = k) \implies (s = 0 \wedge i = 0 \wedge j = 1 \wedge k = 1)$ fails and we generate several counterexamples: say $s = 0$, $j = k$, and $i, k \in \{1, 2, 3, 4, 5\}$. These are 25 counterexamples, and we run some tests from these counterexamples. Two rows of the data matrix A corresponding to these tests are shown below:

1	s	i	j	k	si	sj	sk	ij	ik	jk	...
1	0	3	5	5	0	0	0	15	15	25	...
1	3	3	4	5	9	12	15	12	15	20	...

(2.12)

By computing the null space, we obtain the candidate invariant $I \equiv s + ij = ik$.

Next, we check whether I is an invariant by checking the following conditions:

$$(s = 0 \wedge j = k) \Rightarrow (s + ij = ik) \tag{2.13}$$

$$(s + ij = ik \wedge j > 0 \wedge s' = s + i \wedge j' = j - 1) \Rightarrow s' = i(k - j') \tag{2.14}$$

Both these predicates are valid, and thus $s = i(k - j)$ is the desired loop invariant. Note that these constraints are quite simple: one possible strategy is to just substitute value of s' and j' in the

consequent, in terms of s and j, by using the antecedent. Such simple constraints can be efficiently handled by the recent optimizations in decision procedures for non-linear arithmetic [82]. The cost of solving such constraints can be quite high in general, but we believe that the cost of solving constraints generated from programs occurring in practice is manageable.

In summary, we have informally described how our technique works over two example programs with fairly non-trivial algebraic invariants. Our approach is data driven in that it operates over a data matrix. This has the advantage that our guess procedure is independent of the complexity of the program in contrast to approaches based on static analysis: The guess phase only depends on the number of variables and not on how the variables are used in the program. Finally, our check procedure employs state-of-the-art decision procedures for non-linear arithmetic as a blackbox.

2.2 Preliminaries

We consider programs belonging to the following language of *while programs*:

$$\mathcal{S} \ ::= \ x{:=}M \mid \mathcal{S}; \mathcal{S} \mid \texttt{if } B \texttt{ then } \mathcal{S} \texttt{ else } \mathcal{S} \mid \texttt{while } B \texttt{ do } \mathcal{S}$$

where x is a variable over a countably infinite sort *loc* of memory locations, M is an expression, and B is a boolean expression. Expressions in this language are either of type `int` or `bool`.

A *monomial* α over the variables $\vec{x} = x_1, \ldots x_n$ is a term of the form $\alpha(\vec{x}) = x_1^{k_1} x_2^{k_2} \ldots x_n^{k_n}$. The *degree* of a monomial is $\sum_{i=1}^{n} k_i$. A *polynomial* $f(x_1, \ldots, x_n)$ defined over n variables $\vec{x} = x_1, \ldots, x_n$ is a weighted sum of monomials and has the following form.

$$f(\vec{x}) = \sum_k w_k x_1^{k_1} x_2^{k_2} \ldots x_n^{k_n} = \sum_k w_k \alpha_k \tag{2.15}$$

where $\alpha_k = x_1^{k_1} x_2^{k_2} \ldots x_n^{k_n}$ is a monomial. We are interested in polynomials over integers, that is, $\forall k \ . \ w_k \in \mathbb{Z}$. The *degree* of a polynomial is the maximum degree over its constituent monomials: $max_k \ \{degree(\alpha_k) \mid w_k \neq 0\}$.

An *algebraic equation* is of the form $f(\vec{x}) = 0$, where f is a polynomial. Given a loop $L =$ `while` B `do` S defined over variables $\vec{x} = x_1, \ldots, x_n$ together with a precondition φ, a *loop invariant* I is the strongest predicate such that $\varphi \Rightarrow I$ and $\{I \wedge B\} S \{I\}$. Any predicate I satisfying these two conditions is an invariant for L. In this chapter, we will focus on *algebraic invariants* for a loop. An algebraic invariant $\mathcal{I}$ is of the form $\wedge_i f_i(\vec{x}) = 0$, where each f_i is a polynomial over the variables $\vec{x}$ of the loop.

The next section reviews matrix algebra that is a crucial component of our guess-and-check algorithm. The reader is referred to [75] for an excellent introduction to matrix algebra.

2.2.1 Matrix Algebra

Let $A \in \mathbb{Q}^{m\times n}$ denote a *matrix* with m rows and n columns, with entries from the set of rational numbers $\mathbb{Q}$. Let $x \in \mathbb{Q}^n$ denote a *vector* with n rational number entries. Then x denotes an $n \times 1$ column matrix. The vector x can also be represented as a row matrix $x^T \in \mathbb{Q}^{1\times n}$, where T is the matrix transpose operator. In general, the transpose of a matrix A, denoted A^T is obtained by interchanging the rows and columns of A. That is, $\forall A \in \mathbb{Q}^{m\times n}.(A^T)_{ij} = A_{ji}$. For example,

$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \in \mathbb{Q}^{2\times 3}$, $x = \begin{bmatrix} 8 \\ 9 \\ 10 \end{bmatrix} \in \mathbb{Q}^3$ is a vector,

and $x^T = \begin{bmatrix} 8 & 9 & 10 \end{bmatrix}$, $A^T = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \in \mathbb{Q}^{3\times 2}$.

Given two matrices $A \in \mathbb{Q}^{m\times n}$ and $B \in \mathbb{Q}^{n\times p}$, their product is the matrix C defined as follows:

$$C = AB \in \mathbb{Q}^{m\times p}$$

where the element corresponding to the i^{th} row and j^{th} column $C_{ij} = \sum_{k=1}^{n} A_{ik}B_{kj}$.

If $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \in \mathbb{Q}^{2\times 3}$, and $B = \begin{bmatrix} 7 & 8 \\ 9 & 10 \\ 11 & 12 \end{bmatrix}$, then $C = AB = \begin{bmatrix} 58 & 64 \\ 139 & 154 \end{bmatrix}$.

The *inner product* of two vectors x and y, denoted $\langle x, y\rangle$, is the product of the matrices corresponding to x^T and y which is defined as:

$$x^T y = \sum_{i=1}^{n} x_i y_i \tag{2.16}$$

If $x = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$, and $y = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$, then the inner product $\langle x, y\rangle = 32$.

Given a matrix $A \in \mathbb{Q}^{m\times n}$ and a vector $x \in \mathbb{Q}^n$, their product $y = Ax$ defines a linear combination of the columns of A with coefficients given by x. Alternatively, for a vector $w \in \mathbb{Q}^m$, the product $v = w^T A$ defines a linear combination of the rows of A with coefficients given by the vector w.

A set of vectors $\{x_1, x_2, \ldots, x_n\}$ is *linearly independent* if no vector in this set can be written as a linear combination of the remaining vectors. Conversely, any vector which can be written as a linear combination of the remaining vectors is said to be *linearly dependent*. Specifically, if

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i \tag{2.17}$$

for some $\{\alpha_1, \alpha_2, \ldots, \alpha_{n-1}\}$, then x_n is said to be linearly dependent on $\{x_1, x_2, \ldots, x_{n-1}\}$. Otherwise, it is independent of $\{x_1, x_2, \ldots, x_{n-1}\}$. For example, the set of vectors

$$\left\{ \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix}, \begin{bmatrix} 2 \\ 5 \\ 9 \end{bmatrix}, \begin{bmatrix} -3 \\ 9 \\ 3 \end{bmatrix} \right\}$$

is not linearly independent as

$$\begin{bmatrix} -3 \\ 9 \\ 3 \end{bmatrix} = 33 \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} - 18 \begin{bmatrix} 2 \\ 5 \\ 9 \end{bmatrix} \tag{2.18}$$

The *column rank* of a matrix A is the largest number of columns of A that form a linearly independent set. Analogously, the *row rank* of a matrix A is the largest number of rows of A that form a linearly independent set. It can be easily seen that the column rank of the matrix $B = \begin{bmatrix} 1 & 2 & -3 \\ 3 & 5 & 9 \\ 5 & 9 & 3 \end{bmatrix}$ is 2, and this follows from Equation 2.18.
From the fundamental theorem of linear algebra [75], we know that for every matrix A, its row rank equals its column rank and is referred to as the *rank* of the matrix A. Therefore, the rank of the matrix B above is equal to 2.

The *span* of a set of vectors $\{x_1, x_2, \ldots, x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, x_2, \ldots, x_n\}$. Therefore,

$$span(\{x_1, x_2, \ldots, x_n\}) = \{v \mid v = \sum_{i=1}^{n} \alpha_i x_i, \alpha_i \in \mathbb{Q}\} \tag{2.19}$$

If $\{x_1, x_2, \ldots, x_n\}$, $x_i \in \mathbb{Q}^n$ is a set of n linearly independent vectors, then $span(\{x_1, x_2, \ldots, x_n\}) = \mathbb{Q}^n$. Thus, any vector $v \in \mathbb{Q}^n$ can be written as a linear combination of vectors in the set $\{x_1, x_2, \ldots, x_n\}$. More generally, for any $Q = span(x_1, \ldots, x_n) \subseteq \mathbb{Q}^n$, if every vector $v \in Q$ can be written as a linear combination of vectors from a linearly independent set $B = \{b_1, b_2, \ldots, b_k\}$, and B is minimal, then B forms a *basis* of Q, and k is called the *dimension* of Q.
The *range* of a matrix $A \in \mathbb{Q}^{m \times n}$ is the span of the columns of A. That is,

$$range(A) = \{v \in \mathbb{Q}^m \mid v = Ax, x \in \mathbb{Q}^n\} \tag{2.20}$$

The dimension of $range(A)$ is also equal to $rank(A)$. The *null space* of a matrix $A \in \mathbb{Q}^{m \times n}$ is the

set of all vectors that equal to 0 when multiplied by A. More precisely,

$$\mathit{NullSpace}(A) = \{x \in \mathbb{Q}^n \mid Ax = 0\} \tag{2.21}$$

The dimension of $\mathit{NullSpace}(A)$ is called its *nullity*. For instance, the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{bmatrix}$$

has a null space determined by the span of the following set of vectors:

$$\left\{ \begin{bmatrix} 2 \\ -3 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -2 \\ 1 \\ 0 \end{bmatrix} \right\}$$

with $\mathit{nullity}(A) = 2$.

From the fundamental theorem of linear algebra [75], for any matrix $A \in \mathbb{Q}^{m \times n}$, we also know the following.

$$\mathit{rank}(A) + \mathit{nullity}(A) = n \tag{2.22}$$

2.3 The Guess-and-Check Algorithm

The Guess-and-Check algorithm is described in Figure 2.3. The algorithm takes as input a while program L, a precondition φ on the inputs to L, and an upper bound d on the degree of the desired invariant, and returns an algebraic loop invariant $\mathcal{I}$. If $L = \texttt{while}\ B\ \texttt{do}\ S$, then recall that $\mathcal{I}$ is the strongest predicate such that

$$\varphi \Rightarrow \mathcal{I} \text{ and } \{\mathcal{I} \wedge B\} S \{\mathcal{I}\} \tag{2.23}$$

As the name suggests, Guess-and-Check consists of two phases.

1. *Guess phase* (lines 5–13): this phase processes the data in the form of concrete program states at the loop head to compute a data matrix, and uses linear algebra techniques to compute a candidate invariant.

2. *Check phase* (line 15): this phase uses an off-the-shelf decision procedure for checking if the candidate invariant computed in the guess phase is indeed a true invariant (using the conditions in Equation 2.23) [82].

GUESS-AND-CHECK
Input:
– while program L.
– precondition φ.
– bound on the degree d.
Returns: A loop invariant $\mathcal{I}$ for L.

```
1: x⃗ := vars(L)
2: Tests := TestGen(φ, L)
3: logfile := []
4: repeat
5:     for t⃗ ∈ Tests do
6:         logfile := logfile :: Execute(L, x⃗ = t⃗)
7:     end for
8:     A := DataMatrix(logfile, d)
9:     B := Basis(NullSpace(A))
10:    if B = ∅ then
11:        //No non-trivial algebraic invariant return true
12:    end if
13:    I := CandidateInvariant(B)
14:    (done, t⃗) := Check(I)
15:    if ¬done then
16:        Tests := {t⃗}
17:    end if
18: until done return I
```

Figure 2.3: GUESS-AND-CHECK computes an algebraic invariant for an input while program L with a precondition φ.

The GUESS-AND-CHECK algorithm works as follows. In line 1, $\vec{x}$ represents the input variables of the while program L. The procedure *TestGen* is any test generation technique that generates a set of test inputs *Tests* each of which satisfy the precondition φ. Alternatively, our technique could also employ an existing test suite for *Tests*. The variable *logfile* maintains a sequence of concrete program states at the loop head of L. Line 3 initializes *logfile* to the empty sequence. Lines 4–19 perform the main computation of the algorithm. First, the program L is executed over every test $\vec{t} \in$ *Tests* via the call to *Execute* in line 6. *Execute* returns a sequence of program states (variable to value mapping) at the loop head and this is appended to *logfile*. Note that this can also include the states which violate the loop guard. The function *DataMatrix* (line 8) constructs a matrix A with one row for every program state in *logfile* and one column for every monomial from the set of all monomials over $\vec{x}$ whose degree is bounded above by d (as informally illustrated in Section 2.1). The $(i, j)^{th}$ entry of A is the value of the j^{th} monomial evaluated over the program state represented by the i^{th} row.

Next, using off-the-shelf linear algebra solvers, we compute the basis for the null space of A in line 9. As we will see in Section 2.3.1, Theorem 1, the candidate invariant $\mathcal{I}$ can be efficiently

computed from A (line 14). If $\mathcal{B}$ is empty, then this means that there is no algebraic equation that the data satisfies and we return *true*. Otherwise, the candidate invariant $\mathcal{I}$ is given to the checking procedure *Check* in line 15. The procedure *Check* uses off-the-shelf algebraic techniques [82] to check whether $\mathcal{I}$ satisfies the conditions in Equation 2.23. If so, then $\mathcal{I}$ is an invariant and the procedure terminates by returning $\mathcal{I}$. Otherwise, *Check* returns a counter-example in the form of a test input $\vec{t}$ that explains why I is not an invariant – the computation is repeated with this new test input $\vec{t}$, and the process continues until we have found an invariant. Note that when L is executed with $\vec{t}$ then the loop guard might evaluate to *false*. In such a case, the state reaching just before the loop head is added to the log. Hence, the size of *logfile* strictly increases in every iteration.

In summary, the guess and check phases of GUESS-AND-CHECK operate iteratively, and in each iteration if the actual invariant cannot be derived, then the algorithm automatically figures out the reason for this and corrective measures are taken in the form of generating more test inputs (this corresponds to the case where the data generated is insufficient for guessing a sound invariant).

In the next section, we will formally show the correctness of the GUESS-AND-CHECK algorithm—we prove that it is a sound and relatively complete algorithm.

2.3.1 Connections between Null Spaces and Invariants

In the previous section, we have seen how GUESS-AND-CHECK computes an algebraic invariant over monomials $\vec{\alpha}$ which consists of all monomials over the variables of the input while program with degree bounded above by d. The starting point for proving correctness of GUESS-AND-CHECK is the data matrix A as computed in line 8 of Figure 2.3. The data matrix A contains one row for every program state in *logfile* and one column for every monomial in $\vec{\alpha}$. Every entry (i, j) in A is the value of the monomial associated with column j over the program state associated with row i.

An invariant $\mathcal{I} \equiv \wedge_i^k (w_i^T \vec{\alpha} = 0)$ has the property that

$$\text{for each } w_i,\ 1 \leq i \leq k,\ w_i^T a_j = 0 \text{ for each row } a_j \in \mathbb{Q}^n \text{ of } A = \begin{bmatrix} a_1^T \\ a_2^T \\ \vdots \\ a_m^T \end{bmatrix}.$$

In other words, $Aw_i = 0$. This shows that each w_i is a vector in the null space of the data matrix A. Conversely, any vector in $\mathit{NullSpace}(A)$ is a reasonable candidate for being a part of an algebraic invariant.

We make the observation that a candidate invariant will be a true invariant if the dimension of the space spanned by the set $\{w_i\}_{1 \leq i \leq k}$ equals $\mathit{nullity}(A)$. We will assume, without loss of generality, that $\{w_i\}_{1 \leq i \leq k}$ is a linearly independent set. Then, by definition, the dimension of the space spanned by $\{w_i\}_{1 \leq i \leq k}$ equals k.

Consider an n-dimensional space where each axis corresponds to a monomial of $\vec{\alpha}$. Then the

rows of the matrix A are points in this n-dimensional space. Now assume that $w^T\vec{\alpha} = 0$ is an invariant, that is, $k = 1$. This means that all rows a_j of A satisfy $w^T a_j = 0$. In particular, the points corresponding to the rows of A lie on an $n-1$ dimensional subspace defined by $w^T\vec{\alpha} = 0$. If the data or program states generated by the test inputs *Tests* (line 2 in Figure 2.3) is insufficient, then A might not have rows spanning the $n-1$ dimensions. Therefore, from Equation 2.22, we have $n - \mathit{rank}(A) = \mathit{nullity}(A) \geq 1$ if the invariant is a single algebraic equation. Generalizing this, we can say that $\mathit{nullity}(A)$ is an upper bound on the number of algebraic equations in the invariant. The following lemmas and theorem formalize this intuition.

Lemma 1 (Null space under-approximates invariant)**.** If $\wedge_i^k w_i^T\vec{\alpha} = 0$ is an invariant, and A is the data matrix, then all $w_i \in \mathit{NullSpace}(A)$.

Proof. This follows from the fact that for every w_i, $1 \leq i \leq k$, $Aw_i = 0$. □

Therefore, the null space of the data matrix A gives us the subspace in which the invariants lie. In particular, if we arrange the vectors which form the basis for $\mathit{NullSpace}(A)$ as columns in a matrix V, then $\mathit{range}(V)$ defines the space of invariants.

Lemma 2. If $\wedge_{i=1}^k w_i^T\vec{\alpha} = 0$ is an invariant with the set $\{w_1, w_2, \ldots, w_k\}$ forming a linearly independent set, A is the data matrix and $\mathit{nullity}(A) = k$, then $\{w_i \mid 1 \leq i \leq k\}$ is a basis for $\mathit{NullSpace}(A)$.

Proof. From Lemma 1, we know that $w_i \in \mathit{NullSpace}(A)$, $1 \leq i \leq k$. Since $\{w_i \mid 1 \leq i \leq k\}$ is a linearly independent set of cardinality k, it follows that $\{w_i \mid 1 \leq i \leq k\}$ is also a basis for $\mathit{NullSpace}(A)$. □

Theorem 1. If $\wedge_{i=1}^k w_i^T\vec{\alpha} = 0$ is an invariant with the set $\{w_1, w_2, \ldots, w_k\}$ forming a linearly independent set, A is the data matrix and $\mathit{nullity}(A) = k$, then any basis for $\mathit{NullSpace}(A)$ forms an invariant.

Proof. Let $B = [v_1 \cdots v_k]$ be a matrix with each v_i, $1 \leq i \leq k$ being a column vector, and with $\mathit{span}(\{v_1, \ldots, v_k\})$ equal to $\mathit{NullSpace}(A)$. That is, $\{v_1, \ldots, v_k\}$ is a basis for $\mathit{NullSpace}(A)$. From Lemma 1, we know that every w_i, $1 \leq i \leq k$, lies in $\mathit{span}(\{v_1, \ldots, v_k\})$. This means that every w_i, $1 \leq i \leq k$, can be written as follows.

$$w_i = Bu_i \tag{2.24}$$

for some vector $u_i \in \mathbb{Q}^k$. Therefore, if $\wedge_{j=1}^k v_j^T\vec{\alpha} = 0$, from Equation 2.24, it follows that $w_i^T\vec{\alpha} = 0$, $1 \leq i \leq k$.

From Lemma 2, we know that $\{w_1, w_2, \ldots, w_k\}$ form a basis for $\mathit{NullSpace}(A)$, and therefore every v_j, $1 \leq j \leq k$, can be written as a linear combination of vectors from $\{w_1, w_2, \ldots, w_k\}$. From this, it follows that $\wedge_{i=1}^k w_i^T\vec{\alpha} = 0 \implies v_j^T\vec{\alpha} = 0$ for all $1 \leq j \leq k$. Thus, $\wedge_{i=1}^k w_i^T\vec{\alpha} = 0 \Leftrightarrow \wedge_{j=1}^k v_j^T\vec{\alpha} = 0$. □

Theorem 1 precisely defines the implementation to the call *CandidateInvariant* in line 14 of algorithm Guess-and-Check. Furthermore, Theorem 1 also states that we need to have enough data represented by the data matrix A so that $nullity(A)$ equals k, the dimension of the space spanned by $\{w_i\}_{1 \leq i \leq k}$. If this is indeed the case, then $\mathcal{I} \equiv \wedge_{j=1}^{k} w_j^T \vec{\alpha} = 0$ will be an invariant. On the other hand, if the data is not enough, then Lemma 1 guarantees that the candidate invariant $\mathcal{I}$ is a sound under-approximation of the loop invariant. If the null space is zero-dimensional, then only the trivial invariant *true* constitutes an invariant over conjunction of polynomial equations that has degree less than equal d.

The question of how much data must be generated in order to attain $nullity(A) = k$ is an empirical one. In our experiments, we were able to generate invariants using a relatively small data matrix for various benchmarks from the literature.

2.3.2 Check Candidate Invariants

Computing the null space of the data matrix provides us a way for proposing candidate invariants. The candidates are complete; they do not miss any algebraic equations. But they might be unsound. They might contain spurious equations. To obtain soundness, we will use a decision procedure analogous to the technique proposed in [131].

Theorem 2 (Soundness)**.** If the algorithm Guess-and-Check terminates and the underlying decision procedure for checking candidate invariants *Check* is sound, then it returns an invariant.

Proof. Using Lemma 1, we know that the candidate invariant always under-approximates the true loop invariant. Using the fact that the variable *done* is assigned *true* iff the candidate $\mathcal{I}$ is an invariant, the result is immediate. □

Next, we prove that the algorithm Guess-and-Check terminates.

Theorem 3 (Termination)**.** If the underlying decision procedure *Check* is sound and complete, then the algorithm Guess-and-Check will terminate after at most n iterations, where n is the total number of monomials whose degree is bounded by d.

Proof. Let $A \in \mathbb{Q}^{m \times n}$ be the data matrix computed in line 8 in the Guess-and-Check algorithm. If the candidate invariant $\mathcal{I}$ computed in line 14 of Figure 2.3 is an invariant (that is, $done = true$), then Guess-and-Check terminates.

Therefore, let us assume that I is not an invariant, and let $\vec{t}$ be the test or counterexample that violates the candidate invariant as computed in line 15 of the algorithm. As a result, Guess-and-Check adds $\vec{t}$ to A resulting in a matrix $\hat{A}$. By construction, we also know that $\vec{t} \notin range(A^T)$. Therefore, it follows that $rank(\hat{A}) = rank(A) + 1$. More generally, adding a counter-example to the data matrix A necessarily increases its rank by 1. From Equation 2.22, we know that the rank

of A is bounded above by n, which implies that GUESS-AND-CHECK will terminate in at most n iterations. □

Note that since we are concerned with integer manipulating programs, a sound and complete decision procedure for *Check* cannot exist: the queries are in Peano arithmetic which is undecidable. However, for our experiments, we found that the Z3 [43] SMT solver sufficed (see Section 2.6). Z3 has limited support for non-linear integer arithmetic: It combines extensions on top of simplex and reduction to SAT (after bounding) for these queries. One might try to achieve completeness for GUESS-AND-CHECK by giving up soundness. Just as [25, 120, 125], if we interpret program variables as real numbers then Z3 does have a sound and complete decision procedure for non-linear real arithmetic [82] that has been demonstrated to be practical. Since Z3 supports both non-linear integer and real arithmetic, we can easily combine or switch between the two, if desired (see Section 2.6).

2.3.3 Nested Loops

GUESS-AND-CHECK easily extends to nested loops, while maintaining soundness and termination properties. Given a program with M loops, we construct data matrices for each loop. Let the number of columns of the data matrix of i^{th} loop be denoted by n_i. We run tests and generate candidate invariants $\vec{I}$ at all loop heads. Next, the candidate invariants are checked simultaneously. For checking the candidate invariant of an outer loop, the inner loop is replaced by its candidate invariant and a constraint is generated. For checking the inner loop, the candidate invariant of the outer loop is used to compute a pre-condition. If a counter-example is obtained then it generates more data and invariant computation is repeated. We continue these guess and check iterations until the check phase passes for all the loops; thus, on termination the output consists of sound invariants for all loops. Also, the initial candidate invariants $\vec{I}$ are under-approximations of the actual invariants by Lemma 1, a property that is maintained throughout the procedure and allows us to conclude that when the procedure terminates the output invariants are the strongest possible over algebraic equations. To prove termination, note that each failed decision procedure query increases the rank of some data matrix for some loop, which implies that the number of decision procedure queries which can fail is bounded by $\sum_{i=1}^{M} n_i$. Hence, if $N = max\ n_i$ then the total number of decision procedure queries is bounded by M^2N.

The next subsection describes a heuristic to remove unnecessary higher degree monomials which results in smaller data matrices, and therefore offers greater scalability.

2.3.4 Removing higher degree monomials

Consider a situation in which we are interested in the invariant $z = y^3 \wedge x = z^2$, and the bound on the degree of the desired loop invariant is $d = 3$. Since GUESS-AND-CHECK will consider all possible

```
1: (x,y,i) := (1,z,0)
2: assume(s=0 && j=k);
3: while(i<n)
4:   (x,y,i) := (x*z+1,y*z,i+1)
```

Figure 2.4: Counterexample to the heuristic in Section 2.3.4.

monomials of degree less than or equal to d, it will also consider the monomial $\alpha \equiv x^3$. As a result, we have $\alpha = y^{18}$ and this high degree monomial is unlikely to be a part of the invariant when $d = 3$.

In order to avoid such monomials with an "implicit" high degree, we make a slight modification to the definition of the data matrix A used by the Guess-and-Check algorithm. We add a column (without loss of generality, let this be the last column) to A representing an additional ghost variable ι. This ghost variable ι plays the role of a loop counter in the while program. Therefore, the value of ι is also part of the program state and is added to *logfile* in line 6 of Figure 2.3.

Using the value of the ghost variable ι, we can discard monomials which grow at a rate $\omega(\iota^d)$ with the number of loop iterations. It should be noted that this heuristic does not always apply. For instance, consider two variables which grow very quickly with respect to the loop counter but have a linear relationship with each other. Discarding monomials corresponding to these quickly growing variables might result in missing a lower degree invariant. For example, consider the program of Fig. 2.4 adapted from [103]. This program has the loop invariant `x(z-1)=y-1`. If we let the upper bound on the degree $d = 2$, then `x` and `y` grow at a rate much greater than ι^2. But we cannot discard the monomials formed from `x` and `y` if we want to get the desired invariant. Hence this heuristic can decrese the precision: if the invariant contains a monomial α which we discarded then we will obtain a weaker invariant which does not contain α. Soundness and termination are unaffected.

If this heuristic is applicable, then we will discard the columns of the data matrix A corresponding to the monomials which grow at a rate $\omega(\iota^d)$. Note that it is important to discard these quickly growing monomials from an implementation standpoint as well. For our example, when we execute the loop for generating A, α will take the values y^{18}. This will quickly overflow finite bit numbers and will not allow us to obtain meaningful data.

We will now describe a simple technique for identifying and eliminating quickly growing monomials from the data matrix A. We modify the definition of the data matrix A such that its last column (in this case, the n^{th} column) maintains the value of the ghost loop counter ι for every program state corresponding to a row of A. For every monomial $\alpha_j \in \vec{\alpha}$, we consider the tuples $\{(log(\iota(k)), log(\alpha_j(k))) \mid 1 \leq k \leq m\}$, where $\iota(k)$ denotes the value of ι in k^{th} row or program state in the data matrix A. If we plot these points in $\mathbb{R}^2$, then the slope of the line passing through these points reflects the rate of growth of α_j with respect to the loop counter. For example, if y is a loop counter and $z = y^3$ is a loop invariant, then the monomial $\alpha = z^2$ will produce a line of slope 6. The best fit line passing through a set of points in $\mathbb{R}^2$ can be easily obtained using standard linear algebra techniques [143].

Next, from A, we discard the columns corresponding to the ghost variable and the monomials which give a line of slope more than d in the log-log plot and the rest of the computation proceeds as described by the algorithm Guess-and-Check.

2.4 Richer Theories

An interesting question is whether the algorithm Guess-and-Check generalizes to richer theories beyond polynomial arithmetic. This is indeed possible and entails careful design of the representation of data. For instance, if we want to infer invariants in the theory of linear arithmetic and arrays, we can have an additional column in the data matrix for values obtained from arrays. Similarly, we can have a variable which stores the value returned from an uninterpreted function and assign it a column in the data matrix. So it is possible to use our technique to infer conjunction of equalities in richer theories too if we know the constituents of the invariants. This is analogous to invariant generation techniques based on templates [35, 125].

In order to illustrate how the Guess-and-Check technique would work for programs with arrays, consider the example program shown in Figure 2.5. We want to prove that the assertion in line 6 holds for all inputs to the program. Assume that we log the values of $a[i]$ and i after every iteration and that the degree bound is $d = 1$. The data matrix that Guess-and-Check constructs will have two columns and let us assume that we run a single test with input $n = 4$ which results in the data matrix rows corresponding to program states induced by this input at the loop head in the program as shown below.

$$A = \begin{array}{|c|c|}\hline i & a[i] \\ \hline 0 & 0 \\ 1 & 1 \\ 2 & 2 \\ 3 & 3 \\ \hline \end{array} \tag{2.25}$$

The null space of A is defined by the basis vector $B = [1, -1]^T$, and therefore we obtain the invariant $a[i] = i$ which is sufficient to prove that the assertion holds.

Our approach of using a dynamic analysis technique to generate data in the form of concrete program states and augmenting it with a decision procedure to obtain a sound technique is a general one. We can take the method for discovering array invariants or polynomial inequalities of [107] and extend it to a sound procedure in a similar fashion.

```
1:  (i,a[0]) = (0,0);
2:  while (i < n) do
3:    i := i+1;
4:    a[i] := a[i-1]+1;
5:  done
6:  assert(a[n] == n);
```

Figure 2.5: Example with equality invariant over arrays.

2.5 From Algebraic to Linear Invariants

Conventional invariant generation techniques for linear equalities [85] do not handle disjunctions. Using disjunctive completion to obtain disjunctions of equalities entails a careful design of the widening operator. Techniques for generation of non-linear invariants can generate algebraic invariants that are equivalent to a boolean combination of linear equalities. But if these invariants are to be consumed by a tool that understands only linear arithmetic, it is important to obtain the original linear invariant from the algebraic invariant. For example, verification engines like [64] are based on linear arithmetic and cannot use non-linear predicates for predicate abstraction. It is not obvious how this step can be performed since the discovered polynomials might not factor into linear factors.

Since our approach is data driven, we can solve this problem using standard machine learning techniques. Here is another perspective on converting algebraic to linear invariants. Assume that the algebraic invariant is equivalent to a boolean combination of linear equalities. Express this linear invariant in DNF form. For instance, suppose we have the DNF formula $y = -x \vee y = x$. The rows of the data matrix A are satisfying assignments of this DNF formula. Hence, each row satisfies some disjunct: each row of A satisfies $y = -x$ or $y = x$. If we create partitions of our data such that the states in each partition satisfy the same disjunct, then all the states of a single partition will lie on a subspace: they will satisfy some conjunction of linear equalities. The aim is to find the subspaces in which the states lie. Since a subspace represents a conjunction of linear equalities, a disjunction of all such subspaces can represent an invariant that is a boolean combination of linear equalities.

The problem of obtaining boolean combinations of linear equalities that a given data matrix satisfies is called subspace segmentation in the machine learning community. This problem arises in applications such as face clustering, video segmentation, motion segmentation, and several algorithms have been proposed over the years. In this section we will apply the algorithm of Vidal, Ma, and Sastry [147] to obtain linear invariants from algebraic invariants. The main insight is that the derivative of the polynomials constituting the algebraic invariant evaluated at a program state characterizes the subspace in which the state lies.

The derivative of the polynomial corresponding to the algebraic invariant for Figure 2.2, that is, $x^2 - y^2$ is $[2x, -2y]$: the first entry is partial derivative w.r.t. x and the second entry is the partial derivative w.r.t. y. Running the program with test input $x \in \{-1, 1\}$ for say 4 iterations each will

results in a data matrix A with 10 rows. The first and last rows are shown:

$$A = \begin{array}{|c|c|c|c|c|c|} \hline 1 & x & y & y^2 & x^2 & xy \\ \hline 1 & -1 & 1 & 1 & 1 & -1 \\ \hline 1 & 5 & 5 & 25 & 25 & 25 \\ \hline \end{array} \tag{2.26}$$

Evaluating the derivative at first state of A gives us $[-2, -2]$. This shows that the first state belongs to $-2x-2y = 0$ i.e. $x = -y$. Evaluating at the last state gives us $[10, -10]$, which shows that the last state belongs to $10x - 10y = 0$ or $x = y$. The other 8 states of A (not shown in Equation 2.26) also belong to $x = y$ or $x = -y$ and we return the disjunction of these two predicates as the candidate invariant. The relationship between the boolean structure of a linear invariant and its equivalent algebraic invariant can be described as follows: the number of conjunctions in the linear invariant (in CNF form) corresponds to the number of conjunctions in the algebraic invariant, and the number of disjunctions in the linear invariant (in DNF form) corresponds to the degree of the algebraic invariant.

