Invariant Relations: An Alternative Tool to Analyze Loops

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Abstract

Since their introduction more than four decades ago, invariant assertions have, justifiably, dominated the analysis of while loops, and have been the focus of sustained research interest in the seventies and eighties, and renewed interest in the last decade. In this paper, we tentatively submit an alternative concept for the analysis of while loops, explore its attributes, and its relationship to invariant assertions.

Keywords

Invariant assertions, invariant functions, invariant relations, loop invariants, program analysis, program verification, while loops, loop functions.

1 Introduction

In [10], Hoare introduced the concept of an *invariant assertion* as a useful tool in the analysis of while loops. The study of invariant assertions, and their use in the analysis of while loops, have been the focus of active research in the seventies and eighties, and the subject of renewed interest in the last few years [1, 3–5, 7, 8, 11, 13, 14, 20]. In this paper we introduce an alternative concept to the analysis of while loops, namely the concept of *invariant relation*. Also, we explore the attributes of invariant relations, and their relationship to invariant assertions and to loop semantics. Specifically,

- Whereas an invariant assertion is an assertion that holds after any number of iterations of the loop (including zero iterations, i.e. at the precondition), an invariant relation is a relation that holds between any two states, say s and s', that are separated by an arbitrary number of iterations (including zero).
- Whereas an invariant assertion is dependent not only on the loop, but also on the context of the loop (as captured by its pre-condition and post-condition), an invariant relation is intrinsic to the loop, and does not depend on where the loop is used.

- Whereas invariant assertions are useful to prove the correctness of a loop with respect to a specification in the form of a precondition/ postcondition pair, invariant relations are useful to compute or approximate the function of a loop.
- Given an invariant relation and a precondition, we can generate an invariant assertion; on the other hand, all invariant assertions can be derived from invariant relations.
- Given an invariant assertion, we can generate an invariant relation from it; but not all invariant relations stem from invariant assertions.
- At the LIPAH laboratory, University of Tunis, we are developing / evolving an automated tool that generates invariant relations of while loops written in C-like languages, using pre-stored patterns that represent programming knowledge and domain knowledge. This tool uses a divide-and-conquer discipline that keeps the generation effort virtually linear in the size of the loop.
- We are also evolving and maintaining a tool, programmed in Mathematica (©Wolfram Research), that uses the invariant relations generated above to compute or approximate the function of the while loop.

In section 2 we briefly introduce the mathematical background that will be needed subsequently for our discussions. In section 3 we introduce the concept of *invariant relation* and briefly present the main results pertaining to the properties of invariant relations and their relationship to invariant assertions [12]. In section 4 we discuss how invariant relations can be used to compute or approximate loop functions, and in section 5 we illustrate our tool's performance, and compare it with other tools we know of (that generate invariant assertions). Finally in section 6 we summarize and assess our main finding and identify future research directions.

2 Relational Mathematics

2.1 Elements of Relations

2.1.1 Definitions and Notations

We consider a set S defined by the values of some program variables, say x, y and z; we typically denote elements of S by s, and we note that s has the form $s = \langle x, y, z\rangle$. We use the notation $x(s)$, $y(s)$, $z(s)$ to denote the x-component, y-component and z-component of s. We may sometimes use x to refer to x(s) and x' to refer to $x(s')$, when this raises no ambiguity. We refer to elements s of S as *program states* and to S as the *state space* (or *space*, for short) of the program that manipulates variables x, y and z. Given a program g on state space S, we use functions on S to capture the function that the program defines from its initial states to its final states, and we use relations on S to capture functional specifications that we may want the program to satisfy. To this effect, we briefly introduce elements of relational mathematics. A relation on S is a subset of the cartesian product $S \times S$. Constant relations on some set S include the *universal* relation, denoted by L, the *identity* relation, denoted by I, and the *empty* relation, denoted by $\emptyset$.

2.1.2 Operations on Relations

Because relations are sets, we apply the usual set theoretic operations between relations: union ($\cup$), intersection ($\cap$), complement ($\overline{R}$), cartesian product ($\times$). Operations on relations also include the *converse*, denoted by $\widehat{R}$, and defined by $\widehat{R} = \{(s,s')|(s',s) \in R\}$; and the *product* of relations R and R', denoted by $R \circ R'$ (or RR'), and defined by $R \circ R' = \{(s,s')|\exists s'' : (s,s'') \in R \wedge (s'',s') \in R'\}$. We admit without proof that $\widehat{RR'} = \widehat{R'}\widehat{R}$ and that $\widehat{\widehat{R}} = R$. Given a predicate t, we denote by $I(t)$ the subset of the identity relation defined as $I(t) = \{(s,s')|s' = s \wedge t(s)\}$ and by T the relation defined as $T = \{(s,s')|t(s)\}$; by definition, we have $I(t) = I \cap T$ and $T = I(t) \circ L$. The *pre-restriction* (resp. *post-restriction*) of relation R to predicate t is the relation $\{(s,s')|t(s) \wedge (s,s') \in R\}$ (resp. $\{(s,s')|(s,s') \in R \wedge t(s')\}$). We admit without proof that the pre-restriction of a relation R to predicate t can be written as $I(t) \circ R$ or $T \cap R$, and the post-restriction of relation R to predicate t can be written as $R \circ I(t)$ or $R \cap \widehat{T}$.

