Dynamic Symbolic Execution of Higher-Order Functions

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The effectiveness of concolic testing deteriorates as the size of programs increases. A promising way out is to concolic-test programs in a component-by-component fashion, e.g., one function or class at a time. Alas, this idea hits an important roadblock in modern languages such as JavaScript, Python, and Racket. In these languages, components expect functions, objects, and even classes as inputs. The crux of the problem is that existing concolic testing techniques cannot faithfully capture the complex interactions between a higher-order program and its inputs in order to distill it in a first-order formula that an SMT solver can work with.

In this paper, we take the first step towards solving the problem; we offer a design, semantics, and prototype for concolic testing of higher-order functions. Inspired by work on higher-order symbolic execution, our model constructs inputs for higher-order functions with a canonical shape. This enables the concolic tester to keep track of which pieces of the control-flow path of the higher-order function depend on the shape of its input and which do not. The concolic tester encodes the pieces that do not depend on the shape of the input as a first-order formula. Subsequently, similar to a first-order concolic tester, it leverages an SMT solver to produce another input with the same shape but that explores a different control-flow path of the higher-order function. As a separate dimension, the concolic tester iteratively explores the canonical shapes for the input and, investigating all the ways a higher-order function can interact with its input, searching for bugs.

To validate our design, we prove that if a higher-order function has a bug, our concolic tester will eventually construct an input that triggers the bug. Using our design as a blueprint, we implement a prototype concolic tester and confirm that it discovers bugs in a variety of higher-order programs from the literature.

1 INTRODUCTION

Concolic testing (Cadar and Engler 2005; Godefroid et al. 2005) explores a program’s behavior in a gradual fashion to discover bugs. First, the concolic tester supplies a random input to the program under test (hereafter the user program) and monitors how the random input forces the user program evaluation down a specific control-flow path. The concolic tester records this path as a first-order formula and uses an SMT solver to induce a new input that is designed to force the user program to take a different control-flow path. The process repeats until the concolic tester discovers a bug or times out. In effect, concolic testing enhances random testing with symbolic execution to guide input generation to hard-to-reach corners of the control flow of a program.

Testament to the success of the technique is the number and diversity of its adaptations to (i) different languages and platforms: CUTE (Sen et al. 2005) and CREST (Burnim and Sen 2008) for C, KLOVER (Li et al. 2011) for C++, jCUTE (Sen and Agha 2006) and JDart (Dimjašević et al. 2015) for Java, Jalangi (Sen et al. 2013) and SymJS (Guodong et al. 2014) for JavaScript and CutEr (Giantsios et al. 2015) for Erlang, Pex (Tillmann and Halleux 2008) for .NET, KLEE for LLVM (Cadar et al. 2008); and (ii) different application domains: security (Godefroid et al. 2008, 2012), mobile apps (Anand et al. 2012), database applications (Emmi et al. 2007), concurrent programs (Farzan et al. 2013; Razavi et al. 2012), embedded systems (Kim and Kim 2011), GPU programming (Li et al. 2012) and deep learning (Sun et al. 2018). However, not all is coming up roses. When the size of a program increases,

\footnote{We underline the first occurrence of each new technical term.}

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so does the number of control-flow paths that the concolic tester needs to explore. As a result concolic testing of large programs becomes ineffective and misses bugs.

An alternative to applying concolic testing to a whole program is to test program components. Unfortunately, existing concolic testers are not prepared to effectively test components of programs written in modern higher-order languages like JavaScript, Python and Racket. When concolic testers deal with programs that consume functions or objects, they fall back to heuristics (Koopman and Plasmeijer 2006; Li et al. 2017; Selakovic et al. 2018) or are unable to call back into higher-order values (Giantsios et al. 2015). In general, there are inputs that existing concolic testers cannot generate and these inputs are necessary to explore all of the behavior of a higher-order program.

The reason for this limitation is fundamental; concolic testers rely on SMT solvers that can only deal with first-order formulas. Specifically, in a higher-order setting, inputs affect not only the control-flow of the user program but the user program itself may affect the control-flow of its inputs. This inter-dependency implies that a control-flow path of a higher-order program cannot be described as a symbolic formula of constraints based solely on the first-order properties of the program’s inputs. The control flow of the program also depends on the behavior of the inputs.

Starting from this observation, our contribution is the design of a concolic tester for higher-order programs in a functional, dynamically-typed setting. Our key insight is that it is possible to split the search for a bug in two levels: at one level we describe entire classes of behavior of the input, and at the second level we exploit the solver to search within a specific pattern of behavior.

In essence, the formulas capture the first-order properties of the values that flow between the user program and its input, for a fixed control structure of the input. Thus, just like for first-order code, an SMT solver can produce inputs that explore different control-flow paths in the user program. Intuitively, the concolic tester and the user program are in a conversation and we use the SMT solver to search the space of the first-order properties of the values they exchange after deciding on the “strategy” the concolic tester follows to produce its answers.

To explore all of the behavior of the user program, however, the concolic tester must also explore different patterns of behavior of the input. That is, it must explore all the different strategies the concolic tester can employ in the conversation with the user program. Specifically, this search level varies the higher-order control structure of values that the concolic tester sends to the user program. Building on work on higher-order symbolic execution (Nguyén et al. 2014, 2015, 2017), we design a canonical form for functions that captures all possible patterns of control structure as different syntactic shapes of the body of a function. Starting from the simplest shape, the constant function, we gradually evolve the structural complexity of the inputs. In sum, the SMT-driven exploration of the first-order aspects of the inputs and the orthogonal evolution of their shape work hand-in-hand to explore the space of the higher-order function inputs to the user program.

Our design comes with a formal model that justifies it. The model specifies a concolic tester for a functional language and describes how the tester can evolve an initial, random input to explore different parts of the behavior of the user program. We validate our design idea in two ways:

- We prove that if a higher-order program in our model has a bug, then our model eventually constructs an input that triggers the bug;
- We provide a prototype concolic tester based on the model and use it to uncover bugs in examples from the literature on concolic testing and symbolic execution.

The remainder of the paper is organized as follows. Section 2 and section 3 revisit the two foundations of our work: first-order concolic testing and function forms with canonical control structure. Section 4 builds on these two elements to demonstrate how our higher-order concolic tester gradually evolves inputs to discover a bug in a concrete higher-order example. Section 5 introduces the formal model for our concolic tester and section 6 establishes its formal correctness.
properties. Section 7 describes our prototype implementation and how we use it to discover bugs in a corpus of examples from the literature. Finally, Section 8 places our results in the context of related work.

2 A REFRESHER ON FIRST-ORDER CONCOLIC TESTING

The central idea behind first-order concolic testing is beautifully simple. The concolic tester generates a first set of random inputs for the user program and uses them to run the program in two modes at the same time. The concrete mode is the same as ordinary evaluation. The symbolic one constructs a symbolic formula that represents the path of the control-flow of the program that the generated inputs exercise. After the concolic tester obtains the formula, it negates one of its pieces and asks an SMT solver to produce, if possible, a model for the tweaked formula. The model corresponds to a new set of inputs that cause the user program to follow a different control-flow path than the one due to the original inputs — exactly the control-flow path that corresponds to the tweaked formula. The concolic tester repeats this process and systematically examines the control-flow graph of the user program until it eventually discovers a bug or crosses a pre-defined time or memory threshold.

To make the discussion concrete, consider the following example:

\[
\text{let } z = 2 \times X \text{ in (cond [(z < Y) \text{ error}]
[\text{else 1}]})
[\text{else 0}]\]

Here, the inputs are represented using the variables \(X\) and \(Y\). The goal of the concolic tester is to generate \(X\) and \(Y\) that trigger the \text{error}. In other words the concolic tester has to cause both \(2 \times X < Y\) and \(17 < X\) to be true.

Let’s assume that the concolic tester generates an initial set of inputs where \(X = 0\) and \(Y = 1\), which do not meet the above conditions and fail to trigger the error. In the concrete mode of the concolic tester, the initial inputs imply that \(z\) becomes 0. At the same time, with its symbolic mode, the concolic tester also tracks that 0 is the result of the expression \(2 \times X\). In general, any concrete value computed by primitive operators comes with an expression trace indicating how the concrete value relates to the inputs of the example. For example, the expression \(z < Y\) from the outer \text{cond} expression evaluates to value 1 with trace \(2 \times X < Y\).

Using the expression traces, the concolic tester produces an ordered list of path constraints containing the concrete values and the associated expression traces that determine whether the test of a branch in a conditional expression is true or not. For the above specific inputs and our example, the concolic tester records:

\[
[\langle 1, \langle 2 \times X < Y \rangle \rangle, \\
\langle 0, \langle 17 < X \rangle \rangle] \]

In this list the first path constraint corresponds to the outer \text{cond} expression and captures that the test of the \text{cond} evaluates to concrete value 1 with expression trace \(2 \times X < Y\), while the test of the inner \text{cond} expression produces 0 with trace \(17 < X\). The order of the path constraints matches the evaluation of the example and they induce the symbolic formula that represents the control-flow path of the example for inputs where \(X = 0\) and \(Y = 1\):

\[2\text{In the example and the remainder of the paper, we use 1 and 0 to for true and false respectively.}\]
Put differently, the two inputs we examine reveal two alternative control-flow paths for the concolic tester to explore — each corresponds to negating one of the two clauses of the above formula. Figure 1 depicts the current control-flow path and the two alternatives as a tree with leaves containing the outcome of the example in each case.