Now we explain why this approach works. We sketch the proof from [147] for the case when there is a single algebraic equation $f(\vec{x}) = 0$, that is, the invariant is a disjunction of linear equalities. The case of multiple algebraic equations is similar. Say the invariant is $\vee_i w_i^T \vec{x} = 0 \Leftrightarrow \left(\prod_i w_i^T \vec{x}\right) = 0 \equiv f(\vec{x}) = 0$. The derivative of $f(\vec{x})$, denoted by $\nabla f(\vec{x})$, is a vector of $|\vec{x}|$ elements where the l^{th} element of the vector is a partial derivative with respect to the l^{th} variable:

$$\left(\nabla f(\vec{x})\right)_l = \frac{\partial f(\vec{x})}{\partial x_l}.$$

Now using,

$$\nabla \left(f(\vec{x}) g(\vec{x})\right) = \left(\nabla f(\vec{x})\right) g(\vec{x}) + f(\vec{x}) \left(\nabla g(\vec{x})\right)$$

and

$$\nabla w^T \vec{x} = \left[\frac{\partial w_1 x_1}{\partial x_1}, \ldots, \frac{\partial w_n x_n}{\partial x_n}\right]^T = w \text{ where } |\vec{x}| = n$$

we obtain:

$$\nabla f(\vec{x}) = \nabla \left(\prod_i w_i^T \vec{x}\right) = \sum_i w_i \prod_{j \neq i} (w_j^T \vec{x})$$

Say a program state a satisfies $w_k^T a = 0$. Then $(\nabla f)(a)$ is a scalar multiple of w_k because $\prod_{j \neq i} w_j^T a = 0$ for $i \neq k$. Hence evaluating the derivative at a program state provides the subspace in which the state lies. For more details, the interested reader is referred to [147]. Next we remove from A the states that lie in the same subspace. If A still contains a program state then we can repeat by finding the derivative at that state. In the end we get a collection of subspaces that contain every state of the original data-matrix. A union of these subspaces gives us a boolean combination of linear equalities.

Theorem 4. Given an algebraic invariant $\mathcal{I} = \mathit{NullSpace}(A)$ equivalent to a linear invariant, the procedure of [147] finds a linear invariant equivalent to $\mathcal{I}$.

Note that this conversion is unsound if no equivalent linear invariant exists. Hence the linear predicate should be checked for equivalence with the algebraic invariant; this check can be performed using a decision procedure. Note that we are able to easily incorporate the technique of [147] with Guess-and-Check as our technique is data driven. Also, this conversion just requires differentiating polynomials symbolically, that can be performed linearly in the size of the invariant, and evaluating the derivative at all points in the data matrix. The latter operation is just a matrix multiplication. Hence this algorithm is quite efficient.

2.6 Experimental Evaluation

We evaluate the Guess-and-Check algorithm on a number of benchmarks from the literature on generation of algebraic invariants [120, 121, 125]. All experiments were performed on a 2.5GHz Intel i5 processor system with 4 GB RAM running Ubuntu 10.04 LTS.

Benchmarks The benchmarks over which we evaluated the Guess-and-Check algorithm are from a number of recent research papers on inferring algebraic invariants. These are shown in the first column of Table 4.1. The first three programs are benchmarks from [125]. The first program, `Mul2`, multiplies two numbers by repeated addition. The second program, `LCM/GCD`, computes the great common divisor and least common multiple of two numbers. `Div` divides two numbers to obtain a quotient and a remainder. The next two programs are from [120]. `Bezout` uses extended Euclid's algorithm to compute Bezout's coeffecients. `Factor` finds a divisor of a number. The next three programs are examples from [121]. `Prod` is a different way of multiplying two numbers. `Petter` computes the sum $\sum_i i^5$. `Dijkstra` [44] computes least common multiple and greatest commom divisor of two numbers simultaneously. The next eight programs are examples in [113]. `Cubes` computes the cube of a number. The programs `geoReihe1/2/3` compute geometric sums. The program `potSumm1/2/3/4` computes $\sum_i i^x$, where $x \in \{0, 1, 2, 3\}$.

These programs were implemented in C for data generation. Programs such as `potSumm4`, `Petter`, and `geoReihe3` required the removal of higher degree monomials because some of the monomials overflowed C integers (see Section. 2.3.4).

Evaluation Our approach can be described as a combination of the following components:

1. Test case generation engine: Generally, the programs have tests and we can leverage the existing tests for the purpose of data generation. If these tests are insufficient then the check phase can generate new tests.

Name	#vars	deg	Data	#and	Guess time (s)	Check time (s)	Total time (s)
Mul2	4	2	75	1	0.0007	0.010	0.0107
LCM/GCD	6	2	329	1	0.004	0.012	0.016
Div	6	2	343	3	0.454	0.134	0.588
Bezout	8	2	362	5	0.765	0.149	0.914
Factor	5	3	100	1	0.002	0.010	0.012
Prod	5	2	84	1	0.0007	0.011	0.0117
Petter	2	6	10	1	0.0003	0.012	0.0123
Dijkstra	6	2	362	1	0.003	0.015	0.018
Cubes	4	3	31	10	0.014	0.062	0.076
geoReihe1	3	2	25	1	0.0003	0.010	0.0103
geoReihe2	3	2	25	1	0.0004	0.017	0.0174
geoReihe3	4	3	125	1	0.001	0.010	0.011
potSumm1	2	1	5	1	0.0002	0.011	0.0112
potSumm2	2	2	5	1	0.0002	0.009	0.0092
potSumm3	2	3	5	1	0.0002	0.012	0.0122
potSumm4	2	4	10	1	0.0002	0.010	0.0102

Table 2.1: Evaluation for inference of algebraic invariants. `Name` is the name of the benchmark; `#vars` is the number of variables in the benchmark; `deg` is the user specified maximum possible degree of the discovered invariant; `Data` is the number of times the loop under consideration is executed over all tests; `#and` is the number of algebraic equalities in the discovered invariant; `Guess` is the time taken by the guess phase of Guess-and-Check in seconds. `Check` is the time in seconds taken by the check phase of Guess-and-Check to verify that the candidate invariant is actually an invariant. The last column represents the total time taken by Guess-and-Check.

2. Program instrumentation: We need to add instrumentation to print the memory state of the program to a log. Standard compiler infrastructures like LLVM [29] can facilitate this task.

3. Linear algebra engine: A variety of engines, like SAGE [139] and MATLAB can compute the null space of a matrix.

4. Loop body to a constraint: This can be considered as a source to source transformation and tools like HAVOC [11] can compile programs written in C to SMT-LIB constraints.

5. Theorem prover: This is an off-the-shelf SMT solver which can reason about non-linear arithmetic [1, 43].

6. Feedback mechanism: We need to extract satisfying assignments from the theorem prover and append them to our data log. This assumes the completeness of the prover: if the formula is SAT the the prover can return a satisfying assignment.

Next, we describe our implementation and our experimental results of Table. 4.1. The second column of Table 4.1 shows the number of variables in each benchmark program. The third column shows the upper bound for the degree of the polynomials in the inferred invariant. The fourth column

shows the number of rows of the data matrix. The data or tests were generated naively; each input variable was allowed to take values from 1 to N where N was between 5 and 20 for the experiments. Hence if there were two input variables we had N^2 tests. These tests were executed till termination.

While it is possible to generate tests more intelligently (e.g., by generating counterexamples for failed invariants as suggested in Section 2.1), using inputs from a very small bounding box demonstrates the generality of our technique by not tying it to any symbolic execution engine. Note that including all the states reaching the loop head, over all tests, can include redundant states that do not affect the output. Since the algorithms for null space computation are quite efficient, we do not attempt to identify and remove redundant states. If needed, heuristics like considering a random subset of the states [107] can be employed to keep the size of data matrices small. The fifth column shows the number of algebraic equations in the discovered loop invariant. For most of the programs, a single algebraic equation was sufficient. The null space and the basis computations were performed using off-the-shelf linear algebra algorithms in MATLAB. Guess-and-Check finds the same invariants as reported in the earlier papers [113, 120, 121, 125]. For the programs `Div` and `Cubes`, the invariants found had some redundancy. For instance, we obtained the following three invariants for the program `Div`.

$$\begin{aligned} y1 * y3 + y2 * y4 &= y3 * x1 \\ x2 * y3 &= y2 \\ y1 + x2 * y4 &= x1 \end{aligned}$$

These invariants are linearly independent. Using the cancellation laws of multiplication, it can be seen that the third invariant $x1 = y1 + x2 * y4$ follows from the other two. Since these algorithms for computing null spaces operate on raw data, with no knowledge of what the data represents, they will not be able to remove redundancy caused by more complex axioms of arithmetic, such as those corresponding to non-linear operations like multiplications and divisions. The best they can do to remove redundancy is to ensure linear independence. Techniques like Gröbner bases can be used to remove redundancy. Alternatively, a decision procedure can be used to remove redundant algebraic equations [107]. The time (in seconds) taken by the guess phase of Guess-and-Check is reported in the sixth column of Table 4.1.

The reader might notice that our implementation is significantly faster when `#and` equals one. This is due to an implementation trick. MATLAB provides two algorithms for computing the null space of a matrix. The first is a numerical algorithm which has been significantly optimized. The second is an exact algorithm over the rationals which is comparatively slower. Our implementation first tries to use the faster numerical algorithm for computing the null space and the nullity. If the nullity is one, then it is very simple to obtain a vector in the null space which has all its coordinates as exact integers from the numerical output. This process is not so obvious when nullity is more

than one. Since we need to supply an exact predicate to the check step, we use the slow exact algorithm when the nullity is more than one.

For example, consider the following matrix:

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}$$

On executing `null(A)` in MATLAB (the optimized numerical algorithm), we get, within 0.0002 seconds, that the null space is spanned by the vector $[-0.7071, 0.7071]^T$. From this we can conclude that the null space is spanned by the vector $[-1, 1]^T$. On executing `null(A,'r')` in MATLAB (the slower exact algorithm), we get within 0.0007 seconds that the null space is spanned by $[-1, 1]^T$. Hence using the faster numerical algorithm explains why our implementation is significantly faster when `#and` is one.

We use Z3 [43] for checking that the proposed invariants are actually invariants (implementation of *Check* procedure in the Guess-and-Check algorithm). Theorem prover Z3 was able to easily handle the simple queries made by Guess-and-Check, because once an invariant has been obtained, the constraint encoding that the invariant is inductive is quite a simple constraint to solve and our naively generated tests were sufficient to generate an actual invariant. For all programs, except `Div`, we declare the variables as integers. So even though these queries are in Peano arithmetic, and can contain integer division and modulo operators, the decision procedure is able to discharge them. For `Div` the invariant that [125] finds is inductive only if the variables are over reals. When we execute Guess-and-Check on `Div`, where the queries are in Peano arithmetic, we obtain the trivial invariant *true* after three guess-and-check iterations. Next, we lift the variables to reals when querying Z3. Now, we discover the invariant found by [125] in one guess-and-check iteration and this is the result shown in Table 4.1. By the soundness of our approach, we conclude that an approach producing a non-trivial algebraic invariant for this benchmark can be unsound for integer manipulating programs containing division or modulo operators.

Finally, the time taken by Guess-and-Check on these benchmarks is comparable to the state-of-the-art correct-by-construction invariant generation techniques [25]. Since these benchmarks are small and the time taken by both our technique and [25] is less than a second on these programs, a comparison of run times may not be indicative of performance of either approach on larger loops. For these benchmarks, our algorithm is significantly faster than any algorithm using Gröbner bases. For instance, on the benchmark `factor`, [121] takes 55.4 seconds, while [120] takes 2.61 seconds. We discover the same invariant in 0.012 seconds. However, the exact timings must be taken with a grain of salt (we are running on a newer generation of hardware). We leave the collection of a hard benchmark suite for algebraic invariant generation tools as future work.

2.7 Related Work

The work described in this chapter can be seen as an instantiation of the framework described in [152]. This framework has previously been instantiated with predicate abstraction and three valued logic [122]. In this chapter, we instantiated this framework with a different abstraction, algebraic equations.

Next, we place the Guess-and-Check algorithm in the context of existing work on discovering algebraic loop invariants. Sankaranarayanan et al. [125] describe a constraint based technique that uses user-defined templates for computing algebraic invariants. Their objective is to find an instantiation of these templates that satisfies the constraints and this corresponds to an invariant. The constraints that they use contains quantifiers and therefore the cost of solving them is quite high.

Müller-Olm et al. [34, 103] define an abstract interpretation based technique which is sound and generates all possible algebraic invariants which can be obtained by combination of user provided monomials. Rodríguez-Carbonell et al. [120] also describe an abstract interpretation based technique for discovering algebraic invariants. In order to ensure termination, they rely on a widening operator which is precise enough to generate all invariants whose degree is bounded by a user defined constant. They also empirically evaluate their technique which works very well on a number of small benchmark programs. The same authors, in subsequent work [121], under some technical assumptions on program syntax, provide a fully automatic, sound, complete, and terminating algorithm, which was later extended by Kovács [89].

All of the above mentioned techniques require the heavy technical machinery of Gröbner bases [41] and require restrictions on program syntax, some of which are quite technical, in order to achieve soundness. Recently, Nguyen et al. [107] have proposed a dynamic analysis for inference of candidate invariants. They do not provide any formal characterization of the output of their algorithm and do not prove any soundness or completeness theorems. Their technique has reasonable running time and assumes an upper bound on the degree as input. As noted in [107], our approach can also take advantage of the number of approaches on test case generation developed specifically for the purpose of dynamic invariant generation [72, 73, 150].

More recently, Cachera et al. [25] have extended the work of Müller-Olm et al. [103] to provide an abstract interpretation based algorithm which handles a richer but still somewhat restricted program syntax and achieves a fixpoint in one iteration as opposed to an unknown number of iterations of [103]. Their approach has reasonable running time and requires the degree as input. In contrast, our technique does not require any restriction on program syntax explicitly. We shift the burden of checking an invariant to a decision procedure [82]. In other words, we can handle any program which our decision procedure can handle. This allows us to handle programs with say division and modulo operations, which no existing abstract interpretation based technique is capable of handling: Cachera et al. removed these operators manually [25]. The soundness and completeness of our algorithm follows from the soundness and completeness of the underlying decision procedure.

Moreover, together with these theoretical guarantees, our technique has been implemented and evaluated over a number of benchmarks with encouraging results.

Some other related work includes the following: Amato et al. [4] analyze data from program executions to tune their abstract interpretation. Bagnara et al. [9] introduce new variables for monomials and generate linear invariants over them by abstract interpretation. Inference of linear equalities (as opposed to algebraic equalities) is well studied [40]. The InvGen tool can solve matrix equations to infer linear equalities [71]. The Daikon tool [49] generates likely invariants from tests and templates. In the context of Daikon, it is interesting to note from [108] that very few test cases suffice for invariant generation. Indeed, this has been our experience with the Guess-and-Check as well.

In contrast to all the other techniques which fall into the category of "correct by construction" techniques, the guessing phase of the Guess-and-Check algorithm will not miss any invariant but can produce spurious ones. The spurious invariants can be removed by running more tests, or in a more systematic fashion by using a decision procedure. Assuming the decision procedure can handle queries which encode the text of the program as constraints, we can get rid of these spurious algebraic equations. Since reasoning about non-linear arithmetic is a hard problem in general, our checking procedure has a high complexity, but as our experiments indicate, the hard cases happen rarely in practice. In contrast to the technique in [125] where the constraint solver solves synthesis constraints for invariant inference, the check phase of our algorithm constructs constraints for verifying whether the given candidate invariant is actually an invariant. These constraints are much simpler than the ones for directly synthesizing invariants which reduces the load on the decision procedure and thus makes the Guess-and-Check approach very efficient in practice.

Chapter 3

Binary Equivalence

In the previous chapter, we described a technique to infer equality invariants. In this chapter we show how this technique aids in constructing formal proofs of equivalence.

Equivalence checking of loops is a fundamental problem with potentially significant applications, particularly in the area of compiler optimizations. Unfortunately, the current state of the art in equivalence checking is quite limited: given two assembly loops, no previous technique is capable of verifying equivalence automatically, even if they differ only in the application of standard loop optimizations. In this chapter, we discuss the first practically useful, automatic, and sound equivalence checking engine for loops written in x86.

Proofs of equivalence at the binary level are more desirable than proofs at the source or RTL level, because such proofs minimize the trusted code base. For example, a bug in the code generator of a compiler can invalidate a proof performed at the RTL level or we can have a "what you see is not what you execute" (WYSINWYX) phenomenon [10] and the generated binary can deviate from what is intended in the source.

Existing techniques for proving equivalence can be classified into three categories: sound algorithms for loop-free code [6, 42, 51, 52, 97]; algorithms that analyze finite unwindings of loops or finite spaces of inputs [79, 90, 112, 117]; algorithms that require knowledge of the particular transformations used for turning one program into another [101, 140] and the order in which the transformations have been applied [60, 105, 115]. In contrast, our approach to handling equivalence checking of loops does not assume any knowledge about the optimizations performed.

We have implemented a prototype version of our algorithm in a system called DDEC (Data-Driven Equivalence Checker). This tool checks the equivalence of two loops written in x86 assembly. In outline the tool works as follows. First, DDEC guesses a *simulation relation* [105]. Roughly speaking, a simulation relation breaks two loops into a set of pairs of loop-free code fragments. Logical formulas associated with each pair describe the relationship of the input states of the fragments to the output states of the fragments. Second, DDEC generates verification conditions encoding

the x86 instructions contained in each loop-free fragment as SMT [43] constraints. Finally, DDEC constructs queries which verify that the guessed relationships between the code fragments in fact hold. By construction, if the queries succeed they constitute an inductive proof of equivalence of the two loops.

It is worth stressing that DDEC works directly on unmodified binaries for x86 loops. The x86 instruction set is large, complex, and difficult to analyze statically. The key idea that makes DDEC effective in practice, and even simply feasible to build, is that the process of guessing a simulation relation (step 1 above) is constructed not via static code analyses, but by using data collected from test cases. Because DDEC is data driven, it is able to directly examine the precise net effect of code sequences without first going through a potentially lossy abstraction step. Of course, the use of test cases is an under-approximation and may not capture all possible loop behaviors. Nonetheless, DDEC is sound; a lack of test coverage may cause equivalence checking to fail, but it cannot result in the unsound conclusion that two loops are equivalent when they are not.

While our main result is simply a sound and effective approach to checking the equivalence of loops, we also show that sufficiently powerful equivalence checking tools such as DDEC have novel applications. In particular, we are able to verify the equivalence of binaries produced by completely different compiler toolchains. For a representative set of benchmarks, we automatically prove the equivalence of code produced by CompCert and `gcc` (with optimizations enabled), which allows us to certify the correctness of the entire `gcc` compilation or, conversely, to produce more performant CompCert code. Additionally, we extend the applicability of Stoke [126], a superoptimizer for straight-line programs, to loops. We replace Stoke's validator by DDEC and the resulting implementation is able to perform optimizations beyond Stoke's original capabilities, in fact producing verified code which is comparable in performance to `gcc -O3`.

DDEC is not without limitations. In particular, DDEC restricts the expressiveness of invariants required for a proof to be conjunctions of linear or nonlinear equalities. However, for most interesting intra-procedural optimizations, simple equalities appear to be sufficiently expressive [105, 119, 140]. DDEC is also currently unable to reason about floating point computations, simply because the current generation of off-the-shelf SMT solvers do not support floating point reasoning. Floating point reasoning is orthogonal to our contributions; when even limited floating point reasoning becomes available, DDEC can incorporate it immediately. However, the current state of the art limits the demonstration of DDEC to loops that work only with non-floating point values.

We begin by providing a detailed, but informal, worked example (Section 3.1), which is followed by a presentation of the equivalence checking algorithm (Section 3.2). Next we describe the implementation of DDEC (Section 3.3). Our evaluation (Section 3.4) shows DDEC is competitive with the state of the art in equivalence checking and presents the novel applications described above. Discussions of related work, limitations, and future work are included in Section 3.5.

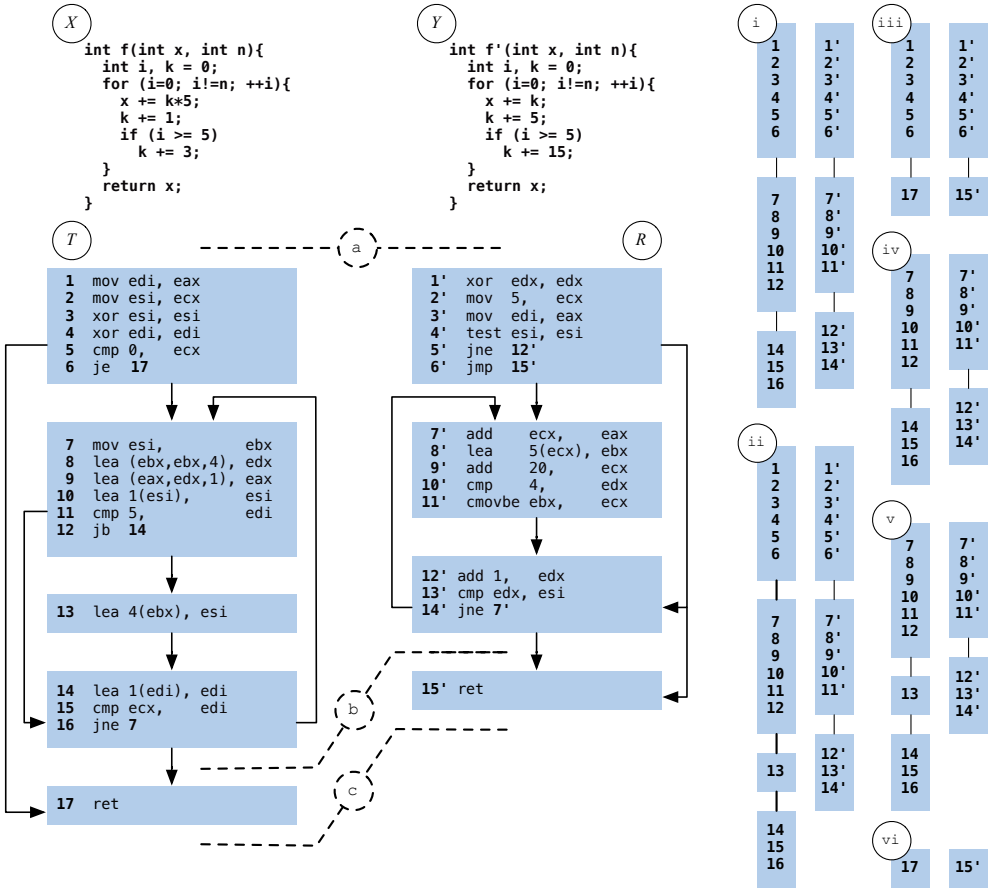


Figure 3.1: Equivalence checking for two possible compilations: (A) no optimizations applied either by hand or during compilation, (B) optimizations applied. Cutpoints (a,b,c) and corresponding paths (i-vi) are shown.

3.1 A Worked Example

Figure 4.1 shows two versions of a function taken from [140]. The straightforward implementation X is optimized using a strength reduction [7] to produce the code Y; corresponding x86 assembly codes $\mathcal{T}$ and $\mathcal{R}$ are shown beneath each source code function. We use primes ($'$) to represent program points and registers corresponding to the optimized code, which we call the *rewrite* R, and unprimed quantities for those corresponding to the unoptimized code, which we call the *target* T, throughout the chapter. The generation of $\mathcal{R}$ also involves some low level compiler optimizations such as the use of an x86 conditional-move (instruction $11'$ of $\mathcal{R}$) to eliminate a jump (instruction 12 of $\mathcal{T}$). We are unaware of any fully automatic technique capable of verifying the equivalence of $\mathcal{T}$ and $\mathcal{R}$. Nonetheless, our goal is to verify equivalence in the absence of source programs, manually written

expert rules for equivalence, source code of the compiler(s) used, and compiler annotations—in other words, given only the two assembly programs and no other information. All of these features are necessary requirements to check equivalence at the assembly level when no knowledge is available about the relationship between the two codes. This situation arises, for example, in verifying the correctness of STOKE optimizations [126].

To verify that $\mathcal{T}$ and $\mathcal{R}$ are equivalent, we must confirm that whenever $\mathcal{T}$ and $\mathcal{R}$ begin execution in identical machine states and $\mathcal{T}$ runs to completion, $\mathcal{R}$ is guaranteed to terminate in the same machine state as $\mathcal{T}$ and with the same return value. In this example, which does not use memory, we limit our discussion of machine states to a valuation of the subset of hardware registers that the two codes use: `eax`, `ebx`, `ecx`, `esi`, and `edi` (our technique does not make this assumption in general and handles memory reads and writes soundly). We also assume that we know which registers are live on exit from the function, which in this case is just the return value `eax`. We stress that the following discussion takes place entirely at the assembly level and does not assume any information about the sources X or Y.

We use the well-known concept of a *cutpoint* [145] to decompose equivalence checking of two loops into manageable sub-parts. A cutpoint is a pair of program points, one in each program. Cutpoints are chosen to divide the loops into loop-free segments. The cutpoints in Figure 1, labeled `a`, `b`, and `c`, segment the programs as follows: 1) the code from `a` to `b` excluding the backedge of the loop, 2) the code that starts from `b`, takes the backedge once, and comes back to `b`, and 3) the code that starts from `b`, exits the loop, and terminates at `c`. Using these three cutpoints, we can produce an inductive proof of equivalence which proceeds as follows. Our goal is to show that the executions of $\mathcal{T}$ and $\mathcal{R}$ move together from one cutpoint to the next and that at each cutpoint, certain invariants are guaranteed to hold. The required invariants at `a` and `c` follow directly from the problem statement. At point `a`, we require that $\mathcal{T}$ and $\mathcal{R}$ agree on the initial machine states. Similarly at point `c`, we require that $\mathcal{T}$ and $\mathcal{R}$ agree on the return value stored in `eax`.

We now encounter two major difficulties in producing a proof of equivalence. The first problem we encounter is identifying the invariant that must hold at `b`. This invariant, I, is a relation between the machine states of T and R. In this chapter, we consider invariants that consist of equality relationships between elements of the two machine states. Once we have identified the appropriate invariant I, an inductive proof would take the following form:

1. If $\mathcal{T}$ and $\mathcal{R}$ begin in `a` with identical machine states and transition immediately to `c`, they terminate with identical return values.
2. If $\mathcal{T}$ and $\mathcal{R}$ begin in `a` with identical machine states and transition to `b`, they both satisfy I.
3. If $\mathcal{T}$ and $\mathcal{R}$ begin in `b` satisfying I, and return to `b`, then I still holds.
4. If $\mathcal{T}$ and $\mathcal{R}$ begin in `b` satisfying I and transition to `c`, they terminate with identical return values.

However, this proof is still incomplete. It does not guarantee that if $\mathcal{T}$ makes a transition, then $\mathcal{R}$ makes the same transition: we do not for instance want $\mathcal{T}$ to transition from `a` to `b` while $\mathcal{R}$ transitions from `b` to `c`. The proof can be completed as follows.

Every transition between cutpoints is associated with some instructions of $\mathcal{T}$ and $\mathcal{R}$: these are the instructions, or *code paths*, which need to be executed to move from one cutpoint to the next. For example, in moving from cutpoint `b` to `c`, $\mathcal{T}$ and $\mathcal{R}$ execute the instructions shown in code paths `vi` of Figure 4.1. A code path p_A of $\mathcal{T}$ *corresponds* to a code path p_B of $\mathcal{R}$ if they start and end at the same cutpoints and when $\mathcal{T}$ executes p_A then $\mathcal{R}$ executes p_B. Figure 4.1 shows a complete set of corresponding paths: `i` and `ii` are associated with transition `a-b`, `iii` is associated with `a-c`, `iv` and `v` are associated with `b-b` and `vi` is associated with `b-c`. We need to check that when $\mathcal{T}$ executes a code path then $\mathcal{R}$ can only execute the corresponding paths. Identifying these corresponding paths is a second major difficulty. The question of what invariants hold at `b` is crucial, as these must be strong enough to statically prove that the execution of $\mathcal{R}$ follows the corresponding paths of $\mathcal{T}$ and that the executions of both $\mathcal{T}$ and $\mathcal{R}$ proceed through the same sequence of cutpoints.

Our solution to both problems, identifying the equalities that hold at `b` and the corresponding paths of the two programs, is to analyze execution data. We identify corresponding paths by matching program traces for both loops on the same test inputs against the set of cutpoints. We observe the instructions executed by $\mathcal{T}$ and $\mathcal{R}$ in moving from one cutpoint to the next and label them as corresponding. For example, for a test case with initial state `edi` $= 0$ and `esi` $= 1$, $\mathcal{T}$ begins its execution from `a` and executes instructions `1` to `16` to reach `b`. It then exits the loop and transitions from `b` to `c` by executing instruction `17`. $\mathcal{R}$ begins its execution from `a` and executes instructions $\texttt{1}'$ to $\texttt{14}'$ to reach `b`. It then executes instruction $\texttt{15}'$ to reach `c`. From this test case, we observe that code paths with instructions `1` to `16` correspond to instructions $\texttt{1}'$ to $\texttt{14}'$ (`i`) and `17` corresponds to $\texttt{15}'$ (`vi`).

The equality conditions at `b` can be determined by inserting instrumentation at `b` to record the values of the live program registers for both programs and observing the results. For a test input where `edi` $= 0$ and `esi` $= 2$, we obtain the following matrix where each row corresponds to the values in live registers when both programs pass through `b`:

$$\begin{bmatrix} \texttt{eax} & \texttt{esi} & \texttt{edi} & \texttt{ecx} & \texttt{eax}' & \texttt{ecx}' & \texttt{edx}' & \texttt{esi}' \\ 0 & 1 & 1 & 2 & 0 & 5 & 1 & 2 \\ 5 & 2 & 2 & 2 & 5 & 10 & 2 & 2 \end{bmatrix}$$

The first row says that when $\mathcal{T}$ reaches `b` for the first time the registers have the values shown in columns `eax` , `esi`, `edi`, and `ecx`; when $\mathcal{R}$ reaches `b` for the first time, the registers have values shown in $\texttt{eax}'$, $\texttt{ecx}'$, $\texttt{edx}'$, and $\texttt{esi}'$. The second row shows the values of registers when `b` is reached the second time, i.e., in the next iteration of $\mathcal{T}$ and $\mathcal{R}$. Using standard linear algebra techniques (Section 2.3.1), it is possible to extract the following relationships, which are sufficient candidates

for the equalities which must hold at `b`: $\texttt{eax} = \texttt{eax}'$, $5 * \texttt{esi} = \texttt{ecx}'$, $\texttt{edi} = \texttt{edx}'$, and $\texttt{ecx} = \texttt{esi}'$. Chapter 2 describes the use of linear algebra on test data for invariant inference and its limitations. The process may generate spurious equality relationships in the guess phase [107], however these can be systematically eliminated using a theorem prover in the check phase [129]. We note that this method assumes that equality relationships are sufficient to prove program equivalence and we do not, for example, consider invariants which contain inequalities. Previous work on translation validation [105, 140] makes the same assumption, which we find to be largely sufficient in practice (see Section 3.4).

Although it is possible that the tests used to generate these values do not produce sufficient coverage, and that either more corresponding paths exist, or spurious equality relationships are discovered at `b`, the consequence is simply that the proof will fail, and we will report that the two functions may be different. We may then reattempt the proof with more test cases, but a lack of test data cannot cause an unsound result. Barring this possibility, almost all of the limitations of DDEC can be mapped to the restricted expressiveness of invariants. Better invariant generation techniques will only improve performance.

3.2 Algorithm

We now present a formal description of the algorithm sketched in Section 3.1. We assume we are given two functions $\mathcal{T}$ and $\mathcal{R}$, each containing one natural loop and no function calls. We infer a candidate *simulation relation* consisting of cutpoints and linear equalities as invariants. Then we check whether the candidate is an actual simulation relation, and if so then we have a proof of equivalence. We consider functions containing multiple loops, calling other functions, and inference of non-linear invariants in Section 3.2.1.

As is standard, we make a distinction between $\mathcal{T}$, the *target* or reference code, and $\mathcal{R}$, the *rewrite* or proposed replacement for the target $\mathcal{T}$. A program *state* consists of a valuation of registers, current stack frame, and memory. The memory consists of the whole virtual memory except the current stack frame. Generally, we will refer to the state at a program point; in such instances we will limit the state to only the live elements. We first define a suitable notion of equality:

Definition 1. Target $\mathcal{T}$ is *equivalent* to rewrite $\mathcal{R}$ if for all states s both of the following hold: (i) if executing $\mathcal{T}$ from initial state s terminates in state s' without aborting, then executing $\mathcal{R}$ from initial state s also terminates in state s' without aborting; and (ii) if $\mathcal{T}$ diverges when execution is started from s, then so does $\mathcal{R}$.