The *domain* of relation R is defined as $dom(R) = \{s|\exists s' : (s,s') \in R\}$. The *range* of relation R is denoted by $rng(R)$ and defined as $dom(\widehat{R})$. We admit without proof that for a relation R, $RL = \{(s,s')|s \in dom(R)\}$ and $LR = \{(s,s')|s' \in rng(R)\}$. The *nucleus* of relation R is the relation denoted by $\mu(R)$ and defined as $R\widehat{R}$. The n^{th} power of relation R, for natural number n, is denoted by R^n and defined by: $R^0 = I$, For $n > 0$, $R^n = R^{n-1} \circ R$. We define the *transitive closure* of relation R as the relation denoted by R^+ and defined by $R^+ = \{(s,s')|\exists n > 0 : (s,s') \in R^n\}$. We define the *reflexive transitive closure* of relation R as the relation denoted by R^* and defined by $R^* = R^+ \cup I$.

We apply the following conventions with regards to operator precedence: unary operators (complement, inverse, closures) are applied first; they are followed by relational product, then intersection, then union.

2.1.3 Properties of Relations

We say that R is *deterministic* (or that it is a *function*) if and only if $\widehat{R}R \subseteq I$, and we say that R is *total* if and only if $I \subseteq R\widehat{R}$, or equivalently, $RL = L$. A relation R is said to be *rectangular* if and only if $R = RLR$. We are interested in two special types of rectangular relations: relations satisfying $RL = R$ are called *vectors*; relations satisfying $LR = R$ are called *invectors* (inverse of a vector). In set theoretic terms, a vector on set S has the form $C \times S$, and an invector has the form $S \times C$, for some subset C of S. Vector $C \times S$ can also be written as $I(C) \circ L$.

A relation R is said to be *reflexive* if and only if $I \subseteq R$, *transitive* if and only if $RR \subseteq R$ and *symmetric* if and only if $R = \widehat{R}$. We admit without proof that the transitive closure of a relation R is the smallest transitive superset of R; and that the reflexive transitive closure of relation R is the smallest reflexive transitive superset of R. A relation R is said to be *inductive* if and only if it can be written as $R = \overline{A} \cup \widehat{A}$ for some vector A; we leave it to the reader to check that if A is written as $\{(s,s')|\alpha(s)\}$, then $\overline{A} \cup \widehat{A}$ can be written as $\{(s,s')|\alpha(s) \Rightarrow \alpha(s')\}$.

2.2 Refinement Ordering

We define an ordering relation on relational specifications under the name *refinement ordering*:

Definition 1 *A relation R is said to* refine *a relation R' if and only if*

$$RL \cap R'L \cap (R \cup R') = R'.$$

We denote this relation by $R \sqsupseteq R'$ or $R' \sqsubseteq R$. In order to present an intuitive interpretation of refinement, we introduce the definition of program function: Given a program g on space S, we let G be the function defined as:

$$G = \{(s, s')| \text{ if } g \text{ starts execution in state } s \text{ then it terminates in state } s'\}.$$

We admit that, modulo traditional definitions of total correctness [6, 9, 17, 19], the following propositions hold:

- A program g is correct with respect to a specification R if and only if $G \sqsupseteq R$.
- $R \sqsupseteq R'$ implies that any program correct with respect to R is correct with respect to R'.

In other words, R refines R' if and only if R represents a stronger requirement than R'.

2.3 Lattice Properties

We admit without proof that the refinement relation is a partial ordering. In [2] Boudriga et al. analyze the lattice properties of this ordering and find the following results:

- Any two relations R and R' have a greatest lower bound, which we refer to as the *meet*, denote by $\sqcap$, and define by: $R \sqcap R' = RL \cap R'L \cap (R \cup R')$.
- Two relations R and R' have a least upper bound if and only if they satisfy the following condition (which we refer to as the *consistency condition*): $RL \cap R'L = (R \cap R')L$. Under this condition, their least upper bound is referred to as the *join*, denoted by $\sqcup$, and defined by: $R \sqcup R' = \overline{RL} \cap R' \cup \overline{R'L} \cap R \cup (R \cap R')$. Intuitively, the join of R and R', when it exists, behaves like R outside the domain of R', behaves like R' outside the domain of R, and behaves like the intersection of R and R' on the intersection of their domain. The consistency condition ensures that the domain of their intersection is identical to the intersection of their domains.
- Two relations R and R' have a least upper bound if and only if they have an upper bound.
- The lattice of refinement admits a *universal lower bound*, which is the empty relation.
- The lattice of refinement admits no *universal upper bound*.
- Maximal elements of this lattice are total deterministic relations.

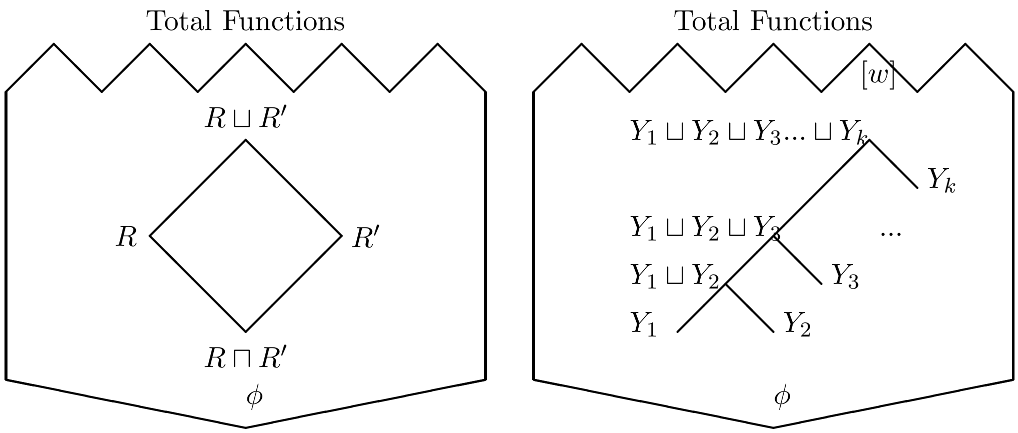
Figure 1 (a) shows the overall structure of the lattice of specifications.

