

Learning to Explore Paths for Symbolic Execution

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ABSTRACT

Symbolic execution is a powerful technique that can generate tests steering program execution into desired paths. However, the scalability of symbolic execution is often limited by path explosion, i.e., the number of symbolic states representing the paths under exploration quickly explodes as execution goes on. Therefore, the effectiveness of symbolic execution engines hinges on the ability to select and explore the right symbolic states.

In this work, we propose a novel learning-based strategy, called LEARCH, able to effectively select promising states for symbolic execution to tackle the path explosion problem. LEARCH directly estimates the contribution of each state towards the goal of maximizing coverage within a time budget, as opposed to relying on manually crafted heuristics based on simple statistics as a crude proxy for the objective. Moreover, LEARCH leverages existing heuristics in training data generation and feature extraction, and can thus benefit from any new expert-designed heuristics.

We instantiated LEARCH in KLEE, a widely adopted symbolic execution engine. We evaluated LEARCH on a diverse set of programs, showing that LEARCH is practically effective: it covers more code and detects more security violations than existing manual heuristics, as well as combinations of those heuristics. We also show that using tests generated by LEARCH as initial fuzzing seeds enables the popular fuzzer AFL to find more paths and security violations.

CCS CONCEPTS

• **Software and its engineering** → **Software testing and debugging**; • **Security and privacy** → **Software security engineering**.

KEYWORDS

Symbolic execution; Fuzzing; Program testing; Machine learning

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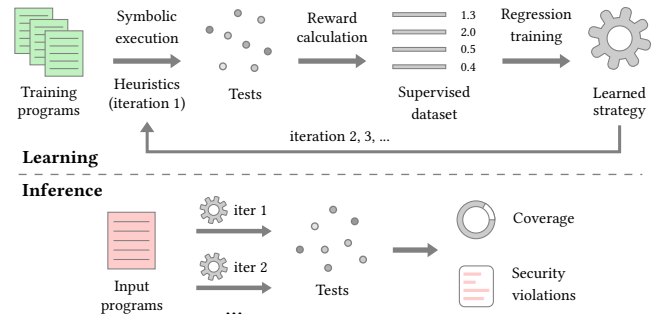


Figure 1: Our recipe for learning a state selection strategy.

1 INTRODUCTION

Symbolic execution [18, 44] is a promising program analysis technique widely used in many security-related tasks, such as analyzing protocol implementations [23, 24, 53], validating hardware design [76], securing smart contracts [49, 55], and detecting cache timing leaks [36]. Most prominently, symbolic execution has been extensively used for automatic test generation to exercise program paths and identify security violations [8, 16, 17, 22, 68], and is by now an established industrial practice for software testing at Microsoft [34], IBM [6], NASA [52], and other organizations.

At a high level, symbolic execution works by representing program inputs as symbolic variables, exploring program paths symbolically, and collecting path constraints that capture conditions over the input variables that must hold to steer the program along a given path. These constraints can be fed into an external constraint solver to construct a concrete test case. The common goal for symbolic execution tools is to generate a test suite that achieves high code coverage over the program's statements within an allocated time budget [16, 52, 74].

Key challenge: path explosion. While powerful, symbolic execution is expensive and difficult to scale to large, real-world programs due to the so-called *path explosion* problem [18]. That is, at each program branch, the (symbolic) state for a given path is forked into two separate states. As a consequence, the number of states is exponential in the number of branches and quickly explodes as the execution reaches deep branches. To cope with this challenge, symbolic execution tools need an effective mechanism to select and execute promising states that achieve the highest coverage and cost the least execution time, while avoiding expensive states that do not improve coverage.

Unfortunately, constructing an ideal state selection is not possible because at the time of picking a state to explore we do not know whether it will indeed improve coverage at a reasonable cost. Ultimately, this decision depends on how the selected state would

unfold as we continue executing it as well as on state selection decisions we make in the future. Due to this fundamental limitation, symbolic execution tools rely on manually designed heuristics, used as a proxy for the ideal selection, that select states based on properties such as instruction count [16], subpath count [48], constraint search depth [52], and hand-crafted fitness [74]. As a result, even though designed by experts, those heuristics can easily get stuck in program parts favoring the measured property and fail to reach other relevant parts that, if covered, would improve code coverage and may identify critical security violations.

LEARCH: a learning-based state selection strategy. In this work, we propose a new *data-driven* approach, called LEARCH (short for Learning-based SEARCH), for learning a state selection strategy that enables symbolic execution tools to efficiently explore the input program. The key idea is to leverage a machine learning regression model that, for each state, estimates a *reward* that directly captures the core objective of the tool – improving more coverage while spending less time producing concrete tests. Based on this model, LEARCH selects the state with the highest estimated reward, as opposed to relying on manual heuristics used as a proxy to maximize the tool’s objective. Importantly, the construction of LEARCH utilizes the knowledge of existing heuristics and can benefit from any advances in the invention of new heuristics.

LEARCH is constructed using an *iterative learning procedure*, as illustrated at the top of Figure 1. At each iteration, we first run symbolic execution on a set of training programs. Notably, instead of exploring states uniformly at random, we leverage different state selection strategies (e.g., manual heuristics at iteration 1) to generate a *diverse* set of tests. Then, for each explored state in the generated tests, we extract a set of high-level features (including the properties used by the heuristics) and calculate a reward based on the overall coverage improvement and time spent exploring the state. This results in a supervised dataset that captures the behaviors of the strategies used in the previous step. Finally, we construct a learned strategy by training a regression model to achieve a small loss on the supervised dataset so that the model can make accurate estimations for the reward. The strategy learned at the current iteration is used to add new supervised data in the next iterations to create additional learned strategies. At inference time (bottom of Figure 1), given an unseen program, we run multiple symbolic execution instances with the learned strategies to generate effective tests used to exercise the program and report security violations.

Instantiation and evaluation. We instantiated LEARCH¹ on the most popular symbolic execution engine KLEE [16]. We evaluated LEARCH on a diverse set of programs, including 52 `coreutils` programs and 10 real-world programs. Our results demonstrate that LEARCH is practically effective: it consistently produced more code coverage (e.g., >20%) and detected more security violations (e.g., >10%) than existing manual heuristics [16, 48], as well as the combinations of individual heuristics. Moreover, we used tests generated by KLEE as initial seeds to run a popular fuzzer, AFL [1, 29]. The initial seeds from LEARCH helped AFL to trigger more paths and security violations than the manual heuristics.

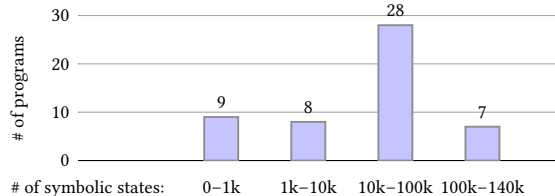


Figure 2: Number of `coreutils` programs grouped by the average number of candidate states available at selection steps.

Main contributions. Our main contributions are:

- LEARCH, a new learning-based state selection strategy for symbolic execution. (Section 3)
- A novel learning framework for constructing multiple learned strategies. (Section 4)
- A complete instantiation of LEARCH on the popular symbolic test generator KLEE. (Section 5)
- An extensive evaluation on a diverse set of programs and various tasks, demonstrating that LEARCH is practically effective and outperforms existing manually designed heuristics. (Section 6)

2 MOTIVATION FOR LEARNING

In this section, we motivate the use of learning for selecting symbolic states by analyzing the results of running KLEE [16] on the 52 `coreutils` programs used as one of the test set in our evaluation. The time limit of KLEE was 1h, and the memory budget was 4GB.