This definition captures the fact that if $\mathcal{T}$ terminates on an input then so does $\mathcal{R}$. Hence, this definition is richer than partial equivalence. Hardware faults can cause an execution to abort. Some common examples of aborting include segmentation faults and floating point exceptions. The asymmetric notion of equality in Definition 1 seems necessary to validate several useful compiler

optimizations. If the target $\mathcal{T}$ aborts on some inputs, optimizing compilers are free to use an $\mathcal{R}$ with any behavior, defined or undefined, on that input. The notion of equality we use is captured in the *verification conditions* (VCs) generated to symbolically compare the behavior of T and R. Since our VCs are in a rich logic, by modifying the VCs that are generated our approach can handle a wide range of specifications of equality, including requiring the target and rewrite to behave identically on every input or allowing the rewrite to differ from the target on any input that causes the target to abort.

Let t be a *code path*, that is, a sequence of instructions in $\mathcal{T}$, r a code path in $\mathcal{R}$, and C the pair $\langle t, r\rangle$. Abusing the notation of Hoare logic, we define proof obligations.

Definition 2. For predicates P and Q and code paths t and r, a proof obligation $\{P\}\langle t, r\rangle\{Q\}$, states that if t starts execution from a state s_1, r start execution from a state s_2, $P(s_1, s_2)$ holds, and t terminates in a final state s_1' without aborting, then r does not abort and for all possible final states s_2' of r, $Q(s_1', s_2')$ holds.

For example

$$\{\texttt{eax} = \texttt{eax}'\}\langle \texttt{mul \$2 eax}, \texttt{shl \$1 eax}\rangle\{\texttt{eax} = \texttt{eax}'\}$$

says if t and r begin with values of `eax` equal and t performs an unsigned multiplication by two and r shifts `eax` left by one bit then the resulting states agree on the value of `eax`. We want to generate sufficiently many proof obligations, such that if they are all satisfied then they constitute an inductive proof of equivalence of $\mathcal{T}$ and $\mathcal{R}$.

3.2.1 Generating Proof Obligations

Each proof obligation $\{P\}C\{Q\}$ has two components: the code paths C and the predicates P and Q on the states of $\mathcal{T}$ and $\mathcal{R}$. We discuss the generation of each component.

Generating Corresponding Paths

We generate corresponding paths t and r for proof obligations using *cutpoints* [145]. A cutpoint n is a pair of program points $\langle \eta_{\mathcal{T}}, \eta_{\mathcal{R}}\rangle$ where $\eta_{\mathcal{T}} \in \mathcal{T}$ and $\eta_{\mathcal{R}} \in \mathcal{R}$. We select cutpoints using the following heuristic: Choose pairs of program points where the corresponding memory states agree on the largest number of values. Cutpoints with higher agreement between the memory states of T and R have simpler invariants than cutpoints where the relationship between the two memory states is more involved.

The cutpoints are discovered using a brute force search that compares the execution data for pairs of program points. We create a candidate cutpoint for every program point pair $\langle \eta_{\mathcal{T}}, \eta_{\mathcal{R}}\rangle$. For every test σ, we find $m^{\sigma}_{\eta_{\mathcal{T}}}$ (resp. $m^{\sigma}_{\eta_{\mathcal{R}}}$), the number of times control flow passes through $\eta_{\mathcal{T}}$ (resp. $\eta_{\mathcal{R}}$) when the execution of $\mathcal{T}$ (resp. $\mathcal{R}$) starts in the state σ. If there do not exist constants a, b s.t.

$\forall\sigma.m^{\sigma}_{\eta_\mathcal{T}} = am^{\sigma}_{\eta_\mathcal{R}} + b$ then $\langle\eta_\mathcal{T}, \eta_\mathcal{R}\rangle$ is rejected as a candidate cutpoint. We also reject candidates for which the number of heap locations in the observed heap states for $\mathcal{T}$ and $\mathcal{R}$ at $\langle\eta_\mathcal{T}, \eta_\mathcal{R}\rangle$ is not a constant across all tests. Note that this operation is possible as we run only terminating tests and thus the memory footprint is bounded. For the remaining candidates, we assign them a penalty representing how different the observed heap states are for $\mathcal{T}$ and $\mathcal{R}$ at $\langle\eta_\mathcal{T}, \eta_\mathcal{R}\rangle$. We pick candidate cutpoints in increasing order of penalty until $\mathcal{T}$ and $\mathcal{R}$ are decomposed into loop free segments. Next, redundant candidates are removed so that the minimum number of program point pairs are selected as candidate cutpoints; a candidate n is redundant if the decomposition is still loop free after removing n. The choice of a minimum set of cutpoints may not be unique and we simply try multiple proofs, with one proof corresponding to every available choice. Multiple cutpoints can be associated with the same program point of $\mathcal{T}$ or $\mathcal{R}$. For example, if a loop unrolling has been performed then there might be several cutpoints sharing the same program point of $\mathcal{T}$.

If satisfactory cutpoints cannot be found then our technique fails, which highlights a limitation of our technique: we fail to prove equivalence for programs which differ from each other at an unbounded number of memory locations. For example, a loop fusion transformation or reordering an array traversal results in loops that cannot be proven equivalent using our method. Handling such loops requires quantified invariants, for which the current state of the art in invariant inference is less mature than for quantifier-free invariants. Generally, the techniques for quantified invariants require manually provided templates; the templates prevent the introduction of an unbounded number of quantified variables. Moreover, theorem provers are not as robust for quantified formulas as they are for quantifier-free formulas.

The set of cutpoints is called a *cutset* $\mathcal{D}$. For every pair of cutpoints n_1 and n_2 in a cutset $\mathcal{D}$, we define a *transition* $\tau \equiv n_1 \triangleright n_2$ from n_1 to n_2. This transition is *associated* with a set of static code paths $\mathcal{P}_1$ of $\mathcal{T}$ and $\mathcal{P}_2$ of $\mathcal{R}$. $\mathcal{P}_1$ and $\mathcal{P}_2$ consists of code paths which go from n_1 to n_2 without passing through some other cutpoint $n_3 \in \mathcal{D}$. The instructions executed for a terminating and non-aborting execution of $\mathcal{T}$ and $\mathcal{R}$ can be represented by a sequence of transitions. For example, in Figure 4.1, let us denote by τ_1 the transition from `a` to `b` and τ_2 from `b` to `c`. Then the execution discussed in Section 3.1 represents the sequence of transitions $\tau_1\tau_2$. Code paths `i` and `ii` of Figure 4.1 are associated with τ_1 and `vi` is associated with τ_2. Now we define corresponding paths formally:

Definition 3. Given a target $\mathcal{T}$, a rewrite $\mathcal{R}$, and a cutset $\mathcal{D}$, a code path t of $\mathcal{T}$ *corresponds to a code path* r *of* $\mathcal{R}$ *if they are associated with the same transition* τ *in* $\mathcal{D}$ *and for some execution* $\tau_1, \ldots, \tau, \ldots, \tau_m$*, for the transition* τ*, if* $\mathcal{T}$ *executes the code path* t *then* $\mathcal{R}$ *executes* r*.*

Now we discuss our data-driven algorithm for generation of corresponding paths. $\mathcal{T}$ and $\mathcal{R}$ are run on a test input and we record the trace of instructions executed in both functions. We analyze this pair of traces to build a set $\mathcal{C}$ of corresponding paths. The algorithm walks over the traces in parallel until a cutpoint is reached in both. The pair of paths taken from the previous pair of cutpoints is added to $\mathcal{C}$. This process is repeated until we reach the end of the traces. We then run the two

functions on another input and repeat the analysis. If test coverage is sufficient, $\mathcal{C}$ will contain all corresponding paths.

We add additional proof obligations to ensure that we have not missed any corresponding paths. For static paths in $\mathcal{T}$ between cutpoints that no test executes, we add an arbitrary path from $\mathcal{R}$ between the same cutpoints as a corresponding path in $\mathcal{C}$. For a path p of $\mathcal{T}$ associated with a transition τ, we add the verification condition that if the target executes p then the rewrite can only execute the paths which correspond to p in $\mathcal{C}$. If these proof obligations fail then this means that our data is insufficient and there are more corresponding paths to be discovered.

Generating Invariants

Following Necula [105], we consider invariants that are equalities over *features*, which are registers, stack locations and a finite set Δ of heap locations. Also as in [105], we replace reads from and writes to stack locations by reads and writes to named temporaries.

We perform a liveness analysis over $\mathcal{T}$ and $\mathcal{R}$ and for each cutpoint (η_1, η_2) obtain the live features (see Section 3.3). Because x86 has sub-registers, these features can be of different bit-widths. For example, it might be that only one byte of a 64-bit register is live. We create a set of matrices, one for each cutpoint (η_1, η_2), whose columns are the live features at η_1 and η_2. If the bit-width of the longest live feature is x bits, we create one column for every x bit live feature. For every live feature of fewer than x bits, we create two columns: one with the feature's value zero-extended to x bits and the other with the value sign-extended. The sign- and zero-extensions are needed because x86 instructions implicitly perform these operations on registers of different bit-widths.

We instrument the functions to record the values of the features at the cutpoints; a snapshot of the state at one cutpoint corresponds to a single matrix row. If the cutpoint (η_1, η_2) is executed m times then we have m rows in the matrix for (η_1, η_2). Note that there are no negative values in the matrices: negative numbers become large positive numbers.

We use techniques described in Chapter 2 to compute the linear equality relationships between features. For the matrix associated with each cutpoint, we compute its nullspace. Recall that, every vector of the nullspace corresponds to an equality relationship between features at that cutpoint for all test inputs. We take a conjunction of equalities generated by all vectors in the basis of the nullspace and return the resulting predicate as a candidate invariant for our candidate simulation relation. For example, if our matrix has three features and two rows:

$$\begin{bmatrix} \texttt{eax} & \texttt{ebx} & \texttt{eax}' \\ 1 & 1 & 1 \\ 2 & 2 & 2 \end{bmatrix}$$

then one possible basis of the nullspace consists of the vectors $[1, -1, 0]$ and $[0, 1, -1]$. These vectors correspond to the equalities $\texttt{eax}*(1)+\texttt{ebx}*(-1)+\texttt{eax}'*0 = 0$ and $\texttt{eax}*0+\texttt{ebx}*(1)+\texttt{eax}'*(-1) = 0$.

Hence the candidate invariant is $\texttt{eax} = \texttt{ebx} \wedge \texttt{ebx} = \texttt{eax}'$. Note that the heap locations, which are not included in features, are implicitly constrained to have identical values for $\mathcal{T}$ and $\mathcal{R}$. Hence, the above invariant includes an implicit equality $H = H'$, that is, for all heap addresses, at the cutpoint, $\mathcal{T}$ and $\mathcal{R}$ have identical values. The cutpoints are labeled with these equalities. One desirable feature of nullspaces is that no sound equality relationship is missed. It can produce spurious equality relationships (for lack of sufficient data) but if an equality holds statically then it will be generated (Lemma 1). Intuitively, this is because every possible equality is contained in the candidate invariant unless there is a test that violates it. In the extreme, when we have zero states in our data then the candidate invariant consists of every possible equality between the features, and hence it also includes the equalities present in the true invariants. We generalize the results in Chapter 2, which uses nullspaces to compute invariants for a single program, to features:

Lemma 3. If x is a set of features at a cutpoint n, and $\mathcal{I}(x)$ is the strongest invariant at n that holds statically and is expressible by conjunctions of linear equalities, then the candidate invariant $I(x)$ obtained by computing the nullspace of test data is a sound under-approximation of $\mathcal{I}$, that is, $I \Rightarrow \mathcal{I}$.

Before we discuss how candidate invariants are checked to see if they are in fact invariants, we briefly digress to discuss how our approach extends to more complex function bodies.

Extensions

Our approach easily generalizes to functions with multiple natural loops, including nested loops. We identify the cutset of $\mathcal{T}$ and $\mathcal{R}$ and identify cutpoints and transitions between two cutpoints if there is a static path from one cutpoint to the other. As is standard, we want every loop to contain at least one cutpoint of the cutset. The algorithm described above for generating proof obligations remains unchanged: run tests, generate corresponding paths, and generate equality relationships at cutpoints.

We can also extend our approach to handle loops that call other functions. The function call is a cutpoint requiring the invariant that the value of arguments and memory is same across $\mathcal{T}$ and $\mathcal{R}$ and after the call we can assume that the memory and return values are equal in the proof obligations. We generate additional obligations to check that the order of function calls is preserved.

Our approach easily extends to generate non-linear equalities of a given degree d for invariants. Following the approach of Chapter 2, we simply create a new feature for every monomial up to the degree d from the existing features. However, non-linear invariants were not required for our equivalence checking tasks (Section 3.4).

3.2.2 Checking Proof Obligations

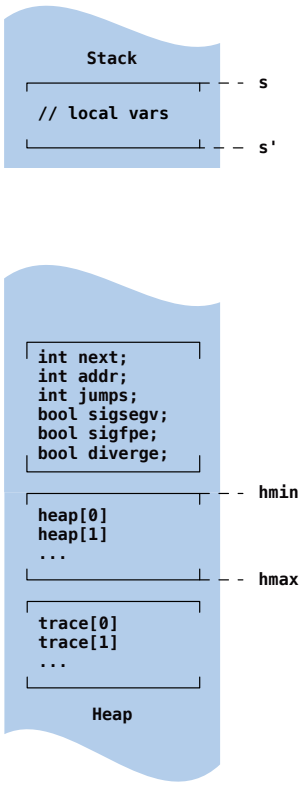
For every transition τ between cutpoints n_1 and n_2 where the candidate invariant at n_1 is equality relationship P, the candidate invariant at n_2 is equality relationship Q, and C is a pair of corresponding paths associated with τ, we construct a proof obligation $\{P\}C\{Q\}$. As noted in Section 3.1, we also generate additional verification conditions or VCs to check that all pairs of corresponding paths are covered. Once the VCs have been obtained, they can be sent to an off-the-shelf theorem prover. These queries are in the quantifier-free theory of bit-vectors. More details about generating VCs can be found in Section 3.3.6. The proof obligations $\{P\}C\{Q\}$ are of three types:

- $\{E\}C\{Q\}$, where E represents exact equivalence between states. Here the corresponding paths are code paths from the start of $\mathcal{T}$ and $\mathcal{R}$ to a cutpoint and Q is the equality relationship associated with that cutpoint.
- $\{P\}C\{Q\}$, where for $C = \langle t, r\rangle$, t and r start at a cutpoint n_1 and end at a cutpoint n_2. P and Q are the equality relationships at n_1 and n_2.
- $\{P\}C\{F\}$, where the corresponding paths start at a cutpoint and end at a return statement of $\mathcal{T}$ and $\mathcal{R}$. Here F expresses that the return values are equal and the memory states are equivalent.

If proof obligation $\{E\}C\{Q\}$ or $\{P\}C\{Q\}$ fails then we can obtain a counter-example from the decision procedure and follow the approach of Chapter 2: If the counter-example violates some equality of Q then we incorporate the data from the counter-example in the appropriate matrix. Next, we recompute the nullspace to obtain new equality relationships satisfying both the data and the counter-example. If the nullspace is just the null vector then we return the trivial invariant *true*. This process systematically guides our data-driven algorithm to generate equality relationships that are actual invariants. It also removes some artifacts of test cases: for example, in all tests some pointer p is assigned the same address a then we can infer a spurious equality relationship that $p = a$. A counter-example can remove this spurious equality. However, if the counter-example satisfies Q then the proof fails; this can happen because r might abort on some state for which t does not.

Note that Chapter 2 has a completeness result (Theorem 2 and Theorem 3), which is possible because it deals with a restricted language with no heap and has no specification to verify. Since DDEC handles memory, the possibility of aborting, and need to prove equivalence, it has only a soundness guarantee:

Theorem 5. If all VCs are proven then the target is equivalent to the rewrite and the cutset and the invariants together constitute a simulation relation.




```
void trace(Code c){
  EMIT(next = 0);
  EMIT(save_callee_save_state());

  foreach (Instr i : c){
    if (mem_deref(i))
      EMIT(addr = deref_addr(i));

    EMIT(record(i, next++));
    EMIT(i);
    EMIT(record(i, next++));
  }
}
```

```
void sandbox(Code c){
  EMIT(next = 0);

  foreach (Instr i : c){
    if (mem_deref(i))
      EMIT(sandbox_addr(i));

    EMIT(record(i, next++));

    if (backedge_jump(i))
      EMIT(sandbox_jump(i));
    else if (is_return(i))
      EMIT(sandbox_return());
    else if (is_mem_deref(i))
      EMIT(sandbox_deref(i));
    else
      EMIT(i);

    EMIT(record(i, next++));
  }
}
```

```
void error(bool bit){
  bit = true;
  restore_callee_saved_state();
  ret;
}
```

```
void sandbox_addr(Instr i){
  addr = deref_addr(i);
  if (addr >= s)
    error(sigsegv);
  if (addr >= s')
    return;
  addr -= hmin;
  if (addr<0 || addr>hmax)
    error(sigsegv);
  addr -= &heap[0];
}
```

```
void record(Instr i, int next){
  foreach (GpReg r : gp)
    trace[next].gp[r] = val(r);
  foreach (XmmReg x : xmm)
    trace[next].xmm[x] = val(x);
  foreach (Flag f : eflags)
    trace[next].ef[f] = val(f);
  if (mem_deref(i)) {
    trace[next].addr = addr;
    trace[next].val = *addr;
  }
}
```

```
void sandbox_jump(Instr jump){
  if (++jumps == max)
    error(diverge);
  jump;
}
```

```
void sandbox_return(Instr ret){
  if (!callee_save_restored())
    error(segv);
  ret;
}
```

```
void sandbox_deref(Instr i){
  i.set_deref_addr(addr);
  i;
}
```

Figure 3.2: Implementation of instrumentation for target and rewrite tracing using a JIT assembler. Targets are assumed safe and instrumented using the `trace()` function. Rewrites are instrumented using the `sandbox()` function which is parameterized by values observed during the execution of the target.

3.3 Implementation

DDEC is a prototype implementation of the algorithm discussed in Section 3.2. We discuss the most important and interesting features of the implementation below.

3.3.1 Liveness Computation

Several components of DDEC require the live variables at a program point. For the most part, liveness is computed using a standard dataflow algorithm, but we note the following modification for the x86 architecture. As mentioned previously, for 64-bit x86 some general purpose registers have subregisters. For example, `dil`, `di`, and `edi` refer to the lowest 8, 16, and 32-bits of `rdi`,

respectively:

$$\texttt{dil} \subset \texttt{di} \subset \texttt{edi} \subset \texttt{rdi}$$

To account for this register aliasing, when calculating the read set of an instruction we include the registers it reads, along with all subsets of those registers. An instruction that reads `di`, for example, also reads `dil`. Similarly, when calculating the write set of an instruction we include the registers it writes, along with all super- and subsets of those registers. Some instructions also produce undefined register values, which are treated as killing any live values.

3.3.2 Testcase Generation

For programs that deal exclusively with stack and register values, DDEC is able to produce tests automatically. Using the control flow graph of the target (recall the distinction between the target and rewrite introduced in Section 3.2), DDEC identifies the set of live-in registers and generates random values as necessary. For programs that dereference heap locations, DDEC requires a user-defined environment in which to execute the target. For large software projects, we expect that a representative set of whole-program tests will exist, and DDEC may simply observe the behavior of the code during normal program execution. When no such inputs exist, a user must provide a small unit test harness which will establish whatever heap structures are necessary to enable the functions to execute correctly.

3.3.3 Target Tracing

To observe the values of live program variables at cut-points, we rely on the ability to instrument the target and observe those values dynamically as they appear under representative inputs. This instrumentation is performed using a custom light-weight JIT assembler for 64-bit x86; the `trace()` function is shown in Figure 3.2. Prior to execution, an array of `trace` states are allocated on the heap. For every instruction executed by the target, we emit a call to the `record()` function to copy the majority of the hardware state (general purpose, SSE, and condition registers) as well as values read from or written to the heap, to the back of the array. Array bounds are tracked (not shown), and in the event of overflow additional capacity is added as necessary. When the target function completes execution, the trace array holds a complete record of the values manipulated by the target in both registers and memory.

Because we already assume that users supply tests for target functions that access data structures in memory, in our prototype we have also assumed that the target is safe and will not crash the machine or corrupt DDEC's state on any of the supplied inputs. This assumption held for the experiments in this chapter, however for a production tool it would be necessary to isolate the target from the tool using well-known but more involved techniques (e.g., emulation).

3.3.4 Rewrite Tracing

The correctness assumptions that we make for the target do not hold for all the rewrites in our experiments. For example, some candidate rewrites can and do dereference invalid memory locations (see Section 3.4.4). Thus, our prototype instruments rewrites using the heavier-weight `sandbox()` function (see Figure 3.2). We can, however, take advantage of information observed in tracing the target to simplify the tracing of the rewrite.

From the execution of the target, we obtain the maximum stack size used along with the minimum and maximum heap addresses that were dereferenced. Using these values, we define stack and heap sandboxes to guard the execution of the rewrite. Specifically, we identify the stack pointer, `s`, which defines the upper bound on the frame used by the rewrite, and from this value identify $\texttt{s}'$, a location which defines a frame no larger than the one used by the target. Similarly, we allocate a heap sandbox array large enough to contain each heap dereference performed by the target without aliasing containing values which are initialized to the live-in memory values dereferenced by the target. Memory dereferences are guarded by the `sandbox_addr()` function, which preserves stack accesses inside the bounds of the stack sandbox, redirects valid heap accesses to the heap sandbox, and traps all other accesses and instead produces a safe premature termination. If necessary, both sandboxes may be scaled by a constant user-defined factor to allow for the possibility of a rewrite with greater memory requirements than the target.

In addition to sandboxing memory accesses, several other behaviors need to be checked to protect DDEC from undefined behavior. First, there is the possibility that the rewrite will go into an infinite loop. This behavior is guarded by a call to `sandbox_jump()`, which counts the number of times that a backedge is taken and causes a premature termination if a bound calculated from the number of backwards jumps taken in the target execution is exceeded. Second, we must guarantee that return instructions take place only after certain invariants specific to the x86 application binary interface have been restored. This property is guaranteed by a call to `sandbox_return()`, which checks that the value of callee-saved registers are restored to the state they held when the rewrite began executing.

3.3.5 Invariant Generation

The invariant can be computed by converting the matrix associated with each cutpoint into Howell normal form [48, 141]. This normal form is an extension of reduced row-echelon form [75] albeit suitable for matrices with bit-vector entries and its computation incurs the same overall cubic-time complexity. Our benchmarks do not rely on overflows and underflows, and therefore we guess the invariants using a standard nullspace computation, for which efficient implementations are available. This simplification is sound as the invariants are still checked via bit-vector reasoning.

DDEC computes invariants using the `nullspace` function of the Integer Matrix Library [27] which is specialized for computing the nullspace of integer and rational matrices using p-adic arithmetic. DDEC uses sixteen random tests to generate data for invariant computation. For the experiments in this chapter, these tests were sufficient for obtaining sound invariants and all necessary corresponding paths. For a production system, a larger number of tests would likely be necessary. However at under 2 ms for each null space computation, we do not expect that this computation would be a bottleneck.

3.3.6 VC Generation

Proof obligations are discharged using Z3 [43]. Because Z3 does not currently provide support for floating point operations, DDEC's ability to reason about such instructions is limited as well. However, Z3 does have a complete algorithm for real numbers and one might be tempted to use this capability to reason about floating point programs. Unfortunately, floating point semantics are not over-approximated by reals—a simple example is the non-associativity of floating point addition. Hence, sound optimizations using real semantics may be unsound using floating point semantics.

We manually encode x86 instructions as Z3 formulas, primarily due to lack of access to formal specification of x86 instructions at the hardware level. For example, some x86 instructions, such as `popcnt`, are informally described by Intel as loops. Wherever possible, we deferred to corresponding loop-free implementations given in A Hacker's Delight [148]. Our formulas precisely model the complexity of the x86 instruction set, which in some cases is quite sophisticated (consider the `crc` instruction, which considers bit-vectors as polynomials in $\mathbb{Z}_2$ and performs a polynomial division). Formula correctness is a necessary prerequisite for proof correctness, and unfortunately, testing is the only available option for ensuring this property. Each formula was tested extensively against hardware semi-automatically to check correctness. In the process we rediscovered known instances in which the x86 instruction set deviates from its specification [58]. For such instances, our formulas encode a sound over-approximation of the observed hardware behavior and the specification.

We generate VCs in the quantifier-free theory of bit-vector arithmetic. Z3 is complete for this theory [149] and is able to soundly analyze the effect of x86 instructions on the machine state with bit-wise precision. When generating constraints, registers are modeled, depending on bit-width, as between 8- and 128-bit bit-vectors. Memory is modeled as two vectors: one of 64-bit addresses and one of corresponding 8-bit values (x86 is byte addressable). For 32-bit x86, addresses are restricted to 32 bits.

DDEC translates proof obligations $\{P\}\langle t, r\rangle\{Q\}$, where P and Q are predicates over registers (the invariants can be more general as described in Section 3.2.1), to a VC as follows. DDEC first asserts the constraint P. It then iterates over the instructions in t, written in SSA form, and for each instruction asserts a constraint which encodes the transformation the instruction induces on the current hardware state. These constraints are chained together to produce a constraint on

the final state of live outputs with respect to t. Analogous constraints are asserted for r. In our implementation, operators that are very expensive for Z3 to analyze, such as bit vector multiplication and division, are replaced by uninterpreted functions constrained by some common axioms. Finally, for all pairs of memory accesses at addresses $\texttt{addr}_1$ and $\texttt{addr}_2$, DDEC asserts additional constraints relating their values: $\texttt{addr}_1 = \texttt{addr}_2 \Rightarrow \texttt{val}_1 = \texttt{val}_2$. These aliasing constraints grow quadratically in the number of addresses, though dependency analysis can simplify the constraints in many cases.

Using these constraints, DDEC constructs a Z3 query which asks whether there exists an initial state satisfying P that causes the two code paths to produce values for live outputs which either violate Q or result in different memory states. If the answer is no, then the obligation is discharged, otherwise the prover produces a counter example, and DDEC fails to verify equivalence. If every VC is discharged successfully, then DDEC has proven that the two functions are equivalent.

Although the implementation described above is correct, it is overly conservative with respect to stack accesses. Specifically, an access to a spill slot [7] will appear indistinguishable from a memory dereference, and Z3 will discover a counter-example in which the input addresses to t and r alias with respect to that slot. As a result, any sound optimized code which eliminates stack traffic will be rejected. We address this issue by borrowing an idea from Necula [105], who solves this problem by replacing spill slots with temporary registers that eliminate the possibility of aliasing between addresses passed as arguments and the stack frame. For well-studied compilers such as `gcc` and CompCert, simple pattern matching heuristics are known to be well-suited to this task [105]. For example, for code compiled with `gcc`, all stack accesses are at constant offsets from the register *rbp*. We can create a new register for *rbp-8*, *rbp-16*, and so on and model loads and stores from the stack frame by loads and stores from these temporaries. Modeling spill slots in this way could result in unsound results if an input address is used to form an offset into the current stack frame. However, this behavior is undefined even in the high-level languages that in theory permit it (e.g., C) and, to the best of our knowledge, existing optimizing compilers are also unsound for such programs.

Given that we have gone to the effort to construct a faithful symbolic encoding of the x86 instruction set, the reader might wonder why we do not simply obtain the simulation relation statically—what does data add? The answer is that inference is harder than checking. Consider an example where we compute the dot product of two 32-bit arrays, where the multiplication of two 32-bit unsigned numbers is used to produce a 64-bit result. Say the target uses Karatsuba's trick [87] and performs three 32-bit *signed* multiplications to obtain a 64-bit result, whereas the rewrite uses a special x86 instruction that performs an *unsigned* multiplication of two 32-bit numbers and directly produces a 64-bit result. A static analysis that attempts to discover the relationship between Karatsuba's trick and the special x86 instruction has a very large search space containing many other plausible proof strategies to sift through, and in fact we know of no inference technique that can reliably perform such reasoning. In contrast, with DDEC the equality simply manifests itself in the data, and knowing that this specific equality is what needs to be checked narrows the

search space to the point that off-the-shelf solvers can verify this fact automatically.

3.4 Experiments

We summarize our experiments with DDEC on a number of benchmarks drawn from both the literature and from existing compiler test suites. In doing so, we demonstrate the relationship between DDEC and the state of the art in translation validation, the use of DDEC in the optimization of a production codebase, and show how DDEC enables the design of novel applications using existing compiler toolchains. Specifically, we use DDEC to combine the correctness guarantees of CompCert with the performance properties of `gcc -O2`, and to extend the applicability of a binary superoptimizer to functions containing loops.

Experiments were performed on a 3.40 GHz Intel Core i7-2600 CPU with 16 GB of RAM. For each experiment we report the number of assembly instructions for target and rewrite, the number of loops contained in each function, the run-time required for DDEC to verify equivalence, and where applicable the observed performance improvement between target and rewrite. Run-times for all experiments were tractable, varying from under a second to several hours, depending on the complexity of the constraints. Memory usage was not an issue and did not exceed 500Mb.

It is worth noting that many of the invariants discovered by DDEC, such as $4 * \texttt{eax} = \texttt{edx}' + 3$ and $10 * \texttt{eax} + \texttt{edx} = \texttt{ecx}'$, were non-trivial. In all cases the run-time required to run tests, infer equality relationships and generate proof obligations was minimal (a few milliseconds) compared to the run-time required to discharge the VCs. Essentially all of DDEC's run-time was spent in Z3 queries.

3.4.1 Micro-benchmarks

In this section, we attempt to provide a detailed comparison between DDEC and techniques based on equality saturation [81, 140]. Equality saturation [140] is a state of the art technique for verifying compiler optimizations which relies on expert-written equality rules, such as "multiplication by two is equivalent to a bit shift". Beginning from both the target and the rewrite, the repeated application of these rules is used to attempt to identify a common representation of both functions, the existence of which implies equality. Unsurprisingly, the technique is precisely as good as the expert rules that it has at its disposal. Missing rules correspond to optimizations for which equivalence cannot be proven. Furthermore, identifying such rules for a CISC architecture such as x86 is a daunting task. As a result, the application of equality saturation has been limited to the verification of optimizations in several intermediate RTL languages.

We compare DDEC to equality saturation using the two motivating examples described in the original paper [140], the first of which appears in Section 3.1; these correspond to the first two rows in Table 3.1. Each example consists of two pairs of programs demonstrating strength reductions. We

Program	LOC	#Loop	Run-time
lerner1a1b	29/26	1	19.39s
lerner3b3c	32/32	2	102.89s
unroll	13/20	1	75.04s
off-by-one	15/14	1	0.13s

Table 3.1: Performance results of DDEC for micro-benchmarks. LOC shows lines of assembly of target/rewrite pair.

Program	Run-time (s)
lerner1a	12.94
lerner3b	53.72
bansal	9.89
chomp	11.00
fannkuch	17.03
knucleotide	6.56
lists	1.40
nsievebits*	36.44
nsieve*	166.31
qsort*	140.87
sha1*	12888.87

Table 3.2: Performance results for CompCert and gcc equivalence checking for the integer subset of the CompCert benchmarks and the benchmarks in this chapter. LOC shows lines of assembly code for the binaries generated by CompCert/gcc. Test is the maximum number of random tests required to generate a proof. A star indicates that a unification of jump instructions was required.

Program	LOC	#Loop	Run-time	Speedup O0/O3
Bansal	9/6	1	44s/5492.75s	1.58x/1.04x
SAXPY	9/9	1	211s/0.62s	9.22x/1.48x

Table 3.3: Performance results for gcc and Stoke+DDEC equivalence checking for the loop failure benchmarks in [126]. LOC shows lines of assembly code for the binaries generated by Stoke/Stoke+DDEC. Run-times for search/verification are shown along with speedups over gcc -O0/O3.

compile each pair with gcc -O0 to both transform the functions into a format that DDEC accepts and to preserve the structure of the original optimizations as best as possible. DDEC successfully proves the equivalence of the resulting binaries.

Equality saturation, in its current form, is unable to handle important optimizations such as loop unrolling [140]. The unroll benchmark in Table 3.1 is an equivalence checking task involving loop unrolling. We take a program which walks over a linked list and unroll it to obtain a new program that walks over two elements in every iteration (Figure 3.3). Hence, we are able to handle optimizations that equality saturation cannot even in the presence of an extensive set of expert written rules.

When given two programs that are semantically different, the process of equality saturation is not guaranteed to terminate. It simply continues applying rules indefinitely in an attempt to prove that the two programs are equal. When given two semantically different programs, DDEC always terminates with a counter-example (Z3 is complete for the VCs we use). Note that counter-examples

```
// Target:
while( p != null ) { p=p->next; ... }

// Rewrite (Unrolled once):
while( p != null ) {
  p=p->next; ...
  if ( p != null ) { p=p->next; ... }
}
```

Figure 3.3: Abstracted codes (target and rewrite) for `unroll` of Table 3.1.

```
// Target:
for ( i = len - 1;     i >= 0; --i ) { ... }

// Rewrite (with off-by-one error):
for ( i = len /*BUG*/; i >= 0; --i ) { ... }
```

Figure 3.4: Abstracted codes (target and rewrite) for `off-by-one` of Table 3.1.

are also possible even for equivalent programs because DDEC is incomplete.

Counter-examples from a failed proof can be used to explain why DDEC believes that a target/rewrite pair are not equivalent. To demonstrate this ability, we take a program which walks backwards over an array and introduce an off-by-one error (Figure 3.4). We compile both programs with `gcc -O0` and use the correct program as the target and the buggy version as the rewrite. When we ask DDEC to prove the equivalence of the two programs, DDEC fails and terminates with a counter-example (`off-by-one` in Table 3.1). Hence, DDEC can be used for finding equivalence bugs. However, in general, it is difficult to map the counter-example at the assembly level to the source code, and especially in the presence of compiler optimizations. A version of DDEC that works on source code and finds equivalence bugs is left as future work.