3 Invariant Relations and Invariant Assertions

In this section, we introduce definitions for invariant relations and invariant assertions, using a uniform relational notation. First, we present a theorem that defines the semantics of loops.

Theorem 1 *Given a while statement of the form $w =$ `while t do b` that terminates for all the states in S. Then its function W is given by (where T is the vector defined by `t` and B is the function of `b`):*

$$W = (T \cap B)^* \cap \widehat{\overline{T}}.$$



(a): Lattice Operations (b): Successive Approximations

Figure 1: Lattice Structure of Refinement

In this paper, we assume that loops terminate for all states in S, i.e. that their function is total; in [18], we discuss why, in theory, this hypothesis does not affect the generality of our study. Also, to illustrate our subsequent discussions, we use a simple running example, which is the following while loop on natural variables n, f, k, such that $1 \le k \le n+1$:

```
w:  while k!=n+1 {f=f*k; k=k+1}.
```

3.1 Invariant Assertions

Traditionally [10, 17], an invariant assertion α for the while loop $w =$ `while t do b` with respect to a precondition/ postcondition pair (p, q) is defined as a predicate on S that satisfies the following conditions: $p \Rightarrow \alpha$, $\{\alpha \wedge t\}b\{\alpha\}$, and $\alpha \wedge \neg t \Rightarrow q$. For the sake of uniformity, we recast these conditions in relational terms, representing the precondition p by the vector $P = \{(s, s')|p(s)\}$, the postcondition q by the vector $Q = \{(s, s')|q(s)\}$, and the predicate α by the vector $A = \{(s, s')|\alpha(s)\}$.

Definition 2 *Given a while statement of the form, $w =$ `while t do b`, an* invariant assertion *for w with respect to precondition P and postcondition Q is a vector A on S that satisfies the following conditions: $P \subseteq A$, $A \cap T \cap B \subseteq \widehat{A}$, and $A \cap \overline{T} \subseteq Q$.*

If we consider the sample loop introduced earlier, and take the precondition $f = 1 \wedge k = 1$ and the postcondition $f = n!$, then we find that $f = (k-1)!$ is an invariant assertion for this program.

3.2 Invariant Relations

Definition 3 *Given a while loop of the form $w =$ `while t do b` on space S, and given a relation R on S, we say that R is an* invariant relation *for w if and only if it is a reflexive and transitive superset of $(T \cap B)$.*

To illustrate this concept, we consider again the loop of the running example, and we submit the following relation:

$$R = \left\{(s,s')|\frac{f}{(k-1)!} = \frac{f'}{(k'-1)!}\right\}.$$

This relation is clearly reflexive and transitive; we leave it to the reader to check that it is a superset of $(T \cap B)$.

3.3 Comparative Analysis

The first question we ask is: can we derive an invariant assertion from an invariant relation?

Proposition 1 *Let w be a while loop on space S and let R be an invariant relation for w. Then $A = \widehat{R}P$ is an invariant assertion for w with respect to the precondition P and the postcondition $Q = \overline{T} \cap \widehat{R}P$.*

Proof. According to Definition 2, we must prove three conditions:

- $P \subseteq \widehat{R}P$,
- $\widehat{R}P \cap T \cap B \subseteq \widehat{\widehat{R}P}$,
- $\widehat{R}P \cap \overline{T} \subseteq \overline{T} \cap \widehat{R}P$.

The first condition stems readily from the reflexivity of R. The second condition is a result from [12]. The third condition is a tautology. **qed**

As an illustration, we consider the invariant relation we had proposed earlier for the sample loop, and we let P be the following vector, representing possible initial conditions of the loop:

$$P = \{(s,s')|f = 1 \wedge k = 1\}.$$

The invariant assertion that we then obtain is the following:

$$\begin{array}{ll}
 & A \\
= & \quad \{ \text{ Proposition 1, symmetry of } R \text{ } \} \\
 & \{(s,s')|\frac{f}{(k-1)!} = \frac{f'}{(k'-1)!}\} \circ \{(s,s')|f = 1 \wedge k = 1\} \\
= & \quad \{ \text{ relational product } \} \\
 & \{(s,s')|\exists s' : \frac{f}{(k-1)!} = \frac{f'}{(k'-1)!} \wedge f' = 1 \wedge k' = 1\} \\
= & \quad \{ \text{ simplification } \} \\
 & \{(s,s')|\frac{f}{(k-1)!} = 1\},
\end{array}$$

which is the invariant assertion we had proposed earlier.

Because invariant relations depend exclusively on the loop whereas invariant assertions depend on the context of the loop in addition to the loop (the context being defined by the precondition and the postcondition), it is difficult to compare them meaningfully. Hence we consider a context-free version of invariant assertions, which we introduce below.

Definition 4 *Given a while loop on space S of the form $w =$ `while t do b`, and given a vector U on S, we say that U is an* inductive assertion *for w if and only if $U \cap T \cap B \subset \widehat{U}$.*

An inductive assertion is an assertion that satisfies the second condition of invariant assertions, but not the first nor the third (both of which refer to its context). The first result that we propose is a generalization of Proposition 1: It provides that, given an invariant relation, we can generate a wide range of inductive assertions from it.