Large number of candidate states. When symbolically executing an input program, KLEE usually forks a large number of states due to branching behaviors such as if-else statements, resolving function pointers, and resolving memory allocation sizes. To measure the number of states produced by KLEE, we ran the tool using the random path search heuristic (`rps`) on the 52 `coreutils` programs and calculated the average number of candidate states at the selection steps, and show the results in Figure 2. For most programs, the number of states produced by KLEE is huge: 28 programs have on average 10k-100k candidate states for selection. For programs larger than `coreutils`, the number of candidate states could be even larger. The enormous search space motivates the need for constructing an effective, fine-grained strategy able to pick promising states instead of relying on simple and crude heuristics.

Limitations of existing manually designed heuristics. Existing heuristics are random or manually designed by experts and typically depend on certain property of the states [16, 48]. They often get stuck in program parts favoring the property but fail to explore other parts. We ran KLEE with a set of existing heuristics and present the average line coverage of the top three heuristics (`rps`, `nurs:depth`, and `sgs`) in the Venn diagram in Figure 3(a). All three heuristics achieved ~540 line coverage. However, no single heuristic significantly outperformed the others. Importantly, the heuristics have non-comparable performance and covered different parts of the program: 499 lines were covered by all heuristics, but the rest 86 lines were covered by different heuristics. Similarly, the capability of detecting security violations (UBSan violations [4] in our work) differs across the heuristics, as shown in Figure 3(b).

¹LEARCH is publicly available at <https://github.com/eth-sri/learch>.

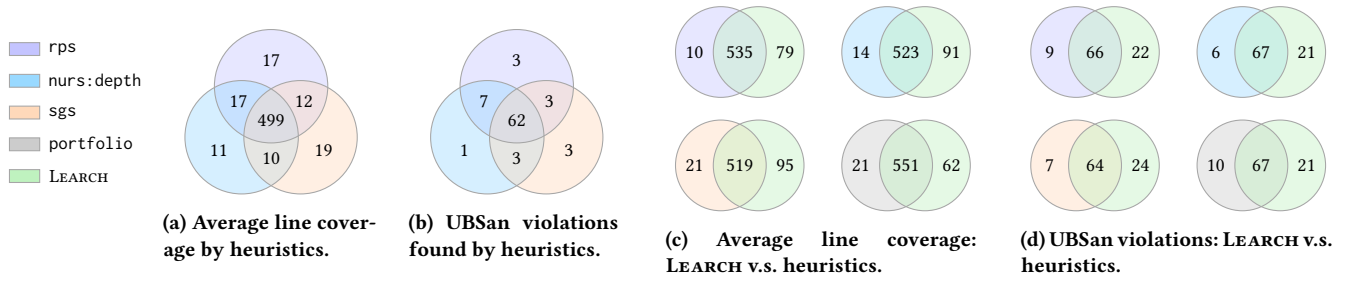


Figure 3: Limitations of existing manually designed heuristics and how LEARCH outperforms them for our coreutils test set.

Opportunities for learning. Based on the results in Figure 3(a) and Figure 3(b), we can compute the *union* of covered lines and detected UBSan violations for the three heuristics. The union achieved 585 line coverage and detected 82 UBSan violations, significantly higher than any individual heuristic. This indicates a promise of constructing an adaptive strategy that subsumes individual heuristics. In fact, the heuristics provide a precious knowledge base that facilitates learning such an adaptive strategy. Namely, the heuristics can be used to generate a diverse training dataset, capturing different selection behaviors, and the properties they rely on can be used as valuable features for a machine learning model. Another key advantage of learning is that while the reward calculation is impossible at inference time, it can be computed for the states explored at training time, from which we can obtain a direct estimator for the final coverage-guided objective. The above insights facilitate and motivate our learning scheme proposed in Figure 1.

To show evidence on the benefits of learning, we constructed another heuristic called `portfolio` by running the three heuristics, each for a third of the total time limit, and combined all produced test cases. We compare LEARCH with the four heuristics in Figure 3(c) and Figure 3(d). In terms of total coverage, LEARCH outperformed all four heuristics. LEARCH was able to cover most code covered by the heuristics, and exclusively covered more code than the heuristics. The same holds for the detection of UBSan violations.

Scope and applicability. Our work focuses on *purely symbolic execution* (i.e., no concrete execution happens during the test generation process), even though our idea may give hints for improving other approaches where it is tricky to select program branches for test generation, such as concolic testing [33, 57, 58, 62] and hybrid testing [27, 69, 75]. We aim to solve the *state selection* problem, while there are many orthogonal approaches for easing path explosion such as state merging [46] and state pruning [13, 14, 21, 70].

3 SYMBOLIC EXECUTION FRAMEWORK

In this section, we first present a general symbolic execution framework parameterized by a state selection strategy and then introduce the LEARCH state selection strategy.

3.1 Symbolic Execution

In Algorithm 1, we show a symbolic execution algorithm called `symExec`, a general version of the one in [48]. `symExec` takes a program `prog` (compiled to low-level instructions such as LLVM IR) and a state selection strategy (`strategy`) as input, and generates a set of

test cases (`tests`). `symExec` symbolically explores the branches of `prog` (different from [16] which explores one instruction each time) and stores the progress in a list of symbolic states (`states`). `strategy` is used to select a state from `states` for execution at each step. When the execution of one program path is finished, a test is generated and added to `tests`. Next, we describe `symExec` step by step.

At Line 2, we initialize `tests` and `states` to be empty. Then, we append `prog`'s initial state which represents the `prog`'s entry block to `states` (Line 3) and calls `update` to update `strategy` (Line 4). `update` is an auxiliary function that is called whenever a new state is added or a pending state is updated. We will discuss `update` later in this section. Next, at Line 5, the main loop for symbolic exploration starts. The loop terminates when `states` becomes empty, i.e., no available state can be explored, or the time limit has been reached. Inside the main loop, we first call `selectState`, another auxiliary function described later, for selecting a state (`state`) from `states` where each state represents a branch under exploration. We continuously execute the instructions of `state` symbolically (Line 8) and meanwhile check if the current execution violates any of the predefined security properties. The execution stops when we encounter an EXIT instruction, a security violation, or a FORK instruction (Line 7). When reaching an EXIT instruction that indicates the end of a program path or detecting a security violation, we call an external constraint solver to construct a new concrete test (Line 10) and remove `state` from `states` so that we stop further execution on `state` (Line 11). FORK instructions indicate a branching point, for which we need to copy `state` to create a forked state `forked` (Line 13). `state` and `forked` then represent the two new branches, respectively. We append `forked` to `states`, and update both `state` and `forked` (Line 14 to Line 16). After the main loop finally finishes, `tests` is returned.

Objective of `symExec`. Given an input program, the objective of running `symExec` with `strategy` is to find a set of concrete tests achieving the maximal coverage within a fixed amount of time:

$$\arg \max_{tests = \text{symExec}(prog, strategy)} \frac{|\bigcup_{t \in tests} \text{coverage}(t)|}{\text{symExecTime}} \quad (1)$$

where `coverage(t)` measures the coverage of test `t` (we use line coverage in this work) and `symExecTime` is the time spent on running `symExec`. Achieving Equation 1 is challenging as the number of pending states is exponential to the number of forks and it is hard to predict what tests and the coverage of the tests a selected state will result in. The key is to construct a state selection strategy that can select the most promising states leading to high-quality tests.