3.4.2 Full System Benchmark

One criticism of DDEC is that it is not purely static: it requires tests. However, we believe that for many systems existing regression tests should suffice. To validate this belief, we perform a case study with OpenSSL. The core computation routine of OpenSSL is big number multiplication: a loop which multiplies n-bit numbers stored as arrays. OpenSSL includes performance tests which use this multiplication loop extensively. For example, the RSA performance test included with OpenSSL executes the core more than fifteen million times.

We instrument OpenSSL to obtain these tests and select sixteen tests at random from the large number performed. We compile the core using `gcc -O0` and `gcc -O3` and use the tests to drive DDEC, which is then able to prove the equivalence in about two hours. We also find that the

maximum time taken by any individual VC is ten minutes. Since checking proof obligations is an embarrassingly parallel task, if we assign a single CPU for every obligation then the proof can be obtained in ten minutes. When we measure the sensitivity of DDEC to the number of tests for this example, we find that 6-8 randomly selected tests are sufficient to obtain a proof.

Hence, for verifying the optimizations of kernels, it seems possible to obtain sufficient tests from existing test suites to drive verification. The tests included with programs might not exercise all parts of the code but they will exercise the performance-critical parts well and hence we believe DDEC can be successfully applied to the performance-critical kernels. Being data-driven, our technique will fail to prove interesting optimizations performed on dead code or the part of code exercised rarely by tests; a static equivalence checking engine for x86, if it existed, could have succeeded here.

3.4.3 CompCert

CompCert is a certified compiler for a subset of the C programming language: it is guaranteed to produce binaries that are semantically equivalent to the input source code. CompCert 1.12, the current version, does not perform loop optimizations and its compilation model does not fit well with CISC architectures such as x86, due to their "paucity of [general purpose] registers" [96].

We use DDEC to verify the equivalence of binaries generated by CompCert and `gcc -O2 -m32`. The `-m32` flag is necessary for compatibility with CompCert, which only produces 32-bit x86 binaries. Furthermore, optimization is restricted to `-O2` because, for these benchmarks, higher optimization levels produce only syntactic differences that do not affect DDEC. In doing so, we are able to extend the correctness guarantees made by CompCert to the more performant but uncertified code generated by `gcc`.

Performance data is shown in Table 3.2 for the integer subset of the CompCert compiler test suite (the benchmarks in the `test/c` directory of the CompCert 1.12 download) and several of the benchmarks described in this section. For the CompCert benchmarks, we profile each program and report results for the one loop (possibly containing other loops) that dominates execution time. The results are encouraging; DDEC is able to prove equivalence in all cases. We note, however, that DDEC did encounter difficulty with some of the benchmarks due to the restrictive logic that it uses. The problem is illustrated by the following example:

Target:

```
if(0<n) {for (i=0; i<n; i++);} return i;
```

Rewrite:

```
if(0<n) {for (i=0; i!=n; i++);} return i;
```

To prove the equivalence of these two functions, DDEC requires the inductive invariant $i = i' \wedge n = n' \wedge i \leq n$. Crucially, $i \leq n$ is inexpressible with equalities. For the final four benchmarks in Table

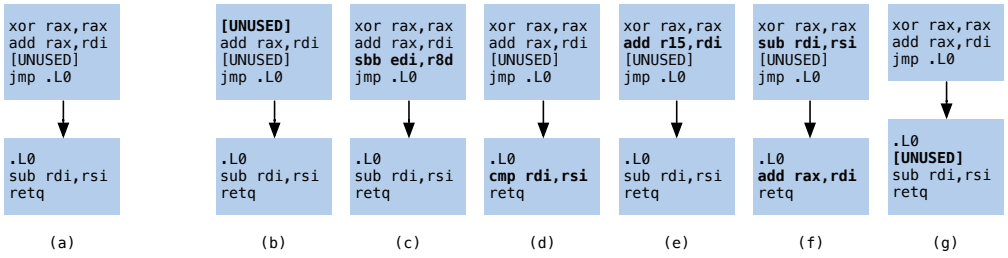


Figure 3.5: STOKE moves applied to a representative code (a). Instruction moves randomly produce the UNUSED token (b) or replace both opcode and operands (c). Opcode moves randomly change opcode (d). Operand moves randomly change operand (e). Swap moves interchange two instructions either within or across basic blocks (f). Resize moves randomly change the allocation of instructions to basic blocks (g).

3.2 (the ones marked with a star), DDEC reported failure due to `gcc` replacing an inequality by a dis-equality. For these benchmarks it was necessary to manually make the test predicates identical before performing a successful equality verification. DDEC can also be combined with an abstract interpreter over binaries [118, 142]: these are capable of finding invariants over state elements of a single program (such as $i \leq n$). The subsequent chapters of this dissertation (Chapter 4 and Chapter 5) also discuss techniques for inequalities. Finally, it is also straightforward to extend DDEC to recognize this common special case.

We note that the long verification time required for `sha1` is due to the large numeric constants used by this cryptographic computation that lead to poor performance in the underlying Z3 theorem prover. We confirmed that if these constants are replaced by small integers the proof obligations are discharged in a few minutes.

3.4.4 STOKE

STOKE [126] is an x86 binary superoptimizer based on the principle that program optimization can be cast as a stochastic search problem. Given a suitable cost function and run for long enough (which may be an extremely long time), STOKE is guaranteed to produce a code with the lowest cost [126]. STOKE performs binary optimization by executing up to billions of small random modifications to a program. For each modification, STOKE evaluates a cost function representing a combination of correctness and performance metrics. STOKE accepts all modifications that decrease the value of this function, and with some probability also accepts modifications that increase the value. Although most of the programs that STOKE considers are ill-formed, the sheer volume of programs that it evaluates leads it in practice to discover correct optimizations. STOKE runs for a user-defined amount of time and returns the lowest cost program that it can prove equivalent to the original program.

Previous work on STOKE demonstrated promising results for loop-free kernels. Beginning from

code compiled using `llvm -O0`, STOKE produces programs that outperform code produced by `gcc -O3` and in some cases outperforms handwritten assembly. Unfortunately, STOKE's application to many interesting high-performance kernels is limited by its inability to reason about equivalence of codes containing loops. We address this limitation by extending STOKE's set of program transformations to include moves which enable loop optimizations and replacing STOKE's equivalence checker by DDEC. Our version of STOKE is able to produce optimizations for the loop benchmarks that could not be fully optimized in [126].

STOKE's underlying program representation is a constant length sequence of 64-bit x86 instructions. STOKE uses a special [UNUSED] token in place of a valid x86 instruction to represent programs that are shorter than this length. STOKE explores candidate rewrites using the following transformations. Instruction moves replace a random instruction with either the [UNUSED] token or with a completely different random instruction. Operand and opcode moves randomly replace the value of a random operand or opcode respectively. And finally, swap moves interchange two instructions at random. STOKE's program transformations are all intra-basic block, and it does not allow moves which modify control flow structure. Our implementation of STOKE remedies these shortcomings by introducing an inter-basic block swap move (Figure 3.5f) and a basic block resizing move (Figure 3.5g), which changes the number of instructions allowed inside a basic block. These simple extensions are sufficient to allow for the exploration of rewrites which include loop-invariant code motion, strength reduction, and most other classic loop optimizations.

The cost function used by STOKE to evaluate transformations includes two terms, a correctness term and a performance term. We leave the correctness term described by [126] unmodified. Candidate rewrites are executed in a memory sandbox on a representative set of tests. Values contained in live memory and registers are compared against the corresponding values produced by the target and penalties are assessed for bits which are incorrect or appear in the wrong location. STOKE approximates the performance of a candidate rewrite by summing the expected latencies of its constituent instructions in nanoseconds. We modify this function to account for loop nesting depth, $\texttt{nd}(\cdot)$ as follows, where w is a constant which we set to 20.

$$\texttt{perf}(C) = \sum_{bb \in C} \sum_{i \in bb} E\big[\texttt{latency}(i)\big] \cdot w^{\texttt{nd}(bb)}$$

We now discuss the failure cases of STOKE: the benchmarks of [126] for which STOKE produces code inferior to `gcc -O3`. The other benchmarks of [126] are loop free and are not relevant here. Our modified version of STOKE is able to produce the two optimizations shown (simplified) in the lower half of Figure 3.6. The optimizations produced by the original version of STOKE are shown above for reference. Figure 3.6a is a linked-list traversal. The kernel iterates over the elements in the list until it discovers a null pointer and multiplies each element by two. Our modified version of STOKE is able to cache the value of the head pointer in a register across loop iterations. Figure

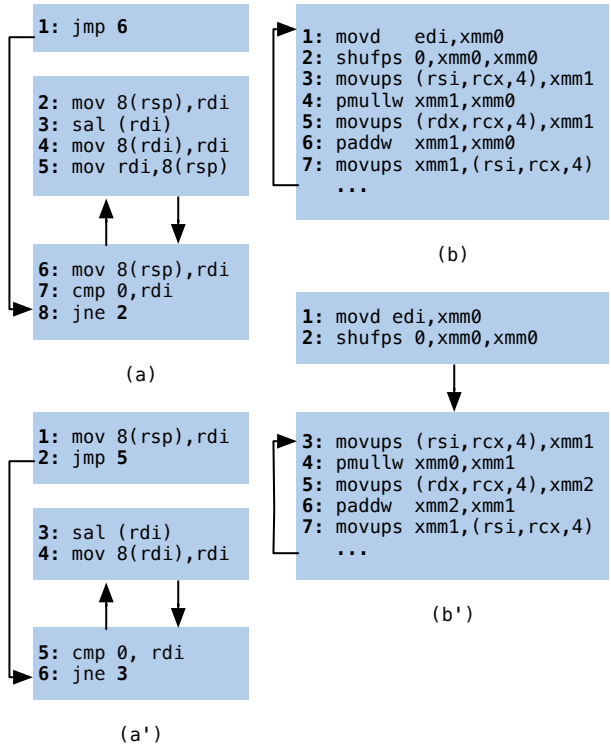


Figure 3.6: Simplified versions of the optimizations produced and verified by our modified version of STOKE. The iteration variable in (`a`) is cached in a register (`a'`). The computation of the 128-bit constant in (`b`) is removed from an inner loop (`b'`).

3.6b performs the BLAS vector function $a \cdot \vec{x} + \vec{y}$. Whereas the original version of STOKE is able to produce an optimization using vector intrinsics, our version is able to further improve on that optimization by first performing a register renaming and removing the invariant computation of a 128-bit constant from the loop. The code motion is not possible if the registers are not suitably renamed first.

Performance data for these experiments are shown in Table 3.3. We note that the time spent verifying `bansal` is significantly greater than what was reported for the COMPCERT benchmarks. This is because STOKE produces 64-bit as opposed to 32-bit x86 binaries, which results in more complex memory equality constraints. The aim of our experiments is to describe the effectiveness of our core ideas and standard heuristics for constraint simplification, which we have not implemented, can be applied to achieve better performance [46]. To illustrate just how important constraint simplification is, for the SAXPY benchmark, following [151] we assumed that distinct memory accesses do not alias and performed slicing on VCs to eliminate constraints that are not relevant to the verification task. The result is that verification requires less than a second, a significant

improvement and the fastest verification time in our benchmark suite. Without these constraint simplifications, DDEC times out after four hours. This suggests that there is substantial room left for further performance optimization of DDEC's generated constraints; however such optimizations increase the size of the trusted code base, which is currently just the circuits for instructions, VC generator, and the theorem prover. Since STOKE starts optimizations from `llvm -O0` compilations, our verification results imply that STOKE+DDEC can produce binaries comparable to `gcc -O3` in performance and provably equivalent to unoptimized binaries generated by `llvm`.

3.5 Related Work

Our approach borrows a number of ideas from previous work on equivalence checking [42], translation validation [105], and software verification [129]. Combining these ideas with our technique for guessing the simulation relation from tests yields the first equivalence checking engine for loops written in x86. Previously, in a closely related work, AXE inferred invariants by pattern matching on tests and used them to prove the equivalence of different implementations of cryptographic routines [135].

Program equivalence checking is an old problem with references that date back to the 1950s. Equivalence checking is common practice in hardware verification, where it is well known that cutpoints play a critical role in determining equality. In sequential equivalence checking, for example, state-carrying hardware elements constitute cutpoints. Equivalence checking of low-level code has also been studied for embedded software [6, 42, 51, 52, 134]. None of these techniques support `while` loops and so are not applicable to our benchmarks.

Our goal is more ambitious than the state of the art in equivalence checking for general purpose languages: DDEC is a practically useful, automatic, and sound procedure for checking equivalence of loops. UC-KLEE [117] performs a bounded model checking that checks equivalence for all inputs up to a certain size. In another version of bounded model checking, differential symbolic execution [112] and SymDiff [90] bound the number of iterations of loops. Semantic Diff [79] checks only whether dependencies are preserved in two procedures. The approach in [97] handles neither while loops nor pointers. Regression verification [59] handles only partial equivalence: it does not deal with termination. As an alternative to DDEC, one can imagine composing two programs into a single program and then using an abstract interpreter [111]. However, the composition of [111] relies on syntactic heuristics that seem difficult to apply to binaries.

Fractal symbolic analysis [101] and translation validation [60, 105, 115] are two techniques that reason about loops in general. Both rely on information about the compiler, such as the specific transformations that the compiler can perform. Hence, these are not directly applicable to the problem of equivalence checking of code of unknown provenance. If one is simply given two assembly programs to check for equivalence there is no "translation" and hence translation validation is not

applicable.

Conceptually, if one tries to port the approach of Necula [105] to x86, then one will need to build a static analysis for x86 which is sound and precise enough to generate simulation relations. This is a decidedly non-trivial engineering task and has never been done (see Section 3.3.6); DDEC sidesteps this issue by using concrete executions (i.e., tests) for finding cutpoints and generalizing from tests to invariants. In addition, the constraints generated by symbolically executing x86 opcodes are complicated enough that we believe that the decision procedure of [105] will fail to infer equalities in most cases. Nonetheless, compiler annotations are a rich source of high level information, and as a result translation validation techniques can handle transformations that DDEC currently cannot, such as reordering traversals over matrices. For DDEC to handle such programs we would need better invariant inference algorithms that can infer quantified invariants fully automatically.

Some of the most recent work on equivalence checking includes random interpretations [65] and equality saturation [140, 144]. The former represents programs as polynomials which it requires to be of low degree. Unfortunately, bit-manipulations and other similar machine-level instructions are especially problematic for this technique. For example, a shift left by one bit has a polynomial of degree 2^{63} for the carry flag. Unlike equality saturation, DDEC does not rely on expert provided equality relationships between program constructs, which would be difficult to produce by hand for a CISC architecture such as x86. Further comparison with equality saturation is in Section 3.4.1.

Chapter 4

Disjunctive Invariants

In the earlier chapters, we restricted the invariants to conjunctions of algebraic equalities. In this chapter, we discuss a Guess-and-Check algorithm to infer arbitrary boolean combinations of inequalities. Therefore, the improvements are two fold: the user does not need to provide a bound on the number of disjunctions (the degree in Chapter 2) and the relationships are in a more expressive class (inequalities subsume equalities). In contrast to previous chapters, we do not aim to find the strongest invariant of the class; the strongest invariants that can be expressed using arbitrary boolean combinations of inequalities have unbounded sizes for infinite state programs. Instead, we are interested in inferring invariants that are strong enough to verify the properties of interest. There is a major difference between these two problem descriptions. The latter includes a program and a property, whereas the former problem is about the strongest invariant of a program and is independent of the property to be checked. Consequently, in addition to reachable states, the algorithms we develop here need additional data that depend on the property to be verified.

To obtain an inference engine for disjunctive invariants, we formalize the problem of safety verification as a learning problem, showing that loop invariants can be regarded as geometric concepts in machine learning. Safety properties define *bad* states: states a program should not reach. Program verification explains why a program's set of reachable (*good*) states is disjoint from the set of bad states. In Hoare Logic, these explanations are predicates that form inductive invariants. Informally, an invariant is a predicate that separates good and bad program states and once we have obtained strong invariants for all the loops, standard VC generation based techniques can be used to generate program proofs. The motivation for using machine learning for invariant inference is twofold: guarantees and expressiveness.

Standard verification algorithms observe some small number of behaviors of the program under consideration and extrapolate this information to (hopefully) get a proof for all possible behaviors of the program. The extrapolation is a heuristic and systematic ways of performing extrapolation are

unknown, except for the cases where they have been carefully designed for a particular class of programs/invariants (e.g., equality invariants in Chapter 2). SLAM [12] generates new predicates from infeasible counter-example traces. Interpolant based techniques [80] extrapolate the information obtained from proving the correctness of finite unwindings of loops. In abstract interpretation [37], fixpoint iterations are performed for a few iterations of the loop and this information is extrapolated using a widening operator. In any of these heuristics, and others, there is no formal characterization of how well the output of the extrapolation strategy approximates the true invariants.

Extrapolation is the fundamental problem attacked by machine learning: A learning algorithm has some finite training data and the goal is to learn a function that generalizes for the infinite set of possible inputs. For classification, the learner is given some examples of good and bad states and the goal is to learn a predicate that separates all the good states from all the bad states. Unlike standard verification approaches that have no guarantees on extrapolation, learning theory provides formal generalization guarantees for learning algorithms. These guarantees are provided in learning models that assume certain oracles. However, it is well known in the machine learning community that extrapolation engines that have learning guarantees in the theoretical models tend to have good performance empirically. The algorithms have been applied in diverse areas such as finance, biology, and vision: we apply learning algorithms to the task of invariant inference.

Standard invariant generation techniques find invariants of a restricted form: there are restrictions on expressiveness that are not due to efficiency considerations but instead due to fundamental limitations. These techniques especially have trouble with disjunctions and non-linearities. Predicate abstraction restricts invariants to a boolean combination of a given set of predicates. Existing interpolation engines cannot generate non-linear predicates [80]. Template based approaches for linear invariants like [71] require a template that fixes the boolean form of the invariant and approaches for non-linear invariants [125] can only find conjunctions of polynomial equalities. Abstract interpretation over convex hulls [40] handles neither disjunctions nor non-linearities. Disjunctions can be obtained by performing disjunctive completion [38, 53], but widening [8] places an ad hoc restriction on the number of disjuncts. Our learning algorithm is strictly more expressive than these previous approaches: It can generate arbitrary boolean combinations of polynomial inequalities (of a given degree). Hence there are no restrictions on the number of disjuncts and we go beyond linear inequalities and polynomial equalities.

Unsurprisingly, our learning algorithm, with such expressive power, has high computational complexity. Next, we show how to trade expressiveness for computational speedups. We construct efficient machine learning algorithms, with formal generalization guarantees, for generating arbitrary boolean combinations of constituent predicates when these predicates come from a given set of predicates (predicate abstraction), when the size of integer constants in the predicates are bounded, or from a given abstract domain (such as boxes or octagons). Note that these efficient algorithms with reduced expressiveness still generate arbitrary boolean combinations of predicates.

Our main insight is to view invariants as geometric concepts separating good and bad states. This view allows us to make the following contributions:

- We show how to use a well known learning algorithm [22] for the purpose of computing candidate invariants. This algorithm is a PAC learner: it has generalization guarantees in the PAC (probably approximately correct) learning model. The learning algorithm makes no assumption about the syntax of the program and outputs a candidate invariant that is as expressive as arbitrary boolean combinations of linear inequalities.
- The algorithm of [22] is impractical. We parametrize the algorithm of [22] by the abstract domain in which the linear inequalities constituting the invariants lie, allowing us to obtain candidates that are arbitrary boolean combinations of linear inequalities belonging to the given abstract domain. We obtain efficient PAC learning algorithms for generating such candidates for abstract domains requiring few variables, such as boxes or octagons and finite domains such as predicate abstraction.
- We augment our learning algorithms with a theorem prover to obtain a sound procedure for computing invariants. This idea of combining procedures for generating likely invariants with verification engines has been previously explored in [108, 129, 131]. We evaluate the performance of this procedure on challenging benchmarks for invariant generation from the literature. We are able to generate invariants, using a small amount of data, in a few seconds per loop on these benchmarks.

The rest of the chapter is organized as follows: We informally introduce our technique using an example in Section 4.1. We then describe necessary background material, including the learning algorithm of [22] (Section 4.2). Section 4.3 describes the main results of this chapter. We first give an efficient algorithm for obtaining likely invariants from candidate predicates (Section 4.3.1). Next, in Section 4.3.1, we obtain efficient algorithms for the case when the linear inequalities constituting the invariant lie in a given abstract domain. In Section 4.3.2, we extend [22] to generate candidates that are arbitrary boolean combinations of polynomial inequalities. Finally, Section 4.3.3 describes our sound procedure for generating disjunctive invariants. Section 4.4 describes our implementation and experiments. Finally, we discuss related work in Section 4.5.

4.1 Overview of the Technique

Consider the program in Figure 4.1 [80]. To prove that the assertion in line 3 is never violated, we need to prove the following Hoare triple:

$$\{x = i \wedge y = j\}\texttt{while (x != 0) do x--; y--}\{i = j \Rightarrow y = 0\}$$

```
1: x := i; y := j;
2: while (x != 0) { x--; y--; }
3: if (i == j) assert (y == 0);
```

Figure 4.1: Motivating example for disjunctive invariants.

In general, to prove $\{P\}$ `while` E `do` S $\{Q\}$, where E is the loop condition and S is the loop body, we need to find a *loop invariant* I satisfying $P \Rightarrow I$, $\{I \wedge E\}S\{I\}$, and $I \wedge \neg E \Rightarrow Q$. Thus, to verify that the program in Figure 4.1 does not violate the assertion, we need a loop invariant I such that $(x = i \wedge y = j) \Rightarrow I$, $\{I \wedge x \neq 0\}S\{I\}$, and $I \wedge x = 0 \Rightarrow (i = j \Rightarrow y = 0)$. The predicate $I \equiv i = j \Rightarrow x = y$ is one such invariant [80].

There is another way to view loop invariants. For simplicity of exposition, we restrict our attention to *correct* programs that never violate assertions (e.g., Figure 4.1). A *state* is a valuation of the program variables, for example $(i, j, x, y) = (1, 0, 1, 0)$. Consider the set of states at the loop head (the `while` statement of Figure 4.1) when the program is executed. All such states are *good* states, that is, states that a correct program can reach. A *bad* state is one that would cause an assertion violation. For example, if we are in the state $(i, j, x, y) = (1, 1, 0, 1)$ at the loop head, then execution does not enter the loop and violates the assertion.

An invariant strong enough to prove the program correct is true for all good states and false for all bad states. Therefore, if one can compute the good states and the bad states, an invariant will be a predicate that *separates* the good states from the bad states. Of course, in general we cannot compute the set of all good states and the set of all bad states. But we can always compute some good and bad states by sampling the program.

To generate samples of good states, we simply run the program on some inputs. If we run the program in Figure 4.1 with the initial state $(1, 0, 1, 0)$, we obtain the good samples $(1, 0, 1, 0)$ and $(1, 0, 0, -1)$. To compute bad states, we can sample from predicates under-approximating the set of all bad states. For Figure 4.1, $(x = 0 \wedge i = j \wedge y \neq 0)$ is the set of bad states that do not enter the loop body and violate the assertion, and $(x = 1 \wedge i = j \wedge y \neq 1)$ is the set of bad states that execute the loop body once and then violate the assertion. Note that such predicates can be obtained from the program using a standard weakest precondition computation. Finally, we find a predicate separating the good and bad samples.

But how can we guarantee that a predicate separating the good samples from the bad samples also separates *all* good states from *all* bad states? In machine learning, formal guarantees are obtained by showing that the algorithm generating these predicates *learns* in some learning model. There are several learning models and in this chapter we use Valiant's PAC (probably approximately correct) model [146]. An algorithm that learns in the PAC model has the guarantee that if it is given enough independent samples then with a high probability it will come up with a predicate that will separate, with high probability, a new freshly drawn good sample from a fresh bad sample. Hence,

under the assumptions of the PAC model, we are guaranteed to find good candidate invariants with high probability. However, just like any other theoretical learning model, the assumptions of PAC model are generally impossible or at least very difficult to realize in practice. We emphasize that in the variety of applications in which PAC learning algorithms are applied, the assumptions of the PAC model are seldom met. Hence, the question whether generalization guarantees in a learning model are relevant in practice is an empirical one. PAC has intimate connections with complexity theory and cryptography and is one of the most widely used models. We demonstrate empirically in Section 4.4 that PAC learning algorithms successfully infer invariants.

Bshouty et al. [22] presented a PAC learning algorithm for geometric concepts (see Section 4.2.2). This algorithm can produce predicates as expressive as arbitrary boolean combinations of linear inequalities. In particular, the invariant required for Figure 4.1 is expressible using this approach. However, this expressiveness has a cost: the algorithm of [22] is exponential in the number of program variables. To obtain polynomial time algorithms in the number of samples and program variables we must restrict the expressiveness. Assume, for example, that we knew the invariant for the program in Figure 4.1 is a boolean combination of octagons (which it is). For octagons, the linear inequalities are of the form $\pm x \pm y \leq c$, where x and y are program variables and c is a constant (Section 4.3.1). We extend [22] to obtain a PAC learning algorithm for obtaining a predicate, separating good and bad samples, that is an arbitrary boolean combination of linear inequalities belonging to a given abstract domain. The time complexity of our algorithm increases gracefully with the expressiveness of the chosen abstract domain (Section 4.3.1). For example, the complexity for octagons is higher than that for boxes.

We augment our learning algorithm with a theorem prover (Section 4.3.3), obtaining a sound algorithm for program verification. Empirically, we show that the predicates discovered by our approach are provably invariants using standard verification engines (Section 4.4).

4.1.1 Finding Invariants for the Example

We now explain how our sound algorithm (Section 4.3.3) for program verification (parametrized by octagons) proves the correctness of the program in Figure 4.1. To sample the good states, assume we run the program on inputs where $i, j \in \{0, 1, 2\}$. As suggested above, we obtain bad states by sampling the predicate representing violations of the assertion after going through at most one loop iteration: $x = 0 \wedge i = j \wedge y \neq 0 \vee x = 1 \wedge i = j \wedge y \neq 1$. In total, for this example, we generated 18 good samples and 24 bad samples. The algorithm of [22] first generates a large set of candidate hyperplanes representing all linear inequalities possibly occurring in the output predicate. We build this set by constructing all possible hyperplanes (of the form $\pm x \pm y = c$) passing through every state. For instance, the state $(2, 2, 0, 0)$ generates twenty four hyperplanes: $x = 0$, $x = y$, $i \pm x = 2$,.... Section 4.3.1 justifies this choice of the set of candidates.

From this large set of hyperplanes, we pick a subset that successfully separates the good and bad

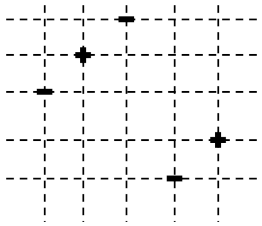


Figure 4.2: Candidate inequalities passing through all states.

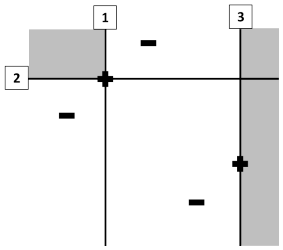


Figure 4.3: Separating good states and bad states using boxes.

samples. Note that every good sample must be separated from every bad sample. Several algorithms can be used to solve this problem. We describe how a standard greedy approach would work. We keep track of the pairs of samples, one good and the other bad, that have not yet been separated by any hyperplane, and repeatedly select from the set of candidate hyperplanes the one that separates the maximum number of remaining unseparated pairs, repeating until no unseparated pairs remain.

We illustrate this process in Figures 4.2 and 4.3. The +'s are the good states, and the −'s are the bad states. Assume that our abstract domain is the box or interval domain, that is, the predicates are inequalities of the form $\pm x \leq c$. We first generate our candidates, that is, hyperplanes of the form $x = c$ passing through all the good and bad states. These corresponds to all possible horizontal and vertical lines passing through all the + and − states as shown in Figure 4.2. Next, from this set of candidate lines, we initially select line 3, separating one good state from three bad states, which is the maximum number of pairs separated by any of the lines. Next, we select line 1 because it separates one good state from two bad states. Finally, we select line 2, separating the final pair of one good state and one bad state. The lines tessellate the space into cells, where each cell is a conjunction of boxes bounding the cell and no cell contains both a good and a bad state. Each shaded cell in Figure 4.3 represents a conjunction of boxes that includes only the good states. The returned predicate is the set of all shaded cells in Figure 4.3, which is a disjunction of boxes.

By a similar process, for the 42 states generated from Figure 4.1 and using the octagon domain, our tool infers the predicate $I \equiv i \leq j+1 \vee j \leq i+1 \vee x = y$ in 0.06 seconds. We annotated the loop of Figure 4.1 with this predicate as a candidate loop invariant and gave it to the BOOGIE [13] program checker. BOOGIE was successfully able to prove that I was indeed a loop invariant and was able to show that the assertion holds. As another example, on parameterizing with the Octahedron [31] abstract domain, our technique discovers the simpler conjunctive loop invariant: $i + y = x + j$ in $0.09s$.

4.2 Preliminaries

This section presents necessary background material, including the learning algorithm of [22]. Our goal is to verify a *Hoare triple* $\{P\}\mathcal{S}\{Q\}$ for the simple language of *while programs* defined as follows:

$$\mathcal{S} ::= \ x{:=}M \mid \mathcal{S}; \mathcal{S} \mid \texttt{if } E \texttt{ then } \mathcal{S} \texttt{ else } \mathcal{S} \mid \texttt{while } E \texttt{ do } \mathcal{S}$$

The while program $\mathcal{S}$ is defined over integer variables, and we want to check whether, for all states s in the precondition P, executing $\mathcal{S}$ with initial state s results in a state satisfying the postcondition Q. In particular, if $L \equiv \texttt{while } E \texttt{ do } S$ is a while program, then to check $\{P\}L\{Q\}$, Hoare logic tells us that we need a predicate I such that $P \Rightarrow I$, $\{I \wedge E\}S\{I\}$, and $I \wedge \neg E \Rightarrow Q$. Such a predicate I is called an *inductive invariant* or simply an *invariant* of the loop L. Once we have obtained invariants for all the loops, then standard techniques can generate program proofs [13]. We first focus our attention on invariants in the theory of *linear arithmetic*:

$$\phi ::= w^T x + d \geq 0 \mid \mathit{true} \mid \mathit{false} \mid \phi \wedge \phi \mid \phi \vee \phi \mid \neg\phi$$

where $w = (w_1, \ldots, w_n)^T \in \mathbb{Q}^n$ is a *point*, an n-dimensional vector of rational number constants. The vector $x = (x_1, \ldots, x_n)^T$ is an n-dimensional vector of variables. The *inner product* $\langle w, x\rangle$ of w and x is $w^T x = w_1 x_1 + \ldots + w_n x_n$. The equation $w^T x + d = 0$ is a *hyperplane* in n dimensions with *slope* w and *bias* d. Each hyperplane *corresponds* to an intersection of two *half-spaces*: $w^T x + d \geq 0$ and $w^T x + d \leq 0$. For instance, $x - y = 0$ is a 2-dimensional hyperplane, $x - y + 2z = 0$ is a 3-dimensional hyperplane, and $x \geq y$ and $x \leq y$ are half-spaces corresponding to the hyperplane $x = y$.

4.2.1 Invariants and Binary Classification

Assume that the Hoare triple $\{P\}\texttt{while } E \texttt{ do } S\{Q\}$ is valid. Let the loop L have n variables $x = \{x_1, \ldots, x_n\}$. Therefore, the precondition $P(x)$ and postcondition $Q(x)$ are predicates over x. If the loop execution is started in a state satisfying P and control flow reaches the loop head after zero or more iterations, then the resulting state is said be *reachable* at the loop head. Denote the set of all reachable states at the loop head by $\mathcal{R}$. Since the Hoare triple is valid, all the reachable states are *good* states. On the other hand, if we execute the loop from a state y satisfying $\neg E \wedge \neg Q$, then we will reach a state at the end of the loop that violates the postcondition, that is, y satisfies $\neg Q$. We call such a state a *bad state*. Denote the set of all bad states by $\mathcal{B}$. Observe that for a correct program, $\mathcal{R} \Rightarrow \neg\mathcal{B}$. Otherwise, any state satisfying $\mathcal{R} \wedge \mathcal{B}$ is a reachable bad state. $\mathcal{R}$ is the strongest invariant, while $\neg\mathcal{B}$ is the weakest invariant sufficient to prove the Hoare triple. Any inductive predicate $\mathcal{I}$ satisfying $\mathcal{R} \Rightarrow \mathcal{I}$ and $\mathcal{I} \Rightarrow \neg\mathcal{B}$ suffices for the proof: $\mathcal{I}$ contains all the good states and does not contain any bad state. Therefore, $\mathcal{I}$ *separates* the good states from the bad

states, and thus the problem of computing an invariant can be formulated as finding a separator between $\mathcal{R}$ and $\mathcal{B}$. In general, we do not know $\mathcal{R}$ and $\mathcal{B}$ – our objective is to compute a separator $\mathcal{I}$ from under-approximations of $\mathcal{R}$ and $\mathcal{B}$. For the Hoare triple $\{P\}$`while` E `do` $S\{Q\}$, any subset of states reachable from P is an under-approximation of $\mathcal{R}$, while any subset of states satisfying, but not limited to, the predicate $\neg E \wedge \neg Q$ is an under-approximation of $\mathcal{B}$.