Proposition 2 *Let w be a while loop on space S and let R be an invariant relation for w and V be an arbitrary vector on S. Then $A = \widehat{R}V$ is an inductive assertion for w.*

This Proposition is due to [12], where it is proved; we content ourselves here with illustrating it. We take the invariant relation

$$R = \{(s, s')|\frac{f}{(k-1)!} = \frac{f'}{(k'-1)!}\},$$

and the following vectors:

$$V_0 = \{(s, s')|f = 1 \wedge k = 1\}\ V_1 = \{(s, s')|f = 1 \wedge k = 2\}\ V_2 = \{(s, s')|f = 2 \wedge k = 3\}$$
$$V_3 = \{(s, s')|f = 6 \wedge k = 4\}\ V_4 = \{(s, s')|f = (k-1)!\}\quad V_5 = \{(s, s')|\tfrac{f}{(k-1)!} = 120\}.$$

If we let A_0, A_1, ... A_5 be the inductive assertions derived from the selected invariant relation by applying vectors V_0, V_1, ... V_5, we find

$$A_0 = A_1 = A_2 = A_3 = A_4 = \{(s, s')|f = (k-1)!\}$$
$$A_5 = \{(s, s')|\tfrac{f}{(k-1)!} = 120\}.$$

The next question that we address is, naturally: can we generate an invariant relation from any inductive assertion. The answer is given by the following proposition.

Proposition 3 *Let A be an inductive assertion for the while loop w; then $R = \overline{A} \cup \widehat{A}$ is an invariant relation for w.*

Proof. By set theory, the condition $T \cap B \cap A \subseteq \widehat{A}$ is equivalent to $T \cap B \subseteq (\overline{A} \cup \widehat{A})$, i.e. R is a superset of $T \cap B$. By construction, $(\overline{V} \cup \widehat{V})$ is reflexive and transitive for any vector V. **qed**

We illustrate this proposition by means of a simple example, using the sample factorial loop. We consider the following inductive assertion,

$$A = \{(s, s')|f = (k-1)!\},$$

and we apply the formula dictated by this Proposition:

$$\begin{array}{ll} & R \\ = & \qquad \{\text{ Proposition 3 }\} \\ & \overline{A} \cup \widehat{A} \\ = & \qquad \{\text{ substitution, simplification }\} \\ & \{(s, s')|f = (k-1)! \Rightarrow f' = (k'-1)!\}. \end{array}$$

Now that we know how to generate an inductive assertion from an invariant relation (Proposition 1) and an invariant relation from an inductive assertion (Proposition 3), can we infer that invariant relations and inductive assertions are equally powerful? The answer is no, because the question we need to pose instead is whether *all* invariant relations can be derived from inductive assertions, and whether *all* inductive assertions can be derived from invariant relations. The following proposition answers the second question.

Proposition 4 *Let w be a while loop on space S and let A be an inductive assertion for w. Then there exists an invariant relation R and a vector V such that $A = \widehat{R}V$.*

The proof of this proposition is given in [12], where R is taken as $\overline{A} \cup \widehat{A}$ and V is taken as A. The interest of this proposition is three-fold: First, it proves that by focusing on generating invariant relations, we cover all possible inductive assertions; Second, it provides a structure for all inductive assertions, as the inverse of an invariant relation composed with a vector; Third, it separates two components of an inductive assertion, namely $\widehat{R}$, which depends exclusively on the loop, and V, which depends on the context (initialization) of the loop.

As to the question of whether any invariant relation can be derived from an inductive assertion, we have no proposition to support the affirmative, and we have reason to believe it is not the case. Consider that according to Proposition 3, the search for inductive assertions is amenable to the search for invariant relations of a certain kind, namely relations that are inductive. Since not all invariant relations are inductive, it is legitimate to infer that invariant relations are a more general concept than inductive assertions.

4 Invariant Relations and Loop Analysis

We are developing and evolving an automated tool that generates invariant relations of while loops, by analyzing their source code (currently in C++, and can trivially be extended to handle other programming languages). Proposition 1 shows how, given an invariant relation and a precondition to a loop, we can constructively generate a postcondition for the loop. While this is an interesting result, it is not the only application of invariant relations, nor the most useful: the following proposition, due to [18], shows that invariant relations can be used to compute or approximate the function of a loop.

Proposition 5 *Let $w =$ `while t do b` be a while loop on space S; let R be an invariant relation for w and let W be the function of w. Then $W \sqsupseteq R \cap \widehat{\overline{T}}$.*

According to this proposition, we can transform an invariant relation of w into a lower bound (in the refinement ordering) of its function W. Consider the lattice structure of refinement shown in Figure 1. We find that maximal elements of this lattice are total deterministic relations; because by hypothesis, W is total and deterministic, it is possible to compute it or approximate using nothing but lower bounds. To this effect, we gather as many invariant relations as we can, from which we generate lower bounds of the loop's function. Then we take the join of all the lower bounds, which we test for totality and determinacy; if it is total and deterministic, then it is the function of the loop, if not it is the best approximation we can derive from the invariant relations at hand. As an illustration, we consider the running sample loop, for which we know the following invariant relation: $R = \{(s,s')|\frac{f}{(k-1)!} = \frac{f'}{(k'-1)!}\}$; from this, we derive the following lower bound

$$Y = \{(s,s')|\frac{f}{(k-1)!} = \frac{f'}{(k'-1)!} \wedge k' = n' + 1\}.$$

This relation is total but is not deterministic, hence we seek another invariant relation for w, say $R = \{(s,s')|n = n'\}$, from which we derive the following lower bound:

$$Y' = \{(s,s')|n = n' \wedge k' = n' + 1\}.$$

Taking the join (in this case, the intersection) of these two lower bounds produces the following (total, deterministic) relation:

$$\{(s,s')|f' = n! \times \frac{f}{(k-1)!} \wedge n' = n \wedge k' = n + 1\}.$$

If this loop is initialized by any segment such as: `k=1; f=1;` or `k=2; f=1;` or `k=3; f=2;` or any segment whose postcondition is $\frac{f}{(k-1)!} = 1 \wedge 1 \leq k \leq n+1$, then the function of the initialized loop is:

$$\{(s,s')|f' = n! \wedge k' = n + 1 \wedge n' = n\}.$$

In the remainder of this section, we consider a number of sample loops; for each loop, we generate the invariant relations derived by our tool, from which we compute the function of the loop (using Proposition 5) and an invariant assertion (using Proposition 1). For the sake of comparison, we show what other tools generate for the same loops, most notably: Aligator [15]; Daikon [7], and LoopFrog [16]. The code is written in C++, with slight modifications: while C++ requires all program constants to be assigned values, we merely declare them as constants, as we want to use them as parameters of the loop function; also, we may sometimes put several statements on the same line, to save space, even though C++ compilers do not allow that.