As the concolic tester does not know which control-flow path results in error, it explores all of them. In order for the example to follow the right-most control-flow path, the test of the outer cond expression needs to become 0. Consequently, the concolic has to generate inputs such that $(2 \times X < Y) = 0$, i.e., the negation of the clause from the first path constraint. The SMT solver responds with the model where $X$ is 1 and $Y$ is 0, giving us our next set of inputs.

Since these inputs do not result in an error, the search continues and the concolic tester negates the second clause and issues a second query

$$(!((2 \times X < Y) = 0)) \land (((17 < X) = 0))$$

The SMT solver responds by assigning $X$ to 18 and $Y$ to 37, causing the program to reach error.

In general terms, given a user program and a set of inputs, the concolic tester runs the program and summarizes, in the form of path constraints, the direction of the control-flow branches the evaluation follows. To explore a different control-flow path, the concolic tester selects a prefix of the given list of path constraints, negates its last element and consults the SMT solver to generate new inputs for the next round of testing. Consequently, with each iteration of the concolic loop, the tester explores an increasing portion of the control-flow graph of the user program until it discovers an error or hits a time or memory limit.

3 CANONICAL FUNCTIONS ARE ALL WE NEED

In the setting of a higher-order functional language, a concolic tester needs to generate not only numbers, but also functions. Fortunately, it is possible to exhaustively exercising all control paths of a higher-order user program, with only a subset of the function terms of the language.

We can describe this subset with a small grammar of canonical functions that restrict the shape of function bodies. In essence, each canonical shape of a functions translates to canonical pattern of interaction between the input and the user program. Intuitively, any generated input first is invoked by the user program, then inspects the results of calls it makes and finally produces a reply. We capture this pattern with a let form followed by a conditional. Of course, the body of the conditional can itself interact (using the above pattern) or it might return a new canonical function. This construction generalizes to arbitrarily higher-order inputs (Nguyễn et al. 2015, 2017).

In the remainder of this section we introduce our canonical functions with a series of examples. The examples demonstrate the key property of the canonical functions: if there is a function that
can trigger a bug in the user program, then there exists a canonical function that also causes the user program to fail. To get started, consider the following user program:

$$\text{(cond } \[(\text{F } 0 < \text{F } 1) \text{ error} \] \[\text{else } 1\])}$$

It is apparent that \text{F} has to be a first-order function from numbers to numbers, but not a constant function, e.g., \(\lambda x. x+4\). However, to reproduce the behavior of this function in this example, the concolic tester does not need to come up with the arithmetic operation \(x+4\). Rather, since the function \text{F} is only applied to 0 and 1, the concolic tester can instead generate the function:

$$\lambda x. (\text{cond } \[(x = 0) 4 \] \[(x = 1) 5\])$$

More generally, if, like in our example, the evaluation of the user program terminates for a particular input, there are only finitely many calls to that input. Thus in the case where the input is a first-order function, it suffices for the concolic tester to produce a cond expression that merely maps arguments from the code under test to the corresponding results of the input without reconstructing the actual computation performed by the input.

The situation is more involved when the input is higher-order itself. Since the input can invoke its argument and then decide how to proceed based on the result(s) of the call(s), the values that the input provides to its argument act, in effect, as new inputs to the user program. The following variant of the previous example displays the issue:

$$\text{(cond } \[(\text{F } (\lambda x. 1) < \text{F } (\lambda y. 2 \times y)) \text{ error} \] \[\text{else } 1\])}$$

A function that can cause this example to fail is \(\text{F} \equiv \lambda g. (g 3) + 10\). However, similar to the previous example, the concolic tester can achieve the same outcome by generating a different function. The necessary details of the shape of the function become evident if we take a closer look at the interaction between the input \(\lambda g. (g 3) + 10\) and the code under test:

To read the diagram, start from the top, considering each line to be an interaction between the user program and it’s input. The first interaction is sending \(\lambda x. 1\) to \text{F}. \text{F} reacts with the application \(g 3\) that transmits 3 back to the user program which replies with 1. Subsequently \text{F} adds 10 to 1 to obtain the result 11 and ends its first interaction with the user program. After this first round of interaction, the user program initiates a second round by sending \(\lambda y. 2 \times y\) to \text{F}. While \text{F} sends again 3 back to the user program, this time the user program multiplies it by 2 and responds with 6. Finally, \text{F} adds 10 to 6 to produce 16, its reply for the second and final interaction.
In this chain of interaction, \( F \) performs two actions: first it sends a number back to the user program, requesting a new number, and then, similar to a first-order function, it maps that number to another number. Thus we can rewrite \( F \) to separate the two actions syntactically:

\[
\lambda g. \text{let } z = g \ 3 \\
\text{in } z + 10
\]

This revamped shape suggests how we can replace the input with a canonical function that behaves just like the input, inducing the same interactions with the user program as the input does. Building on our discussion about first-order function inputs above, we construct a \( \text{cond} \) expression that dispatches on \( z \) and avoid the use of the arithmetic operator:

\[
\lambda g. \text{let } z = g \ 3 \\
\text{in} \ (\text{cond} [(z = 1) \ 11] \\
[(z = 6) \ 16])
\]

In sum, canonical functions can capture all patterns of interaction between the user program and the input despite their strict structure. We revisit canonical functions and their properties formally in section 5 and section 6. In the following section, we discuss how their structure helps generate inputs that uncover bugs in user programs.

4 DIRECTED EVOLUTION OF CANONICAL FUNCTIONS

Canonical functions allow the concolic tester to limit the space of inputs it needs to search to trigger an error. Even better, the structure of our canonical functions makes it possible for the concolic tester to search the space of canonical inputs in a targeted fashion. The concolic loop starts with a constant function. Then, based on the interaction between the input and the user program, the input evolves into a more complex one, at each evolution step hoping to explore a different path of the control-flow of the user program. This process of evolution of the term is guaranteed to find the fittest function: no matter where a bug might be in the program, a canonical input can trigger it. This section explains the evolution of canonical functions by example.

To start, consider the following program where \( F \) is its higher-order input:

\[
\text{(cond} [(F \ (\lambda x. \ 4) + F \ (\lambda y. \ 2 \times y) = 10) \\
(F \ (\lambda w. \ (\text{cond} [(w = 2) \ \text{error}] \\
[\text{else} -1)))]) \\
[\text{else} -2])
\]

The example applies \( F \) to two functions and if the sum of the two applications is equal to 10, it calls \( F \) with a third function which signals an \textit{error}.

The concolic tester starts with the simplest canonical function \( \lambda g. \ (\text{cond} \ [\text{else} \ 0]) \) as the first input for the example. The peculiar shape of the function is due to the shape of canonical functions that requires that their bodies consists of \text{let} and/or \text{cond} expressions. The label \( L_0 \) is a unique identifier for the conditional branch; we expand on the role of branch labels further on. With that input, both calls to \( F \) return to 0 and the example returns -2.

Following our discussion of first-order concolic testing in section 2, the tester records first-order path constraints that encode the control-flow path of the example (but not its inputs). The single constraint here is \( \langle 0, \ (0 + 0 = 10) \rangle \) and indicates that the test of the conditional of the example evaluates to 0 because the sum of the two constants 0 is not equal to 10. On its own this constraint is not sufficient for the concolic tester to generate a new input; it lacks any connection with \( F \).

To remedy this shortcoming, our higher-order concolic tester records constraints about the evaluation of the input that it generates. As each \text{cond} expression inspects the properties of one
specific value (checking to see which integer it is, or if it is a procedure), we record a constraint that captures that value followed by a series of constraints that capture the queries of the value. The former are called test constraints, and they record both a unique label for the cond expression and the value being inspected. The latter are called branch constraints, and they each record three pieces of information: a unique label for the branch, the outcome of its test (if the branch is taken or not), and the expression trace of the outcome. Our running example results into four input-related constraints in addition to the first-order constraint from above:

\[
\langle \text{cond: } l_0, \text{test: } \lambda x. 4 \rangle,
\langle \text{branch: } l_0, 1, \langle 1 \rangle \rangle,
\langle \text{cond: } l_0, \text{test: } \lambda y. 2 \times y \rangle,
\langle \text{branch: } l_0, 1, \langle 1 \rangle \rangle,
\langle 0, \langle 0 + 0 = 10 \rangle \rangle
\]

The input-related constraints form two pairs (that show up on the same line in the list above). The first pair corresponds to the application \(F (\lambda x. 4)\), and the resulting evaluation of \(F\)'s cond expression, while the second corresponds to the application \(F (\lambda y. 2 \times y)\). This grouping of input-related constraints is a general pattern; every execution of a cond expression in the input adds a consecutive block of constraints that starts with a test constraint and ends with a branch constraint whose test evaluates to 1. If this last constraint has the same label as the test constraint of the cond expression, like these two do, evaluation follows the else branch of the cond expression.