Computing separators between sets of points is a well-studied problem in machine learning and goes under the name *binary classification*. The input to the binary classification problem is a set of points with labels from $\{1, 0\}$. Given points and their labels, the goal of the binary classification is to find a *classifier* $C : \mathit{points} \to \{\mathit{true}, \mathit{false}\}$, such that $C(a) = \mathit{true}$, for every point a with label 1, and $C(b) = \mathit{false}$ for every point b with label 0. This process is called *training* a classifier, and the set of labeled points is called the *training data*.

The goal of classification is not to just classify the training points correctly but also to be able to predict the labels of previously unseen points. In particular, even if we are given a new labeled point w, with label l, not contained in the training data, then it should be very likely that $C(w)$ is *true* if and only if $l = 1$. This property is called *generalization*, and an algorithm that computes classifiers that are likely to perform well on unseen points is said to *generalize* well.

If C lies in linear arithmetic, that is, it is an arbitrary boolean combination of half-spaces, then we call such a C a *geometric concept*. Our goal is to apply machine learning algorithms for learning geometric concepts to obtain invariants. The good states, obtained by sampling from $\mathcal{R}$, will be labeled 1 and the bad states, obtained by sampling from $\mathcal{B}$, will be labeled 0. We want to use these labeled points to train a classifier that is likely to be an invariant, separating all the good states $\mathcal{R}$ from all the bad states $\mathcal{B}$. In other words, we would like to compute a classifier that generalizes well enough to be an invariant.

4.2.2 Learning Geometric Concepts

Let R and B be under-approximations of the good states $\mathcal{R}$ and the bad states $\mathcal{B}$, respectively, at a loop head. The classifier $\vee_{r \in R} x = r$ trivially separates R from B. However, this classifier has a large generalization error. In particular, it will *misclassify* every state in $\mathcal{R} \setminus R$; a candidate invariant misclassifies a good state r when $I(r) = \mathit{false}$ and a bad state b when $I(b) = \mathit{true}$. It can be shown if a predicate or classifier grows linearly with the size of training data ($\vee_{r \in R} x = r$ being such a predicate), then such a classifier cannot generalize well. On the other hand, a predicate that is independent of the size of training data can be proven to generalize well [20].

To reduce the size of the predicates, Bshouty et al. [22] frame the problem of learning a general geometric concept as a *set cover* problem. Let X be a set of n points. We are given a set $F \subseteq 2^X$ with k elements such that each element $F_i \in F$ is a subset of X. We say that an element $x \in X$ is *covered* by the set F_i if $x \in F_i$. The goal is to select the minimum number of sets F_i such that each element of X is covered by at least one set. For example, if $X = \{1, 2, 3\}$ and $F = \{\{1, 2\}, \{2, 3\}, \{1, 3\}\}$, then

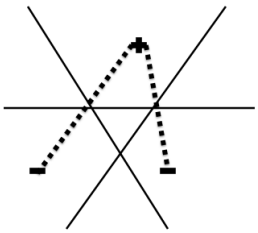


Figure 4.4: Separating three points in two dimensions. The solid lines tessellate $\mathbb{R}^2$ into seven cells. The $-$'s are the bad states and the $+$'s are the good states. The dotted lines are the edges to be cut.

$\{\{1,2\},\{2,3\}\}$ is a solution, and this minimum set cover has a size of two. The set cover problem is NP-complete and we have to be satisfied with approximation algorithms [21, 30]. Bshouty et al. [22] formalize learning of geometric concepts as a set cover problem, solve it using [21], and show that the resulting algorithm PAC learns. Note that experiments of [21] show that the performance of the naive greedy algorithm [30] is similar to the algorithm of [21] in practice. Hence, we use the simple to implement greedy set cover for our implementation (Section 4.4).

We are given a set of samples $V = \{x_i\}_{i=1,\ldots m}$, some of which are good and some bad. We create a bipartite graph $\mathcal{U}$ where each sample is a node and there is an edge between nodes x_+ and x_- for every good sample x_+ and every bad sample x_-. In Figure 4.4, there is one good state, two bad states, and dotted lines represent edges of $\mathcal{U}$. Next, we look for hyperplanes that cut the edges of the graph $\mathcal{U}$. A hyperplane cuts an edge if the two endpoints of the edge lie on different sides of the hyperplane. Note that for every solution, each good sample needs to be separated from every bad sample. This implies that we will need to "cut" every edge in graph $\mathcal{U}$. Intuitively, once we have collected a set S of hyperplanes such that every edge in graph $\mathcal{U}$ is cut by at least one hyperplane in S we can perfectly separate the good and bad samples. The hyperplanes in S tessellate $\mathbb{R}^d$ into a number of cells. (In Figure 4.4, the three solid lines tessellate $\mathbb{R}^2$ into seven cells.) No cell contains both a good sample and a bad sample – if it does, then the edge between a good sample and a bad sample in the cell is not cut by any hyperplane in S. Thus, each cell contains only good samples, or only bad samples, or no samples at all. We can therefore label each cell, as "good" in the first case, "bad" in the second case, and with an arbitrary "don't care" label in the last case.

Each cell is bounded by a set of hyperplanes, and therefore corresponds to an intersection of half-spaces. The "good" region of $\mathbb{R}^d$ (where d is the number of variables in the program) is then a union of cells labeled "good", and hence a union of intersections of half-spaces, that we output. Thus, the union of intersections of half-spaces we output contains all the good samples, no bad samples, and separates all the good from all the bad samples.

This discussion shows that all we need to do is to come up with the set S of hyperplanes that together cut every edge of graph $\mathcal{U}$. To achieve this goal, we consider a universal set of hyperplanes

$\mathcal{F}$ corresponding to all possible partitions of states. Every hyperplane defines a partition of states: some states lie above the plane and some lie below it. $\mathcal{F}$ contains one hyperplane for every possible partition. By Sauer's lemma, such a set $\mathcal{F}$ has cardinality $\mathcal{O}(m^d)$ [22]. We say that an edge is covered by a hyperplane from $\mathcal{F}$ if the hyperplane cuts it. We want to cover all edges of graph $\mathcal{U}$ by these hyperplanes. This set cover problem can be solved in several ways that have comparable performance in practice [21, 30]. The simplest solution is to greedily select the hyperplane from $\mathcal{F}$ that covers the maximum number of uncovered edges of graph $\mathcal{U}$, and repeating the greedy selection until all edges in $\mathcal{U}$ are cut. For Figure 4.4, $\mathcal{F}$ contains three hyperplanes, and graph $\mathcal{U}$ has two edges (edges between $-$'s and $+$'s.). The horizontal plane cuts both the edges and divides the space into two cells: one above and one below. Since the cell above the horizontal plane contains a '+', we will label it "good". Similarly, the cell below is labeled "bad". The output predicate is the half-space above the horizontal hyperplane. If the good and bad samples, total m in number, require a minimum number of s hyperplanes to separate them, then the greedy approach has the guarantee that will compute a predicate that uses $\mathcal{O}(s \log m)$ hyperplanes. Using [21], we can obtain a predicate using $\mathcal{O}(sd \log sd)$ hyperplanes. This implies that the number of inequalities of the classifier approximates the number of the inequalities of the simplest true invariant by a logarithmic factor. Such a relationship between candidate and true invariants appears to be new in the context of invariant inference.

4.2.3 PAC Learning

By enumerating a plane for each partition and performing a set cover, the algorithm of [22] finds a geometric concept that separates the good samples from the bad samples. But how well does it generalize? Bshouty et al. [22] showed that under the assumptions of the PAC model [146] this process is likely to produce a geometric concept that will separate a fresh good sample from a fresh bad samples with high probability. The major assumption of the PAC model is that there is an oracle that knows the true classifier and it generates training data by drawing independent and identically distributed samples from a distribution and assigning them labels, either good or bad, using the true classifier.

Independent samples are theoretically justified as otherwise one can construct data with an arbitrary number of samples by duplicating one sample an arbitrary number of times and then the term "amount of training data" is not well defined. Practically, if one draws a sample randomly from some distribution, then deciding whether it is good or bad is undecidable. Hence such an oracle cannot be implemented and in our experiments we make do with a simple technique for obtaining samples, where the samples are not necessarily independent.

The proof of PAC learning in [22] uses the following result from the seminal paper of Blumer et al. [20].

Theorem 6. If an algorithm outputs f consistent with a sample of size $max\left(\frac{4}{\epsilon}\log\frac{2}{\delta}, \frac{8VC}{\epsilon}\log\frac{13}{\epsilon}\right)$ then f has error at most ϵ with probability at least $1-\delta$.

Intuitively, this theorem states that if an algorithm can separate a large number of good and bad samples then the classifier has a low probability of misclassifying a new sample. Here VC is the Vapnik-Chervonenkis dimension, a quantity determined by the number of hyperplanes in the geometric concepts we are learning and the number of variables. In [22], by using algorithms for set cover that have a good approximation factor [21], Bshouty et al. are able to bound the number of planes in the output predicate f, and hence the quantity VC. Since the output of [22] is consistent with all good and bad samples, given enough samples the algorithm outputs a predicate that is very likely to separate all the good states from all the bad states. For the full proof the reader is referred to [22].

Hence, [22] can produce predicates that are likely to separate all good states and bad states, under PAC assumptions. This is a formal guarantee on the extrapolation we have performed using some good and bad samples, that is, using some finite behaviors of the program. Although this guarantee is in a model, we are unaware of any previous program verification engine with any guarantee, in a model or otherwise, on the heuristic extrapolation they perform. Even though this guarantee is not the best possible guarantee that one would desire, the undecidability of program verification prevents strong results for the problem we consider. It is well known that the PAC learners tend to have good performance in practice for a variety of learning tasks. Our experiments show that the PAC learners we construct have good performance for the task of invariant inference. We believe that by finding candidate invariants separating all good samples from all bad samples and misclassifying unseen points with low probability leads our technique to produce true invariants.

4.2.4 Complexity

If we have m states in d dimensions, then we need to cover $\mathcal{O}(m^2)$ edges of graph $\mathcal{U}$ using $\mathcal{O}(m^d)$ hyperplanes of $\mathcal{F}$. Greedy set cover has a time complexity of $\mathcal{O}(m^2|\mathcal{F}|)$. Considering $\mathcal{O}(m^d)$ hyperplanes is, however, impractical. With a thousand samples for a four variable program, we will need to enumerate 10^{12} planes. Hence this algorithm has a very high space complexity and will run out of memory on most benchmarks of Section 4.4.

Suppose the invariant has s hyperplanes. Hence the good states and bad states can be separated by s hyperplanes. To achieve learning, we require that $\mathcal{F}$ should contain s hyperplanes that separate the good samples and the bad samples – since the planes constituting the invariant could be any arbitrary set, in general we need to select a lot of candidates to ensure this. By adding assumptions about the invariant, the size of $\mathcal{F}$ can be reduced. Say for octagons, for thousand samples and four variables, the algorithm of Section 4.3.1 considers 24000 candidates.

4.2.5 Logic Minimization

The output of the algorithm of Section 4.2.2 is a set S of hyperplanes separating every good sample from every bad sample. As described previously, these hyperplanes tessellate $\mathbb{R}^d$ into cells. Recall

that S has the property that no cell contains both a good state and a bad state.

Now we must construct a predicate containing all good samples and excluding all bad samples. One obvious option is the union of cells labeled "good". But this might result in a huge predicate since each cell is an intersection of half-spaces. Our goal is to compute a predicate with the smallest number of boolean operators such that it contains all the "good" cells and no "bad" cells. Let $\mathcal{H}$ be the set of half-spaces constituting the "good" cells. Define a boolean matrix M with m rows and $|\mathcal{H}|$ columns, and an m-dimensional vector y as follows.

$$\begin{aligned} M(i,j) &= true \Leftrightarrow \{i^{th} state \in j^{th} \text{ half-space of } \mathcal{H}\} \\ y(i) &= true \Leftrightarrow \{i^{th} state \text{ is a good state}\} \end{aligned}$$

This matrix M together with the vector y resembles a partial truth table – the i^{th} row of M identifies the cell in which the i^{th} state lies and $y(i)$ (the label of the i^{th} state) gives the label for the cell (whether it is a cell containing only good states or only bad states). Now, we want to learn the simplest boolean function (in terms of the number of boolean operators) $f : \{true, false\}^{|\mathcal{H}|} \rightarrow \{true, false\}$, such that $f(M_i) = y(i)$ (M_i is the i^{th} row of M). This problem is called logic minimization and is NP-complete. Empirically, however, S has a small number of hyperplanes, at most eight in our experiments, and we are able to use standard exponential time algorithms like the Quine-McCluskey algorithm [99] to get a small classifier.

In summary, we use set covering for learning geometric concepts (Section 4.2.2) to compute predicates with a small number of hyperplanes. Combining this with logic minimization, we compute a predicate with a small number of boolean connectives. Empirically, we find that these predicates are actual invariants for *all* the benchmarks that have an arbitrary boolean combination of linear inequalities as an invariant.

4.3 Practical Algorithms

The algorithm discussed in Section 4.2.2, although of considerable interest, has limited practical applicability because its space and time complexity is exponential in the dimension, which in our case, is the number of program variables (Section 4.2.4). This complexity is not too surprising since, for example, abstract interpretation over the abstract domain of convex hulls [40] is also exponential in the number of variables. In this chapter, we make the common assumption that the invariants come from a restricted class, which amounts to reducing the number of candidate sets for covering in our set cover algorithm. Therefore, we are able to obtain polynomial time algorithms in the number of samples and the dimension to generate classifiers under mild restrictions (Section 4.3.1).

4.3.1 Restricting Generality

Let s denote the number of hyperplanes in the invariant. Then for PAC learning, we say the set $\mathcal{F}$ of candidate hyperplanes is *adequate* if it contains s hyperplanes that completely separate the good samples from the bad samples. Recall that the complexity of the procedure of Section 4.2.2 is $\mathcal{O}(m^2|\mathcal{F}|)$, and therefore a polynomial size set $\mathcal{F}$ makes the algorithm polynomial time. In addition, the set covering step can be parallelized for efficiency [14].

In the following two sections we will give two PAC learning algorithms. The formal proofs that these algorithms learn in the PAC model are beyond the scope of this thesis and are similar to the proofs in [22]. However, we do show the construction of adequate sets $\mathcal{F}$ that coupled with a good approximation factor of set cover [21] give us PAC learning guarantees.

Predicate Abstraction

Suppose we are given a set of predicates $\mathcal{P}$ where each predicate is a half-space. Assume that the invariant is a boolean combination of predicates in $\mathcal{P}$, and checking whether a given candidate I is an invariant is co-NP-complete. If the invariant is an intersection or disjunction of predicates in $\mathcal{P}$, then Houdini [54] can find the invariant in time P^{NP} (that is, it makes a polynomial number of calls to an oracle that can solve NP problems). When the predicates are arbitrary boolean combinations of half-spaces from $\mathcal{P}$, then the problem of finding the invariant is much harder, NP^{NP}-complete [91]. We are not aware of any previous approach that solves this problem.

Now suppose that instead of an exact invariant, we want to find a PAC classifier to separate the good states from the bad states. If the set of candidates $\mathcal{F}$ is $\mathcal{P}$, then this trivially guarantees that there are s hyperplanes in $\mathcal{F}$ that do separate all the good states from the bad states – all we need to do now to obtain a PAC algorithm is to solve a set cover problem [21]. This observation allows us to obtain a practical algorithm. By using the greedy algorithm on m samples, we can find a classifier in time $\mathcal{O}(m^2|\mathcal{P}|)$. Therefore, by relaxing our problem to finding a classifier that separates good samples from bad samples, rather than finding an exact invariant, we are able to solve a NP^{NP} complete problem in time $\mathcal{O}(m^2|\mathcal{P}|)$ time, a very significant improvement in time complexity.

Abstract Interpretation

Simple predicate abstraction can be restrictive because the set of predicates is fixed and finite. Abstract interpretation is another approach to finding invariants that can deal with infinite sets of predicates. For scalable analyses, abstract interpretation assumes that invariants come from restricted abstract domains. Two of the most common abstract domains are boxes and octagons. In boxes, the predicates are of the form $\pm x + c \geq 0$, where x is a program variable and c is a constant. In octagons, the predicates are of the form $\pm x \pm y + c \geq 0$. Note that, by varying c, these form an infinite family of predicates. These restricted abstract domains amount to fixing the set of possible

slopes w of the constituent half-spaces $w^T x + b \geq 0$ (the bias b that corresponds to c, is however free).

Suppose now that we are given a finite set of slopes, that is, we are given a finite set of weight vectors $\Sigma = \{w_i \mid i = 1, \ldots, |\Sigma|\}$, such that the invariant only involves hyperplanes with these slopes. In this case, we observe that we can restrict our attention to hyperplanes that pass through one of the samples, because any hyperplane in the invariant that does not pass through any sample can be translated until it passes through one of the samples and the resulting predicate will still separate all the good samples from the bad samples. In this case, the set $\mathcal{F}$ is defined as follows:

$$\mathcal{F} = \{(w, b) \mid w \in \Sigma \text{ and } w^T x_i + b = 0 \text{ for some sample } x_i \in V\} \tag{4.1}$$

The size of $\mathcal{F}$ is $|\Sigma|m$. Again, this set contains s hyperplanes that separate all the good samples from all the bad samples (the s hyperplanes of the invariant, translated to where they pass through one of the samples), and therefore this set is adequate and coupled with set covering [21] gives us a PAC learning algorithm.

The time complexity for greedy set cover in this case also includes the time taken to compute the bias for each hyperplane in $\mathcal{F}$. There are $|\mathcal{F}| = |\Sigma|m$ such hyperplanes, and finding the bias for each hyperplane takes $\mathcal{O}(d)$ time. The time complexity is therefore $\mathcal{O}(m^2|\mathcal{F}| + d|\mathcal{F}|) = \mathcal{O}(m^3|\Sigma|)$.

If we want to find classifiers over abstract domains such as boxes and octagons, then we can work with the appropriate slopes. For boxes $|\Sigma|$ is $\mathcal{O}(d)$ and for octagons $|\Sigma|$ is $\mathcal{O}(d^2)$. Interestingly, the increase in complexity when learning classifiers as we go from boxes to octagons mirrors the increase in complexity of the abstract interpretation. By adding more slopes we can move to more expressive abstract domains. Also note that the abstract domain over which we compute classifiers is much richer than the corresponding abstract interpretation. Conventional efficient abstract interpretation can only find invariants that are conjunctions of predicates, but we learn arbitrary boolean combinations of half-spaces, that allows us to learn arbitrary boolean combinations of predicates in abstract domains.

Again, we observe that by relaxing the requirement from an invariant to a classifier that separates good and bad samples, we are able to obtain predicates in polynomial time that are richer than any existing symbolic program verification tool we are familiar with.

4.3.2 Non-linear Invariants

Our geometric method of extracting likely invariants carries over to polynomial inequalities. Assume we are given a fixed bound k on the degree of the polynomials. Consider a d-dimensional point $\vec{x} = (x_1, \ldots, x_d)$. We can map $\vec{x}$ to a $\binom{d+k-1}{k}$-dimensional space by considering every possible

monomial involving the components of $\vec{x}$ of maximum degree k as a separate dimension. Thus,

$$\phi(\vec{x}) = (x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d} \mid \sum_i \alpha_i \leq k, \alpha_i \in \mathbb{N}) \tag{4.2}$$

Using the mapping ϕ, we can transform every point $\vec{x}$ into a higher dimensional space. In this space, polynomial inequalities of degree k are linear half-spaces, and so the entire machinery above carries through without any changes. In the general case, when we have no information about the invariant then we will take time exponential in d. When we know the slopes or the predicates constituting the invariants then we can get efficient algorithms by following the approach of Section 4.3.1. Therefore, we can infer likely invariants that are arbitrary boolean combinations of polynomial inequalities of a given degree.

4.3.3 Recovering Soundness

Once we obtain a classifier, we want to use it to construct proofs for programs. But the classifier is not guaranteed to be an invariant. To obtain soundness, we augment our learning algorithm with a theorem prover using a Guess-and-Check loop [129, 131]. We sample, perform learning, and propose a candidate invariant using the set cover approach for learning geometric concepts as described in Section 4.2.2 (the guess step). We then ask a theorem prover to check whether the candidate invariant is indeed an invariant (the check step). If the check succeeds we are done. Otherwise, the candidate invariant is not an invariant and we sample more states and guess again. When we terminate successfully, we have computed a sound invariant. For a candidate invariant I, we make the following queries:

1. The candidate invariant is weaker than the pre-condition $P \Rightarrow I$.
2. The candidate invariant implies the post-condition $I \wedge \neg E \Rightarrow Q$.
3. The candidate invariant is inductive $\{I \wedge E\}S\{I\}$.

If all three queries succeed, then we have found an invariant. Note that since we are working with samples, I is neither an under-approximation nor an over-approximation of the actual invariant. If the first constraint fails, then a counter-example is a good state that I classifies as bad. If the second constraint fails, then a counter-example is a bad state that I classifies as good. If the third constraint, representing inductiveness, fails then we get a pair of states (x, y) such that I classifies x as good, y as bad, and if the loop body starts its execution from state x then it can terminate in state y. Hence if x is good then so is y and (x, y) refutes the candidate I. However, x is unlabeled, i.e., we do not know whether it is a good state or not and we cannot add x and y to samples directly.

Now, we want our learning algorithm to generate a classifier that respects the pair (x, y) of counter-example states: if the classifier includes x then it also includes y. If the invariant has s

hyperplanes then the greedy set cover can be extended to generate a separator between good and bad samples that respects such pairs. The basic idea is to greedily select the hyperplanes which make the most number of pairs consistent. Moreover the number of hyperplanes in the output is guaranteed to be $\mathcal{O}(s(\log m)^2)$: the size of the predicate can increase linearly with the number of pairs. This algorithm can be used to guide our learning algorithm in the case it finds an invariant that is not inductive. Note that the need for this extension did not arise in our experiments. Using a small amount of data, greedy set cover was sufficient to find an invariant. For buggy programs, a good state g, a bad state b, and a sequence of pairs $(x_1, x_2), (x_2, x_3), \ldots, (x_{k-1}, x_k)$ such that $g = x_1$ and $b = x_k$ is an error trace, i.e., certificate for a bug.

When we applied guess-and-check in the previous chapters to infer relevant predicates for verification, we checked for only two out of the three constraints listed above. Hence, these predicates did not prove any program property and moreover they were of limited expressiveness (no disjunctions among other restrictions). Checking fewer constraints coupled with reduced expressiveness made it straightforward to incorporate counter-examples. In contrast, we now must deal with the kinds of counter-examples (good, bad, and unlabeled) for an expressive class of predicates. Handling all three kinds is necessary to guarantee progress, ensuring that an incorrect candidate invariant is never proposed again. However, if the candidates are inadequate then the guess-and-check procedure will loop forever: Inadequacy results in candidate invariants that grow linearly with the number of samples.

If we want to analyze a single procedure program with multiple loops, then we process the loops beginning with the last, innermost loop and working outwards and upward to the first, outermost loop. The invariants of the processed loops become assertions or postconditions for the to-be-processed loops. While checking the candidate invariants, the condition that the candidate invariant should be weaker than the pre-condition is only checked for the topmost outermost loop L and not for others. If this check generates a counter-example then the program is executed from the head of L with the variables initialized using the counter-example. This execution generates new good states for the loops it reaches and invariant computation is repeated for these loops.

4.4 Experimental Evaluation

We have implemented and evaluated our approach on a number of challenging C benchmarks. Greedy set cover is implemented in one hundred lines of MATLAB code. We use HAVOC [11] to generate BOOGIEPL programs from C programs annotated with candidate invariants. Next, BOOGIE [13] verification condition generator operates on the BOOGIEPL programs to check the candidate invariants by passing the verification conditions to Z3 theorem prover [43]. All experiments were performed on a 2.67GHz Intel Xeon processor system with 8 GB RAM running Windows 7 and MATLAB R2010b.

Program	LOC	#Loops	#Vars	#Good	#Bad	Learn(s)	Check(s)	Result
fig6 [64]	16	1	2	3	0	0.030	1.04	OK
fig9 [64]	10	1	2	1	0	0.030	0.99	OK
prog2 [64]	19	1	2	10	0	0.034	1.00	OK
prog3 [64]	29	1	4	8	126	0.106	1.05	OK
test [64]	30	1	4	20	0	0.162	1.00	OK
ex23 [78]	20	1	2	111	0	0.045	1.05	OK
sas07 [61]	20	1	2	103	6112	2.64	1.02	OK
popl07 [66]	20	1	2	101	10000	2.85	0.99	OK
get-tag [71]	120	2	2	6	28	0.092	1.04	OK
hsort [71]	47	2	5	15	435	0.19	1.05	OK
maill-qp [71]	92	1	3	9	253	0.11	1.05	OK
msort [71]	73	6	10	9	77	0.093	1.12	OK
nested [71]	21	3	4	49	392	0.24	0.99	OK
seq-len1 [71]	44	6	5	36	1029	0.32	1.04	PRE
seq-len [71]	44	6	5	224	3822	4.39	1.04	OK
spam [71]	57	2	5	11	147	1.01	1.05	OK
svd [71]	50	5	5	150	1708	4.92	0.99	OK
split	20	1	5	36	4851	FAIL	NA	FAIL
div [125]	28	2	6	343	248	2.03	1.04	OK

Table 4.1: Evaluation of GUESS-AND-CHECK for disjunctive invariants. `Program` is the name, `LOC` is lines, `#Loops` is the number of loops, and `#Vars` is the number of variables in the benchmark. `#Good` is the maximum number of good states, `#Bad` is the maximum number of bad states, and `Learn` is the maximum time of the learning routine over all loops of the program. `Check` is time by BOOGIE for proving the correctness of the whole program and `Result` is the verdict: OK is verified, FAIL is failure of our learning technique, and PRE is verified but under certain pre-conditions.

Implementation notes Our implementation analyzes single procedure C programs with integer variables and assertions. Since all these programs contain loops, we need to compute invariants that are strong enough to prove the assertions. For every loop, our technique works as follows: first, we instrument the loop head to log the values of the variables in scope. Next, we run the program till termination on some test inputs to generate data. All internal non-deterministic choices, such as non-deterministic tests on branches, are randomly selected. All states reaching the loop head are stored in a matrix `good`. We then compute the null space of `good` to get the sub-space J in which the good states lie: J represents the equality relationships that the good states satisfy. Working in the lower dimensional sub-space J improves the performance of our algorithms by effectively reducing d, the number of independent variables.

Next, from the loop body, we statically identify the predicate B representing the states that will violate some assertion after at most one iteration of the loop. We then sample the bad states from the predicate $B \wedge J$. The good and bad samples are then used to generate the set of candidate hyperplanes $\mathcal{F}$ using the specified slopes—octagons are sufficient for all programs except `seq-len`.

We perform another optimization: we restrict the candidates to just the octagons passing through

the good states, thus reducing the number of candidates. Note that this optimization still leads to an adequate set of candidates and we retain our learning guarantees. Next, using the greedy algorithm, we select the hyperplanes that separate the good from the bad states, and return a set of half-spaces $\mathcal{H}$ and a partial boolean function f: $f(b_1, \ldots, b_{|\mathcal{H}|})$ that represents the label of the cell that lies inside the half-spaces for which b_i's are *true* and outside the half-space for which b_i is *false*. This algorithm is linear in the number of bad states and its complexity is governed almost entirely by the number of good states. For our benchmarks, $|\mathcal{H}|$ was at most 8. We use the Quine-McCluskey algorithm for logic minimization (Section 4.2.5) that returns the smallest total boolean function g that agrees with f. Conjoining the predicate obtained using g and $\mathcal{H}$ with J yields a candidate invariant. This invariant is added as an annotation to the original program that is checked with BOOGIE for assertion violations.

Evaluation The overall approach is the following: generate data, learn a candidate invariant, and check the candidate invariant using BOOGIE. If BOOGIE approves the candidate then we have successfully found an invariant. If the candidate is not an invariant, we generate more data until we discover counter-examples to the candidate. Next, we run the learner again with the counter-examples as additional data.

An important empirical question regarding this approach is that how much data is sufficient to obtain a sound invariant. To answer this question, we adopt the following method for generating data: we run the programs on all possible inputs s.t. all input variables have their values between $[-1, N]$ where N is initially zero. This process generates good states at the loop head. Next we generate bad states and check whether our first guess is an invariant. If not then we continue generating more bad states and checking if the guess is an invariant. If we have generated 10,000 bad states and still have not found an invariant then we increment N by one and repeat the process. We are able to obtain a sound invariant within four iterations of this process for our linear benchmarks; `div` needs ten iterations: it needs more data as the (non-linear) invariant is found in a higher dimensional space.

Now we explain our approach of sampling bad states given a set of good states. Each variable x at the loop head takes values in some range $[L_x, M_x]$ for the good states. To sample the bad states, we exhaustively enumerate states (in the subspace in which the good states lie) where the value of each variable x varies over the range $[L_x, M_x]$. For deterministic programs with finite number of reachable states, any enumerated state that is unreachable is labeled bad. For others, bad states are generated by identifying the enumerated states satisfying the predicate B representing bad states. Because this process can enumerate a very large number of states unless the range or number of variables is small, we incrementally enumerate the states until we generate 10,000 bad states. The results in Table 4.1 show the number of good states (column 5) and bad states (column 6) that yield a sound invariant.

We observe that only a few good states are required for these benchmarks, which leads us to

believe that existing test suites of programs should be sufficient for generating sound invariants. We observe that our sampling strategy based on enumeration generates many bad states that do not remain useful for the later iterations of the algorithm. The candidate invariant is mainly determined by the bad states that are close to the good states and not those that are further away and play no role in determining the good state/bad state boundary. The complexity of our algorithm is governed mainly by the good states, due to our optimizations, and hence accumulating superfluous bad states is not an issue for these benchmarks. Since the candidate inequalities are determined by the good and bad states, the good and bad samples should be generated with the goal of including the inequalities of the invariants in the set of candidates. Note that we use a naive strategy for sampling. Better strategies directed towards the above goal are certainly possible and may work better.

The benchmarks that we used for evaluating our technique are shown in the first column (labeled `Program`) of Table 4.1. Lee-Yannakakis partition refinement algorithm [94] does not work well on `fig6`; Synergy [64] fails to terminate on `fig9`; `prog2` has a loop with a large constant number of iterations and predicate abstraction based tools like Slam take time proportional to the number of loop iterations. The program `prog3` requires a disjunctive invariant. For `test` we find the invariant $y = x + lock$: Slam finds the disjunctive invariant $(x = y \Rightarrow lock = 0 \wedge x \neq y \Rightarrow lock = 1)$. For `ex23`, we discovered the invariant $z = counter + 36y$. This is possible because the size of constants are bounded only for computing inequalities: the equalities in J have no restriction on the size of constants. Such relationships are beyond the scope of tools performing abstract interpretation over octagons [92]. The equalities in J are sufficient to verify the correctness of the benchmarks containing a zero in column `#Bad` of Table 4.1. The programs `sas07` and `popl07` are deterministic programs requiring disjunctive invariants. We handle these without using any templates [71]. The programs `get-tag` through `svd` are the benchmarks used to evaluate the template based invariant generation tool InvGen [71]. As seen from Table 4.1, we are faster than InvGen on half of these programs, and slower on the other half.

We modify `seq-len` to obtain the benchmark `seq-len1`; the program `seq-len1` assumes that all inputs are positive. We are able to find strong invariants for the loops, using octagons for slopes, that are sufficient to prove the correctness of this program. These invariants include sophisticated equalities like $i + k = n0 + n1 + n2$. Since we proved the correctness by assuming a pre-condition on inputs, the `Result` column says PRE. Next, we analyze `seq-len`, that has no pre-conditions on inputs, using octagons as slopes. We obtain a separator that has as many linear inequalities as the number of input states; such a predicate will not generalize. For this example, there is no separator small in size if we restrict the domain of our slopes to octagons. Therefore, we add slopes of hyperplanes that constitute invariants of `seq-len1` and similar slopes to our bag of slopes. We are then able to prove `seq-len` correct by discovering invariants like $i + k \geq n0 + n1 + n2$. This demonstrates how we can find logically stronger invariants in specialized contexts.

The `split` program requires an invariant that uses an interpreted function *iseven*. Our approach fails on this program as the desired invariant cannot be expressed as an arbitrary boolean combinations of half-spaces. For the `div` program, the objective is to verify that the computed remainder is less than the divisor and the quotient times divisor plus remainder is equal to dividend. Using the technique described in Section 4.3.2 with a degree bound of 2, we are able to infer a invariant that proves the specification.

4.5 Related Work

In this section, we compare our approach with existing techniques that generate invariants composed of inequalities. A discussion of techniques that infer equality invariants can be found in Section 2.7.

Linear invariant generation tools that are based on abstract interpretation [37, 40], constraint solving [35, 71], or probabilistic inference [66] cannot handle arbitrary boolean combinations of half-spaces. Similar to us, Clousot [93] improves its performance by conjoining equalities and inequalities over boxes. Some approaches like [50, 53, 61, 66, 68, 98, 124] can handle disjunctions, but they restrict the number of disjunctions by widening, manual input, or trace based heuristics. In contrast, [57] handles disjunctions of a specific form.