4.1 Sequential Loop Body

We consider the following loop, whose loop body consists of a sequence of assignment statements to numeric variables; note that function f is not declared explicitly, as we do not need to know its explicit expression to analyze the loop.

```
#include <iostream> #include <math.h> using namespace std;  float f (float z);
int main ()  {const int e, g, cN; const float a, m, b, c, d;     // constants
int h, i, j, k, l, n, p, xx, yy; float x, y, z, u, v, w, q, r, s, t;  // vars
int aa[cN]; int ab[cN];                                               //arrays
while (k>=7)    {j=j+aa[i]; i=i+n; l=l+ab[n]; n=n-k; k=k-7; yy=xx*yy; x=a+m*x;
y=a*pow(y,m); t=t+b*w; n=n+k+6; s=s+c*z; z=z+b; u=a*u+m; v=v-c; w=d*w; q=q+r;
r=f(r); h=h+g*p; p=p/e; i=i-n;}}
```

Our tool finds the following function for this loop (where $\frac{k}{7}$ designates the integer division of k by 7 and $mod(k,7)$ designates the remainder of the integer division of k by 7):

$$W = \left\{ (s,s')| \begin{array}{c} d>0 \wedge d \neq 1 \wedge a \neq 0 \wedge a \neq 1 \wedge e>0 \wedge e \neq 1 \wedge m \geq 2 \wedge k \geq 0 \wedge \\ k' = mod(k,7) \wedge aa' = aa \wedge ab' = ab \wedge i' = i + \frac{k}{7} \wedge \\ r' = f^{\frac{k}{7}}(r) \wedge j' = j + \Sigma_{H=i}^{i-1+\frac{k}{7}} aa[H] \wedge z' = z + b\frac{k}{7} \wedge \\ l' = l + \Sigma_{H=1+n-\frac{k}{7}}^{n} ab[H] \wedge n' = n - \frac{k}{7} \wedge \\ y' = y^{m^{\frac{k}{7}}} a^{\frac{m^{\frac{k}{7}}-1}{m-1}} \wedge p' = e^{-\frac{k}{7}} p \wedge h' = \frac{h-eh+e(-1+e^{-\frac{k}{7}})gp}{1-e} \wedge \\ q' = q + \Sigma_{H=1}^{n} f^H(r) - \Sigma_{H=1}^{n-\frac{k}{7}} f^H(f^{\frac{k}{7}}(r)) \wedge \\ s' = \frac{1}{2}(2s - bc\frac{k}{7} + 2cz\frac{k}{7} + bc\frac{k}{7}^2) \wedge t' = t + bw\frac{d^{\frac{k}{7}}-1}{d-1} \wedge \\ u' = \frac{-m+a^{\frac{k}{7}}(m+(a-1)u)}{a-1} \wedge xx' = xx \wedge yy' = xx^{\frac{k}{7}} yy \wedge \\ v' = v - c\frac{k}{7} \wedge w' = d^{\frac{k}{7}} w \wedge x' = \frac{-a+m^{\frac{k}{7}}(a+(m-1)x)}{m-1} \end{array} \right\}.$$

Execution of Aligator on this program is possible only after we delete the array statements, the function calls, and the statements `y=a*y**m` and `i=i-n`; when we delete these statements, the execution yields the following invariant assertion:

$$c \times q + r \times v = 5 \times r \wedge b \times v + c \times z = 5 \times b + c \wedge b \times q + r = r \times z \wedge 2 \times s + (v-5) \times (1+z) = b \times (v-5).$$

Execution of Daikon was only possible after we instantiated all the constants, initialized all the variables, and defined function f, which we did as follows:

```
const int e=2, g=1; cN=21;  const float a=2., m=2., b=1., c=1., d=2.;
int i=1, n=20, j=0, k=150, p=20, h=0, l=0, xx=5, yy=2;
float x=0., y=2., z=1., v=5., w=1., s=0., t=0., u=0., q=0., r=1.;
int aa[cN] = {2,8,10,38,15,0,3,6,23,90,57,14,46,175,23,19,0,16,22,17,72};
int ab[cN] = {12,50,4,9,6,3,0,22,19,12,15,2,0,0,8,1,42,12,5,3,0};
float f (float z) {return z+1;};
```

Then, Daikon generates the following invariant assertion:

$$i+n = 21 \wedge 7 \times i + k = 157 \wedge 7 \times n + 10 = k \wedge z + v = 6 \wedge w - t = 1 \wedge 2 \times w = x + 2 \wedge 2 \times t = x \wedge$$

$$z = r \wedge s = q \wedge x = u \wedge x\%a = 0 \wedge yy\%e = 0 \wedge e \in aa[].$$

As for LoopFrog, it produces the following assertion:

$$zz \leq r \wedge k \leq n \wedge r = z \wedge t = w \wedge u = x.$$

For the sake of comparison, we generate an invariant assertion from our invariant relation (the same invariant relation we used to generate the loop function, above), using Proposition 1; for the precondition, we take the initialization presented above, and we instantiate the constants to the values presented above. We find the following invariant assertion (represented by a vector), where

ϕ represents the fractional part of a number.