Because of the pattern of the input-related constraints, the concolic tester can infer that the default input ignores its argument \(g\) for both applications. This opens up a possibility for how the concolic tester can generate a new input that influences the example in a different way. That is, the input can evolve to one that interacts with \(g\). The simplest one simply checks if \(g\) is a function:

\[
\lambda g. (\text{cond } \langle \text{procedure?}(g) e^* \rangle l_1 \langle \text{else } 0 \rangle l_0)
\]

where \(e^*\) stands for the various ways the input proceeds after establishing that \(g\) is indeed a function.

There are two general options for \(e^*\) based on the shape of canonical functions. The first is for the input to ignore what it has learned about \(g\), and simply return a constant number, a constant function, or a variable in scope (in this case, the only such variable is \(g\) itself). Alternatively, the input can call \(g\) (or in fact any other function in scope) which translates to an \(e^*\) of the form:

\[
\text{let } z = g v^* \text{ in } (\text{cond } \langle \text{else } 0 \rangle l_2 \langle \text{else } 0 \rangle l_0)
\]

Any of the above options could trigger the error in the example. Thus the concolic tester may have to ultimately explore all of them. However, for the sake of the discussion, we assume that the concolic tester picks a constant function and stashes away the rest for future consideration. Consequently the concrete input for the next iteration of the concolic loop is

\[
\lambda g. (\text{cond } \langle \text{procedure?}(g) \rangle (\text{let } z = g X \text{ in } (\text{cond } \langle \text{else } 0 \rangle l_2 \langle \text{else } 0 \rangle l_0)) l_1 \langle \text{else } 0 \rangle l_0)
\]

Here, instead of some concrete value, \(g\) is applied to \(X\). This is an important piece of the design of our higher-order concolic tester. In essence, \(X\) is an additional input that the concolic tester controls and can use to further affect the evaluation of the example. In other words, the evolution of the shape of the input aims to offer to the concolic tester new channels through which it can influence the example.

If we assume that the concolic tester randomly picks the initial value of \(X\) to be 3, the application \(F (\lambda x. 4)\) reduces to the \(I\) branch of \(F\), producing the input-related constraints \(\langle \text{cond: } I_0, \text{test: } \lambda x. 4 \rangle\)
and \(\langle\text{branch}: I_1, 1, \{1\}\rangle\). The latter indicates that the procedure\((g)\) test succeeds, i.e., its result is 1. Next, the application \(g\ X\) inside branch \(I_1\) returns 4 and the nested cond expression follows the else branch with label \(I_1\), which induces the input-related constraints \(\langle\text{cond}: I_2, \text{test}: \{4\}\rangle\) and \(\langle\text{branch}: I_2, 1, \{1\}\rangle\). The second application of \(F\), \(F\ (\lambda y. 2 \times y)\), proceeds in a similar manner. In summary, we obtain the following new list of path constraints:

\[
\begin{align*}
\langle\text{cond}: I_0, \text{test}: \lambda x. 4\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle\text{cond}: I_2, \text{test}: \{4\}\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle\text{cond}: I_0, \text{test}: (\lambda y. 2 \times y)\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle\text{cond}: I_2, \text{test}: (2 \times X)\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle 0, \{0 + 0 = 10\}\rangle
\end{align*}
\]

It is worth noting that, in contrast to all the other test constraints so far, the second test constraints for the nested cond expression (with label \(I_2\)) includes an expression trace \(\langle2 \times X\rangle\) instead of the actual value 6. This is because the tests in this cond expression inspect a first-order value. Hence the concolic tester keeps track of how the value depends on first-order inputs so that it can adjust those inputs to affect what branch of the cond expression that the evaluation follows.

With this second list of constraints, the input can evolve further. For example, the input constraints for the nested cond expression of \(F\) indicate that \(F\) ignores the result of the application \(g\ X\) and goes straight to the else branch with label \(I_5\). Hence, as above, the concolic tester can tweak the shape of \(F\) so that its nested cond expression inspects the result of \(g\ X\). The test constraint \(\langle\text{cond}: I_0, \text{test}: \{4\}\rangle\) shows one way to do so; the concolic tester can add a new clause to the nested cond expression that tests if \(z = 4\) and forces the evaluation to avoid the else branch. As before, the concolic tester has a number of choices for the new clause of the nested cond expression and eventually it may have to explore them all. This time we opt to continue the discussion by having the new clause return a random number that we represent as yet a new input \(Y\):

\[
\lambda g. (\text{cond [procedure?}(g) \\
(\text{let } z = g\ X \\
\text{in (cond [z = 4] Y_3)}^{I_3} \\
[\text{else 0}])^{I_3}))^{I_3}
\]

Assuming that \(X\) is equal to 3, as above, and \(Y_3\) is randomly set to 0, we obtain this third list of path constraints from the evaluation of the example:

\[
\begin{align*}
\langle\text{cond}: I_0, \text{test}: \lambda x. 4\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle\text{cond}: I_2, \text{test}: \{4\}\rangle, \\
\langle\text{branch}: I_3, 1, \{4 = 4\}\rangle, \\
\langle\text{cond}: I_0, \text{test}: (\lambda y. 2 \times y)\rangle, \langle\text{branch}: I_1, 1, \{1\}\rangle, \\
\langle\text{cond}: I_2, \text{test}: (2 \times X)\rangle, \langle\text{branch}: I_1, 0, \{2 \times X = 4\}\rangle, \langle\text{branch}: I_2, 1, \{1\}\rangle, \\
\langle 0, \{Y_3 + 0 = 10\}\rangle
\end{align*}
\]

The list is roughly the same as the one from the previous input except for three constraints. The first difference is that the fourth constraint is a test constraint that indicates that the nested cond expressions of \(F\) follows branch \(I_1\) for the first application of \(F\). Next, the second to last constraint is a new branch constraint that indicates that the nested cond expressions of \(F\) fails to follow branch \(I_2\) for the first application of \(F\), since \(2 \times X\) is not equal to 4. Finally, the last constraint records that
the the test of the cond expression of the example still evaluates to 0 but that the result depends on the input $Y_s$ specifically that $Y_s+0 = 10$.

At this point, the concolic tester could focus on the first-order constraint $\langle 0, (Y_s+0 = 10) \rangle$ and ask the SMT solver to come up with a value for $Y_s$ that flips the test of the cond expression. Instead, we opt for a different choice that focuses on the input-related constraints and, pushing the evolution of the shape of the input further.

In particular, the concolic tester can use the test constraint $\langle \text{cond: } l_2, \text{test: } \langle 2 \times X \rangle \rangle$ to further refine the shape of $F$. This constraint is part of the group of constraints that correspond to the second application of $F$ which imply that for the second application of $F$, evaluation again follows the else branch of the nested cond expression of the input. Thus the concolic tester can extend the nested cond expression with a new branch with the test $z = 2 \times X$:

$$
\lambda g. \text{cond} \left[ \text{procedure?}(g) \right]
\begin{array}{l}
\text{let } z = g X \\
in \text{cond} \left[ (z = 4) \ Y_s \right]^{l_1} \\
(\langle z = 2 \times X \rangle \ Y_s)^{l_1} \\
[\text{else } 0]^{l_1}
\end{array}
$$

where both $Y_s$ and $Y_t$ are the constant number 0.

Note that this step of input evolution is that the test of the new branch uses the expression trace $2 \times X$ instead of an actual number. This is necessary because this branch should handle the result of the application $g \ X$ when $g$ is $\lambda y. 2 \times y$ for all values of $X$ and not just when $X$ is 3.

At the same time, this evolution establishes a connection between the input $X$ and the test of the cond expression through the new input $Y_s$ which has important repercussions for the concolic loop. Specifically, running the example with the new input produces the list of path constraints:

$$
\langle\langle \text{cond: } l_0, \text{test: } \langle l x. 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle, \langle\langle \text{cond: } l_1, \text{test: } \langle 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 4 = 4 \rangle \rangle, \langle\langle \text{cond: } l_0, \text{test: } \langle l y. 2 \times y \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle, \langle\langle \text{cond: } l_2, \text{test: } \langle 2 \times X \rangle \rangle, \langle \text{branch: } l_1, 0, \langle 2 \times X = 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 2 \times X = 2 \times X \rangle \rangle, \langle 0, \langle Y_s + Y_t = 10 \rangle \rangle \rangle
$$

Hence, the concolic tester has two ways ($Y_s$ and $Y_t$) to affect the cond expression in the example. It can ask the SMT solver to come up with values for $Y_s$, $Y_t$ and $X$, using the negation of the only first-order constraint, i.e., $Y_s+Y_t = 10$. However, due to the second to last branch constraint it has to also constrain the SMT solver, ensuring that $(2 \times X = 4)$ is false. Unfortunately, this constraint makes it impossible for the SMT solver to derive $X=2$ which is necessary to trigger the bug. In fact, exactly for this reason, this shape of input is a dead-end.