Algorithm 1: Branch-based symbolic execution

```
1 Procedure symExec(prog, strategy)
   Input : prog, an input program.
           strategy, a state selection strategy.
   Output: tests, a set of generated test cases.
2 tests ← emptySet(); states ← emptyList()
3 states.append(prog.initialState)
4 update(prog.initialState, strategy)
5 while states.size > 0 and !TIMEOUT do
6   state ← selectState(states, strategy)
7   while state.inst ≠ EXIT and !state.foundViolation and
   state.inst ≠ FORK do
8     executeInstruction(state)
9   if state.inst = EXIT or state.foundViolation then
10    tests.add(generateTest(state))
11    states.remove(state)
12  else // state.inst = FORK
13    forked ← doFork(state)
14    states.append(forked)
15    update(state, strategy)
16    update(forked, strategy)
17 return tests
```

3.2 State Selection Strategy

Next, we formally define a state selection strategy.

Definition 1 (State selection strategy). A *state selection strategy* is a mapping from symbolic states to real value scores that measure the importance of the states for exploration. To apply a state selection strategy in symExec, we need two auxiliary functions described at a high level below:

- **selectState**: The inputs of **selectState** are a list of pending symbolic states *states* and a state selection strategy *strategy*. Each time invoked (Line 6 of Algorithm 1), **selectState** leverages the importance scores returned by *strategy* to select a state from *states* for the next exploration step. **selectState** can be deterministic or probabilistic, e.g., normalizing the scores into a probability distribution and drawing a sample from the distribution.
- **update**: When a new pending state is added (Lines 4 and 16 of Algorithm 1) or a currently pending state enters a new branch (Line 15 of Algorithm 1), **update** is called to update the internal mechanics of *strategy* for computing the importance scores and also the scores themselves.

The detailed implementation of **selectState** and **update** depends on each specific strategy. Next, we provide the depth-first search (DFS) strategy in KLEE [16] as an example.

Example 1. The DFS strategy always selects the state representing the deepest path before exploring other paths.

- **strategy**: maps each pending state to its depth, i.e., the number of forks executed for the path that the state explores.
- **selectState**: selects the state with the largest depth.
- **update**: updates the depth of the input state.

Algorithm 2: LEARCH’s update function

```
1 Procedure update(state, strategy)
   Input: state, the state to update.
           strategy, the LEARCH strategy.
2 state.feature ← extractFeature(state)
3 reward ← strategy.predict(state.feature)
4 strategy.setReward(state, reward)
```

Ideal objective of a state selection strategy. In symExec, a selected state can produce different new states and finally different tests, depending on the program logic and subsequent selection decisions. Ideally, at **selectState**, we would want to consider the overall effect of each pending state (i.e., the states and tests produced from the state) and select states leading to tests that not only achieve higher coverage but also cost less time to obtain, such that symExec’s objective in Equation 1 is achieved. This criterion can be summarized in the **reward** function defined as:

$$\text{reward}(\textit{state}) = \frac{|\bigcup_{t \in \textit{testsFrom}(\textit{state})} \text{coverage}(t)|}{\sum_{d \in \textit{statesFrom}(\textit{state})} \text{stateTime}(d)} \quad (2)$$

where **testsFrom**(*state*) and **statesFrom**(*state*) return the set of tests and the set of symbolic states originating from *state*, respectively. **stateTime**(*d*) returns the time spent on state *d*, including execution time, constraint solving time, etc. Intuitively, **reward** measures *state* by the total amount of coverage achieved by the tests involving *state* divided by the total amount of time symExec spends on *state* and the states produced from *state*. Then, an ideal strategy would always select the state with the highest reward.

However, it is hard to exactly compute **reward** at each **selectState** step, because the states and the tests produced from *state* depend on future selections that are unknown at the current step. That is, we usually cannot calculate **testsFrom**(*state*) and **statesFrom**(*state*) ahead of time before symExec finishes. Due to this limitation, existing heuristics [16, 48] typically compute importance scores for states based on a certain manually designed property, as a proxy for **reward**. As a result, they often get stuck at certain program parts and cannot achieve high coverage.

3.3 A Learned State Selection Strategy: LEARCH

Now we introduce the LEARCH strategy. The core component of LEARCH is a machine learning regression model $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}$ learned to estimate the reward in Equation 2 for each pending state. To achieve this, LEARCH extracts a vector of *n* features for the input state with a function called **extractFeature** and invokes φ on the *n*-dimensional features. The choices of the features and φ are discussed in Section 5.1.

The **selectState** function of LEARCH greedily selects the state with the highest estimated reward, i.e.:

$$\textit{state} = \arg \max_{s \in \textit{states}} \textit{strategy}.\text{getReward}(s).$$

We also considered probabilistic sampling but found that the greedy one performed better. LEARCH’s **update** function is presented in Algorithm 2. At Line 2, we call **extractFeature** to extract the features for the input state. At Line 3, we leverage φ to predict a reward for the state. Then at Line 4, the learned strategy updates the reward

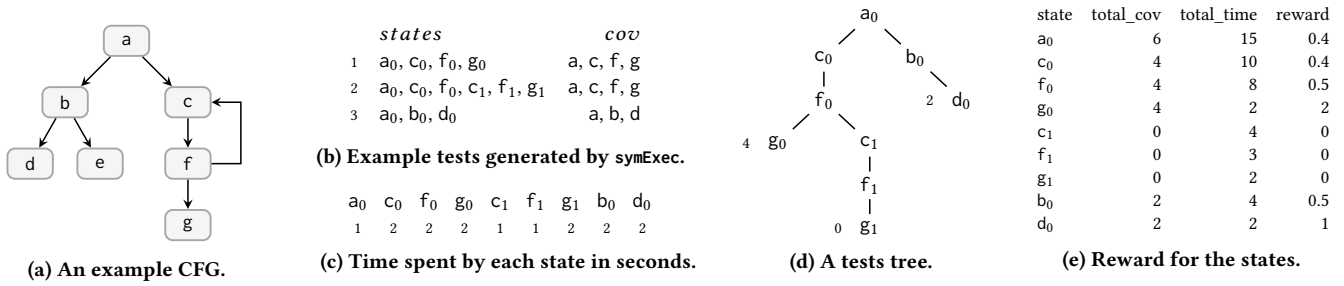


Figure 4: An example on assigning a reward to explored states of the tests generated by symExec.

of the state. Note that the expensive feature extraction and reward prediction are done once per update. In `selectState`, we only read the predicted rewards, avoiding unnecessary re-computations.

Benefits of a learned strategy. Different from existing heuristics [16, 48], the LEARCH strategy makes decisions based on multiple high-level features (including the ones from the heuristics) and directly estimates Equation 2 to optimize for Equation 1. Therefore, LEARCH can effectively explore the input program and rarely gets stuck. As a result, LEARCH achieves higher coverage and detects more security violations than manually designed heuristics.