$$A = \left\{ (s,s')| \begin{array}{c} i \geq 1 \wedge n \leq 20 \wedge \phi(1.4427log(p)) = 0.321928 \wedge \\ aa = [2,8,10,38,15,0,3,6,23,90,57,14,46,175,23,19,0,16,22,17,72] \wedge \\ ab = [12,50,4,9,6,3,0,22,19,12,15,2,0,0,8,1,42,12,5,3,0] \wedge \\ xx = 5 \wedge j + \Sigma_{H=i}^{21} aa[H] = 656 \wedge l + \Sigma_{H=1}^{n} ab[H] = 225 \wedge \\ q + \Sigma_{H=1}^{n} f^H(r) = \Sigma_{H=1}^{20} f^H(1) \wedge \\ 1.4427nlog(xx) + 1.4427log(yy) = 47.4386 \wedge \\ i + n = 21 \wedge 7i + k = 157 \wedge 2^i = x + 2 \wedge 2^i = 1 + 1.4427log(y) \wedge i = z \wedge \\ 2^i = u + 2 \wedge i + v = 6 \wedge w = 0.52^i \wedge f^{21-i}(r) = f^{20}(1) \wedge \\ i + \lfloor \frac{log(p)}{log(2)} \rfloor = 5 \wedge s - 0.5(z-1)z = 0 \wedge t - w = -1 \wedge h + 2p = 40 \end{array} \right\}.$$

4.2 Non Trivial Calculations

We consider the following loop, which manipulates numeric variables, and includes non trivial numeric computations.

```
#include <iostream> #include <math.h> using namespace std;          // header
int fact (int n);               // body not shown; computes the factorial of n
int main () { const int  cN, ca;   int i, j, fb, nc, np;  float x, x1, x2, x3;
while (j!=cN) {j=j+i;  nc=fb;  fb=np+nc;  np=nc;  x2=x2+pow((x-ca),i)/fact(i);
       x3=x3+pow(x,i)/fact(i); x1=x1+pow(x,j)/fact(j); i=i+1; j=j-i;}}
```

Our method produces the following function for this loop:

$$W = \left\{ (s,s')| \begin{array}{c} j \geq cN \wedge x' = x \wedge j' = cN \wedge \\ x1' = \frac{x1\Gamma(1+cN)\Gamma(1+j) - e^x\Gamma(1+j)\Gamma(1+cN,x) + e^x\Gamma(1+cN)\Gamma(1+j,x)}{\Gamma(1+j)\Gamma(1+cN)} \wedge \\ x2' = \frac{e^{-ca}(e^{ca}x2\Gamma(i)\Gamma(i+j-cN) - e^x\Gamma(i+j-cN)\Gamma(i,x-ca) + e^x\Gamma(i)\Gamma(i+j-ca,x-ca)}{\Gamma(i)\Gamma(i+j-cN)} \wedge \\ x3' = \frac{x3\Gamma(i)\Gamma(i+j-cN) - e^x\Gamma(i+j-cN)\Gamma(i,x) + e^x\Gamma(i)\Gamma(i+j-cN,x)}{\Gamma(i)\Gamma(i+j-cN)} \wedge \\ fb' = np \times Fib(j-cN) + fb \times Fib(j+1-cN) \wedge i' = i + j - cN \wedge \\ nc' = np \times Fib(j-cN-1) + fb \times Fib(j-cN) \wedge \\ np' = np \times Fib(j-cN-1) + fb \times Fib(j-cN) \end{array} \right\},$$

where Γ is Euler's Gamma function and Fib is Fibonacci's function. In order to generate an invariant assertion for this loop, we need to choose a vector P that represents initial conditions (as per Proposition 1). We let P be defined by the following initial conditions: $i = 1 \wedge j = 30 \wedge fb = 1 \wedge nc = 1 \wedge np = 1 \wedge x1 = x2 = x3 = 0$. This yields the following invariant assertion:

$$A = \left\{ (s,s')| \begin{array}{c} i \geq 1 \wedge j \leq 30 \wedge i + j = 31 \wedge x = 3 \wedge np = Fib(i) \wedge fb = Fib(i+1) \wedge \\ x2 = 2.71828\frac{\Gamma(i,1)}{\Gamma(i)} - 1 \wedge x3 = 20.0855\frac{\Gamma(i,3)}{\Gamma(i)} \wedge x1 = 20.0855(1 - \frac{\Gamma(j+1,3)}{\Gamma(j+1)}) \end{array} \right\}.$$

Aligator could not process this loop; when we removed all the statements that it could not parse, it produced the following assertion (where variable names indexed by zero designate the initial value of the variable)

$$i^2 + 2j + i_0 = i + i_0^2 + 2j_0 \wedge x2 + \frac{(x-ca)^{i_0}}{ca + ca^2 - 2ca \times x + (x-1)x} = x2_0 \wedge x3 + \frac{x^{i_0+1}}{x-1} = x3_0.$$

Daikon did not object to any statement, and produced $i + j - 31 = 0$.

4.3 Non Trivial Control Structures

We consider the following loop, which has nested if then else statements in its loop body:

```
#include <iostream> using namespace std;
int main () {int x, z, t;  float y;
while (x!=1) {if (x%4==0) {x=x/4; y=y*4; z=z+2; t=t-2;}
      else {if (x%2==0) {x=x/2; y=y*2; z=z+1; t=t-1;}
    else {x=x-1; y=y+y/x;}}}}
```

Our tool returns the following function for this loop:

$$W = \left\{(s, s')|x' = 1 \wedge y' = x \times y \wedge z' = z + \lfloor\frac{log(x)}{log(2)}\rfloor \wedge t' = t - \lfloor\frac{log(x)}{log(2)}\rfloor\right\}.$$

We apply Proposition 1 to the invariant relation generated for this loop, using the precondition P defined by $x = 30 \wedge y = 2 \wedge z = 0 \wedge t = 20$, and we find the following invariant assertion (represented by a vector):

$$A = \{(s, s')|xy = 60 \wedge z + \lfloor log_2(x)\rfloor = 4 \wedge t - \lfloor log_2(x)\rfloor = 16\}.$$

Aligator and Daikon both find $t + z = 20$.