As a result, the concolic server is better off backtracking to the second input from above:

$$
\lambda g. \text{cond} \left[ \text{procedure?}(g) \right]
\begin{array}{l}
\text{let } z = g X \\
in \text{cond} \left[ (z = 4) \ Y_s \right]^{l_1} \\
[\text{else } 0]^{l_1}
\end{array}
$$

where $X$ and $Y_s$ are equal to 3 and 0 respectively. With this input, the evaluation of the example produces these path constraints (duplicated from earlier):
Thus, the concolic tester can ask the SMT solver for help with determining a new value for \( Y_s \), the input it has a first-order constraint for. Subsequently the SMT solver derives that when \( Y_s \) is 10, the result of \( Y_s + 0 = 10 \) flips.

With a new value for \( Y_s \) in hand and the same shape for \( F \), the concolic tester evaluates the example and, as usual, records a new list of path constraints:

\[
[\langle \text{cond: } l_0, \text{test: } \lambda x. 4 \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle \text{cond: } l_1, \text{test: } \langle 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 4 = 4 \rangle \rangle,
\langle \text{cond: } l_0, \text{test: } \lambda y. 2 \times y \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle \text{cond: } l_1, \text{test: } \langle 2 \times X \rangle \rangle, \langle \text{branch: } l_0, 0, \langle 2 \times X = 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle 1, \langle Y_s + 0 = 10 \rangle \rangle,
\langle \text{cond: } l_0, \text{test: } \lambda w. \text{(cond } [(w = 2) \text{ error} [\text{else -1}])] \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle 0, \langle X = 2 \rangle \rangle,
\langle \text{cond: } l_1, \text{test: } \langle -1 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle]
\]

Since the value of \( Y_s \) makes the test of the \text{cond} expression true, the evaluation reaches the third application of \( F \) and through that the test of the \text{cond} expression of \( \lambda w. \text{(cond } [(w = 2) \text{ error} [\text{else -1}])] \). This test contributes the new first-order constraint \( \langle 0, \langle X = 2 \rangle \rangle \). Unfortunately, if the concolic tester asks the the SMT solver to tweak the input so that \( X \) is equal to 2, the solver reports that the formula is unsatisfiable since \( X = 2 \) from the new first-order constraint clashes with the fact that \( 2 \times X = 4 \) is false from the second to last branch constraint.

To make progress here, the concolic tester can take a step back and and force the evaluation of the second application of \( F \) in the example to follow branch \( l_1 \) instead of the else branch. To do so, the tester truncates its list of path constraints and inserts at the end a new branch constraint as if the test of branch \( l_1 \) would have succeeded for the second application of \( F \). This targeted branch constraint modification produces:

\[
[\langle \text{cond: } l_0, \text{test: } \lambda x. 4 \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle \text{cond: } l_1, \text{test: } \langle 4 \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 4 = 4 \rangle \rangle,
\langle \text{cond: } l_0, \text{test: } \lambda y. 2 \times y \rangle, \langle \text{branch: } l_1, 1, \langle 1 \rangle \rangle,
\langle \text{cond: } l_1, \text{test: } \langle 2 \times X \rangle \rangle, \langle \text{branch: } l_1, 1, \langle 2 \times X = 4 \rangle \rangle]
\]

The concolic tester translates the modified constraints into a formula, asks the SMT solver for a model and the solver replies that \( X \) is equal to 2.

Consequently, the concolic tester tries again the previous input

\[
\lambda g. \text{(cond } [\text{procedure?}(g)\text{)}
\begin{align*}
\text{let } z &= g \text{ } X \\
\text{in } &\text{(cond } [(z = 4) \text{ } Y_s]\text{[1]} \\
\text{[else 0]}\text{[1]}\text{)]}\text{[1]}
\end{align*}
\]

but where \( X \) is equal to 2 and \( Y_s \) remains equal to 0, as before. The resulting path constraints are:
[⟨cond: l0, test: λx. 4⟩, ⟨branch: l1, 1, ⟨⟩⟩,
⟨cond: l1, test: ⟨⟩⟩, ⟨branch: l1, 1, ⟨⟩⟩,
⟨cond: l2, test: ⟨⟩⟩, ⟨branch: l1, 1, ⟨⟩⟩,
⟨cond: l2, test: ⟨⟩⟩, ⟨branch: l3, 1, ⟨⟩⟩,
⟨cond: l0, test: (λy. 2×y)⟩, ⟨branch: l1, 1, ⟨⟩⟩,
⟨cond: l2, test: ⟨⟩⟩, ⟨branch: l3, 1, ⟨⟩⟩,
⟨0, ⟨Y3 + Y3 = 10⟩⟩]

With the next iteration of the concolic loop, the concolic tester can perform one more SMT query. The query adjusts Y3 to 5 to achieve Y3 + Y3 = 10. As a result the evaluation reaches again the cond expression in (λw. (cond [(w = 2) error] [else -1])) and since X is already equal to 2, the input finally triggers the error.

To sum up, the example shows how our higher-order concolic tester evaluates a program under test and records both first-order and input-related constraints. It feeds the first-order ones to an SMT solver the same way a first-order concolic tester uses the constraints it records to explore the control-flow graph of the program under test. The input-related ones, which are a distinguishing feature of our design, help the concolic tester to evolve the input iteratively and introduce further ways the input can influence the evaluation of the user program. The subsequent section makes these insights precise with a formal model.

Remark on Completeness. Before though we conclude this section, we briefly discuss a subtle point about the inputs that our concolic tester produces through evolution. The astute reader may have observed that λf. (let z = f 2 in 5), a simpler input than the one our concolic tester generates, can also reveal the error in our running example. The ability of the concolic tester to produce inputs like the one for our running example — that call their arguments (maybe more than once), inspect the result of the call(s) and, then based on that, decide on the value to return — is critical and, without it, we would not be able to explore all possible behavior of the user program. For instance, consider the following variant of our example:

\[
\text{(cond } [(F (\lambda x. 4) = 0) \\
\quad \text{(cond } [(F (\lambda y. 2 \times y) = 10) \text{ error}] \\
\quad \text{[else -1]])] \\
\text{[else -2])}
\]

Here, the input cannot trigger the error unless it can distinguish the two call sites of F and thus it must be able to distinguish the two functions that are passed to F. And, clearly, the only way to distinguish them is to call them. Indeed this is exactly what concolic-generated input does:

\[
\lambda g. (\text{cond } [\text{procedure?}(g) \\
\quad \text{(let } z = g X \\
\quad \text{in (cond } [(z = 4) Y_3]_{l_3} \\
\quad \quad [(z = 2 \times X) Y_4]_{l_4} \\
\quad \quad \text{[else 0]})]_{l_1} \\
\quad \text{[else 0]})_{l_0})
\]

Put differently, it is not sufficient that a higher-order concolic tester call user program functions simply to discover errors in them. It must also be able to call given functions in order to force the user program to expose all of its possible behavior.

5 FORMALIZING HIGHER-ORDER CONCOLIC TESTING

The formal model of our higher-order concolic tester consists of three pieces: (i) the language of user programs, (ii) a concolic machine that evaluates a user program for a given input and produces the corresponding list of path constraints, and (iii) the input evolution process that uses the list of
path constraints to construct a new input for the user program for the next iteration of the concolic loop.

Figure 2 puts these three pieces together and shows how they form the concolic loop. First, a user program \( e \) goes through an instrumentation step that translates it into the corresponding concolic program \( e \). Instrumentation requires also the construction of a store \( \sigma \) that maps each free variable \( X \) of \( e \) to a number \( n \) or a canonical function \( \lambda x. \text{conds}_x \). In the initial store, concolic variables map to a random number or the default canonical function \( \lambda x. (\text{cond [else 0]} lis) \). Put differently the store codifies the input for the user program. Given the store, the concolic machine evaluates the result of the instrumentation, \( e \), using three registers: the store \( \sigma \), the list of path constraints \( \pi \) (that is initially empty) and the concolic program \( e \). If the result of the evaluation is not an error, the final content \( \pi \) of the middle register together with the store \( \sigma \) become the seed for the evolution of the input. Specifically, the \( \text{evolve} \) metafunction uses them to compute a new store \( \sigma' \) and the concolic loop proceeds with this new input to the next iteration until it discovers an error in the user program.

Section 5.1 details the syntax of user programs, the syntax of concolic programs, the instrumentation step that translates the former to the latter and the operation of the concolic machine. Section 5.2 concludes this section with a formal description of the evolution of new inputs.

### 5.1 From User Programs to Concolic Evaluation

The language of user programs is a typical dynamic functional language based on the call-by-value \( \lambda \)-calculus. Figure 3 collects the constructs of the language that include numbers \( n \), \text{error}, multi-way conditional expressions \text{cond}, and concolic variables \( X \) which as we discuss in the previous sections correspond to the inputs of a program. For closed user programs, i.e., those without concolic or other
free variables, we define a standard call-by-value reduction semantics with reduction relation $\rightarrow_s$. The complete definition of the language of the user programs is in the supplementary material.