Predicate abstraction based tools are geared towards computing arbitrary boolean combinations of predicates [2, 12, 16, 18, 63, 64]. Among these, Yogi [64] uses test cases to determine where to refine its abstraction However, just like [104], it uses the trace and not the concrete states generated by a test. InvGen [71] uses test cases for constraint simplification, but they do not generalize from tests with provable generalization guarantees. In a separate work, we ran support vector machines [114], a widely used machine learning algorithm, in a Guess-and-Check loop to obtain a sound interpolation procedure [131]. However, [131] cannot handle disjunctions and computed interpolants need not be inductive.

Existing tools for non-linear invariant generation can produce invariants that are conjunctions of polynomial equalities [25, 34, 89, 103, 107, 120, 121, 125] or candiadate invariants that are conjunctions of polynomial inequalities [107]. We soundly infer invariants that are arbitrary boolean combinations of polynomial inequalities.

Finally, in Chapter 2, we provided soundness and termination guarantees for generating polynomial equalities as invariants. A termination proof was possible as the Guess-and-Check loop there can return the trivial invariant *true*: it is not required to find invariants strong enough to prove some property of interest, which is our goal here.

Chapter 5

General Invariant Inference

In the earlier chapters we discussed invariant inference for integer manipulating programs. In this chapter, we discuss a general invariant inference based engine based on decision procedures. The idea of using decision procedures for invariant inference is not new [47, 71]. However, this approach has been applied previously only in domains with some special structure, e.g., when the VCs belong to theories that admit quantifier elimination, such as linear rational arithmetic (Farkas' lemma) or linear integer arithmetic (Cooper's method). For general inference tasks, such theory-specific techniques do not apply, and the use of decision procedures for such tasks has been restricted to invariant checking: to prove or refute a given manually provided candidate invariant.

Guess-and-Check provides a general framework that, given a procedure for checking invariants, uses that checker to produce an invariant inference engine for a given language of possible invariants. We apply Guess-and-Check to various classes of invariants; we use it to generate inference procedures that prove safety properties of numerical programs, prove non-termination of numerical programs, prove functional specifications of array manipulating programs, prove safety properties of string manipulating programs, and prove functional specifications of heap manipulating programs that use linked list data structures. The two main characteristics of our approach are

- The decision procedure is only used to check a program annotated with candidate invariants (in contrast to approaches that use the decision procedure directly to infer an invariant).
- We uses a randomized search algorithm to search for candidate invariants. Empirically, the search technique is effective for generating good candidates for various classes of invariants.

The use of a decision procedure as a checker for candidate invariants is also not novel [55, 56, 83, 88, 110, 129, 130]. The main contribution of this chapter is a general and effective search procedure that makes a general framework feasible. The use of randomized search is motivated by its recent success in program synthesis [3, 126] and recognizing that invariant inference is also a synthesis task. More specifically, our contributions are:

- We describe a GUESS-AND-CHECK based framework that iteratively invokes randomized search and a decision procedure to perform invariant inference. The randomized search combines random walks with hill climbing and is an instantiation of the well-known Metropolis Hastings MCMC sampler [28].
- We empirically demonstrate the generality of our search algorithm. We use randomized search for finding numerical invariants, *recurrent sets* [70], universally quantified invariants over arrays, invariants over string operators, and invariants involving reachability predicates for linked list manipulating programs. These studies show that invariant inference is amenable to randomized search.
- Randomized search is effective only when done efficiently. We describe optimizations that allow us to obtain practical randomized search algorithms for invariant inference.

Even though we expect the general inference engines based on randomized search to be inferior in performance to the domain specific invariant inference approaches, our experiments show that randomized search has competitive performance with the more specialized techniques (by which we mean that the specialized techniques are not the obvious winners in any performance comparison, not that randomized search is consistently faster). This outcome does not prove that randomized search will always be competitive with techniques tuned to a particular domain, but does show that randomized search is worth evaluating, as it is usually simple to implement. The rest of the chapter is organized as follows. We describe our search algorithm in Section 5.1. Next, we describe inference of numerical invariants in Section 5.2, universally quantified invariants over arrays in Section 5.3, string invariants in Section 5.4, and invariants over linked lists in Section 5.5. Finally, we discuss related work in Section 5.6.

5.1 Preliminaries

An imperative program annotated with invariants can be verified by checking some *verification conditions* (VCs), which must be discharged by a decision procedure. As an example, consider the following program:

$$\texttt{assume}\ P; \texttt{while}\ B\ \texttt{do}\ S\ \texttt{od}; \texttt{assert}\ Q$$

The loop has a pre-condition P. The entry to the loop is guarded by the predicate B and S is the loop body (which, for the moment, we assume to be loop-free). We assert that the states obtained after execution of the loop satisfy Q. Given a loop invariant I, we can prove that the assertion holds if the following three VCs are valid:

$$P \Rightarrow I; \quad \{I \wedge B\}S\{I\}; \quad I \wedge \neg B \Rightarrow Q \tag{5.1}$$

Given a *candidate invariant* C, a decision procedure checks the conditions of Equation 5.1. Since there are three conditions for a predicate to be an invariant, there are three queries that need to be discharged to check a candidate. Each query, if it fails, generates a different kind of counterexample. We discuss these next.

The first condition states that for any invariant I, any state that satisfies P also satisfies I. However, if $P \wedge \neg C$ has a satisfying assignment g, then $P(g)$ is *true* and $C(g)$ is *false* and hence g proves C is not an invariant. We call any state that must be satisfied by an actual invariant, such as g, a *good* state. Now consider the second condition of Equation 5.1. A *pair* (s, t) satisfies the property that s satisfies B and if the execution of S is started in state s then S can terminate in state t. Since an actual invariant I is inductive, it should satisfy $I(s) \Rightarrow I(t)$. Hence, a pair (s, t) satisfying $C(s) \wedge \neg C(t)$ proves C is not an invariant. Finally, consider the third condition. A satisfying assignment b of $C \wedge \neg B \wedge \neg Q$ proves C is inadequate to discharge the post-condition. For an adequate invariant I, $I(b)$ should be *false*. We call a state that must not be satisfied by an adequate invariant, such as b, a *bad* state. Hence, given an incorrect candidate invariant and a decision procedure that can produce counterexamples, the decision procedure can produce either a good state, a pair, or a bad state as a counterexample to refute the candidate.

Problems other than invariant inference can also be reduced to finding some unknown predicates to satisfy some VCs [62]. Consider the following problem: prove that the loop `while` B `do` S `od` goes into non-termination if executed with input i. One can obtain such a proof by demonstrating a *recurrent set* [24, 70] I which makes the following VCs valid.

$$I(i); \quad \{I \wedge B\}S\{I\}; \quad I \Rightarrow B \tag{5.2}$$

Our inference algorithm consumes such VCs with some unknown predicates. We use the term *invariant* for any such unknown predicate that we want to infer. In the rest of this section, we focus on the case when we need to infer a single predicate. The development here can be easily generalized to the case where we need to infer multiple predicates.

Our search algorithm is based on Markov Chain Monte Carlo (MCMC) sampling. Specifically, we use the Metropolis Hastings algorithm, which we describe next.

5.1.1 Metropolis Hastings

We denote the verification conditions by V, the unknown invariant by I, a candidate invariant by C, the set of predicates that satisfy V by $\mathcal{I}$ (more than one predicate can satisfy V), and the set of all possible candidates C by $\mathcal{S}$.

We view inference as a cost minimization problem. For each predicate $P \in \mathcal{S}$ we assign a non-negative cost $c_V(P)$ where the subscript indicates that the cost depends on the VCs. Suppose the cost function is designed to obey $C \in \mathcal{I} \Leftrightarrow c_V(C) = 0$. Then by minimizing c_V we can find an

Search(J: Initial candidate)
Returns: A candidate C with $c_V(C) = 0$.

```
1: C := J
2: while c_V(C) ≠ 0 do
3:     m := SampleMove(rand())
4:     C' := m(C)
5:     c_o := c_V(C), c_n := c_V(C')
6:     if c_n < c_o or e^{-γ(c_n - c_0)} > rand()/RANDMAX then
7:         C := C'
8:     end if
9: end whilereturn C
```

Figure 5.1: Metropolis Hastings for cost minimization.

invariant. In general, c_V is highly irregular and not amenable to exact optimization techniques. In this chapter, we use a MCMC sampler to minimize c_V.

The basic idea of a Metropolis Hastings sampler is given in Figure 5.1. The algorithm maintains a current candidate C. It also has a set of *moves*. A move, $m : \mathcal{S} \mapsto \mathcal{S}$, *mutates* a candidate to a different candidate. The goal of the search is to sample candidates with low cost. By applying a randomly chosen move, the search transitions from a candidate C to a new candidate C'. If C' has lower cost than C we keep it and C' becomes the current candidate. If C' has higher cost than C, then with some probability we still keep C'. Otherwise, we undo this move and apply another randomly selected move to C. Using these random mutations, combined with the use of the cost function, the search moves towards low cost candidates. We continue proposing moves until the search *converges*: the cost reduces to zero.

The algorithm in Figure 5.1, when instantiated with a suitable proposal mechanism (*SampleMove*) and a cost function (c_V), can be used for a variety of optimization tasks. If the proposal mechanism is designed to be *symmetric* and *ergodic* then the algorithm in Figure 5.1 has interesting theoretical guarantees.

A proposal mechanism is *symmetric* if the probability of proposing a transition from C_1 to C_2 is equal to the probability of proposing a transition from C_2 to C_1. Note that the cost is not involved here: whether the proposal is accepted or rejected is a different matter. Symmetry just talks about the probability that a particular transition is proposed from the available transitions.

A proposal mechanism is *ergodic* if there is a non-zero probability of reaching every possible candidate C_2 starting from any arbitrary candidate C_1. That is, there is a sequence of moves, $m_1, m_2, \ldots, m_k$, such that the probability of sampling each m_i is non-zero and $C_2 = m_k(\ldots(m_1(C_1)\ldots)$. This property is desirable because it says that it is not impossible to reach $\mathcal{I}$ starting from a bad initial guess. If the proposal mechanism is symmetric and ergodic then the following theorem holds [5]:

Theorem 7. In the limit, the algorithm in Figure 5.1 samples candidates in inverse proportion to

their cost.

Intuitively, this theorem says that the candidates with lower cost are sampled more frequently. A corollary of this theorem is that the search always converges. The proof of this theorem relies on the fact that the *search space* $\mathcal{S}$ should be finite dimensional. Note that MCMC sampling has been shown to be effective in practice for extremely large search spaces and, with good cost functions, is empirically known to converge well before the limit is reached [5]. Hence, we design our search space of invariants to be a large but finite dimensional space that contains most useful invariants by using templates. For example, our search space of disjunctive numerical invariants restricts the boolean structure of the invariants to be a DNF formula with ten disjuncts where each disjunct is a conjunction of ten linear inequalities. This very large search space is more than sufficient to express all the invariants in our numerical benchmarks.

Theorem 7 has limitations. The guarantee is only asymptotic and convergence could require more than the remaining lifetime of the universe. However, if the cost function is arbitrary then it is unlikely that any better guarantee can be made. In practice, for a wide range of cost functions with domains ranging from protein alignment [106] to superoptimization [126], MCMC sampling has been demonstrated to converge in reasonable time. Different cost functions do result in different convergence rates. Empirically, cost functions that provide feedback to the search have been found to be useful [126]. If the search makes a move that takes it closer to the answer then it should be rewarded with a decrease in cost. Similarly, if the search transitions to something worse then the cost should increase. We next present our cost function.

5.1.2 Cost Function

Consider the VCs of Equation 5.1. One natural choice for the cost function is

$$c_V(C) = 1 - \mathit{Validate}(V[C/I])$$

where $\mathit{Validate}(X)$ is 1 if predicate X is valid and 0 otherwise. We substitute the candidate C for the unknown predicate I in the VCs and if the VCs are valid then the cost is zero and otherwise the cost is one. This cost function has the advantage that a candidate with cost zero is an invariant. However, this cost function is a poor choice for two reasons:

1. Validation is slow. A decision procedure takes several milliseconds in the best case to discharge a query. For a random search to be effective we need to be able to explore a large number of proposals quickly.

2. This cost function does not give any incremental feedback. The cost of all incorrect candidates is one, although some candidates are clearly closer to the correct invariant than others.

Empirically, search based on this cost function times out on even the simplest of our benchmarks. Instead of using a decision procedure in the inner loop of the search, we use a set of concrete program states that allows us to quickly identify incorrect candidates. As we shall see, concrete states also give us a straightforward way to measure how close a candidate is to a true invariant.

Recall from the discussion of Equation 5.1 that there are three different kinds of interesting concrete states. Assume we have a set of good states G, a set of bad states B, and a set of pairs Z. The data elements encode constraints that a true invariant must satisfy. A good candidate C should satisfy the following constraints:

1. It should separate all the good states from all the bad states: $\forall g \in G. \forall b \in B. \neg(C(g) \Leftrightarrow C(b))$.
2. It should contain all good states: $\forall g \in G. C(g)$.
3. It should exclude all bad states: $\forall b \in B. \neg C(b)$.
4. It should satisfy all pairs: $\forall (s,t) \in Z. C(s) \Rightarrow C(t)$.

For most classes of predicates it is easy to check whether a candidate satisfies these constraints for given sets G, B, and Z without using decision procedures. For every violated constraint, we assign a penalty cost. In general, we can assign different weights to different constraints, but for simplicity, we weigh them equally. The reader may notice that the first constraint is subsumed by constraints 2 and 3. However, we keep it as a separate constraint as it encodes the amount of data that justifies a candidate. If a move causes a candidate to satisfy a bad state (which it did not satisfy before) then intuitively the increase in cost should be higher if the initial candidate satisfied many good states than if it satisfied only one good state. The third constraint penalizes equally in both scenarios (the cost increases by 1) and in such situations the first constraint is useful. The result is a cost function that does not require decision procedure calls, is fast to evaluate, and can give incremental credit to the search: the candidates that violate more constraints are assigned a higher cost than those that violate only a few constraints.

$$\begin{aligned} c_V(C) \quad = \quad & \textstyle\sum_{g \in G} \sum_{b \in B} \left(\neg C(g) * \neg C(b) + C(g) * C(b) \right) \\ & + \textstyle\sum_{g \in G} \neg C(g) + \sum_{b \in B} C(b) \\ & + \textstyle\sum_{(s,t) \in Z} C(s) * \neg C(t) \end{aligned} \tag{5.3}$$

In evaluating this expression, we interpret *false* as zero and *true* as one. The first line encodes the first constraint, the second line encodes the second and the third constraints, and the third line encodes the fourth constraint.

This cost function has one serious limitation: Even if a candidate has zero cost, still the candidate might not be an invariant. Once a zero cost candidate C is found, we check whether C is an invariant using a decision procedure; note this decision procedure call is made only if C satisfies all the constraints and therefore has at least some chance of actually being an invariant. If C is not an

invariant one of the three parts of Equation 5.1 will fail and if the decision procedure can produce counterexamples then the counterexample will also be one of three possible kinds. If the candidate violates the first implication of Equation 5.1 then the counterexample is a good state and we add it to G. If the candidate violates the second implication then the counter example is a pair that we add to Z, and finally if the candidate violates the third implication then we get a bad state that we add to B. We then search again for a candidate with zero cost according to the updated data. Thus our inference procedure can be thought of as a counterexample guided inductive synthesis (CEGIS) procedure [136], in particular, as an ICE learner [56]. Note that a pair (s, t) can also contribute to G or B. If $s \in G$ then t can be added to G. Similarly, if $t \in B$ then s can be added to B. If a state is in both G and B then we abort the search. Such a state is both a certificate of the invalidity of the VCs and of a bug in the original program.

Not all decision procedures can produce counterexamples; in fact, in many more expressive domains of interest (e.g., the theory of arrays) generating counterexamples is impossible in general. In such situations the data we need can also be obtained by running the program. Consider the program point η where the invariant is supposed to hold. Good states are generated by running the program with inputs that satisfy the pre-conditions and collecting the states that reach η. Next, we start the execution of the program from η with an arbitrary state σ; i.e., we start the execution of the program "in the middle". If an assertion violation happens during the execution then all the states reaching η, including σ, during this execution are bad states. Otherwise, including the case when the program does not terminate (the loop is halted after a user-specified number of iterations), the successive states reaching η can be added as pairs. Note that successive states reaching the loop head are always pairs and may also be pairs of good states, bad states, or even neither.

The cost function of Equation 5.3 easily generalizes to the case when we have multiple unknown predicates. Suppose there are n unknown predicates $I_1, I_2, \ldots, I_n$ in the VCs. We associate a set of good states G_i and bad states B_i with every predicate I_i. For pairs, we observe that VCs in our benchmarks have at most one unknown predicate symbol to the right of the implication and one unknown predicate symbol to the left (both occurring positively), implying that commonly n^2 sets of pairs suffices: a set of pairs $Z_{i,j}$ is associated with every pair of unknown predicates I_i and I_j. A candidate $C_1, \ldots, C_n$ satisfies the set of pairs $Z_{i,j}$ if $\forall (s, t) \in Z_{i,j}.C_i(s) \Rightarrow C_j(t)$. For the pair $(s, t) \in Z_{i,j}$, if $s \in G_i$ then we add t to G_j and if $t \in B_j$ then we add s to B_i. Each of G_i, B_i, and $Z_{i,j}$ induces constraints and a candidate is penalized by each constraint it fails to satisfy.

In subsequent sections we use the cost function in Equation 5.3 and the search algorithm in Figure 5.1, irrespective of the type of program (numeric, array, string, or list) under consideration. What differs is the instantiation of Guess-and-Check with different decision procedures and search spaces of invariants. Since a proposal mechanism dictates how a search space is traversed, different search spaces require different proposal mechanisms. In general, when Guess-and-Check is instantiated with a search space, the user must provide a proposal mechanism and a function

eval that evaluates a predicate in the search space on a concrete state, returning *true* or *false*. The function *eval* is used to evaluate the cost function; for the search spaces discussed in this chapter, the implementation of *eval* is straightforward and we omit it. We discuss the proposal mechanisms for each of the search spaces in some detail in the subsequent sections.

5.2 Numerical Invariants

We describe the proposal mechanism for inferring numerical invariants. Suppose $x_1, x_2, \ldots, x_n$ are the variables of the program, all of type $\mathbb{Z}$. A program state σ is a valuation of these variables: $\sigma \in \mathbb{Z}^n$. For each unknown predicate of the given VCs, the search space $\mathcal{S}$ is formulas of the following form:

$$\bigvee_{i=1}^{\alpha} \bigwedge_{j=1}^{\beta} \left(\sum_{k=1}^{n} w_k^{(i,j)} x_k \ \leq \ t^{(i,j)} \right)$$

Hence, predicates in $\mathcal{S}$ are boolean combinations of linear inequalities. We refer to w's as *coefficients* and t's as *constants*. The possible values that w's can take are restricted to a finite bag of coefficients $W = \{w_1, w_2, \ldots, w_{|W|}\}$. In our evaluation, the set $W = \{-1, 0, 1\}$ suffices. If needed, heuristics described in [4] can be used to obtain W. The possible values of t's are valuations of expression trees with leaves from a finite bag of constants $F = \{f_1, f_2, \ldots, f_{|F|}\}$. Binary multiplication and addition constitute the internal nodes of the expression trees. In our evaluation, the bag F contain all of the statically occurring constants in the program and their negations. The expression trees are created by the GEN-E procedure (Figure 5.2). Possible expression trees include $f_1 \times f_2$, $(f_1 + f_2) + f_3$, etc.

For our experiments, for the benchmarks that require conjunctive invariants we set $\alpha = 1$ and $\beta = 10$ and for those that require disjunctive invariants we set $\alpha = \beta = 10$. This search space, $\mathcal{S}$, is sufficiently large to contain invariants for all of our benchmarks.

5.2.1 Proposal Mechanism

We use $y \sim Y$ to denote that y is selected uniformly at random from the set Y and $[a : b]$ to denote the set of integers in the range $\{a, a+1, \ldots, b-1, b\}$. Unless stated otherwise, all random choices are derived from uniform distributions. Before a move we make the following random selections: $i \sim [1 : \alpha]$, $j \sim [1 : \beta]$, and $k \sim [1 : n]$ .We have the following three moves, each of which is selected with probability $\frac{1}{3}$:

- Coefficient move: select $l \sim [1 : |W|]$ and update $w_k^{(i,j)}$ to W_l.
- Constant move: update $t^{(i,j)}$ to GEN-E(F) (Figure 5.2).
- Inequality move: With probability $1 - \rho$, apply constant move to $t^{(i,j)}$ and coefficient move to $w_h^{(i,j)}$ for all $h \in [1 : n]$. Otherwise (with probability ρ) remove the inequality by replacing it with *true*.

These moves are motivated by the fact that prior empirical studies of MCMC have found that a proposal mechanism that has a good mixture of moves that make minor and major changes to a candidate leads to good results [126]. The first two moves make small changes and the last move can change an inequality completely.

This proposal mechanism is symmetric and ergodic. Using inequality moves we can transform any predicate in $\mathcal{S}$ to any other predicate in $\mathcal{S}$. For proving symmetry observe that the moves are themselves symmetric: if a move mutates C_1 to C_2 with probability p then the same move also updates C_2 to C_1 with probability p. It is easy to see that if all the moves are symmetric then the proposal mechanism is symmetric. Combining this proposal mechanism with the cost function in Equation 5.3 and the procedure in Figure 5.1 provides us a search procedure for numerical invariants. We call this procedure `MCMC` in the empirical evaluation of Section 5.2.3. Next, we describe two variations of this procedure.

In the first variation, we accept every move irrespective of the cost. The search terminates when a zero cost candidate is found. The resulting procedure is a pure random walk through the search space. The motivation for considering this variation is that it helps us evaluate the benefit of the cost function. We call this search strategy `Pure` in the evaluation in Section 5.2.3.

In the second variation, we further constrain the search space. The user provides templates to restrict the constituent inequalities of the candidate invariants. As an example, suppose we have a program with two variables x_1 and x_2 and the user restricts the invariants to boolean combinations of intervals. The inequalities must then be of the from $x_1 \leq d$, $x_1 \geq d$, $x_2 \leq d$, and $x_2 \geq d$. In general, the user can restrict the coefficients using other abstract domains like octagons [102] (bounds on sum or difference of at most two variables $\pm x_i \pm x_j \leq d$), octahedra [31] (bounds on all possible sums or differences of variables $\sum_i \pm x_i \leq d$), etc. In this variation, our moves need to ensure that the inequalities in the candidate invariants satisfy the templates. Hence, we need to modify the coefficient moves. The constant moves remain unchanged.

We replace the coefficient move with a template move: Select an inequality and replace all the coefficients with coefficients from a randomly chosen selection of coefficients permitted by the template. For example, for intervals, $x_1 \leq 2$ can be mutated to $-x_2 \leq 2$ by a template move. The inequality move applies a constant move and a template move. This variation is called `Templ` in the evaluation in Section 5.2.3.

5.2.2 Example

We give a simple example to illustrate the moves. Suppose we have two variables x_1 and x_2, $\alpha = \beta = 1$, the initial candidate is $C \equiv 0{*}x_1 + 0{*}x_2 \leq 0$, $W = \{0, 1\}$, and $F = \{0, 1\}$. Then a coefficient move leaves C unchanged with probability 0.5 and mutates it to $1{*}x_1 + 0{*}x_2 \leq 0$ or $0{*}x_1 + 1{*}x_2 \leq 0$ with probability 0.25 each. A constant move selects a new constant t (by calling Figure 5.2) to be one of $\{0, 1\}$ with probability 0.25 each, one of $\{0{+}1, 1{+}0, 0{+}0, 1{+}1, 1{\times}0, 0{\times}1, 0{\times}0, 1{\times}1\}$ with probability

GEN-E(F: An array of integers)
Returns: An integer.

```
1: t := r(F); O:={+, ×, ⊥, ⊥};
2: o := r(O);
3: while o ≠ ⊥ do
4:     f := r(F); t := o(t, f); o := r(O);
5: end while
6: return t
```

Figure 5.2: Generate a random expression tree using leaves in F and operators in O; $r(A)$ returns an element selected uniformly at random from the array A.

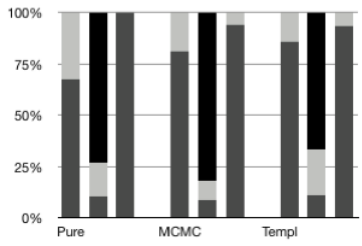


Figure 5.3: Statistics for three different randomized searches applied to the `cgr2` benchmark.

$\frac{1}{32}$ each, etc., and mutates C to $0*x_1+0*x_2 \leq t$ with the associated probability. An inequality move applies a constant move and a coefficient move to each coefficient. If we use intervals as templates then the possible values of the coefficients are $\{(0,0),(0,1),(0,-1),(1,0),(-1,0)\}$. Hence a template move leaves C unchanged with probability 0.2 and mutates it to $-x_1 \leq 0$, $x_1 \leq 0$, $-x_2 \leq 0$, or $x_2 \leq 0$ with probability 0.2 each. With templates, an inequality move applies a template move and a constant move.

5.2.3 Evaluation

We start with no data: $G = B = Z = \emptyset$. The initial candidate invariant J is the predicate in $\mathcal{S}$ that has all the coefficients and the constants set to zero: $\forall i,j,k.w_k^{(i,j)} = 0 \wedge t^{(i,j)} = 0$. The cost is evaluated using Equation 5.3 and when a candidate with cost zero is found then the decision procedure Z3 [43] is called. If Z3 proves that the candidate is indeed an invariant then we are done. Otherwise, Z3 provides a model. For better feedback, we ask Z3 for at most five distinct models. We extract counter-examples (good states, bad states, or pairs) from the models, they are incorporated in the data and the search is restarted with J as the initial candidate. A *round* consists of one search-and-validate iteration: finding a predicate with zero cost and asking Z3 to prove/refute it.

Observe that since the search space is finite-dimensional, we can also use a decision procedure to search for a candidate invariant. This direction was pursued in recent work by Garg et al. [56].

Program	Z3-H	ICE	[130]	[71]	Pure	MCMC	Templ
cgr1 [68]	0.0	0.0	0.2	0.1	0.0	0.0	0.0
cgr2 [68]	0.0	7.3	?	?	0.4	0.4	0.5
fig1 [68]	0.0	0.1	?	?	0.1	0.3	0.3
w1 [68]	0.0	0.0	0.2	0.1	0.0	0.0	0.0
fig3 [64]	0.0	0.0	0.1	0.1	0.0	0.0	0.0
fig9 [64]	0.0	0.0	0.2	0.1	0.0	0.0	0.0
tcs [80]	TO	1.4	0.5	0.1	0.7	0.0	0.0
ex23 [78]	?	14.2	?	?	TO	0.0	0.0
ex7 [78]	0.0	0.0	0.4	?	0.0	0.0	0.0
ex14 [78]	0.0	0.0	0.2	?	0.0	0.0	0.0
array [15]	0.0	0.3	0.2	?	1.0	0.6	0.9
fil1 [15]	0.0	0.0	0.4	0.1	0.0	0.0	0.0
ex11 [15]	0.0	0.6	0.2	0.1	0.0	0.0	0.0
trex1 [15]	0.0	0.0	0.4	0.1	0.0	0.0	0.0
monniaux	5.14	0.0	1.0	0.2	0.0	0.0	0.0
nested	0.0	?	1.0	0.0	0.1	0.2	0.0

Table 5.1: Inference of numerical invariants for proving safety properties.

Similar to us, they bound the search space to a finite set and iteratively invoke search and validate phases. Instead of using randomized search, they rely on Z3 to find an instantiation of the coefficients and the constants. Hence by comparing our approach against theirs, we can compare systematic search using a decision procedure with a randomized search.

The results of these comparisons are in Table 5.1. The first column is the name of the benchmark. For each benchmark, the problem is to find an invariant strong enough to discharge assertions in the program. All benchmarks except monniaux and nested are part of the benchmark suite described in [56]. The additional benchmarks are described below. Many of these benchmarks are flagship examples used by the respective papers to motivate a new technique for invariant inference. Five of these benchmarks require disjunctive invariants. The Z3-H column shows the time taken by Z3-Horn [74] in seconds. Z3-Horn is a decision procedure inside Z3 for solving VCs with unknown predicates. We observe that it is the fastest method for most of the programs. However, it crashes on ex23 (? in the table), is slow for monniaux, and times out on tcs (TO in the table). The ICE column shows the search-and-validate approach of [56]. While slower, it is able to handle the benchmarks that trouble Z3-Horn. The fourth column evaluates the geometric machine learning algorithm of Chapter 4 to search for candidate invariants and the next column is InvGen [71] a symbolic invariant inference engine that uses concrete data for constraint simplification. Columns ICE, [130], and [71] have been copied verbatim from [56] and the reader is referred to [56] for details.

The experiments in the last three columns (Pure, MCMC, and Templ) are performed on a 2.2 GHz Intel i7 with 4GB of memory. The experiments we compare to in Table 5.1 and in the rest of the chapter were performed on a variety of machines. Our goal in reporting performance numbers is not

to make precise comparisons, but only to show that Guess-and-Check has competitive performance with other techniques. Indeed, we observe that the time measurements of the Guess-and-Check searches in Table 5.1 are competitive with previous techniques. It is also worth emphasizing that because Guess-and-Check is a stochastic technique, there is variation in the timing on repeated executions using the same input. Moreover, we have observed that it is usual for some runs to never succeed and timeout eventually. The numbers reported in this chapter are the best of ten runs. We report the fastest time, rather than another statistic such as the median, because a natural approach to using randomized search in practice is to run many searches in parallel and the first search to succeed determines the running time.

The `Pure` column shows the time taken by the pure random walk of Section 5.2.1. The time is the total time of all the rounds including the time for both search and validation. The naive expectation is that the unguided search of `Pure` would fail for most of the benchmarks. However, the pure random walk is able to find the invariants for almost all the benchmarks including the ones on which the other tools fail. Moreover, the time required is comparable to the other tools. This observation suggests that the search space of numerical invariants is amenable to randomized search. Intuitively, there are many solutions in the search space and there are many possible sequences of transitions leading from one predicate to the other.

The `MCMC` column shows the effect of MCMC search that is guided by the cost function. The expectation is that it should perform much better than the pure random walk. We note that this expectation does not always hold (for `cgr2`, `fig1`, and `nested`). The reason is that MCMC search is slower. The pure random walk makes over a million proposals per second. On the other hand, MCMC search, with its overhead of computing the cost, is roughly an order of magnitude slower. Hence, even though MCMC search requires fewer proposals to converge for all the benchmarks in Table 5.1, it can take more time than the pure random walk. In Section 5.5.2, we show that `Pure` does not scale to more sophisticated search spaces and the cost function is essential. Also `Pure` times out on `ex23`: the reason is the absence of a cost function that guides the search towards the expression trees required for this benchmark.

The last column, `Templ`, shows the time when we manually provide templates to the search. The possible choices of templates are octagons and octahedra. Again, the expectation is that template based search should perform much better than `MCMC`. However, the templates adversely affect the desirable property of the MCMC proposal mechanism that there should be a good mixture of moves making small and large changes to the candidates.

Over all the benchmarks and all the different randomized searches fewer than 100 data points (good, bad, and pairs) and fewer than 30 rounds are sufficient to discover the invariant. The graph in Figure 5.3 shows some of the statistics for `cgr2`. We do not discuss the statistics for the other benchmarks as they are all quite similar and do not add additional insight.

The results in Figure 5.3 are divided into three groups. Each group corresponds to a different

Program	Z3-H	Pure	MCMC	Templ
term1	0.01	0.02	0.02	0.02
term2	TO	0.02	0.03	0.02
term3	TO	0.03	0.03	0.03
term4	0.01	0.03	0.05	0.02
term5	0.02	0.05	0.02	0.02
term6	TO	0.03	0.03	0.05

Table 5.2: Inference results for non-termination benchmarks.

randomized inference engine. In each group the first bar represents the percentage of time spent in search (bottom) versus validation (top). All three approaches spend most of their time in search. The second bar shows the good states (bottom), bad states (middle), and pairs (top) as percentages of the number of data elements. The number of pairs is higher than the number of good or bad states. The third bar shows the number of proposals accepted (bottom) and rejected (top) as the percentage of total proposals. `Pure` accepts everything and the others reject only a small fraction of proposals.

The benchmark `monniaux`[1] illustrates a limitation of Z3-Horn.

```
for(i=0;i<1000;i++);assert(i<=10000);
```

Intuitively, Z3-Horn is based on under-approximating strongest post-conditions and the large constant in the loop bound results in slow convergence. Empirically, for this example, the time taken by Z3-Horn appears to grow quadratically with the loop bound. On the other hand, the time taken by randomized search is independent of the size of the constants and is able to quickly find the invariant.

The benchmark `nested` has nested loops and cannot be handled by the implementation for simple loops described in [56]. Z3-Horn terminates on this example but instead of finding the simple invariants $i \geq 0$ and $0 \leq i < n \wedge 0 \leq j$, discovered by randomized search, it finds an existentially quantified invariant that cannot be consumed by most tools.