4.4 Non Integer Data

We consider the following loop, which performs a fixpoint computation on real numbers; the interesting aspect of this loop is that it is not inductive, i.e. it is not maintaining any invariant property as it converges towards the fixpoint. Hence its loop invariant gives no clue as to what it is doing.

```
#include <iostream>  #include <math.h>
int main () {float x, y, z;  while (fabs(y-x)!=0) {y=x; x=1+z/x;}}
```

Our algorithm finds a trivial invariant relation for this loop, which is $R = L$; by applying Proposition 5, we find the lower bound $Y_0 = \widehat{\widehat{T}}$. But this is not sufficient; in fact our algorithm also systematically generates another lower bound, which does not depend on any invariant relation, to the effect that if the loop body is executed at least once, then the range of the loop body's function is necessarily a superset of the range of W. The combination of these lower bounds yields:

$$W \sqsupseteq \{(s, s')|x = y \wedge s' = s\}$$

$$\cup\{(s, s')|x \neq y \wedge 1 + 4z \geq 0 \wedge x' = \frac{1 + \sqrt{1 + 4z}}{2} \wedge y' = \frac{1 + \sqrt{1 + 4z}}{2} \wedge z' = z\}$$

$$\cup\{(s, s')|x \neq y \wedge 1 + 4z \geq 0 \wedge x' = \frac{1 - \sqrt{1 + 4z}}{2} \wedge y' = \frac{1 - \sqrt{1 + 4z}}{2} \wedge z' = z\}.$$

Indeed, this program has two fixpoints, and it converges to one or the other depending on the initial value x. Note that because this relation is not deterministic (though it is total), we cannot say that it equals W; we can only say that it is refined by W. Aligator finds no loop invariant, since it cannot identify a recurrence relation. Daikon, which merely inspects the execution of the code to produce likely invariants, finds: $x \neq y \wedge x > z \wedge y > z$.

4.5 Non Numeric Data

We consider the following program, which handles data of type list.

```
#include <iostream>  #include <list>  using namespace std;   //   header
int main ()  {list <int> l1, l2, l3;   int x;            // declarations
while (!l2.empty()) {l1.push_back(l2.front()); l3.push_front(l2.front());
                     x=x+l2.front(); l2.pop_front();}}
```

Our tool produces the following function for this loop:

$$W = \{(s, s')|l2' = () \wedge l1' = l1.l2 \wedge l3' = \widehat{l2}.l3 \wedge x' = x + \Sigma(l2)\},$$

where the dot represents list concatenation, the hat represents list inversion, and Σ represents list summation. Application of Proposition 1 with the precondition $l1 = (12, 2, 12) \wedge l2 = (8, 10, 3, 6, 4) \wedge l3 = (7, 8, 5, 9) \wedge x = 1$ yields the following invariant assertion:

$$A = \{(s, s')|l1.l2 = (12, 2, 12, 8, 10, 3, 6, 4) \wedge x + \Sigma(l2) = 32 \wedge \widehat{l2}.l3 = (4, 6, 3, 10, 8, 7, 8, 5, 9)\}.$$

Neither Aligator nor Daikon can process this program.

5 Generating Invariant Relations

While in the previous section we discussed how to use invariant relations, in this section we discuss how to generate them. The detailed discussion of the algorithm is beyond the scope of this paper; we will content ourselves with presenting the main premises and mathematical results behind its design. As we recall, an invariant relation is a reflexive transitive superset of the function of the loop body; because the interest of invariant relations is that they approximate the reflexive transitive closure of $(B \cap T)$, which is the *smallest* reflexive transitive superset of $(B \cap T)$, it is easy to see why smaller invariant relations are better. The following proposition gives us an idea how to obtain small invariant relations.

Proposition 6 *Let w be a while loop on space S and let R and R' be invariant relations for w; then $R \cap R'$ is an invariant relation for w.*

Proof. The intersection of two reflexive relations is reflexive; the intersection of two transitive relations is transitive; and the intersection of two supersets of $(B \cap T)$ is a superset of $(B \cap T)$. **qed**

So that we can generate smaller invariant relations by taking the intersection of not-so-small invariant relations. As for how to generate elementary invariant relations, consider that in order to find supersets of $(B \cap T)$, it helps to write it as an intersection, such as:

$$(B \cap T) = B_1 \cap B_2 \cap B_3 \cap ... \cap B_n.$$

Because then, any superset of B_1 is a superset of $(B \cap T)$; any superset of $B_1 \cap B_2$ is a superset of $(B \cap T)$; any superset of $B_1 \cap B_2 \cap B_3$ is a superset of $(B \cap T)$; etc. This gives us a priceless divide-and-conquer strategy: we can derive invariant relations for an arbitrarily large loop, once the function of its loop body is written as an intersection, by looking at one term at a time, or two at a time, or three at a time, etc. In practice, our algorithm proceeds as follows:

- The source code is mapped into a notation that rewrites the function of the loop body as an intersection; when the loop body is merely a sequence of assignments, this can be done by eliminating sequential dependencies. When the loop body has a more complex control structures, we invoke a more general procedure, which we discuss subsequently.
- We deploy a pattern-matching algorithm that matches the terms of the intersection one a time, then two at a time, then three at a time against pre-stored patterns (called the *recognizers*) for which we store the corresponding invariant relation pattern. Whenever a match is successful, we instantiate the invariant relation pattern to obtain an actual invariant relation. So far, we have limited ourselves to looking at no more than three terms at a time in order to control the combinatorics of the pattern-matching step; but as we consider more complex programs, we are envisioning to increase the number of terms that need to be considered.
- We take the intersection of all the invariant relations that are generated, to obtain a smaller invariant relation.