4 LEARNING STATE SELECTION STRATEGIES

While a learned strategy can be effective, it is non-obvious how to learn the desired strategy. This is because a supervised dataset consisting of explored states and their ground-truth reward for training the machine learning model φ is not explicitly available. Next, we introduce techniques for extracting such a supervised dataset from the tests generated by symExec, from which φ can be obtained with off-the-shelf learning algorithms.

4.1 Assigning a Reward to Explored States

Given a set of training programs, we run symExec to obtain a set of tests where each test consists of a list of explored states and covers certain code. From the tests, we construct a novel representation of the tests, called *tests trees*, whose nodes are the explored states, and leverage the trees to calculate a reward for the explored states. Note that the calculation of Equation 2 is feasible during training because symExec has already finished for the training programs. Finally, a supervised dataset is built for training φ . Next, we describe how to achieve this step by step.

First, we formally define tests in our context.

Definition 2 (Test). A *test* generated by symExec for an input program is a tuple $(states, input, cov)$. *states* is a list of symbolic states $[state_0, state_1, \dots, state_n]$ selected by `selectState` at Line 6 of Algorithm 1. Each state represents an explored branch and the branch represented by $state_i$ is followed by the branch represented by $state_{i+1}$ in the control flow graph of the program. Therefore, *states* indicates the program path induced by *test*. *input* is a concrete input for the input program and is constructed by solving the path constraints of $state_n$ with a constraint solver. The concrete execution of *input* follows the path indicated by *states* and achieves coverage *cov*.

Example 2. In Figure 4(a), we show the control flow graph (CFG) of an example program. The CFG consists of seven basic blocks and seven edges, and the edges between nodes *f* and *c* represent a loop. We symbolically execute the example program and generate three tests shown in Figure 4(b). Test 1 and 2 execute the loop once and twice, respectively, both covering block *a*, *c*, *f*, and *g* (i.e., the results of the coverage function in Equations 1 and 2). Test 3 does not execute the loop but explores states a_0 , b_0 , and d_0 , covering blocks *a*, *b*, and *d*. Note that for the examples, we show basic block coverage for simplicity. In our implementation, we used line coverage. We record the time spent by symExec on each state (i.e., the results of the `stateTime` function in Equation 2) in Figure 4(c).

After generating tests for a training program, we construct a tests tree defined in the following.

Definition 3 (Tests tree). Given a series of tests $[test^0, test^1, \dots, test^m]$ for a program, we construct a *tests tree* whose nodes are the explored states of the tests (i.e., those in the *states* field). For each $test^i$, we go over all pairs of states $state_j^i$ and $state_{j+1}^i$ and set $state_j^i$ as the parent of $state_{j+1}^i$ in the tree.

Example 3. In Figure 4(d), we show a tests tree constructed from the tests in Figure 4(b). Each tree path from the root to a leaf corresponds to the explored states of a test. For example, the left-most path $a_0-c_0-f_0-g_0$ consists of the states of test 1. At the left-hand side of each leaf node, we annotate the number of new blocks covered by the corresponding test. For instance, test 1 covers four new blocks: *a*, *c*, *f*, and *g*. Then, test 2 does not yield new coverage because the four blocks covered by test 2 were already covered by test 1 before. Test 3 covers two new blocks: *b* and *d*.

The tests tree representation recovers the hierarchy of the explored states and provides a structure for conveniently calculating `testsFrom(state)` and `statesFrom(state)` by considering the descendants and the paths of each explored *state*, respectively. As a result, the reward can be efficiently computed.

Calculate a reward for explored states. To calculate a reward (Equation 2) for each *state*, we need to calculate the numerator, i.e., the total coverage achieved by all tests involving *state*, and the denominator, i.e., the total amount of time spent by *state* and its descendants. We compute those information with the tests trees in a bottom-up recursive fashion.

To compute the numerator `totalCov` for each *state*, we compute the coverage achieved by the tests involving *state*. This is equal

Algorithm 3: Generating a supervised dataset

```
1 Procedure genData(progs, strategies)
  Input :progs, a set of training programs.
          strategies, a set of state selection strategies.
  Output: dataset, a supervised dataset.
2 dataset  $\leftarrow$  emptySet()
3 for strategy in strategies do
4   for prog in progs do
5     tests  $\leftarrow$  symExec(prog, strategy)
6     newData  $\leftarrow$  dataFromTests(tests)
7     dataset  $\leftarrow$  dataset  $\cup$  newData
8 return dataset
```

to summing up the new coverage (newCov) of all the leaves that are descendants of $state$ in the tests trees and can be done in a recursive way as follows:

$$\text{totalCov}(state) = \begin{cases} \text{newCov}(state) & \text{if } state \text{ is a leaf,} \\ \sum_{c \in \text{children}(s)} \text{totalCov}(c) & \text{otherwise.} \end{cases}$$

To compute the denominator totalTime , we sum up the time spent on the considered state and its descendants via the following recursive equation:

$$\text{totalTime}(state) = \text{stateTime}(state) + \sum_{c \in \text{children}(s)} \text{totalTime}(c)$$

Then the reward can be computed by $\text{reward}(state) = \frac{\text{totalCov}(state)}{\text{totalTime}(state)}$.

Example 4. For each $state$ in Figure 4(d), we compute totalTime , totalCov , and reward in Figure 4(e).

4.2 Strategy Learning Algorithms

We now present the final algorithms for learning LEARCH.

Generate a supervised dataset. In Algorithm 3, we present a procedure named genData for generating a supervised dataset. The inputs of genData are a set of training programs $progs$ and a set of state selection strategies. First, at Line 2, we initialize the supervised dataset ($dataset$) to an empty set. Then, for each strategy in $strategies$ and each program in $progs$ (the loops from Line 3 to Line 7), we run symExec to generate a set of tests $tests$ (Line 5). Next, at Line 6, a new supervised dataset is extracted from the tests with the techniques described in Section 4.1. The new dataset is added to $dataset$ (Line 7). After the loops finish, $dataset$ is returned.

Iterative learning for producing multiple learned strategies.

While a single learned strategy is already more effective than existing heuristics [16, 48], we found that using multiple models during inference time can improve the tests generated by symExec even more (a form of ensemble learning). This is because the space of symbolic states is exponentially large and multiple strategies can explore a more diverse set of states than a single strategy. We propose an iterative algorithm called iterLearn in Algorithm 4 that trains multiple strategies. To incorporate the knowledge of existing heuristics into LEARCH, we treat them as an input ($strategies$) to iterLearn and leverage them in the data generation process.

Algorithm 4: Iterative learning

```
1 Procedure iterLearn(progs, strategies, N)
  Input :progs, a set of training programs.
          strategies, a set of manual heuristics.
          N, the number of training iterations.
  Output: learned, a set of learned strategies.
2 dataset  $\leftarrow$  emptySet(); learned  $\leftarrow$  emptySet()
3 for i  $\leftarrow$  1 to N do
4   newData  $\leftarrow$  genData(progs, strategies)
5   dataset  $\leftarrow$  dataset  $\cup$  newData
6   newStrategy  $\leftarrow$  trainStrategy(dataset)
7   learned.add(newStrategy)
8   strategies  $\leftarrow$  {newStrategy}
9 return learned
```

iterLearn first initializes a supervised dataset $dataset$ and a set of learned strategies $learned$ to empty sets (Line 2). Then it starts a loop from Line 3 to Line 8 with N iterations. For each iteration, genData (Algorithm 3) is called to generate new supervised data using $strategies$ (Line 4) and the new data is added to $dataset$ (Line 5). Then, a new strategy $newStrategy$ is trained at Line 6. To achieve this, we run an off-the-shelf learning algorithm on $dataset$, represented by the trainStrategy function. Then, $newStrategy$ is added to $learned$ (Line 7). At Line 8, we assign $newStrategy$ as the only element in $strategies$. This indicates that genData is called with the manual heuristics only at the first loop iteration. After the first loop iteration, the learned strategy obtained from the previous iteration is used to generate new supervised data. After the loop finishes, we return the N learned strategies.