Figure 4 shows the definition of the concolic language. The syntax of concolic programs (in the left-hand side of the figure) deviates from that of user programs in two points: (i) it combines and generalizes numbers and concolic variables into traced values (t) and (ii) it adds an additional log-and-sequence construct (log(label, e, e) ; e).

As we discuss in section 2 and section 4, an expression trace t describes how a number depends on the inputs of the program. That is a number may be directly the value of a concolic variable X, or a constant number n, or the negation of a trace !t (since we use 0 and 1 as booleans), or the result of an operation op t1 t2. In a concolic program we represent a number with trace t as (t), and we recompute the actual numerical value when needed. In effect, traced values allow us to “concolically” multiplex the concrete and the symbolic evaluation of programs.

The log-and-sequence construct (log(label, e, e) ; e) instructs the concolic machine to extend its current list of path constraints with a new constraint. For the new constraint the machine uses the first three arguments of the construct and we revisit the details of how it does so further on. After the machine adds the new constraint to its list of path constraints, concolic evaluation continues with e.

Before delving into the details of how the instrumentation translates user programs to concolic ones, we discuss the concolic machine M. The right-hand side of figure 4 defines the states of the machine as a triplet of a store $\sigma$, a list of path constraints $\pi$ and a concolic program e. As we discuss above $\sigma$ encodes the inputs of the user program and maps the program’s concolic variables to either numbers n or concolic functions $\lambda x. \text{conds}_x$. The body of the latter, $\text{conds}_x$, follows the informal description from section 3 and section 4. Formally $\text{conds}_x$ is a cond expression that has either just an else branch that returns the default value 0 or, in addition to the else branch it also has branches that inspect variable x. In particular, the latter branches test whether x is a procedure or whether it is equal to a number. Each branch, including the else branch, has a unique identifying label l. The body of a branch other than the else branch is either a variable or a concolic function.

\[
\begin{align*}
  t & ::= X | n | !t | \text{op } t t \\
  e & ::= (t) | \text{error} | x | (\lambda x. e) \\
      & | \text{op } e \text{ op } e \ e \\
      & | (\text{cond } [e e] ... [\text{else } e]) \\
      & | (\log(\text{label}, e, e); e) \\
  v & ::= (t) | (\lambda x. e) \\
  E & ::= [] \\
      & | \text{op } E | \text{op } E e | \text{op } v E \\
      & | E e | v E \\
      & | (\text{cond } [E e] [e e] ... [\text{else } e]) \\
      & | (\log(\text{label}, E, e); e) \\
      & | (\log(\text{label}, v, E); e) \\
  M & ::= \langle \sigma, \pi, e \rangle \\
  \sigma & : X \rightarrow n \text{ or } \lambda x. \text{conds}_x \text{e} \\
  \text{conds}_x & ::= (\text{cond } [\text{else } 0]) \\
      & | (\text{cond } [\text{procedure?}(x) \ e] \ e) \\
      & | [(x = t) \ e] \\
      & | [\text{else } 0] \\
  e^* & ::= (\text{let } z = f v^* \text{ in } \text{conds}_x) | v^* \\
  v^* & ::= x | X | (\lambda x. \text{conds}_x) \\
  \pi & ::= \text{list of } p \\
  p & ::= \langle \text{label}, 0, v \rangle | \langle \text{label}, 1, v \rangle | \langle l, 2, v \rangle \\
  \text{label} & ::= l | \text{user}
\end{align*}
\]

Fig. 4. The Syntax of the Concolic Language and the Definition of the Concolic Machine
or a \texttt{let} expression that calls some function \texttt{f} in scope and makes the result \texttt{z} available to a nested \texttt{conds_{x}} expression.~\textsuperscript{3}

The list of path constraints \(\pi\) consists of three kinds of constraints \(\pi\). The first are of the form \(\langle \text{user}, \ 0, \ v \rangle\) and record the result \(n\) (0 or 1) of a test in a \texttt{cond} expression of the user program together with its expression trace — recall that traces are embedded in the representation of first-order values in the concolic language. These constraints are akin to the first-order constraints from section 4 such as \(\langle 0, \ 0+0 = 10 \rangle\). The other two kinds correspond to the input-related constraints from section 4. In the model, branch constraints are of the form \(\langle l, \ 0, \ v \rangle\) and, as before, record whether the test from branch \(l\) of a \texttt{cond} expression in an input succeeds or fails together with the (traced) result of the test. Test constraints take the form \(\langle l, \ 2, \ v \rangle\) and they record that all the tests of a \texttt{cond} expression whose \texttt{else} branch has label \(l\) may inspect value \(v\).

The instrumentation meta-function \(\mathcal{I}\) consumes a store \(\sigma\) and a user program \(e\) and produces an equivalent concolic program \(e\) that has \texttt{log} expressions at the appropriate places to record path constraints. Figure 5 shows the interesting cases of \(\mathcal{I}[\sigma, e]\) while the remaining ones recur structurally on \(e\). The interesting cases are those concerning numbers, \texttt{cond} expressions and concolic variables. For a number \(n\), the instrumentation embeds \(n\) in a traced value. For a \texttt{cond} expression, it transforms the expression in a mostly recursive manner except that it injects a \texttt{log} expression for the result of the test of each branch that records it together with its expression trace.~\textsuperscript{4} The injected \texttt{log} expression generates a first-order constraint as we discuss above.

\textsuperscript{3}We use \texttt{let} \(x = e;\) in \(e;\) as shorthand for (\((\lambda x.\ e)\) \(e;\))

\textsuperscript{4}!!z, is a double negation that turns \texttt{z}; to 1 if it is a number other than 0.

\begin{figure}[h]
\begin{center}
\begin{align*}
\mathcal{I} &: \sigma \ e \rightarrow e \quad \text{(interesting cases)} \\
\mathcal{I}[\sigma, n] &= \langle n \rangle \\
\mathcal{I}[\sigma, X] &= \langle X \rangle \quad \text{where } \sigma(X) = n \\
\mathcal{I}[\sigma, F] &= \mathcal{I}_e[\lambda x. \ \text{conds}_x] \quad \text{where } \sigma(F) = (\lambda x. \ \text{conds}_x) \\
\mathcal{I}[\sigma, (\text{cond } [e_1, e_2] \ldots ] \ [\text{else } e_1]\rangle] &= (\text{cond } [(\text{let } z_i = \mathcal{I}[\sigma, e_i] \text{ in } (\text{log(user, } !!z_i, z_i; z_i))) \mathcal{I}[\sigma, e_1] \ldots \ [\text{else } \mathcal{I}[\sigma, e_1]\rangle]) \\
\mathcal{I}_e &: e^* \rightarrow e \quad \text{(interesting cases)} \\
\mathcal{I}_e[X] &= \langle X \rangle \\
\mathcal{I}_e[\lambda x. \ \text{conds}_x] &= \lambda x. \ \mathcal{I}_e[x, \ \text{conds}_x] \\
\mathcal{I}_e[(\text{let } x = f v^* \text{ in } \text{conds}_x)] &= (\text{let } x = f (\mathcal{I}_e[v^*]) \text{ in } \mathcal{I}_e[x, \ \text{conds}_x]) \\
\mathcal{I}_e &: x \ \text{conds}_x \rightarrow e \quad \text{(the interesting case)} \\
\mathcal{I}_e[x, (\text{cond } [\text{procedure?}(x) \ e_2]^{l_i}) = (\text{let } z = \text{procedure?}(x) \text{ in } (\text{log}(l_i, z, z); z)) \mathcal{I}_e[e_2] \ldots \ \text{[else } 0]^{l_i}]] &= (\text{cond } [(\text{let } z_1 = \mathcal{I}[\sigma, e_1] \text{ in } (\text{log}(l_i, !!z_1, z_1; z_1))) \mathcal{I}_e[e_1] \ldots \ [\text{else } (\text{log}(l_i, 0, 0); 0))])}
\end{align*}
\end{center}
\end{figure}
The cases for a concolic variable $X$ are the most involved. If the store $\sigma$ maps $X$ to a number then, the instrumentation simply embeds $X$ in a traced value similar to the case for numbers. However, if $\sigma$ maps $X$ to a canonical function, the instrumentation cannot turn $X$ to the corresponding traced value. After all, expression traces aim to capture formulas that the concolic tester records in path constraints so that it can use them to issue queries to the SMT solver. Thus they have to refer strictly to variables that hold first-order data. Consequently, $\mathcal{I}$ delegates to two further meta-functions $\mathcal{I}_e$ and $\mathcal{I}_c$ that produce an instrumented function that gets substituted for the concolic variable in the concolic program.

The $\mathcal{I}_e$ meta-function is similar to $\mathcal{I}^5$ except that it calls $\mathcal{I}_c$ for the instrumentation of a cond expression and passes along to it the value its tests may inspect. In turn, $\mathcal{I}_c$ adds at the beginning of the cond expression a log expression that records a test path constraint for the conditional expression and then similar to $\mathcal{I}$, it injects a log expression in each branch of the cond expression to record branch constraints.