Since the randomized searches and Z3-Horn work with VCs, we can directly apply them to problems beyond invariant inference. Consider the problem addressed by the tool Looper [24]: Does a loop go into non-termination when executed with an input i? A certificate of non-termination is a *recurrent set* [70], a predicate that ensures the validity of the VCs in Equation 5.2. We consider the benchmarks for proving non-termination from TnT [70] and Looper in Table 5.2. Since these papers do not include performance results, we compare randomized search with Z3-Horn.

In Table 5.2, Z3-Horn is fast on half of the benchmarks and times out after thirty minutes on the other half. This observation suggests the sensitivity of symbolic inference engines to the search heuristics and the usefulness of Theorem 7. For half the benchmarks, the post-condition

[1] http://stackoverflow.com/questions/17547132/slow-invariant-inference-with-horn-clauses-in-z3

computation of Z3-Horn diverges. Randomized search, with no such systematic strategy and an asymptotic convergence guarantee, successfully handles all the benchmarks in less than a second.

5.3 Arrays

We consider the inference of universally quantified invariants over arrays. A program state for an array manipulating program contains the values of all the numerical variables and the arrays in scope. Given an invariant, existing decision procedures are robust enough to check that it indeed is an actual invariant. But in our experience, the decision procedures generally fail to find concrete counterexamples to refute incorrect candidates. This situation is a real concern, because if our technique is to be generally applicable then it must deal with the possibility that the decision procedures might not always be able to produce counterexamples to drive the search. Fortunately, there is a solution to this problem. As outlined in Section 5.1.2, the good states, the bad states, and the pairs required for search can be obtained from program executions.

We use an approach similar to [55, 130] to generate data. Let Σ_k denote all states in which all numerical variables are assigned values $\leq k$, all arrays have sizes $\leq k$, and all elements of these arrays are also $\leq k$. We generate all states in Σ_0, then Σ_1, and so on. To generate data, we run the loop with these states (see Section 5.1.2). To refute a candidate invariant, states from these runs are returned to the search. For our benchmarks, we did not need to enumerate beyond Σ_4 before an invariant was discovered. Better testing approaches are certainly possible [73].

We now define a search space of invariants to simulate the *fluid updates* abstraction for reasoning about arrays [45]. This abstraction is concerned with points-to relationships given by triples $(f[u], \phi, g[v])$, with the interpretation that ϕ is satisfied when $f[u]$ points to $g[v]$. In [45] both may relationships ($f[u] = g[v] \Rightarrow \phi$) and must relationships ($\phi \Rightarrow f[u] = g[v]$) are used. The must relationships suffice for our benchmarks and we discuss only these here. If $x_1, \ldots, x_n$ are the numerical variables of the program and f and g are array variables, then we are interested in array invariants of the following form:

$$\forall u, v. T(x_1, x_2, \ldots, x_n, u, v) \Rightarrow f[u] = g[v] \tag{5.4}$$

The variables u and v are universally quantified variables and T is a numerical predicate in the quantified variables and the variables of the program. Using this template, we reduce the search for array invariants to numerical predicates $T(x_1, x_2, \ldots, x_n, u, v)$.

The search for T proceeds as described in Section 5.2. For all our benchmarks, the search space with $\alpha = 1$ and $\beta = 10$ suffices. The only significant difference between this search and the search in Section 5.2 is in the evaluation of the cost function. Since T has quantified variables, the evaluation of the cost function is more expensive: when evaluating whether a state satisfies a candidate, each quantified variable results in a loop. When applying moves, quantified and free variables are treated identically.

Program	[45]	Z3-H	ARMC	Dual	Pure	MCMC	Templ
init	0.01	0.06	0.15	0.72	0.06	0.02	0.01
init-nc	0.02	0.08	0.48	6.60	0.05	0.15	0.02
init-p	0.01	0.03	0.14	2.60	0.01	0.01	0.01
init-e	0.04	TO	TO	TO	TO	TO	TO
2darray	0.04	0.18	?	TO	0.02	0.41	0.02
copy	0.01	0.04	0.20	1.40	0.87	0.80	0.02
copy-p	0.01	0.04	0.21	1.80	0.09	0.13	0.01
copy-o	0.04	TO	?	4.50	TO	TO	0.50
reverse	0.03	0.12	2.28	8.50	TO	3.48	0.03
swap	0.12	0.41	3.0	40.60	TO	TO	0.21
d-swap	0.16	1.37	4.4	TO	TO	TO	0.51
strcpy	0.07	0.05	0.15	0.62	0.01	0.02	0.01
strlen	0.02	0.07	0.02	0.20	0.01	0.01	0.01
memcpy	0.04	0.20	16.30	0.20	0.02	0.03	0.01
find	0.02	0.01	0.08	0.38	2.23	0.30	0.02
find-n	0.02	0.01	0.08	0.39	0.07	0.95	0.01
append	0.02	0.04	1.76	1.50	TO	TO	0.12
merge	0.09	0.04	?	1.50	TO	TO	0.41
alloc-f	0.02	0.02	0.09	0.69	0.07	0.10	0.01
alloc-nf	0.03	0.03	0.13	0.42	0.49	0.14	0.07

Table 5.3: Inference results for array manipulating programs

5.3.1 Evaluation

The principal difference between the evaluation here and in Section 5.2.3 is that there is no feedback between the search and the decision procedure. We manually wrote harnesses for generating data and then produced enough data that the search discovers a numerical predicate T that is an invariant of the array manipulating program. For all benchmarks, at most 150 data elements were sufficient to obtain an invariant. Just as in Section 5.2.3, we consider three variations of the search for T: `Pure` is a pure random walk, `MCMC` uses the cost function, and `Templ` restricts the inequalities in T to a user supplied abstract domain.

We evaluate these randomized search algorithms on the benchmarks of [45] in Table 5.3. The VCs for these benchmarks were obtained from the repository of the competition on software verification.[2] The first column is the name of the program. We have omitted benchmarks with bugs from the original benchmark set; these bugs are triggered during data generation. The second column shows the time taken by analyzing these benchmarks using the fluid updates abstraction [45]. Using a specialized abstract domain leads to a very efficient analysis, but the scope of the analysis is limited to array manipulating programs that have invariants given by Equation 5.4.

In [19], the authors use templates to reduce the task of inferring universally quantified invariants

[2]https://svn.sosy-lab.org/software/sv-benchmarks/trunk/clauses/QALIA/

for array manipulating programs to numerical invariants and show results using three different back-ends: Z3-Horn [74], Armc [62], and Duality [100]. These are reproduced verbatim as columns `Z3-H`, `ARMC`, and `Dual` of Table 5.3. Details about these columns can be found in the original text [19]. Note that the benchmark `init-e` requires a divisibility constraint that none of these back-ends or our search algorithms currently support.

The next three columns describe our randomized searches. The time measurements are the total time to search (with sufficient data) and validate an invariant. We observe that `Pure` times out on several benchmarks, which suggests that these problems are harder than those for numerical invariants. Moreover, whenever the pure random search times out, both Armc and Duality take more than a second. Hence, there seems to be some correlation between which verification tasks are difficult for different techniques. Another factor that adversely affects the randomized searches is that, due to the quantified variables, the evaluation of the cost function is slower than the evaluation of the cost function for numerical candidates.

The surprising result is that `Pure` still terminates quickly on the majority of the benchmarks. The next column shows that `MCMC` also times out on several benchmarks (these are a subset of benchmarks on which `Pure` times out). For these benchmarks, as shown by the last column, just specifying the abstract domain in which the linear inequalities in the invariant belong suffices to make the search terminate in under a second. Moreover, `Templ` is faster than both Armc and Duality on all the benchmarks of Table 5.3. These results suggest that randomized search is a suitable technique for inference of universally quantified invariants over arrays and can generate results competitive with state-of-the-art symbolic inference techniques.

5.4 Strings

Consider the string manipulating program of Figure 5.4 that computes the string $({}^{i}\mathtt{a})^{i}$. To validate its assertions, the invariants must express facts about the contents of strings, integers, and lengths of strings; we are unaware of any previous inference technique that can infer such invariants. The string operations such as *length* (compute the length of a string), *indexof* (find the position of a string in another string), *substr* (extract a substring between given indices), etc., intermix integers and strings and pose a challenge for invariant inference. However, the decision procedure Z3-str [153] can decide

```
i := 0; x := "a";
while(non_det()){ i++; x := "(" + x + ")"; }
assert( x.length == 2*i+1 );
if(i>0) assert( x.contains( "(a)" ) );
```

Figure 5.4: A program that intermixes strings and integers.

	Figure 5.4	`replace`	`index`	`substring`
`Pure`	342.6	0.01	0.06	0.5
`MCMC`	0.8	0.02	0.06	0.05
Z3-STR	0.03	TO	114.6	0.01

Table 5.4: Inference results for string manipulating programs. The time taken (in seconds) by pure random search, by MCMC search, and by Z3-STR (for proving the correctness of the invariants) are shown.

formulas over strings and integers. We use GUESS-AND-CHECK to construct an invariant inference procedure from Z3-STR.

A program state contains the values of all the numerical and the string variables. The search space $\mathcal{S}$ consists of boolean combinations of predicates that belong to a given bag $\mathcal{P}$ of predicates: $\bigvee_{j=1}^{\alpha} \left(\bigwedge_{k=1}^{\beta} P_k^j \right)$ where $P_k^j \in \mathcal{P}$. The bag $\mathcal{P}$ is constructed using the constants and the predicates occurring in the program. We set $\alpha = 5, \beta = 10$, and for Figure 5.4, $\mathcal{P}$ has predicates $x.contains(y)$, $y_1 = y_2$, $w_1 i + w_2 x.length + w_3 \leq 0$ where $y \in \{x, \text{“}\texttt{a}\text{”}, \text{“(”}, \text{“)”}, \text{“(}\texttt{a}\text{)”}\}$ and $w \in [-2 : 2]$. A move replaces a randomly selected P_k^j with a randomly selected predicate from $\mathcal{P}$. The current counterexample generation capabilities of Z3-STR are unreliable and we generate data using the process explained in Section 5.3. (At most 25 data elements were sufficient to obtain an invariant.) For Figure 5.4, randomized search discovers the following invariant and discharges the assertions:

$$\big(x = \text{“}\texttt{a}\text{”} \wedge i = 0\big) \vee \big(x.contains(\text{“(}\texttt{a}\text{)”}) \wedge x.length = 2i + 1\big)$$

Due to the absence of an existing benchmark suite for string-manipulating programs, our evaluation is limited to a few handwritten examples shown in Table 5.4. The program `replace` uses *replace* (replace the first occurrence of a string with another) in addition to the string operations present in Figure 5.4. This program checks that repeatedly replacing `"a"` by `"aa"` in a loop increases the length by the number of loop iterations. For this program Z3-STR times out in validating the candidate invariant. We confirmed that the candidate is an invariant manually. The program `index` uses *indexof* in addition to the string operations in `replace`. This program replaces all occurrences of one string by another and checks the relationship between the length of the output string and the number of iterations. Finally, `substring` uses *substr* and in this benchmark we prove that a loop which constructs an `http` request does not modify the domain name.

An alternative to GUESS-AND-CHECK for proving these examples requires designing a new abstract interpretation [36, 37], which entails designing an abstract domain that incorporates both strings and integers, an abstraction function, a widening operator, and abstract transfer functions that are precise enough to find disjunctive invariants like the one shown above. Such an alternative requires significantly greater effort than instantiating GUESS-AND-CHECK. In our implementation, both the proposal mechanism and the *eval* function, required to instantiate GUESS-AND-CHECK, are

under 50 lines of C++ each.

5.5 Relations

In this section we define a proposal mechanism to find invariants over relations. We are given a program with variables $x_1, x_2, \ldots, x_n$ and some relations $R_1, R_2, \ldots, R_m$. A program state is an evaluation of these variables and these relations. For example, consider the program state $i = 1, j = 2, pts = \{(1,2),(2,1)\}, eq = \{(1,1),(2,2)\}$ where pts is the points-to relation and eq is the equality relation. In this state i and j point to two heap cells that form a circularly linked list. The invariants are composed of variables and such relations. The search space consists of predicates F given by the following grammar:

$$\begin{array}{rcll} \textit{Predicate } F & ::= & \bigwedge_{i=1}^{\theta} F_i & \\ \textit{Formula } F^i & ::= & \bigwedge_{j=1}^{\delta} G_j^i & \\ \textit{Subformula } G^i & ::= & \forall u_1, u_2, \ldots, u_i.T & \\ \textit{QF Predicate } T & ::= & \bigvee_{k=1}^{\alpha} \bigwedge_{l=1}^{\beta} L_l^k & \\ \textit{Literal } L & ::= & A \mid \neg A & \\ \textit{Atom } A & ::= & R(V_1, \ldots, V_a) & a = \textit{arity}(R) \\ \textit{Argument } V & ::= & x \mid u \mid \kappa & \end{array} \tag{5.5}$$

A predicate in the search space is a conjunction of formulas F_i. The subscript of F_i denotes the number of quantified variables in its subformulas. A subformula is a quantified predicate with its quantifier free part T expressed in DNF. Each atomic proposition of this DNF formula is a relation whose arguments can be a variable of the program (x), a quantified variable (u), or some constant (κ) like *null*. We focus our attention on universally quantified predicates. Predicates with existential quantifiers and arbitrary alternations can also be incorporated easily in the search, but validating such candidates is much harder [138]. The variables *in scope* of a relation in a predicate are the program variables and the quantified variables in the associated subformulas.

Next we define the moves of our proposal mechanism. We select a move uniformly at random from the list below and apply it to the current candidate C. As usual, we write "at random" to mean "uniformly at random".

1. Variable move: Select an atom of C at random. Next, select one of the arguments and replace it with an argument selected at random from the variables in scope and the constants.

2. Relation move: Select an atom of C at random and replace its relation with a relation selected at random from the set of relations of the same arity. The arguments are unaffected.

3. Atom move: Select an atom of C at random and replace its relation with a relation selected at random from all available relations. Perform variable moves to fill the arguments of the new

relation.

4. Flip polarity: Negate a literal selected at random from the literals of C.

5. Literal move: Perform an atom move and flip polarity.

These moves are ergodic: using atom moves and flipping polarity it is possible to transform any candidate C_1 into any other candidate C_2. Moreover, these moves are symmetric and hence the proposal mechanism satisfies symmetry.

Next, we evaluate the MCMC algorithm in Figure 5.1 with this proposal mechanism and the cost function of Equation 5.3. We also evaluate a pure variation in which all moves are accepted. We do not evaluate a "template" variation as the relations can be seen as templates and it is unclear what additional template restrictions could be added.

5.5.1 Lists

We use the relational proposal mechanism to prove functional properties of linked list manipulating programs. The heap is composed of cells and each cell either contains *null* or the address of another cell. The reachability relation $n^*(i, j)$ holds if the cell pointed to by j can be reached from i using zero or more pointer dereferences. While writing post-conditions to express functional properties, it is useful to talk about the reachability relation that holds before the program begins execution. We denote this binary relation by $\_n^*$. Using these relations, the predicates in our search space are universally quantified formulas over these reachability relations for linked list manipulating programs.

A recently published decision procedure is complete for such candidates via a reduction of such formulas to boolean satisfiability [76]. It takes a program annotated with invariants as input and checks the assertions. We use this decision procedure as our validator and randomized search to find invariants for some standard singly linked list manipulating programs. The evaluation of [76] shows that it can handle relations and hence can validate a variety of programs that have been hand-annotated with invariants. During our evaluation of various verification tasks, we observed that such decision procedures for advanced logics are not able to accept all formulas in their input language. Hence, sometimes we must perform some equality-preserving simplifications on the candidate invariants our search discovers. Currently we perform this step manually when necessary, but the simplifications could be automated.

5.5.2 Evaluation

For defining the search space using Equation 5.5 we set $\alpha = \beta = \delta = 5$ and $\theta = 2$, which is sufficient to express the invariants for all of our benchmarks. Our evaluation results on the benchmarks of [76] are in Table 5.5. The first column lists the programs, all of which perform basic manipulations of singly linked lists. The program `delete` removes a specific element of the list, `deleteall` deletes

Program	#G	#R	Search	Valid	Proposed	Accepted	[77]
delete	50	2	0.20	0.04	4437	3949	9.32
delete-all	20	7	1.03	0.13	8482	7225	37.35
filter	50	26	10.41	0.11	160489	126389	55.53
last	50	3	0.90	0.04	98064	87446	7.49
reverse	20	54	55.11	0.08	582665	484208	146.42

Table 5.5: Inference results for list manipulating programs.

all the elements, `filter` deletes some specific elements if present in the list, `last` returns the last element of the list, and `reverse` is in-place reversal. The invariants for these programs are subtle and easy to get wrong.

Since these invariants are complex, pure random walk times out on all of these benchmarks. Hence, we show the results for only the MCMC search. Recall from Section 5.1.2 that it is easy to obtain good states: just run the program and collect the reachable states. However, it is more difficult to obtain bad states. We run our benchmarks on lists of length up to five to generate an initial set of good states, the size of which is shown in the column `G`. Starting from a non-empty set of good states results in faster convergence than starting from an empty set. Next, we start our search with zero bad states and zero pairs and generate candidate invariants. If the candidate is not an invariant we get a counterexample, which is added to the data (see discussion in Section 5.5.1). The number of rounds for the search to converge to an invariant is shown in the column `R`. The next four columns show the statistics of the last (and also the most expensive) round, the one that produces an invariant. The column `Search` shows the time taken by the search to infer an invariant. The column `Valid` shows the time taken by the validator to validate the invariant discovered by the search. The next two columns show the number of proposals made (`Proposed`) and the number of proposals accepted (`Accepted`) by the search. Observe that the search converges in less than a million proposals for all the benchmarks.

On comparing these results with those for array invariants, we note that the time taken by the search is higher. However, with arrays we were able to execute many more proposals per second. The maximum number of proposals for the results in Table 5.3 are about seven hundred thousand (`MCMC` for `reverse`) which is more than the number of proposals for any benchmarks in Table 5.5. Note that shape analyses like TVLA [122] can also handle the benchmarks in Table 5.5 within seconds. The last column of Table 5.5 is a recent invariant inference engine for lists that also uses the decision procedure of [76]. However, due to the intermediate manual steps in our evaluation, we cannot perform a direct comparison.

On analyzing the invariants discovered by the search, we observe that they are different from the invariants in the manually annotated benchmarks of [76]. Consider the benchmark `reverse`. The variable h is the head of the initial list, i is the head of the remaining list to be reversed, and j is

the head of the reversed list. The pre-condition is that the heap contains only the linked list and nothing else. The program is as follows:

```
i = h; j = null; while (i != null) { k=*i; *i=j; j=i; i=k; }
```

For `reverse` the search discovers the following invariant:

$$\forall u(u \neq null \Rightarrow (n^*(i,u) \vee n^*(j,u)))$$
$$\forall u,v(n^*(u,v) \Rightarrow (\neg\_n^*(i,u) \wedge \_n^*(v,u) \vee \_n^*(u,v) \wedge \neg\_n^*(u,j)))$$

The decision procedure of [76] is able to validate this invariant and uses it to show that `reverse` correctly reverses a linked list. Note that this invariant is more succinct and difficult to comprehend than the invariant written by hand in [76]:

$$\forall u(u \neq null \Rightarrow (n^*(i,u) \Leftrightarrow \neg n^*(j,u)))$$
$$\forall u,v(n^*(i,u) \Rightarrow (n^*(u,v) \Leftrightarrow \_n^*(u,v)))$$
$$\forall u,v(n^*(j,u) \Rightarrow (n^*(u,v) \Leftrightarrow \_n^*(v,u)))$$

This easier to understand invariant says that every node is either in the partially reversed list or the to be reversed list. In the to be reversed list, the reachability relation is unchanged and in the partially reversed list the reachability relation is reverse of the initial.

Since the decision procedure of [76] is complete, it is able to consume and verify any unusual invariants that the search produces. Generally the decision procedures for more advanced data structures are not so robust that they can consume arbitrary candidates. Often, one needs to write the invariants with care and might even need to provide additional axioms or lemmas to verify more advanced data structure manipulating programs [116]. Once the state of the art of these decision procedures improve, we can apply randomized search for these programs too. We do not need a complete decision procedure as we can generate data by running the programs, just as we do for arrays and strings. But the decision procedure should be robust enough to handle arbitrary candidate invariants automatically.

5.6 Related Work

The goal of this chapter is a framework to obtain inference engines from decision procedures. Guess-and-Check is parametrized by the language of possible invariants. This characteristic is similar to TVLA [122], which is a parametric shape analysis. TVLA requires specialized heuristics (focus, coerce, etc.) to maintain precision. We do not require these heuristics and this generality aids us in obtaining inference procedures for verification tasks beyond shape analysis. Guess-and-Check is a template-based analysis that does not use decision procedures to instantiate the templates and limits their use to checking an annotated program. We do not rely on decision procedures to compute a

predicate cover [69], or for fixpoint iterations [54, 137], or on Farkas' lemma [17, 35, 68, 71]. Hence, GUESS-AND-CHECK is applicable to various decision procedures, including the incomplete procedures (Section 5.3 and Section 5.4).

Most techniques for invariant inference are symbolic analyses that trade generality for effective techniques in specific domains [16, 26, 47, 71, 77, 84]. We are not aware of any symbolic inference technique that has been successfully demonstrated to infer invariants for the various types of programs that we consider (numeric, array, string, and list). We have shown that invariant search using concrete data and general search procedures such as Metropolis Hastings has the potential to be a general solution to obtain inference procedures from checking procedures. We discuss the related techniques that learn invariants from concrete data and compare them with randomized search.

Concrete states can help maintain precision by aiding the computation of the best abstract transformers [118]. However, this approach suffers from irrecoverable imprecision as it relies on widening heuristics for termination. In contrast, randomized search can always recover from excessive under or over approximations, but only provides an asymptotic guarantee of termination if an invariant exists. The inference algorithm for numerical invariants described in [56] uses decision procedures to search for candidate invariants. It is not clear whether decision procedures can effectively search for good candidates that satisfy data over quantified domains. There are several automata-based approaches for learning invariants [33, 55, 56]. It is unclear whether automata can express numerical invariants. Domain-specific search procedures like these seem unsuitable for a general framework for obtaining inference procedures from checking procedures.

Algorithmic learning [83, 88] based approaches also iteratively invoke search and validate phases. They use a CDNF learning algorithm that requires membership queries (is a conjunction of atomic predicates contained in the invariant) and equivalence queries (is the candidate an invariant). Since the invariant is unknown, the membership queries are resolved heuristically. In contrast, GUESS-AND-CHECK does not require membership queries. Other techniques that use concrete data to guide verification include [4, 64, 67, 104].

We are unaware of the any previous work that uses Metropolis Hastings sampler for invariant inference. In a related work, [66] uses Gibbs sampling for inference of numerical invariants. However, the inference works directly on the program (it computes pre-conditions and post-conditions) as opposed to concrete data. Handling programs with pointers and arrays is left as an open problem by [66].

We use efficiency to guide the choice of parameters for randomized search. E.g., in our evaluations, we set γ in Figure 5.1 to $log_e\ 2$. Systematic approaches described in [132] can also be used for setting such parameters.

MCMC based search has been found to be useful in superoptimization [126], where the goal is to infer an assembly program that satisfies some concrete input/output examples. MCMC search has also been used in program testing to achieve better coverage [123]. A randomized scheduler is used

to find concurrency bugs in [23].

Chapter 6

Conclusion

In this thesis, we have discussed loop invariant inference techniques that combine static analysis and machine learning. We break down the problem of invariant inference into two phases. In the *guess* phase, the loop is executed on a few inputs and the observed program states are logged. These logs constitute our *data*. Subsequently, a learner guesses a candidate invariant from the data. In the *check* phase, a static analysis proves whether the candidate invariant is an actual invariant or not. In the former case, the inference succeeds. In the latter case, we repeat the process with additional data.

This Guess-and-Check approach helps us achieve new results. Chapter 2 describes a sound and relatively complete algorithm for inference of algebraic invariants that finds correct invariants (if the SMT solver can answer all queries correctly) and the inferred invariant is the best possible in the given class. In contrast, all previous tools for inferring algebraic equality invariants unsoundly approximate integral program variables by real-valued variables. Chapter 3 describes DDEC, the first equivalence checker for x86. The key idea that makes DDEC effective in practice, and even simply feasible to build, is that the process of guessing a simulation relation is constructed not via static code analyses, but by using data collected from tests. Chapter 4 presents the first invariant inference technique that does not place any ad-hoc restriction on the number of disjunctions while also guaranteeing that invariants are of bounded size. Naive approaches tend to generate a very large or even an unbounded number of disjunctions, leading to non-terminating analyses. Therefore, to ensure tractability, all previous analyses use a user-provided or an ad-hoc bound on the number of disjunctions. Chapter 5 presents an approach to infer arbitrary invariants. Instantiating the Guess-and-Check approach with MCMC samplers as learners and suitable SMT solvers yields inference engines for many classes, including those for which invariant inference techniques were previously unknown.

A common theme of these chapters is the observation that the decomposition of invariant inference into two phases substantially simplifies the architecture of a verifier and leads to simpler

implementations. The learners are just data crunching algorithms that are easy to implement. For checking, we use off-the-shelf SMT solvers and take advantage of recent advances in automatic theorem proving.

Although this thesis focuses on loop invariants, it is possible to leverage the data-driven techniques for many other inference tasks. For example, consider the problem of program termination. Termination proofs are based on inferring *variants* or ranking functions. We have used data to infer ranking functions in [110]. Data has also assisted us in proving race freedom and deadlock freedom of aggressively optimized GPU programs [128]. We explored connections between program analyses and statistical machine learning in [132], and these connections helped significantly improve the performance of an industrial strength device-driver verifier. We believe that data-driven techniques can significantly enhance the state of the art in many other verification tasks.

Since data-driven techniques are very different from the symbolic techniques routinely used in verification, the Guess-and-Check based inference engines have different strengths and weaknesses compared to traditional static analyses. Intuitively, a purely static analysis is governed by a proof goal and tries to infer logic formulas that would help the proof go through. In contrast, the learner observes concrete states and mines patterns that are apparent in the data and produces them as candidate invariants. The learners studied in machine learning are often guided by Occam's razor and aim to generate the simplest hypotheses that explain the data. A Guess-and-Check approach succeeds if the simple patterns are sufficient for the proof. Since programmers/compilers reason about the correctness of the code they generate, in many cases, the invariants are indeed simple and the candidates guessed via learning are useful. However, some verification tasks can require invariants that are larger than the programs themselves and a purely static analysis can perform better than Guess-and-Check for such cases.

There are several domains where the data-driven techniques described in this thesis are currently inapplicable, such as verification of models or abstract specifications. Such models are usually not executable, and data generation fails. In verification using interactive theorem provers, it is typical to construct a proof and an implementation together. Therefore, unless the proof has been completed, an executable program is not available, and data cannot be generated. Rich symbolic techniques for data generation can help alleviate some of these concerns. Finally, the invariants considered in this thesis can be inferred by simple learners and consumed by SMT solvers. More expressive invariants pose a challenge for both the existing learners and the existing checkers; these would require new techniques beyond this thesis.

Bibliography

[1] Behzad Akbarpour and Lawrence C. Paulson. MetiTarski: An automatic theorem prover for real-valued special functions. *J. Autom. Reasoning*, 44(3):175–205, 2010.

[2] Aws Albarghouthi, Arie Gurfinkel, and Marsha Chechik. Craig interpretation. In *Static Analysis - 19th International Symposium, SAS 2012, Deauville, France, September 11-13, 2012. Proceedings*, pages 300–316, 2012.

[3] Rajeev Alur, Rastislav Bodík, Garvit Juniwal, Milo M. K. Martin, Mukund Raghothaman, Sanjit A. Seshia, Rishabh Singh, Armando Solar-Lezama, Emina Torlak, and Abhishek Udupa. Syntax-guided synthesis. In *Formal Methods in Computer-Aided Design, FMCAD 2013, Portland, OR, USA, October 20-23, 2013*, pages 1–8, 2013.

[4] Gianluca Amato, Maurizio Parton, and Francesca Scozzari. Discovering invariants via simple component analysis. *J. Symb. Comput.*, 47(12):1533–1560, 2012.

[5] Christophe Andrieu, Nando De Freitas, Arnaud Doucet, and Michael I Jordan. An introduction to MCMC for machine learning. *Machine learning*, 50(1-2):5–43, 2003.

[6] Tamarah Arons, Elad Elster, Limor Fix, Sela Mador-Haim, Michael Mishaeli, Jonathan Shalev, Eli Singerman, Andreas Tiemeyer, Moshe Y. Vardi, and Lenore D. Zuck. Formal verification of backward compatibility of microcode. In *Computer Aided Verification, 17th International Conference, CAV 2005, Edinburgh, Scotland, UK, July 6-10, 2005, Proceedings*, pages 185–198, 2005.

[7] David F. Bacon, Susan L. Graham, and Oliver J. Sharp. Compiler transformations for high-performance computing. *ACM Comput. Surv.*, 26(4):345–420, 1994.

[8] Roberto Bagnara, Patricia M. Hill, and Enea Zaffanella. Widening operators for powerset domains. *STTT*, 9(3-4):413–414, 2007.

[9] Roberto Bagnara, Enric Rodríguez-Carbonell, and Enea Zaffanella. Generation of basic semi-algebraic invariants using convex polyhedra. In *Static Analysis, 12th International Symposium, SAS 2005, London, UK, September 7-9, 2005, Proceedings*, pages 19–34, 2005.

[10] Gogul Balakrishnan and Thomas W. Reps. WYSINWYX: What you see is not what you eXecute. *ACM Trans. Program. Lang. Syst.*, 32(6), 2010.

[11] Thomas Ball, Brian Hackett, Shuvendu K. Lahiri, Shaz Qadeer, and Julien Vanegue. Towards scalable modular checking of user-defined properties. In *Verified Software: Theories, Tools, Experiments, Third International Conference, VSTTE 2010, Edinburgh, UK, August 16-19, 2010. Proceedings*, pages 1–24, 2010.

[12] Thomas Ball and Sriram K. Rajamani. The SLAM toolkit. In *Computer Aided Verification, 13th International Conference, CAV 2001, Paris, France, July 18-22, 2001, Proceedings*, pages 260–264, 2001.

[13] Michael Barnett, Bor-Yuh Evan Chang, Robert DeLine, Bart Jacobs, and K. Rustan M. Leino. Boogie: A modular reusable verifier for object-oriented programs. In *Formal Methods for Components and Objects, 4th International Symposium, FMCO 2005, Amsterdam, The Netherlands, November 1-4, 2005, Revised Lectures*, pages 364–387, 2005.

[14] Bonnie Berger, John Rompel, and Peter W. Shor. Efficient NC algorithms for set cover with applications to learning and geometry. *J. Comput. Syst. Sci.*, 49(3):454–477, 1994.

[15] Dirk Beyer. Competition on Software Verification (SV-COMP) benchmarks. https://svn. sosy-lab.org/software/sv-benchmarks/tags/svcomp13/loops/.

[16] Dirk Beyer, Thomas A. Henzinger, Ranjit Jhala, and Rupak Majumdar. The software model checker Blast. *STTT*, 9(5-6):505–525, 2007.

[17] Dirk Beyer, Thomas A. Henzinger, Rupak Majumdar, and Andrey Rybalchenko. Invariant synthesis for combined theories. In *Verification, Model Checking, and Abstract Interpretation, 8th International Conference, VMCAI 2007, Nice, France, January 14-16, 2007, Proceedings*, pages 378–394, 2007.

[18] Dirk Beyer, Thomas A. Henzinger, Rupak Majumdar, and Andrey Rybalchenko. Path invariants. In *Proceedings of the ACM SIGPLAN 2007 Conference on Programming Language Design and Implementation, San Diego, California, USA, June 10-13, 2007*, pages 300–309, 2007.

[19] Nikolaj Bjørner, Kenneth L. McMillan, and Andrey Rybalchenko. On solving universally quantified Horn clauses. In *Static Analysis - 20th International Symposium, SAS 2013, Seattle, WA, USA, June 20-22, 2013. Proceedings*, pages 105–125, 2013.

[20] Anselm Blumer, Andrzej Ehrenfeucht, David Haussler, and Manfred K. Warmuth. Learnability and the Vapnik-Chervonenkis dimension. *J. ACM*, 36(4):929–965, 1989.

[21] Hervé Brönnimann and Michael T. Goodrich. Almost optimal set covers in finite VC-dimension. *Discrete & Computational Geometry*, 14(4):463–479, 1995.

[22] Nader H. Bshouty, Sally A. Goldman, H. David Mathias, Subhash Suri, and Hisao Tamaki. Noise-tolerant distribution-free learning of general geometric concepts. In *Proceedings of the Twenty-Eighth Annual ACM Symposium on the Theory of Computing, Philadelphia, Pennsylvania, USA, May 22-24, 1996*, pages 151–160, 1996.

[23] Sebastian Burckhardt, Pravesh Kothari, Madanlal Musuvathi, and Santosh Nagarakatte. A randomized scheduler with probabilistic guarantees of finding bugs. In *Proceedings of the 15th International Conference on Architectural Support for Programming Languages and Operating Systems, ASPLOS 2010, Pittsburgh, Pennsylvania, USA, March 13-17, 2010*, pages 167–178, 2010.