Note that our learning pipeline is general and can be extended to optimizing for other objectives (e.g., detecting heap errors) just by choosing an appropriate reward function (e.g., the number of heap access visited during execution) and designing indicative features. Moreover, LEARCH employs an offline learning scheme, i.e., training is done beforehand and the learned strategies are not modified at inference time. One natural future work item is to extend LEARCH with online learning where we utilize already explored states of the input program to improve the strategies at inference time. Online learning can help LEARCH generalize better to programs that are drastically different from the training programs.

5 INSTANTIATING LEARCH ON KLEE

In this section, we describe how to instantiate LEARCH in KLEE [16]. For more implementation details, please refer to LEARCH’s open source repository at <https://github.com/eth-sri/learch>. While LEARCH is general and can be applied to other symbolic execution frameworks, we chose KLEE because it is widely adopted in many applications, including hybrid fuzzing [27] and others [23, 24, 36, 53, 76]. We believe the benefits of LEARCH can be quickly transferred to the downstream applications and other systems [8, 22, 52, 68, 74].

5.1 Features and Model

We describe the features and the machine learning model of LEARCH.

Table 1: Features for representing a symbolic state *state*.

Feature	Description
stack	Size of <i>state</i> 's current call stack.
successor	Number of successors of <i>state</i> 's current basic block.
testCase	Number of test cases generated so far.
coverage	(1) Number of new instructions covered by <i>state</i> 's branch. (2) Number of new instructions covered along <i>state</i> 's path. (3) Number of new source lines covered by <i>state</i> 's branch. (4) Number of new source lines covered along <i>state</i> 's path.
constraint	Bag-of-word representation of <i>state</i> 's path constraints.
depth	Number of forks already performed along <i>state</i> 's path.
cpicnt	Number of instructions visited in <i>state</i> 's current function.
icnt	Number of times for which <i>state</i> 's current instruction has been visited.
covNew	Number of instructions executed by <i>state</i> since the last time a new instruction is covered.
subpath	Number of times for which <i>state</i> 's subpaths [48] have been visited. The length of the subpaths can be 1, 2, 4, or 8.

Features. In Table 1, we list the features extracted for a symbolic state (*state*) by `extractFeature` at Line 2 of Algorithm 2. Feature `stack` calculates the size of *state*'s current call stack. The larger the call stack size, the deeper the execution goes into. Feature `successor` calculates the number of successors that *state*'s current basic block has. The more successors, the more paths the state can lead to. The next two features capture the execution progress. Feature `testCase` returns the number of already generated test cases. The `coverage` feature tracks the new instruction and line coverage achieved by *state*'s latest branch and the program path already explored by *state*, respectively. The states with more new coverage should be explored first. Feature `constraint` is a 32-dimensional vector containing the bag-of-word representation of the path constraints of *state*. To extract the bag-of-word representation, we go over each path constraint that is represented by an expression tree and traverse the tree to obtain the count of each node type.

The last five statistics are borrowed from existing expert-designed heuristics [16, 48]. By including them as features of LEARCH, we enable LEARCH to learn the advantages of those heuristics. Feature `depth` calculates the number of forks that happened along *state*'s path. Feature `cpicnt` records the number of instructions executed inside *state*'s current function. Feature `icnt` is the number of times for which the current instruction of *state* is executed. Feature `covNew` records the last newly covered instruction for *state* and calculates its distance to the current instruction. For feature `subpath`, we track the subpaths of *state* (i.e., the last branches visited by *state*'s path [48]) and return the number of times for which the subpaths have been explored before. The fixed length of the subpaths is a hyperparameter and we used 1, 2, 4, and 8, as done in [48].

Model selection. LEARCH requires a machine learning model that transforms the features described above to an estimated reward (Line 3 of Algorithm 2). Any regression model can be adopted in our setting. We leverage the feedforward neural network model as it yielded good results in practice. We also tried simpler linear regression and more complicated recurrent neural networks, but

found that feedforward networks achieved the best results. More results on model selection are discussed in Section 6.6.

Leverage multiple learned strategies. As described in Section 4.2, we apply ensemble learning to train N models and construct N strategies. To apply the N strategies during inference time, we simply divide the total time budget into N equal slots, run KLEE with each learned strategy independently on one slot, and union the tests from all the runs. This results in tests that achieve higher coverage and detect more security violations than using a single strategy for the full time budget. This is because different learned strategies can explore an even more diverse set of program parts. Moreover, KLEE usually generates tests quickly in the beginning and saturates later. One time slot is usually already enough for a learned strategy to generate a reasonably good set of tests.

5.2 Security Violations

An important aspect of symbolic execution tools is to detect violations of program properties that can lead to security issues. The original KLEE detects certain types of errors. However, we found that it usually only reports failures of the symbolic execution model such as errors of the symbolic memory model, reference of external objects, and unhandled instructions. Those errors are usually not triggered concretely and do not lead to security violations.

In this work, we leverage Clang's Undefined Behavior Sanitizer (UBSan) [4] to instrument the input program and label five kinds of security violations, listed below:

- *Integer overflow*: checks if the arithmetic operations overflow. The operations include addition, subtraction, multiplication, division, modulo, and negation of signed and unsigned integers.
- *Oversized shift*: checks if the amount shifted is equal to or greater than the bit-width of the variable shifted, or is less than zero.
- *Out-of-bounds array reads/writes*: checks if the indices of array reads and writes are equal to or greater than the array size.
- *Pointer overflow*: checks if pointer arithmetic overflows.
- *Null dereference*: detects the use of null pointers or creation of null dereferences.

When any UBSan violation happens, a specific function is called. We added handlers for capturing those functions and generating a concrete test case triggering the violations, except for integer overflows which has already been supported by KLEE. As a result, KLEE is able to generate reproducible concrete tests for the above violations. We note that KLEE is not restricted to UBSan violations but the difficulty of supporting more violations depends on the implementation of the handlers. For example, it would take a significant amount of effort to support the AddressSanitizer [63] in KLEE so we consider it as a future work item.

6 EXPERIMENTAL EVALUATION

We present an extensive evaluation of LEARCH aiming to answer the following questions:

- Can LEARCH cover more code than existing manual heuristics?
- Can LEARCH discover more security violations?
- Can LEARCH generate better initial seeds for fuzzing?
- What is the impact of LEARCH's design choices?

Table 2: The statistics of the programs used as test sets. MainLOC represents the main program lines without neither internal nor external library code, i.e., the lines of the source file containing the main function. ELOC represents the total executable lines in the final executable after KLEE’s optimizations, including internal libraries within the package but excluding external library code that KLEE automatically links. The numbers for coreutils were averaged from all 52 test programs.