We conclude this section with a discussion of the reduction rules for concolic evaluation. From figure 6, Rule $[R\text{-APP}]$ is the standard call-by-value $\beta$-reduction. The next two rules, $[R\text{-TRACE1}]$ and $[R\text{-TRACE2}]$, reduce primitive operators and produce appropriate expression traces. When the given operator is one of integer? or procedure?, $[R\text{-TRACE1}]$ inspects the tag of its argument and produces $\langle 1 \rangle$ if the tag is the right one and $\langle 0 \rangle$ otherwise. When the given operator is not a predicate, $[R\text{-TRACE2}]$ constructs an expression trace from the given operator and the traces of the operands. Rule $[R\text{-LOG}]$ appends a new path constraint to the list of path constraints $\pi$ of the machine and then proceeds with the $e$ expression. The new path constraint contains the label from the first argument of log, the number that corresponds to the traced value of the second argument and the traced value of the third argument. The next three rules, $[R\text{-ELSE}]$, $[R\text{-TRUE}]$ and $[R\text{-FALSE}]$ govern the evaluation of cond expressions. If the number that corresponds to the $\langle 0 \rangle$ test expression of the first branch of the cond expression is non-zero, $[R\text{-TRUE}]$ reduces the cond expression to the body of the first branch. Otherwise, $[R\text{-FALSE}]$ drops the first branch. When the given cond expression only contains the $\langle 1 \rangle$se branch, $[R\text{-ELSE}]$ proceeds with its body. Finally, rules $[R\text{-ERROR}]$ and $[R\text{-CTX}]$ introduce the compatible closure of the reduction relation (modulo errors).

### 5.2 Evolving New Inputs

Once it obtains a list of path constraints $\pi$ from the concolic evaluation of a user program (after instrumentation), the concolic tester uses meta-function evolve to modify the current input $\sigma$. Figure 8 through figure 10 present the formal definition of evolve$[\sigma, \pi]$ as a non-deterministic process that describes all the valid next inputs after an iteration of the concolic loop. The meta-function also returns a new list of path constraints $\pi'$ that, as we show in section 6, predicts the path constraints produced by the evaluation of the user program with input $\sigma'$. Figure 7 provides a summary of the auxiliary metafunctions that evolve employs. The update meta-function offers an interface to the SMT solver while the rest compute information about the contexts of the store $\sigma$. The supplementary material contains their complete definitions.

Figure 8 presents the first three rules of evolve. The first rule, $[M\text{-PREFIX}]$, allows the concolic tester to cut off any suffix from the list of path constraints and focus on the remaining prefix. The next

---

5In contrast to $\mathcal{I}$, $\mathcal{I}_e$ has a single case for concolic variables $X$. This is because by construction concolic variables in canonical functions point to first-order data. We return to that point further on when we discuss the evolution of inputs.
two rules, \([\text{M-False}]\) and \([\text{M-True}]\), handle the situation where the remaining list, \(\pi\), ends with a (first-order) path constraint logged from a conditional expression in the user program. These two rules negate the last path constraint and, with \(update\), consult the SMT solver for a solution that satisfies the negated list of path constraints \(\pi'\).

The next three rules, \([\text{M-NewProc1}]\), \([\text{M-NewProc2}]\) and \([\text{M-NewInt}]\) in figure 9 handle the insertion of new branches in the conditional expression of inputs. As we mention in section 4, when \(\pi\) ends with a list of path constraints of the form \([l_k, 2, v], (l_i, 1, t)\), there must be a corresponding canonical function in \(\sigma\) with a conditional expression with just an \(\text{else}\) branch with label \(l_i\). In
update : σ π → σ
Given a store σ and a list of path constraints π, encodes the path constraints as an SMT query, invokes the SMT solver and updates the store with the solution. The encoding of the list of path constraints into the query involves (i) asserting all first-order constraints in the list; (ii) asserting the expression traces from the branch constraints in the list if the branches’ tests succeed or their negation if they fail and (iii) asserting a constraint per conditional expression in the store that entails the branches of the conditional are disjoint.

bound : C° → x
bound⟦C°[(λx. [])]⟧ = x
bound⟦C°[(let x = f v° in [])]⟧ = x
Given a canonical context s that ends with a λ-abstraction or a let-binding, extracts the variable introduced by the innermost binder.

Δ ⊂ {x, y, z, . . . } stands for any finite subset of non-concolic variables.
enumerateb : σ Δ Δ p → a set of ⟨σ, e° ⟩
genome b  : σ Δ Δ p → a set of ⟨σ, e° ⟩
Given a store, two sets of variables, computes the set of new branch bodies, creating fresh concolic variables and mapping them to numbers in the resulting store as needed. The bodies of the new branches can refer to any variables in the first set while let expressions can apply any the of variables in the second set.

locals : C° → Δ
Given a canonical context d, computes the set of all variables in scope in the hole.

localsp : C° → Δ
Given a canonical context of variables in scope in the whole that are bound to functions.

Fig. 7. Metafunctions Used by evolve to Update Inputs and Compute Auxiliary Information

Fig. 8. Evolving New Inputs (i): Negating Branches in User Programs

this case either rule [M-NEWPROC1] or rule [M-NEWPROC2] inserts a new procedure? clause to this conditional expression, depending on whether the tests of this conditional expression inspect a value that is a function or a number. If the suffix of π indicates that the conditional expression has more than one branches and the tests of the conditional expression inspect a number, rule [M-NEWINT] inserts a new branch using the expression trace of the number. For the body of the new branch, the rules pick one of the options we discuss in section 4. using meta-function enumerateb.
if for some \(F \in \text{dom}(\sigma)\), \(\sigma(F) = C'[(\text{cond } \text{else } 0)]\)

and \(\pi = \pi_1 \leftrightarrow [\langle l_1, 2, (\lambda x. e)\rangle, \langle l_1, 1, \langle 1 \rangle \rangle] :\)

let \(y = \text{bound}(C')\)

pick any \(\langle \sigma_1, e' \rangle \in \text{enumerate}_b[\sigma, \text{locals}[C'], \{y\} \cup \text{locals}_p[C']]\)

let fresh \(l \notin \text{labels}(\sigma_1, e')\)

\(\pi' = \pi_1 \leftrightarrow [\langle l_1, 2, (\lambda x. e)\rangle, \langle l_1, 1, \langle 1 \rangle \rangle] \)

\begin{equation}
\text{do } \sigma_1' \leftarrow \sigma_1[F \mapsto C'[(\text{cond } [\text{procedure}?e' \text{else } y = t] \text{else } 0)]'] \right] \quad [\text{M-NEWPROC1}]
\end{equation}

\(\langle \sigma', \pi' \rangle \in \text{evolve}[\sigma, \pi]\)

if for some \(F \in \text{dom}(\sigma)\), \(\sigma(F) = C'[(\text{cond } \text{else } 0)]\)

and \(\pi = \pi_1 \leftrightarrow [\langle l_1, 2, (t)\rangle, \langle l_1, 1, \langle 1 \rangle \rangle] :\)

let \(y = \text{bound}(C')\)

pick any \(\langle \sigma_1, e' \rangle \in \text{enumerate}_b[\sigma, \text{locals}[C'], \{y\} \cup \text{locals}_p[C']]\)

let fresh \(l \notin \text{labels}(\sigma_1, e')\)

\(\pi' = \pi_1 \leftrightarrow [\langle l_1, 2, (t)\rangle, \langle l_1, 0, (0)\rangle, \langle l_1, 1, \langle 1 \rangle \rangle] \)

\begin{equation}
\text{do } \sigma_2' \leftarrow \sigma_1[F \mapsto C'[(\text{cond } [\text{procedure}?e' \text{else } (y = t)] \text{else } 0)]'] \right] \quad [\text{M-NEWPROC2}]
\end{equation}

\(\langle \sigma', \pi' \rangle \in \text{evolve}[\sigma, \pi]\)

if for some \(F \in \text{dom}(\sigma)\),

\(\sigma(F) = C'[(\text{cond } [\text{procedure}?e' \text{else } 0)]')' \}

and \(\pi = \pi_1 \leftrightarrow [\langle l_1, 2, (t)\rangle, \langle l_1, 0, (0)\rangle, \langle l_1, 0, (t = t)\rangle, ..., \langle l_1, 1, \langle t = t \rangle \rangle] :\)

pick any \(\langle \sigma_1, e' \rangle \in \text{enumerate}_b[\sigma, \text{locals}[C'], \text{locals}_p[C']]\)

let fresh \(l \notin \text{labels}(\sigma_1, e')\)

\(\pi' = \pi_1 \leftrightarrow [\langle l_1, 2, (t)\rangle, \langle l_1, 0, (0)\rangle, \langle l_1, 0, (t = t)\rangle, ..., \langle l_1, 1, \langle t = t \rangle \rangle] \)

\begin{equation}
\text{do } \sigma_2' \leftarrow \sigma_1[F \mapsto C'[(\text{cond } [\text{procedure}?e' \text{else } 0)]')' \}