[24] Jacob Burnim, Nicholas Jalbert, Christos Stergiou, and Koushik Sen. Looper: Lightweight detection of infinite loops at runtime. In *ASE 2009, 24th IEEE/ACM International Conference on Automated Software Engineering, Auckland, New Zealand, November 16-20, 2009*, pages 161–169, 2009.

[25] David Cachera, Thomas P. Jensen, Arnaud Jobin, and Florent Kirchner. Inference of polynomial invariants for imperative programs: A farewell to Gröbner bases. In *Static Analysis - 19th International Symposium, SAS 2012, Deauville, France, September 11-13, 2012. Proceedings*, pages 58–74, 2012.

[26] Cristiano Calcagno, Dino Distefano, Peter W. O'Hearn, and Hongseok Yang. Compositional shape analysis by means of bi-abduction. In *Proceedings of the 36th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2009, Savannah, GA, USA, January 21-23, 2009*, pages 289–300, 2009.

[27] Zhuliang Chen and Arne Storjohann. A BLAS based C library for exact linear algebra on integer matrices. In *Symbolic and Algebraic Computation, International Symposium ISSAC 2005, Beijing, China, July 24-27, 2005, Proceedings*, pages 92–99, 2005.

[28] Siddhartha Chib and Edward Greenberg. Understanding the Metropolis-Hastings algorithm. *The American Statistician*, 49(4):327–335, 1995.

[29] Chris Lattner and Vikram Adve. The LLVM Instruction Set and Compilation Strategy. Tech. Report UIUCDCS-R-2002-2292, CS Dept., Univ. of Illinois at Urbana-Champaign, Aug 2002.

[30] V Chvatal. A greedy heuristic for the set-covering problem. *Mathematics of Operations Research*, 4(3):233–235, 1979.

[31] Robert Clarisó and Jordi Cortadella. The octahedron abstract domain. In *Static Analysis, 11th International Symposium, SAS 2004, Verona, Italy, August 26-28, 2004, Proceedings*, pages 312–327, 2004.

[32] Edmund M. Clarke, Orna Grumberg, Somesh Jha, Yuan Lu, and Helmut Veith. Counterexample-guided abstraction refinement. In *Computer Aided Verification, 12th International Conference, CAV 2000, Chicago, IL, USA, July 15-19, 2000, Proceedings*, pages 154–169, 2000.

[33] Jamieson M. Cobleigh, Dimitra Giannakopoulou, and Corina S. Pasareanu. Learning assumptions for compositional verification. In *Tools and Algorithms for the Construction and Analysis of Systems, 9th International Conference, TACAS 2003, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2003, Warsaw, Poland, April 7-11, 2003, Proceedings*, pages 331–346, 2003.

[34] Michael Colón. Approximating the algebraic relational semantics of imperative programs. In *Static Analysis, 11th International Symposium, SAS 2004, Verona, Italy, August 26-28, 2004, Proceedings*, pages 296–311, 2004.

[35] Michael Colón, Sriram Sankaranarayanan, and Henny Sipma. Linear invariant generation using non-linear constraint solving. In *Computer Aided Verification, 15th International Conference, CAV 2003, Boulder, CO, USA, July 8-12, 2003, Proceedings*, pages 420–432, 2003.

[36] Giulia Costantini, Pietro Ferrara, and Agostino Cortesi. Static analysis of string values. In *Formal Methods and Software Engineering - 13th International Conference on Formal Engineering Methods, ICFEM 2011, Durham, UK, October 26-28, 2011. Proceedings*, pages 505–521, 2011.

[37] Patrick Cousot and Radhia Cousot. Abstract interpretation: A unified lattice model for static analysis of programs by construction or approximation of fixpoints. In *Conference Record of the Fourth ACM Symposium on Principles of Programming Languages, Los Angeles, California, USA, January 1977*, pages 238–252, 1977.

[38] Patrick Cousot and Radhia Cousot. Systematic design of program analysis frameworks. In *Conference Record of the Sixth Annual ACM Symposium on Principles of Programming Languages, San Antonio, Texas, USA, January 1979*, pages 269–282, 1979.

[39] Patrick Cousot, Radhia Cousot, Jérôme Feret, Laurent Mauborgne, Antoine Miné, David Monniaux, and Xavier Rival. The ASTRÉE analyzer. In *Programming Languages and Systems, 14th European Symposium on Programming, ESOP 2005, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2005, Edinburgh, UK, April 4-8, 2005, Proceedings*, pages 21–30, 2005.

[40] Patrick Cousot and Nicolas Halbwachs. Automatic discovery of linear restraints among variables of a program. In *Conference Record of the Fifth Annual ACM Symposium on Principles of Programming Languages, Tucson, Arizona, USA, January 1978*, pages 84–96, 1978.

[41] David A. Cox, John Little, and Donal O'Shea. *Ideals, Varieties, and Algorithms - An Introduction to Computational Algebraic Geometry and Commutative Algebra.* Undergraduate texts in mathematics. Springer, 1997.

[42] David W. Currie, Alan J. Hu, and Sreeranga P. Rajan. Automatic formal verification of DSP software. In *Proceedings of the 37th Conference on Design Automation, Los Angeles, CA, USA, June 5-9, 2000. ACM, 2000*, pages 130–135, 2000.

[43] Leonardo Mendonça de Moura and Nikolaj Bjørner. Z3: an efficient SMT solver. In *Tools and Algorithms for the Construction and Analysis of Systems, 14th International Conference, TACAS 2008, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2008, Budapest, Hungary, March 29-April 6, 2008. Proceedings*, pages 337–340, 2008.

[44] Edsger W. Dijkstra. *A Discipline of Programming.* Prentice-Hall, 1976.

[45] Isil Dillig, Thomas Dillig, and Alex Aiken. Fluid updates: Beyond strong vs. weak updates. In *Programming Languages and Systems, 19th European Symposium on Programming, ESOP 2010, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2010, Paphos, Cyprus, March 20-28, 2010. Proceedings*, pages 246–266, 2010.

[46] Isil Dillig, Thomas Dillig, and Alex Aiken. Small formulas for large programs: On-line constraint simplification in scalable static analysis. In *Static Analysis - 17th International Symposium, SAS 2010, Perpignan, France, September 14-16, 2010. Proceedings*, pages 236–252, 2010.

[47] Isil Dillig, Thomas Dillig, Boyang Li, and Kenneth L. McMillan. Inductive invariant generation via abductive inference. In *Proceedings of the 2013 ACM SIGPLAN International Conference on Object Oriented Programming Systems Languages & Applications, OOPSLA 2013, part of SPLASH 2013, Indianapolis, IN, USA, October 26-31, 2013*, pages 443–456, 2013.

[48] Matt Elder, Junghee Lim, Tushar Sharma, Tycho Andersen, and Thomas W. Reps. Abstract domains of affine relations. *ACM Trans. Program. Lang. Syst.*, 36(4):11:1–11:73, 2014.

[49] Michael D. Ernst, Jeff H. Perkins, Philip J. Guo, Stephen McCamant, Carlos Pacheco, Matthew S. Tschantz, and Chen Xiao. The daikon system for dynamic detection of likely invariants. *Sci. Comput. Program.*, 69(1-3):35–45, 2007.

[50] Manuel Fähndrich and Francesco Logozzo. Static contract checking with abstract interpretation. In *Formal Verification of Object-Oriented Software - International Conference, FoVeOOS 2010, Paris, France, June 28-30, 2010, Revised Selected Papers*, pages 10–30, 2010.

[51] Xiushan Feng and Alan J. Hu. Automatic formal verification for scheduled VLIW code. In *Proceedings of the 2002 Joint Conference on Languages, Compilers, and Tools for Embedded Systems & Software and Compilers for Embedded Systems (LCTES'02-SCOPES'02), Berlin, Germany, 19-21 June 2002*, pages 85–92, 2002.

[52] Xiushan Feng and Alan J. Hu. Cutpoints for formal equivalence verification of embedded software. In *EMSOFT 2005, September 18-22, 2005, Jersey City, NJ, USA, 5th ACM International Conference On Embedded Software, Proceedings*, pages 307–316, 2005.

[53] Gilberto Filé and Francesco Ranzato. Improving abstract interpretations by systematic lifting to the powerset. In *Logic Programming, Proceedings of the 1994 International Symposium, Ithaca, New York, USA, November 13-17, 1994*, pages 655–669, 1994.

[54] Cormac Flanagan and K. Rustan M. Leino. Houdini, an annotation assistant for esc/java. In *FME 2001: Formal Methods for Increasing Software Productivity, International Symposium of Formal Methods Europe, Berlin, Germany, March 12-16, 2001, Proceedings*, pages 500–517, 2001.

[55] Pranav Garg, Christof Löding, P. Madhusudan, and Daniel Neider. Learning universally quantified invariants of linear data structures. In *Computer Aided Verification - 25th International Conference, CAV 2013, Saint Petersburg, Russia, July 13-19, 2013. Proceedings*, pages 813–829, 2013.

[56] Pranav Garg, Christof Löding, P. Madhusudan, and Daniel Neider. ICE: A robust framework for learning invariants. In *Computer Aided Verification - 26th International Conference, CAV 2014, Held as Part of the Vienna Summer of Logic, VSL 2014, Vienna, Austria, July 18-22, 2014. Proceedings*, pages 69–87, 2014.

[57] Khalil Ghorbal, Franjo Ivancic, Gogul Balakrishnan, Naoto Maeda, and Aarti Gupta. Donut domains: Efficient non-convex domains for abstract interpretation. In *Verification, Model Checking, and Abstract Interpretation - 13th International Conference, VMCAI 2012, Philadelphia, PA, USA, January 22-24, 2012. Proceedings*, pages 235–250, 2012.

[58] Patrice Godefroid and Ankur Taly. Automated synthesis of symbolic instruction encodings from I/O samples. In *ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI '12, Beijing, China - June 11 - 16, 2012*, pages 441–452, 2012.

[59] Benny Godlin and Ofer Strichman. Regression verification. In *Proceedings of the 46th Design Automation Conference, DAC 2009, San Francisco, CA, USA, July 26-31, 2009*, pages 466–471, 2009.

[60] Benjamin Goldberg, Lenore D. Zuck, and Clark W. Barrett. Into the loops: Practical issues in translation validation for optimizing compilers. *Electr. Notes Theor. Comput. Sci.*, 132(1):53–71, 2005.

[61] Denis Gopan and Thomas W. Reps. Guided static analysis. In *Static Analysis, 14th International Symposium, SAS 2007, Kongens Lyngby, Denmark, August 22-24, 2007, Proceedings*, pages 349–365, 2007.

[62] Sergey Grebenshchikov, Nuno P. Lopes, Corneliu Popeea, and Andrey Rybalchenko. Synthesizing software verifiers from proof rules. In *ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI '12, Beijing, China - June 11 - 16, 2012*, pages 405–416, 2012.

[63] Bhargav S. Gulavani, Supratik Chakraborty, Aditya V. Nori, and Sriram K. Rajamani. Automatically refining abstract interpretations. In *Tools and Algorithms for the Construction and Analysis of Systems, 14th International Conference, TACAS 2008, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2008, Budapest, Hungary, March 29-April 6, 2008. Proceedings*, pages 443–458, 2008.

[64] Bhargav S. Gulavani, Thomas A. Henzinger, Yamini Kannan, Aditya V. Nori, and Sriram K. Rajamani. SYNERGY: a new algorithm for property checking. In *Proceedings of the 14th ACM SIGSOFT International Symposium on Foundations of Software Engineering, FSE 2006, Portland, Oregon, USA, November 5-11, 2006*, pages 117–127, 2006.

[65] Sumit Gulwani. Program analysis using random interpretation. In *Ph.D. Dissertation, UC-Berkeley*, 2005.

[66] Sumit Gulwani and Nebojsa Jojic. Program verification as probabilistic inference. In *Proceedings of the 34th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2007, Nice, France, January 17-19, 2007*, pages 277–289, 2007.

[67] Sumit Gulwani and George C. Necula. Discovering affine equalities using random interpretation. In *Conference Record of POPL 2003: The 30th SIGPLAN-SIGACT Symposium on Principles of Programming Languages, New Orleans, Louisisana, USA, January 15-17, 2003*, pages 74–84, 2003.

[68] Sumit Gulwani, Saurabh Srivastava, and Ramarathnam Venkatesan. Program analysis as constraint solving. In *Proceedings of the ACM SIGPLAN 2008 Conference on Programming*

Language Design and Implementation, Tucson, AZ, USA, June 7-13, 2008, pages 281–292, 2008.

[69] Sumit Gulwani, Saurabh Srivastava, and Ramarathnam Venkatesan. Constraint-based invariant inference over predicate abstraction. In *Verification, Model Checking, and Abstract Interpretation, 10th International Conference, VMCAI 2009, Savannah, GA, USA, January 18-20, 2009. Proceedings*, pages 120–135, 2009.

[70] Ashutosh Gupta, Thomas A. Henzinger, Rupak Majumdar, Andrey Rybalchenko, and Ru-Gang Xu. Proving non-termination. In *Proceedings of the 35th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2008, San Francisco, California, USA, January 7-12, 2008*, pages 147–158, 2008.

[71] Ashutosh Gupta, Rupak Majumdar, and Andrey Rybalchenko. From tests to proofs. In *Tools and Algorithms for the Construction and Analysis of Systems, 15th International Conference, TACAS 2009, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2009, York, UK, March 22-29, 2009. Proceedings*, pages 262–276, 2009.

[72] Neelam Gupta and Zachary V. Heidepriem. A new structural coverage criterion for dynamic detection of program invariants. In *18th IEEE International Conference on Automated Software Engineering (ASE 2003), 6-10 October 2003, Montreal, Canada*, pages 49–59, 2003.

[73] Michael Harder, Jeff Mellen, and Michael D. Ernst. Improving test suites via operational abstraction. In *Proceedings of the 25th International Conference on Software Engineering, May 3-10, 2003, Portland, Oregon, USA*, pages 60–73, 2003.

[74] Krystof Hoder and Nikolaj Bjørner. Generalized property directed reachability. In *Theory and Applications of Satisfiability Testing - SAT 2012 - 15th International Conference, Trento, Italy, June 17-20, 2012. Proceedings*, pages 157–171, 2012.

[75] Kenneth Hoffman and Ray Kunze. *Linear Algebra*. Prentice Hall, second edition, 1971.

[76] Shachar Itzhaky, Anindya Banerjee, Neil Immerman, Aleksandar Nanevski, and Mooly Sagiv. Effectively-propositional reasoning about reachability in linked data structures. In *Computer Aided Verification - 25th International Conference, CAV 2013, Saint Petersburg, Russia, July 13-19, 2013. Proceedings*, pages 756–772, 2013.

[77] Shachar Itzhaky, Nikolaj Bjørner, Thomas W. Reps, Mooly Sagiv, and Aditya V. Thakur. Property-directed shape analysis. In *Computer Aided Verification - 26th International Conference, CAV 2014, Held as Part of the Vienna Summer of Logic, VSL 2014, Vienna, Austria, July 18-22, 2014. Proceedings*, pages 35–51, 2014.

[78] Franjo Ivancic and Sriram Sankaranarayanan. NECLA Static Analysis Benchmarks http://www.nec-labs.com/research/system/systems_SAV-website/small_static_bench-v1.1.tar.gz.

[79] Daniel Jackson and David A. Ladd. Semantic diff: A tool for summarizing the effects of modifications. In *Proceedings of the International Conference on Software Maintenance, ICSM 1994, Victoria, BC, Canada, September 1994*, pages 243–252, 1994.

[80] Ranjit Jhala and Kenneth L. McMillan. A practical and complete approach to predicate refinement. In *Tools and Algorithms for the Construction and Analysis of Systems, 12th International Conference, TACAS 2006 Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2006, Vienna, Austria, March 25 - April 2, 2006, Proceedings*, pages 459–473, 2006.

[81] Rajeev Joshi, Greg Nelson, and Keith H. Randall. Denali: A goal-directed superoptimizer. In *Proceedings of the 2002 ACM SIGPLAN Conference on Programming Language Design and Implementation (PLDI), Berlin, Germany, June 17-19, 2002*, pages 304–314, 2002.

[82] Dejan Jovanovic and Leonardo Mendonça de Moura. Solving non-linear arithmetic. In *Automated Reasoning - 6th International Joint Conference, IJCAR 2012, Manchester, UK, June 26-29, 2012. Proceedings*, pages 339–354, 2012.

[83] Yungbum Jung, Soonho Kong, Bow-Yaw Wang, and Kwangkeun Yi. Deriving invariants by algorithmic learning, decision procedures, and predicate abstraction. In *Verification, Model Checking, and Abstract Interpretation, 11th International Conference, VMCAI 2010, Madrid, Spain, January 17-19, 2010. Proceedings*, pages 180–196, 2010.

[84] Yamini Kannan and Koushik Sen. Universal symbolic execution and its application to likely data structure invariant generation. In *Proceedings of the ACM/SIGSOFT International Symposium on Software Testing and Analysis, ISSTA 2008, Seattle, WA, USA, July 20-24, 2008*, pages 283–294, 2008.

[85] Michael Karr. Affine relationships among variables of a program. *Acta Inf.*, 6:133–151, 1976.

[86] James C. King. Symbolic execution and program testing. *Commun. ACM*, 19(7):385–394, 1976.

[87] Donald E. Knuth. *The Art of Computer Programming, Volume II: Seminumerical Algorithms, 2nd Edition*. Addison-Wesley, 1981.

[88] Soonho Kong, Yungbum Jung, Cristina David, Bow-Yaw Wang, and Kwangkeun Yi. Automatically inferring quantified loop invariants by algorithmic learning from simple templates.

In *Programming Languages and Systems - 8th Asian Symposium, APLAS 2010, Shanghai, China, November 28 - December 1, 2010. Proceedings*, pages 328–343, 2010.

[89] Laura Kovács. A complete invariant generation approach for P-solvable loops. In *Ershov Memorial Conference*, pages 242–256, 2009.

[90] Shuvendu K. Lahiri, Chris Hawblitzel, Ming Kawaguchi, and Henrique Rebêlo. SYMDIFF: A language-agnostic semantic diff tool for imperative programs. In *Computer Aided Verification - 24th International Conference, CAV 2012, Berkeley, CA, USA, July 7-13, 2012 Proceedings*, pages 712–717, 2012.

[91] Shuvendu K. Lahiri and Shaz Qadeer. Complexity and algorithms for monomial and clausal predicate abstraction. In *Automated Deduction - CADE-22, 22nd International Conference on Automated Deduction, Montreal, Canada, August 2-7, 2009. Proceedings*, pages 214–229, 2009.

[92] Gaël Lalire, Mathias Argoud, and Bertrand Jeannet. The Interproc Analyzer. http://pop-art.inrialpes.fr/people/bjeannet/bjeannet-forge/interproc/index.html.

[93] Vincent Laviron and Francesco Logozzo. Subpolyhedra: a family of numerical abstract domains for the (more) scalable inference of linear inequalities. *STTT*, 13(6):585–601, 2011.

[94] David Lee and Mihalis Yannakakis. Online minimization of transition systems (extended abstract). In *Proceedings of the 24th Annual ACM Symposium on Theory of Computing, May 4-6, 1992, Victoria, British Columbia, Canada*, pages 264–274, 1992.

[95] Xavier Leroy. A formally verified compiler back-end. *J. Autom. Reasoning*, 43(4):363–446, 2009.

[96] Xavier Leroy. The CompCert C verified compiler documentation and users manual, 2013.

[97] Takeshi Matsumoto, Hiroshi Saito, and Masahiro Fujita. Equivalence checking of C programs by locally performing symbolic simulation on dependence graphs. In *7th International Symposium on Quality of Electronic Design (ISQED 2006), 27-29 March 2006, San Jose, CA, USA*, pages 370–375, 2006.

[98] Laurent Mauborgne and Xavier Rival. Trace partitioning in abstract interpretation based static analyzers. In *Programming Languages and Systems, 14th European Symposium on Programming,ESOP 2005, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2005, Edinburgh, UK, April 4-8, 2005, Proceedings*, pages 5–20, 2005.

[99] E. J. McCluskey. Minimization of boolean functions. *Bell Systems Technical Journal*, 35(6):1417–1444, 1956.

[100] Kenneth McMillan and Andrey Rybalchenko. Combinatorial approach to some sparse-matrix problems. Technical report, Microsoft Research, 2013.

[101] Vijay Menon, Keshav Pingali, and Nikolay Mateev. Fractal symbolic analysis. *ACM Trans. Program. Lang. Syst.*, 25(6):776–813, 2003.

[102] Antoine Miné. The octagon abstract domain. *Higher-Order and Symbolic Computation*, 19(1):31–100, 2006.

[103] Markus Müller-Olm and Helmut Seidl. Computing polynomial program invariants. *Inf. Process. Lett.*, 91(5):233–244, 2004.

[104] Mayur Naik, Hongseok Yang, Ghila Castelnuovo, and Mooly Sagiv. Abstractions from tests. In *Proceedings of the 39th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2012, Philadelphia, Pennsylvania, USA, January 22-28, 2012*, pages 373–386, 2012.

[105] George C. Necula. Translation validation for an optimizing compiler. In *Proceedings of the 2000 ACM SIGPLAN Conference on Programming Language Design and Implementation (PLDI), Vancouver, British Columbia, Canada, June 18-21, 2000*, pages 83–94, 2000.

[106] Andrew F Neuwald, Jun S Liu, David J Lipman, and Charles E Lawrence. Extracting protein alignment models from the sequence database. *Nucleic Acids Research*, 25(9):1665–1677, 1997.

[107] ThanhVu Nguyen, Deepak Kapur, Westley Weimer, and Stephanie Forrest. Using dynamic analysis to discover polynomial and array invariants. In *34th International Conference on Software Engineering, ICSE 2012, June 2-9, 2012, Zurich, Switzerland*, pages 683–693, 2012.

[108] Jeremy W. Nimmer and Michael D. Ernst. Automatic generation of program specifications. In *Proceedings of the International Symposium on Software Testing and Analysis, July 22-24, Roma, Italy. ACM, 2002*, pages 229–239, 2002.

[109] Aditya V. Nori, Sriram K. Rajamani, SaiDeep Tetali, and Aditya V. Thakur. The Yogi project: Software property checking via static analysis and testing. In *Tools and Algorithms for the Construction and Analysis of Systems (TACAS)*, pages 178–181, 2009.

[110] Aditya V. Nori and Rahul Sharma. Termination proofs from tests. In *Joint Meeting of the European Software Engineering Conference and the ACM SIGSOFT Symposium on the Foundations of Software Engineering, ESEC/FSE'13, Saint Petersburg, Russian Federation, August 18-26, 2013*, pages 246–256, 2013.

[111] Nimrod Partush and Eran Yahav. Abstract semantic differencing for numerical programs. In *Static Analysis - 20th International Symposium, SAS 2013, Seattle, WA, USA, June 20-22, 2013. Proceedings*, pages 238–258, 2013.

[112] Suzette Person, Matthew B. Dwyer, Sebastian G. Elbaum, and Corina S. Pasareanu. Differential symbolic execution. In *Proceedings of the 16th ACM SIGSOFT International Symposium on Foundations of Software Engineering, 2008, Atlanta, Georgia, USA, November 9-14, 2008*, pages 226–237, 2008.

[113] Michael Petter. Berechnung von polynomiellen invarianten. Master's thesis, Fakultät für Informatik, Technische Universität München, 2004.

[114] John C. Platt. Fast training of support vector machines using sequential minimal optimization. *Advances in kernel methods*, pages 185–208, 1999.

[115] Amir Pnueli, Michael Siegel, and Eli Singerman. Translation validation. In *Tools and Algorithms for Construction and Analysis of Systems, 4th International Conference, TACAS '98, Held as Part of the European Joint Conferences on the Theory and Practice of Software, ETAPS'98, Lisbon, Portugal, March 28 - April 4, 1998, Proceedings*, pages 151–166, 1998.

[116] Xiaokang Qiu, Pranav Garg, Andrei Stefanescu, and Parthasarathy Madhusudan. Natural proofs for structure, data, and separation. In *ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI '13, Seattle, WA, USA, June 16-19, 2013*, pages 231–242, 2013.

[117] David A. Ramos and Dawson R. Engler. Practical, low-effort equivalence verification of real code. In *Computer Aided Verification - 23rd International Conference, CAV 2011, Snowbird, UT, USA, July 14-20, 2011. Proceedings*, pages 669–685, 2011.

[118] Thomas W. Reps, Shmuel Sagiv, and Greta Yorsh. Symbolic implementation of the best transformer. In *Verification, Model Checking, and Abstract Interpretation, 5th International Conference, VMCAI 2004, Venice, January 11-13, 2004, Proceedings*, pages 252–266, 2004.

[119] M. Rinard. Credible compilers. Technical report, Massachusetts Institute of Technology, 1999.

[120] Enric Rodríguez-Carbonell and Deepak Kapur. Automatic generation of polynomial invariants of bounded degree using abstract interpretation. *Science of Computer Programming*, 64(1):54–75, 2007.

[121] Enric Rodríguez-Carbonell and Deepak Kapur. Generating all polynomial invariants in simple loops. *Journal of Symbolic Computation*, 42(4):443–476, 2007.

[122] Shmuel Sagiv, Thomas W. Reps, and Reinhard Wilhelm. Parametric shape analysis via 3-valued logic. *ACM Trans. Program. Lang. Syst.*, 24(3), 2002.

[123] Sriram Sankaranarayanan, Richard M. Chang, Guofei Jiang, and Franjo Ivancic. State space exploration using feedback constraint generation and Monte-Carlo sampling. In *Proceedings*

of the 6th joint meeting of the European Software Engineering Conference and the ACM SIGSOFT International Symposium on Foundations of Software Engineering, 2007, Dubrovnik, Croatia, September 3-7, 2007, pages 321–330, 2007.

[124] Sriram Sankaranarayanan, Franjo Ivancic, Ilya Shlyakhter, and Aarti Gupta. Static analysis in disjunctive numerical domains. In *Static Analysis, 13th International Symposium, SAS 2006, Seoul, Korea, August 29-31, 2006, Proceedings*, pages 3–17, 2006.

[125] Sriram Sankaranarayanan, Henny Sipma, and Zohar Manna. Non-linear loop invariant generation using gröbner bases. In *Proceedings of the 31st ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2004, Venice, Italy, January 14-16, 2004*, pages 318–329, 2004.

[126] Eric Schkufza, Rahul Sharma, and Alex Aiken. Stochastic superoptimization. In *Architectural Support for Programming Languages and Operating Systems, ASPLOS '13, Houston, TX, USA - March 16 - 20, 2013*, pages 305–316, 2013.

[127] Rahul Sharma and Alex Aiken. From invariant checking to invariant inference using randomized search. In *Computer Aided Verification - 26th International Conference, CAV 2014, Held as Part of the Vienna Summer of Logic, VSL 2014, Vienna, Austria, July 18-22, 2014. Proceedings*, pages 88–105, 2014.

[128] Rahul Sharma, Michael Bauer, and Alex Aiken. Verification of producer-consumer synchronization in GPU programs. In *Proceedings of the 36th ACM SIGPLAN Conference on Programming Language Design and Implementation, Portland, OR, USA, June 15-17, 2015*, pages 88–98, 2015.

[129] Rahul Sharma, Saurabh Gupta, Bharath Hariharan, Alex Aiken, Percy Liang, and Aditya V. Nori. A data driven approach for algebraic loop invariants. In *Programming Languages and Systems - 22nd European Symposium on Programming, ESOP 2013, Held as Part of the European Joint Conferences on Theory and Practice of Software, ETAPS 2013, Rome, Italy, March 16-24, 2013. Proceedings*, pages 574–592, 2013.

[130] Rahul Sharma, Saurabh Gupta, Bharath Hariharan, Alex Aiken, and Aditya V. Nori. Verification as learning geometric concepts. In *Static Analysis - 20th International Symposium, SAS 2013, Seattle, WA, USA, June 20-22, 2013. Proceedings*, pages 388–411, 2013.

[131] Rahul Sharma, Aditya V. Nori, and Alex Aiken. Interpolants as classifiers. In *Computer Aided Verification - 24th International Conference, CAV 2012, Berkeley, CA, USA, July 7-13, 2012 Proceedings*, pages 71–87, 2012.

[132] Rahul Sharma, Aditya V. Nori, and Alex Aiken. Bias-variance tradeoffs in program analysis. In *The 41st Annual ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL '14, San Diego, CA, USA, January 20-21, 2014*, pages 127–138, 2014.

[133] Rahul Sharma, Eric Schkufza, Berkeley R. Churchill, and Alex Aiken. Data-driven equivalence checking. In *Proceedings of the 2013 ACM SIGPLAN International Conference on Object Oriented Programming Systems Languages & Applications, OOPSLA 2013, part of SPLASH 2013, Indianapolis, IN, USA, October 26-31, 2013*, pages 391–406, 2013.

[134] K. C. Shashidhar, Maurice Bruynooghe, Francky Catthoor, and Gerda Janssens. Verification of source code transformations by program equivalence checking. In *Compiler Construction, 14th International Conference, CC 2005, Held as Part of the Joint European Conferences on Theory and Practice of Software, ETAPS 2005, Edinburgh, UK, April 4-8, 2005, Proceedings*, pages 221–236, 2005.

[135] Eric W. Smith. *Axe, an automated formal equivalence checking tool for programs.* PhD thesis, Stanford University, 2011.

[136] Armando Solar-Lezama, Rodric M. Rabbah, Rastislav Bodík, and Kemal Ebcioglu. Programming by sketching for bit-streaming programs. In *Proceedings of the ACM SIGPLAN 2005 Conference on Programming Language Design and Implementation, Chicago, IL, USA, June 12-15, 2005*, pages 281–294, 2005.

[137] Saurabh Srivastava and Sumit Gulwani. Program verification using templates over predicate abstraction. In *Proceedings of the 2009 ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI 2009, Dublin, Ireland, June 15-21, 2009*, pages 223–234, 2009.

[138] Saurabh Srivastava, Sumit Gulwani, and Jeffrey S. Foster. VS3: SMT solvers for program verification. In *Computer Aided Verification, 21st International Conference, CAV 2009, Grenoble, France, June 26 - July 2, 2009. Proceedings*, pages 702–708, 2009.

[139] W. A. Stein et al. *Sage Mathematics Software (Version 5.0).* The Sage Development Team, 2012. `http://www.sagemath.org`.

[140] Ross Tate, Michael Stepp, Zachary Tatlock, and Sorin Lerner. Equality saturation: a new approach to optimization. In *Proceedings of the 36th ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2009, Savannah, GA, USA, January 21-23, 2009*, pages 264–276, 2009.

[141] Aditya Thakur, Akash Lal, Junghee Lim, and Thomas Reps. Spans in the module (z,n)*. In *Linear and Multilinear Algebra 19*, 1986.

[142] Aditya V. Thakur and Thomas W. Reps. A method for symbolic computation of abstract operations. In *Computer Aided Verification - 24th International Conference, CAV 2012, Berkeley, CA, USA, July 7-13, 2012 Proceedings*, pages 174–192, 2012.

[143] Lloyd N. Trefethen and David Bau. *Numerical linear algebra*. SIAM, 1997.

[144] Jean-Baptiste Tristan, Paul Govereau, and Greg Morrisett. Evaluating value-graph translation validation for LLVM. In *Proceedings of the 32nd ACM SIGPLAN Conference on Programming Language Design and Implementation, PLDI 2011, San Jose, CA, USA, June 4-8, 2011*, pages 295–305, 2011.

[145] A. Turing. Checking a large routine. In *The early British computer conferences*. MIT Press, Cambridge, MA, USA, 1989.

[146] Leslie G. Valiant. A theory of the learnable. *Commun. ACM*, 27(11):1134–1142, 1984.

[147] René Vidal, Yi Ma, and Shankar Sastry. Generalized principal component analysis (GPCA). *IEEE Trans. Pattern Anal. Mach. Intell.*, 27(12):1945–1959, 2005.

[148] Henry S. Warren. *Hacker's Delight*. Addison-Wesley Longman Publishing Co., Inc., Boston, MA, USA, 2002.

[149] Christoph M. Wintersteiger, Youssef Hamadi, and Leonardo Mendonça de Moura. Efficiently solving quantified bit-vector formulas. *Formal Methods in System Design*, 42(1):3–23, 2013.

[150] Tao Xie and David Notkin. Tool-assisted unit test selection based on operational violations. In *18th IEEE International Conference on Automated Software Engineering (ASE 2003), 6-10 October 2003, Montreal, Canada*, pages 40–48, 2003.

[151] Yichen Xie and Alexander Aiken. Scalable error detection using boolean satisfiability. In *Proceedings of the 32nd ACM SIGPLAN-SIGACT Symposium on Principles of Programming Languages, POPL 2005, Long Beach, California, USA, January 12-14, 2005*, pages 351–363, 2005.

[152] Greta Yorsh, Thomas Ball, and Mooly Sagiv. Testing, abstraction, theorem proving: better together! In *Proceedings of the ACM/SIGSOFT International Symposium on Software Testing and Analysis, ISSTA 2006, Portland, Maine, USA, July 17-20, 2006*, pages 145–156, 2006.

[153] Yunhui Zheng, Xiangyu Zhang, and Vijay Ganesh. Z3-str: a z3-based string solver for web application analysis. In *Joint Meeting of the European Software Engineering Conference and the ACM SIGSOFT Symposium on the Foundations of Software Engineering, ESEC/FSE'13, Saint Petersburg, Russian Federation, August 18-26, 2013*, pages 114–124, 2013.