Program	Version	Input format	Binary size	MainLOC	ELOC	KLEE settings for symbolic inputs
coreutils	8.31	various	142 KB	330	1208	-sym-args 0 1 10 -sym-args 0 2 2 -sym-files 1 8 -sym-stdin 8
diff	3.7	cmd + text	548 KB	552	7,739	-sym-args 0 2 2 A B -sym-files 2 50
find	4.7.0	cmd + text	802 KB	256	11,472	-sym-args 0 3 10 -sym-files 1 40 -sym-stdin 40
grep	3.6	cmd + text	587 KB	1,167	9,545	-sym-args 0 2 2 -sym-arg 10 A -sym-files 1 50
gawk	5.1.0	awk + text	1.3 MB	604	24,079	-f A B -sym-files 2 50
patch	2.7.6	cmd + text + diff	466 KB	984	7,007	-sym-args 0 2 2 A B -sym-files 2 50
objcopy	2.36	cmd + elf	4.9 MB	2,513	48,895	-sym-args 0 2 2 A -sym-files 1 100
readelf	2.36	elf	2.4 MB	10,381	28,522	-a A -sym-files 1 100
make	4.3	Makefile	466 KB	883	7,862	-n -f A -sym-files 1 40
cjson	1.7.14	json	83 KB	71	610	A -sym-files 1 100 yes
sqlite	3.33.0	sql commands	2.1 MB	35,691	46,388	-sym-stdin 20

6.1 Evaluation Setup

Now we describe the setup for our experimental evaluation.

Benchmarks. We evaluated LEARCH on coreutils (version 8.31) and 10 real-world programs (listed in Table 2). coreutils is a standard benchmark for evaluating symbolic execution techniques [16, 22, 48, 50]. We excluded 3 coreutils utilities (kill, ptx, and yes) that caused non-deterministic behaviors in our initial experiments. As a result, we used 103 coreutils programs in our evaluation. The 10 real-world programs are much larger than most coreutils programs, deal with various input formats, and are widely used in fuzzing and symbolic execution literature [7, 12, 15, 21, 43, 72].

We randomly selected 51 of the 103 coreutils programs for training LEARCH. The rest 52 coreutils programs and the 10 real-world programs were used as test sets for evaluating LEARCH’s performance on unseen programs. The statistics of both test sets can be found in Table 2. The coreutils test set has overlapping code with the training set as they are from the same package [5]. This represents a common and valid use case where developers train LEARCH on programs from their code base and then run it to test other programs from the same code base. Note that our use case is different from other security tasks based on machine learning such as binary function recognition [5, 10, 67] where sharing of code between train-test splits must be avoided as training on target binaries is impossible due to unavailable source code. The 10 real-world programs are from packages different from coreutils and thus share less code with coreutils. They are used to demonstrate that LEARCH generalizes well across different code bases. That is, once trained (e.g., with coreutils in our evaluation), LEARCH can directly be used to test other software packages.

Baselines. We adopted existing manually crafted heuristics created for KLEE as baselines [16, 48]. We do not compare with [74] because it is not part of KLEE and we did not find its implementation available. We ran all KLEE’s individual heuristics on our coreutils test set and only present the top four due to space limit:

- rss (random state search): each time selects a state uniformly at random from the list of pending states.

- rps (random path search): constructs a binary execution tree where the leaves are the pending states and the internal nodes are explored states that produce the pending states. To select a state, rps traverses the tree in a top-down fashion, picks a child of internal nodes randomly until reaching a leaf, and returns the reached leaf as the selection result. The leaves closer to the root are more likely to be selected.
- nurs:cpicnt and nurs:depth: both are instances of the nurs (non-uniform random search) family. They sample a state from a distribution where the probability of each state is heuristically defined by cpicnt and depth, respectively. See Table 1 and Section 5.1 for the definitions of cpicnt and depth.

We also compare LEARCH with combinations of multiple heuristics:

- sgs (subpath-guided search) [48]: selects a state whose subpath (defined in Table 1 and Section 5.1) was explored least often. To achieve the best results, the authors of [48] ran four independent instances of sgs where subpath lengths were configured to 1, 2, 4, and 8, respectively. Each instance spent a quarter of the total time limit, and then the resulted test cases were combined. We followed this in our evaluation.
- portfolio: a portfolio of four different heuristics: rps, nurs:cpicnt, nurs:depth, and sgs. Like sgs and LEARCH, we ran each heuristic of portfolio as an independent instance that spends a quarter of the total time budget.

Different from Algorithm 1 which selects a state per branch, the original KLEE performs state selection per instruction. In our initial experiments on coreutils, we found that running the heuristics with Algorithm 1 gave better results and thus used Algorithm 1 for all heuristics in our evaluation. This means that our baselines are already stronger than their counterparts in the original KLEE.

KLEE settings. KLEE provides users with options to specify the number and length of symbolic inputs (e.g., command-line arguments, files, stdin, and stdout) to an input program. The symbolic options we used are listed in Table 2. We followed prior works [16, 48] to set symbolic inputs for coreutils programs. For the 10 real-world programs, we configured the symbolic options based on their input formats and prior works [15, 43].

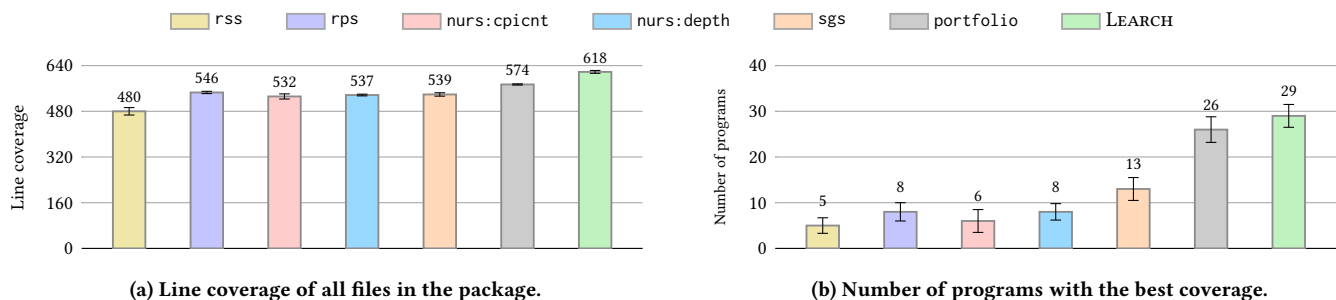


Figure 5: Line coverage of running KLEE with different strategies for 1h on the 52 coreutils testing programs. The numbers were averaged over 20 runs and the error bars represent standard deviations.