[\text{else } 0)]' \right] \quad [\text{M-NEWINT}]
\end{equation}

\(\langle \sigma', \pi' \rangle \in \text{evolve}[\sigma, \pi]\)

\(\text{When the latter introduces a fresh concolic variable as the body of a branch, it always maps it}
\text{to a number in the corresponding store in its result. Thus, inductively, all concolic variables in}
\text{canonical functions hold first-order data as we note above in our discussion of instrumentation.}
\text{The last rule in figure 10, [M-CHANGE], shows how the concolic tester performs targeted branch}
\text{constraint modification. The goal of this rule is to cause the evaluation to follow a particular branch}
\text{of a conditional expression during a call of a canonical function. The rule does so by adjusting branch}
\text{constraints in the argument } \pi \text{ of } \text{evolve. Specifically, it truncates a group of branch constraints from}
\text{a conditional expression and attaches at the end a new branch constraint that would have been}
\text{present in the corresponding store.}
if for some $F \in \text{dom}(\sigma)$,
\[
\sigma(F) = C[\text{cond} \ [\text{procedure}?(y) \ e^1] \ [(y = t) \ e^2] \ ... \ [\text{else} 0]^{\text{h}}]
\]
and $\pi = \pi_i \vdash [\langle l_i, 2, \langle t \rangle \rangle, \langle l_i, 0, \langle 0 \rangle \rangle, \langle l_i, 0, \langle v \rangle \rangle, \ldots, \langle l_i, 1, \langle v \rangle \rangle] :$
pick any $j$ such that $[\langle t_j, 1 \rangle, \ldots, \langle t, 1 \rangle] \vdash$
let $\pi' = \pi_i \vdash [\langle l_i, 2, \langle t \rangle \rangle, \langle l_i, 0, \langle 0 \rangle \rangle, \langle l_i, 0, \langle t = t \rangle \rangle, \ldots, \langle l_i, 1, \langle t = t \rangle \rangle]$
do $\sigma' \leftarrow \text{update}[\sigma, \pi']$

\[
\langle \sigma', \pi' \rangle \in \text{evolve}[\sigma, \pi]
\]

\[\text{[M-CHANGE]}\]

Fig. 10. Evolving New Inputs (iii): Targeted Branch Constraint Modification

there if the evaluation had followed a particular branch of the conditional expression. In detail, the new branch constraint asserts that the traced value $(t)$ that the tests of the conditional expression inspect satisfies one of the tests $y = t$, from the branches of the conditional expression. Lastly, the rule consults the SMT solver for a new store that matches the new list of path constraints.

6 Correctness of Higher-Order Concolic Testing

This section establishes three facts about our concolic tester that together entail its correctness. First, if concolic evaluation of a program triggers a bug so does the evaluation of the program in the user language (soundness). Second, the concolic tester can produce inputs that triggers a bug in the user program, if such input exists (completeness). Third, for each iteration of the concolic loop, the concolic tester produces inputs to explore a specific and selected-in-advance control-flow path of the user program (concolic property). We discuss the formal statements of the three facts and we provide some interesting details about their proofs. The complete formal development with all the proofs is in the supplementary material.

Soundness guarantees that concolic evaluation respects the semantics of the user language. In particular, concolic evaluation does not discover spurious bugs. Thus, the information that the concolic machine collects such as path constraints and expression traces does not affect the behavior of programs. Formally, the Soundness theorem states that for any proper store $\sigma$\textsuperscript{6} if the concolic evaluation of user program $e$ with inputs $\sigma$ reduces to error, the evaluation of $e$ in the user language after retrieving its inputs from $\sigma$ also reduces to error. The metafunction $C[\sigma, X]$ retrieves the input of $e$ bound to $X$ in $\sigma$ by traversing $\sigma$ recursively and turning traced values into their user language counterparts.

\textbf{Theorem 6.1 (Soundness).} For any $e$ with concolic variables $X_1, \ldots, X_n$ and any store $\sigma$ closing $e$, if $\langle \sigma, [], I[\sigma, e] \rangle \rightarrow^* \langle \sigma, \pi, \text{error} \rangle$ then $e[X_i \mapsto C[\sigma, X_i], \ldots] \rightarrow^* \text{error}$.

Completeness captures that if a user program has a bug, our concolic tester finds it through the iterative evolution of initially default inputs. Formally, the Completeness theorem assumes that, for some inputs, the user program returns error and has five conclusions that describe that (1) the concolic loop starts with a store that contains inputs for all concolic variables in a user program; (2) these initial inputs are arbitrary numbers or the default functions (3) each iteration $i$ results in a pair $\langle \sigma_i, \pi_i \rangle$ of a store and a list of path constraints; (4) after the end of iteration $i$ that does not

\textsuperscript{6} A store $\sigma$ is proper if (i) all concolic variables occurring free in canonical functions in $\sigma$ are mapped to numbers by $\sigma$, (ii) all labels in $\sigma$ are unique and (iii) the expression traces in cond expression correspond to distinct numbers. In this section, we only consider proper stores.
trigger an error, evolve uses \( \langle \sigma, \pi \rangle \) to generate \( \langle \sigma_{i+1}, \pi_{i+1} \rangle \); and (5) the concolic loop terminates with the discovery of the error. An interesting point about the fourth conclusion is that it establishes that the list of path constraints \( \pi_{i+1} \) that evolve returns at the end of each iteration \( i \) is equivalent to the actual list that iteration \( i+1 \) of the loop produces. Here, two lists of path constraints are equivalent if they have the same first-order and branch constraints.

**Theorem 6.2 (Completeness).** For any \( e \) with concolic variables \( X_1, \ldots, X_n \), if there exists closed values \( y_1, \ldots, y_n \) in the language of user programs such that none of the values contain error and \( e[X_1 \mapsto y_1, \ldots] \rightarrow^* \) error then there exists a sequence of stores and paths \( \langle \sigma_1, \pi_1 \rangle, \ldots, \langle \sigma_m, \pi_m \rangle \) such that

1. \( \text{dom}(\sigma_i) = \{X_1, \ldots, X_n\} \).
2. For all \( 1 \leq k \leq n \), either \( \sigma_i(X_k) = 0 \) or \( \sigma_i(X_k) = \lambda x. (\text{cond } \text{else } 0)^i \).
3. For all \( 1 \leq i < m \), \( \langle \sigma_i, [], I[\sigma, e] \rangle \rightarrow^* \langle \sigma_i, \pi_i, e \rangle \).
4. For all \( 1 \leq i < m \), there exists a pair \( \langle \sigma_i, \pi_i \rangle \in \text{evolve}[\sigma_i, \pi_i] \) such that \( \pi_i \) is equivalent to a prefix of \( \pi_{i+1} \).
5. \( \langle \sigma_m, [], I[\sigma_m, e] \rangle \rightarrow^* \langle \sigma_m, \pi_m, \text{error} \rangle \).

We prove the Completeness theorem in two steps. First, we show that if there is an error in the user program that an input can trigger, there exists a store \( \sigma \) that contains numbers and canonical functions that also causes the error to manifest. Thus this step validates the definition of canonical functions.

**Lemma 6.3 (Representation Completeness).** Let \( \langle \sigma, \pi \rangle \) be a proper counterexample for a user program \( e \) if \( \text{FV}(e) \subseteq \text{dom}(\sigma) \), \( \langle \sigma, [], I[\sigma, e] \rangle \rightarrow^* \langle \sigma, \pi, \text{error} \rangle \) and \( \pi \) does not contain branch constraints from else branches. For any \( e \) with concolic variables \( X_1, \ldots, X_n \), if there exists closed values \( y_1, \ldots, y_n \) such that no value contains error and \( e[X_1 \mapsto y_1, \ldots] \rightarrow^* \) error then there exists a store \( \sigma \) and path constraints \( \pi \) such that \( \langle \sigma, \pi \rangle \) is a proper counterexample of \( e \).

**Proof Sketch.** To prove Lemma 6.3, we define an intermediate language that contains the union of the user language and the concolic language. The intermediate language also collects details about the interaction between user programs and concolic functions in a global map. Given \( e \) and \( \{v_i\} \), we simulate the reduction sequence of \( e \) with the intermediate language and construct a store \( \sigma \) using the collected information from the global map.

As the second step of the proof of Completeness, we show that the evolution of inputs of the concolic loop produces an input that can trigger the same error as the one an arbitrary \( \sigma \) triggers. As a consequence, the concolic tester only needs to explore inputs it obtains from evolve.

**Lemma 6.4 (Search Completeness).** For any \( e \) with concolic variables \( X_1, \ldots, X_n \), if \( e \) has a proper counterexample then there exists a sequence of stores and paths satisfying Theorem 6.2 (1)-(5).