It is easy to write the function of the loop body as an intersection only if the loop body is made up of a sequence of assignments. When the loop body contains more complex control structures, such as nested if-then-else statements, then the outermost structure of the function of loop body is a union. In that case, we apply the pattern matching algorithm discussed above to each term of the union, to obtain an invariant relation as an intersection of larger invariant relations, of the form:

$$
\begin{array}{l}
R = \\
(R_{1,1} \cap R_{1,2} \cap ...R_{1,n1}) \\
\cup(R_{2,1} \cap R_{2,2} \cap ...R_{2,n2}) \\
\cup... \\
\cup(R_{m,1} \cap R_{m,2} \cap ...R_{m,nm}).
\end{array}
$$

This relation is a superset of the function of the loop body, and it is reflexive; but it is not transitive, as the union of transitive relations is not transitive. To derive an invariant relation from it, we deploy a routine (written in Mathematica, ©Wolfram Research), to merge the terms of this union into a single term, structured as an intersection. The key idea of the routine is to identify common supersets of the terms of the union, and take their intersection. To explain the merger routine, we consider two terms of the union, where each term is the intersection of two terms:

$$R = (R_{11} \cap R_{12}) \cup (R_{21} \cap R_{22}).$$

If we find, for example, that $(R_{21} \cap R_{22}) \subseteq R_{11}$ then we conclude that R_{11} is an invariant relation, since it is reflexive and transitive (by construction), and it is a superset of each term of the union. If, for example, we find also that $(R_{11} \cap R_{12}) \subseteq R_{22}$ then we can infer (for the same reasons as above) that R_{22} is an invariant relation. From which we conclude that $R_{11} \cap R_{22}$ is an invariant relation. As an illustration, consider the following simple loop:

```
while (y!=0) {if (y%2==0) {y=y/2;x=2*x;} else {z=z+x;y=y-1;}}
```

As a reflexive transitive superset of the first branch (which we call B_1), our tool finds $R_1 = R_{11} \cap R_{12}$, where $R_{11} = \{(s, s')|xy = x'y'\}$ and $R_{12} = \{(s, s')|z = z'\}$. As a reflexive transitive superset of the second branch (which we call B_2), our tool finds $R_2 = R_{21} \cap R_{22}$, where $R_{21} = \{(s, s')|x = x'\}$ and $R_{22} = \{(s, s')|z+xy = z'+x'y'\}$. The relation $R = R_1 \cup R_2$ is a superset of $(T \cap B)$ (by construction); and it is reflexive (as the union of reflexive relations); but it is not necessarily transitive (as the union of transitive relations). However, we note that R_{22} is a superset of R_1 (by inspection); on the other hand, it is also a superset of R_2 (any term of an intersection is a superset of the intersection). Hence R_{22} is a superset of $R_1 \cup R_2$; because by construction $R_1 \supseteq B_1$ and $R_2 \supseteq B_2$ we infer that R_{22} is a superset of $B_1 \cup B_2$, which is $(T \cap B)$. On the other hand, because it is generated by our tool, R_{22} is by construction reflexive and transitive. As a reflexive transitive superset of $(T \cap B)$, R_{22} is an invariant relation for the while loop.

6 Concluding Remarks

In this paper, we have briefly introduced the concept of invariant relation, and shown how it can be used to analyze the functional properties of while loops. In particular, we have presented the following results:

- Invariant relations can be used to compute or approximate the function of the loop.
- Invariant relations subsume invariant assertions, in the sense that any invariant assertions can be derived from an invariant relation.
- Any invariant assertion can be structured as the combination of an invariant relation, which is intrinsic to the loop, with the precondition of the loop, which reflects the loop's initialization.
- Invariant relations can be derived from an analysis of the source code of the loop, using a divide-and-conquer algorithm that enables us to handle large loops in nearly linear time.

Our tool for generating invariant relations is based on a pattern matching algorithm that matches pre-stored code patterns, which we call *recognizers*, against a representation of the loop, and generates corresponding invariant relations whenever a match is successful. We believe that the task of computing the function of a loop is essentially a mapping from a domain neutral notation, namely the programming language, to a domain-specific notation, namely the application domain of the program, with its attendant abstractions, notations, axiomatizations, etc. As long as we are handling only numeric data types (integers, reals, etc), then the distinction between programming notation and domain notation is moot, since numeric data types are native to all (C-like) programming languages. But as soon as we need to analyze programs that handle non native data types, we must be able to codify and integrate domain information in order for the tool to carry out a meaningful analysis. In our approach, domain knowledge is codified in the recognizers, and in the axiomatizations that we use after invariant relations are generated to compute the function of the loop.

The examples that we have shown in section 4 show our tool in a favorable light by comparison with other tools, but that is only because we chose the examples according to our current repository of recognizers. In its current status, our prototype tool includes about 50 recognizers, and our algorithm operates by syntactic matching. We envision three important extensions of it:

- Replace the current syntactic matching algorithm by a semantic matching algorithm; whereas we currently match statements of the loop with recognizer patterns token by token, we want to replace this by semantic match, which declares a match if the actual expression and the formal expression are identical, when instantiated by the same variable names. We envision to use Mathematica for this purpose.

- Replace the current repository of recognizers by a set of more general recognizers, and increase the scope of the repository in size (number of recognizers), as well as in genericity (range of code patterns that semantically match each recognizer).

- Develop domain-specific sub-repositories, that can be deployed for code dealing with specific application domains, and would then use domain-specific abstractions, notations, and axiomatizations.

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