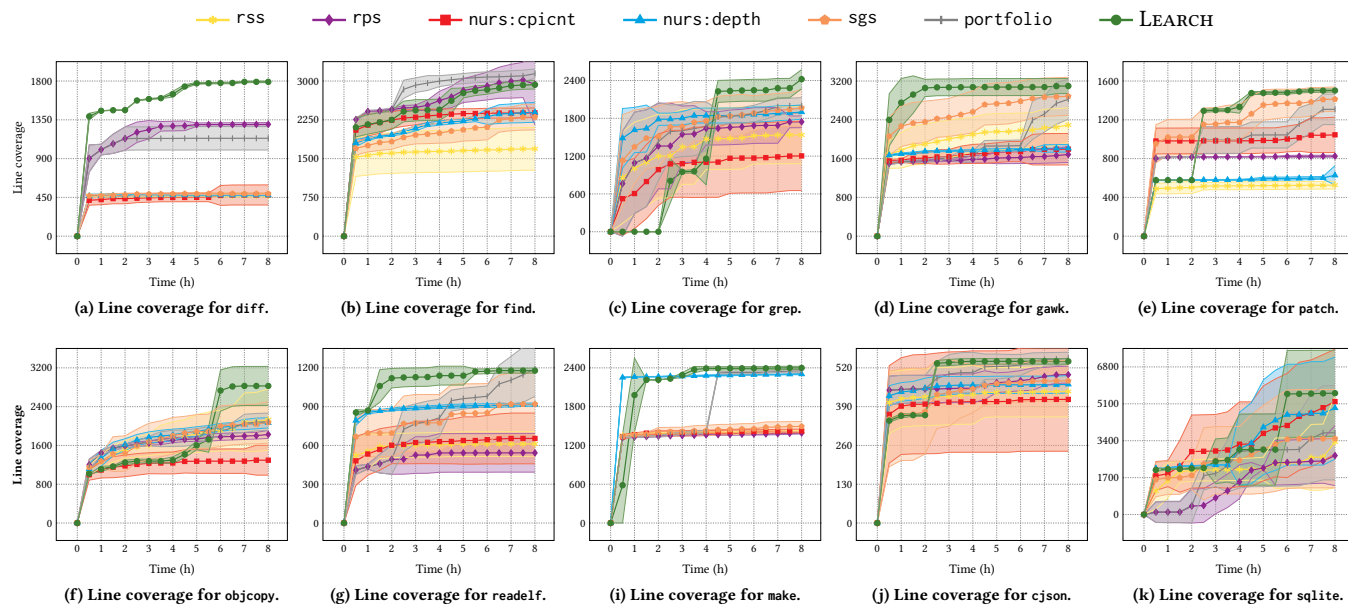


Figure 6: Line coverage for the 10 real-world programs by running KLEE with different strategies for 8h. Mean values and standard deviations over 20 runs are plotted.

When evaluating the `coreutils` test set, we set the time limit to 1h for each search strategy, following [16, 48]. For the real-world programs, the time limit was 8h. The memory limit for all programs was 4GB, which is higher than KLEE’s default budget (2GB) and the limit used by prior works [15, 21]. We did not input any initial seed test to KLEE. Whenever necessary, we repeated our experiments for 20 times and report the mean and standard deviation.

Training and testing LEARCH. We trained LEARCH by running Algorithm 4 on the 51 `coreutils` training programs. The set of initial strategies consisted of `rps`, `nurs:cpicnt`, `nurs:depth`, and `sgs` (with subpath lengths 1, 2, and 4) as these strategies performed the best on the training programs. We ran Algorithm 4 for 4 iterations to train 4 strategies (feedforward networks with 3 linear layers, 64 hidden dimension, and ReLU activations). We did not include more trained strategies because more strategies did not significantly increase LEARCH’s performance. Each iteration spent around 4h (2h on `symExec`, 1h on `dataFromTests`, and 1h on `trainStrategy`). When

running LEARCH on the test set, we ran each strategy for a quarter of the total time limit and combined the resulted test cases.

Versions and platform. We implemented LEARCH on KLEE 2.1 and LLVM 6.0. We used pytorch 1.4.0 for learning. All symbolic execution experiments were performed on a machine with 4 Intel Xeon E5-2690 v4 CPUs (2.60 GHz) and 512 GB RAM. Each KLEE instance was restricted to running on one core. The machine learning models were trained on a machine with RTX 2080 Ti GPUs.

6.2 Code Coverage

In this section, we present our evaluation on code coverage, i.e., line coverage measured with `gcov` [2]. We first report absolute line coverage for all files in the package. Then, we present and discuss the percentage of covered lines.

Line coverage for coreutils programs. In Figure 5(a), we present the coverage of each strategy on the 52 `coreutils` testing programs. On average, LEARCH (green bar) covered 618 lines for all files in the

Table 3: Percentage of covered MainLOCs.

	rss	rps	nurs:cpicnt	nurs:depth	sgs	portfolio	LEARCH
coreutils	66.4	73.1	71.6	71.4	72.0	75.4	76.9
diff	30.3	53.7	31.1	30.6	32.3	50.5	59.1
find	52.1	57.7	58.3	56.0	60.2	61.2	61.0
grep	21.8	29.7	17.1	28.1	29.8	29.7	36.5
gawk	39.2	39.2	39.2	43.0	39.2	43.0	39.2
patch	13.8	19.1	24.4	15.1	33.5	31.9	35.8
objcopy	9.9	9.5	6.0	9.3	8.3	9.8	13.3
readelf	4.8	3.9	5.2	6.5	7.7	9.1	9.0
make	33.3	33.3	33.0	45.2	33.3	45.2	45.2
cjson	79.8	80.2	76.5	79.6	79.7	80.3	80.3
sqlite	8.1	6.3	12.8	11.4	9.2	8.7	14.2

package. The best individual heuristic was `rps` (purple bar), which covered 546 lines. That is, `LEARCH` achieved at least 13% more coverage than any individual heuristic. `portfolio` (purple bar) was the best combined heuristic but still covered 44 lines less than `LEARCH`.

In Figure 5(b), we plot the number of programs where each strategy achieved the best coverage among all the strategies. For ties, we count one for each strategy. For 29 programs, `LEARCH` was the best strategy, outperforming `portfolio` by 3 and other heuristics by a large margin. For the other 23 programs, at least one heuristics performed better than `LEARCH`, but usually only by a small margin. Moreover, we found that `LEARCH` gave more benefits on larger `coreutils` programs. For example, for the largest 5 programs, `LEARCH` achieved ~30% more coverage than `portfolio`, compared to ~8% overall for all 52 programs. For smaller programs, the manual heuristics already covered most parts of the programs so `LEARCH` hardly improved upon them.

Line coverage for real-world programs. In Figure 6, we plot the coverage of each strategy on the 10 real-world programs. To generate the coverage curve for combinations of strategies, we treat independent runs of each strategy sequentially. On average, `LEARCH` covered 2,433 lines while the best manual heuristic, `portfolio`, covered 2,023 lines. Overall, `LEARCH` outperformed all the manual heuristics by >20%.

Judging from the mean values, `LEARCH` was the best strategy for 8 of the 10 real-world programs, except for `cjson` and `find`. For `cjson`, `LEARCH` was the second best, covering 10 lines less than `portfolio`. For `find`, `LEARCH` covered 242 and 191 less lines than `portfolio` and `rps`, respectively. `LEARCH`'s superior performance in code coverage was consistent among the 10 programs while all manual heuristics were unstable. For example, `portfolio` did well on `cjson` and `find` but not on `objcopy` and `sqlite`. Similarly, `sgs` performed well on `gawk` but poorly on `diff`.

For `sqlite`, the standard deviations of all strategies were high. The reason is that, during some runs, the strategies were unable to generate a few important test cases, resulting in thousand of lines less coverage than other runs. This happened the least often for `LEARCH` so `LEARCH`'s mean coverage was the highest.