**Proof Sketch.** Let \( \langle \sigma, \pi \rangle \) denote a proper counterexample of \( e \). First, we show a property of the concolic loop. For any store \( \sigma \), the concolic evaluation of \( e \) with inputs \( \sigma \) either follows the same control-flow path as the evaluation of \( e \) with inputs \( \sigma \) or takes a different branch at some point. By applying evolve to \( \sigma \), and the list of path constraints, we can obtain \( \sigma \), such that the evaluation of \( e \) with inputs \( \sigma \) follows a control-flow path that has one more branch in common with the evaluation
of $e$ with inputs $a$. With this property in hand, we start with a store containing default canonical functions (the ones with the simplest shape) and we use the property to construct a sequence of stores that gradually approximate $a$ until one of them triggers the error in $e$.

The last fact we establish for our concolic tester is necessary for the proof of Lemma 6.4 but also has value on its own. It entails that, at each iteration of its loop, the concolic tester aims to explore a specific control-flow path of the user program and indeed produces new inputs that achieve this goal. We call this property the concolic property. Formally, Theorem 6.5 shows that evaluating the user program with the store constructed by $\text{evolve}$ follows the control-flow path that $\text{evolve}$ predicts with the list of path constraints it returns along the store.

**Theorem 6.5 (Concolic).** Let the non-terminal $ps$ denote the subset of $\pi$ that corresponds to a first-order constraint or a test constraint together with a block of branch constraints. For any $e$ and $\sigma_i$, if

1. $(\sigma_i, [], I[\sigma_i, e]) \rightarrow^* (\sigma_i, \pi_i + ps_i, e)$
2. $\pi_i$ has no branch constraints corresponding to $\text{else}$ in the canonical functions in $\sigma_i$.
3. $(\sigma_2, \pi_i + ps) \in evolve[\sigma_1, \pi_i + ps_i]$.

then $(\sigma_2, [], I[\sigma_2, e]) \rightarrow^* (\sigma_2, \pi_i + ps_2, e)$ such that $\pi_i + ps$ is equivalent to $\pi_i + ps_2$.

**Proof Sketch.** We show by simulation that there exists $e'_i$, $e'_j$, and $\pi_j$ such that

- $\pi_j$ is equivalent to $\pi_i$,
- $(\sigma_j, [], I[\sigma_j, e]) \rightarrow^* (\sigma_j, \pi_j, e'_j) \rightarrow^* (\sigma_j, \pi_j + ps_i, e)$ and
- $(\sigma_2, [], I[\sigma_2, e]) \rightarrow^* (\sigma_2, \pi_j, e'_j)$

Since $\sigma_j$ makes the test of the branch from $ps$ succeed and $e'_i$ and $e'_j$ are built using simulation, we establish that $(\sigma_2, \pi_j, e'_j) \rightarrow^* (\sigma_2, \pi_j + ps_2, e)$ where $ps_2$ is equivalent to $ps$.

7 PROTOTYPE IMPLEMENTATION

To evaluate whether our higher-order concolic tester can find bugs in practice, we built a prototype implementation and used it with higher-order programs of our own devising and programs from the literature. In section 7.1 we describe the prototype implementation and in section 7.2 we report on the programs we tried and how well the implementation can find the bugs they contain.

7.1 Implementation Architecture

At the heart of our prototype is a language built on top of Rosette (Torlak and Bodik 2013, 2014), a framework for constructing domain-specific languages that employ SAT solvers. We start with most of the features from Rosette itself, but use Racket’s domain-specific language support (Felleisen et al. 2018; St-Amour et al. 2017) to adjust Rosette to concolic evaluation. More specifically, we replace Rosette’s conditional expressions (that employ symbolic execution) with ones that compute specific values at conditional tests and in order to avoid exploring both branches of any given conditional. These replacement conditional expressions also record path constraints. We use this language for the concolic evaluation of the programs we aim to test.

To properly test these programs we also need to be able to construct higher-order inputs (as described in section 3 and section 4). To do so, we have designed a data structure that closely follows the grammar for canonical forms. We interpret that data structure, producing higher-order functions that we supply as inputs to the user program, and we compute new instances of the data structure based on the results of calling the SMT solver, leveraging Rosette. Thus, in essence the result forms in the prototype have their own small language. This language is slightly
more general than the description of canonical forms in section 5. Specifically, in addition to unary functions and integers, it also supports lists and booleans.

The programs we set to test, however, use some fairly sophisticated features of Racket that the concolic language in our prototype does not support. To bridge the gap, we added a number of libraries. First, we implemented a rudimentary contract system and a rudimentary complex number library in our concolic adaptation of Rosette. We also implemented a library that provides conversion wrappers to adjust values flowing in and out of the user program. It supports several forms of conversions: it can adjust curried functions to appear as n-ary functions; it can adjust a list of functions to appear as an object, and it also supports a “lump” conversion where integers are translated back and forth to a specific set of interesting constants (typically symbols and strings). This encoding of inputs also enables us to keep the language of the prototype’s canonical forms small (thereby making the evolution of new inputs simpler) while still being able to find bugs in programs that use some of Racket’s more sophisticated features.

As the formal model does not specify an explicit search strategy, the prototype comes with a very naive search strategy. Specifically, we simply follow a breadth-first approach. After each iteration of the concolic loop, we add all possible next evolutions of the input (following \texttt{evolve[σ, π]}, from figure 8, figure 9, and figure 10) in a queue to continue the search.

All together, our prototype is a bit more than 7,000 lines of code (with a bit less than 7,000 lines of code in the prototype’s test suites).

### 7.2 Benchmark Programs

Our benchmark programs come from three sources. The first, and primary source, is Nguyêń et al. (2017)’s work, specifically from the jfp branch of https://github.com/philnguyen/soft-contract. These programs ultimately come from other papers, as cited in figure 11. The second source is CutEr (Giantsios et al. 2017), the tool for concolic testing functional programs in Erlang. We collected all of the test cases in CutEr’s test suite that seem to use higher-order functions and translated them to use our prototype. The last source are small examples that we invented as part of this work; they are in the supplementary material.

Out of 122 benchmarks, our prototype fails to discover bugs in 9 of the programs. These programs can be collected into groups that correspond to specific limitations of our prototype and that explain why our tool fails to test them successfully. First, our search strategy is naive, so one benchmarks
time out after an hour. Second, our prototype does not handle Racket’s `struct` declaration so for five benchmarks the prototype fails to find a bug. Third, our prototype does not generate pairs of inputs when the contract is `any/c` which results in one more failure. Finally, two benchmarks use fairly complex syntactic features of Racket that our prototype cannot accommodate.

8 RELATED WORK

Concolic Testing. CutEr (Giantsios et al. 2015, 2017) is a concolic testing tool for Erlang (Armstrong et al. 2007). It supports the generation of functions, but it is not complete in our sense. More specifically it does not generate inputs that contain calls in their bodies. Palacios and Vidal (2015) proposes an instrumentation approach for concolic testers of functional languages but do not address the generation of higher-order inputs.

Li et al. (2017) extends the design of path constraints with symbolic subtype expressions in order to handle control-flow structure involving polymorphism in object-oriented languages. However, this design only generates inputs using existing classes and does not synthesize new class definitions.

Path explosion remains a central challenge for concolic testing techniques (Baldoni et al. 2018; Cadar and Sen 2013), and it is a challenge that partially motivates our work. Godefroid (2007) approaches the problem by computing function summaries on-the-fly to tame the combinatorial explosion of the search space of control-flow paths. Similarly, Anand et al. (2008) performs symbolic execution compositionally using function summaries. In both cases, due to the first-order nature of the programming languages they are working with, the summaries are first-order and do not include possible higher-order interactions between functions.

FOCAL (Kim et al. 2019) addresses the path explosion problem by breaking programs down into small units to reduce the search space. FOCAL tests units individually and tries to construct a system-level test by refining path constraints using function summaries.

Symbolic Execution. Nguyên et al. (2017) and Tobin-Hochstadt and Horn (2012) introduce higher-order symbolic execution and propose the idea of canonical forms for generating counterexamples. Their work on symbolic execution inspired our approach to higher-order concolic testing. Comparing to their work, our concolic tester incorporates the notion of path constraints to support incremental and systematic search over the control-flow graph of higher-order programs.

Random Testing. QuickCheck (Claessen and Hughes 2000) supports random testing of higher-order functions by using user-provided maps from the input type to integers and from integers to the output type. Koopman and Plasmeijer (2006) improves upon QuickCheck by using a predefined datatype representing the syntax of higher-order functions to generate inputs with richer behavior. LambdaTester (Selakovic et al. 2018) focuses on testing and generating higher-order functions that mutate an object state in order to affect control-flow paths that depend on the object’s state.

Klein et al. (2010) uses the idea of calling higher-order inputs in order to discover bugs in them, combining the output of a function with the input of another. Their techniques target a stateful setting and are designed to work with opaque types.

Program Synthesis. The study of program synthesis for functional languages also faces the challenge of generating higher-order programs. Myth (Osera and Zdancewic 2015) synthesizes higher-order functions that generalize a given set of input-output examples over inductive datatypes. Concolic testing for higher-order functions can be viewed as synthesizing higher-order inputs from an evolving set of examples dynamically collected from the user programs, while having the goal of exposing all control-flow paths.

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7 Personal communication with Kostis Sagonas.
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