Percentage of covered lines. Apart from absolute line coverage, we calculated the percentage of covered lines to investigate how thoroughly the test programs are covered by `KLEE` and the strategies. We measured the percentage of covered MainLOCs and

Table 4: Percentage of covered ELOCs.

	rss	rps	nurs:cpicnt	nurs:depth	sgs	portfolio	LEARCH
coreutils	13.6	15.2	14.7	14.9	14.9	15.7	16.1
diff	1.9	3.3	2.0	2.0	2.0	3.1	3.6
find	1.0	1.1	1.2	1.1	1.2	1.2	1.2
grep	2.3	2.5	1.8	2.9	3.1	3.1	3.9
gawk	0.9	0.9	0.9	1.0	0.9	1.0	0.9
patch	1.7	2.4	3.1	1.9	4.2	4.0	4.5
objcopy	0.5	0.4	0.3	0.4	0.4	0.5	0.6
readelf	1.5	1.2	1.6	2.0	2.5	2.9	2.9
make	3.2	3.2	3.2	4.4	3.2	4.4	4.4
cjson	7.3	7.4	7.0	7.3	7.3	7.4	7.4
sqlite	5.5	4.2	8.8	7.8	6.3	5.9	9.7

ELOCs (mean value from 20 runs). The total number of MainLOCs and ELOCs for each test program can be found in Table 2.

MainLOC was used for measuring coverage in [16, 48] and refers to the main program lines, i.e., the lines of the source file containing the main function. It does not include internal and external library code that can be invoked by multiple programs to avoid counting them multiple times (see [16] for details on the advantages of using MainLOC). The results for MainLOC percentages are presented in Table 3. `LEARCH` achieved the highest coverage for most cases. We can observe that the percentages for all strategies decrease with increasing program size: for small programs such as `coreutils`, `cjson` and `find`, all strategies achieved relatively high coverage (e.g., >60%); while for large programs such as `readelf` and `sqlite`, `KLEE` only covered ~10% MainLOCs.

ELOC, short for executable lines of code, represents the total executable lines in the final executable after `KLEE`'s optimizations. In [16, 48], it was used for measuring program size and included external library code that `KLEE` automatically links. In our work, we use ELOC for measuring coverage and thus excluded external library code that does not belong to the program package. The internal library code from the package was included. The results on the percentage of covered ELOCs are presented in Table 4. `LEARCH` still covered most portions of code for most cases. However, even with the best strategy, `KLEE` covered only a very small portion of code (e.g., <10% for the real-world programs).

Our results on percentage of covered lines show that it is still challenging to scale symbolic executor like `KLEE` to large programs. While `LEARCH` improves on other search strategies, efforts on other directions are also needed, such as reducing memory consumption [15, 21], accelerating constraint solving [9, 28, 32, 61], and executing program fragments instead of the whole program [59, 70].

Summary on generalizability. `LEARCH`'s effectiveness in code coverage demonstrates its generalizability: it generalizes between programs from the same package (i.e., training and testing on `coreutils`). This is because these programs usually share the same code and our learning method can capture this. More interestingly, `LEARCH` also generalizes from a package of smaller programs (i.e., training on `coreutils`) to other packages whose code is different from the training package and programs are much larger (i.e., testing on the real-world programs). This is likely because `LEARCH`'s features capture the importance of symbolic states even for programs different from the training set.

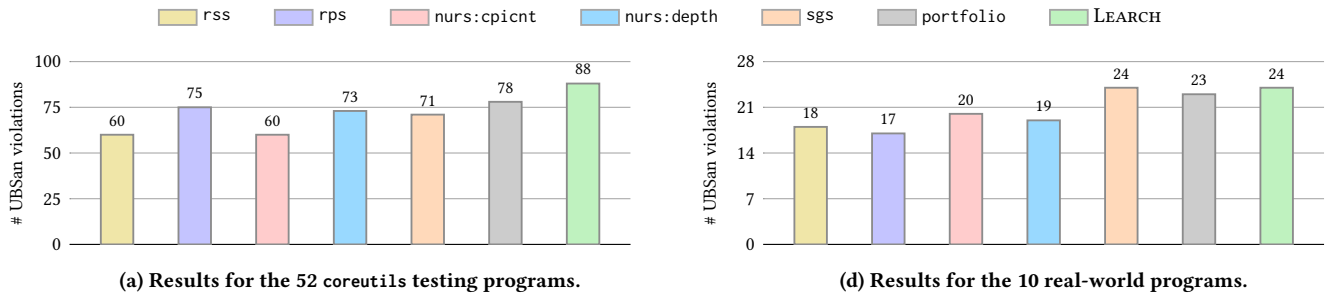


Figure 7: The total number of detected UBSan violations found by KLEE with different strategies.

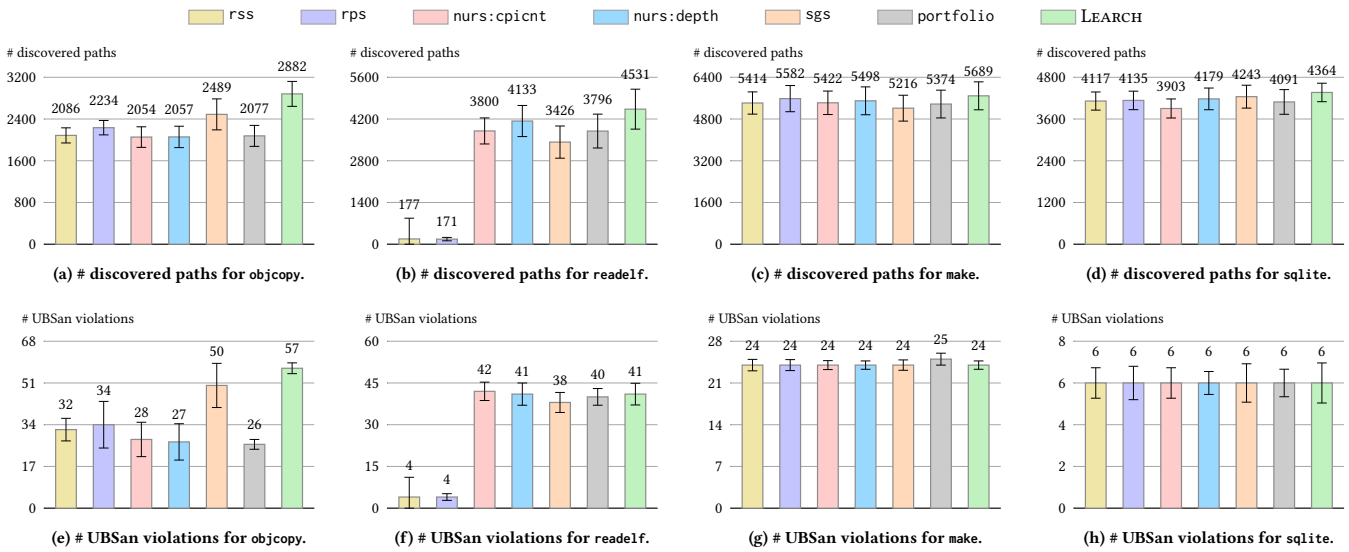


Figure 8: The number of paths and UBSan violations discovered by AFL after 8h using KLEE tests as initial seeds. The numbers were averaged over 20 runs and the error bars represent standard deviations.

6.3 Detecting Security Violations

We ran the strategies on program instrumented with UBSan checkers to evaluate their capability of detecting UBSan violations. All the detected violations are *true positives* because they can be triggered by the generated test cases.

In Figure 7, we present the number of UBSan violations detected by the strategies. For the *coreutils* test set (Figure 7(a)), LEARCH detects 88 violations in total, outperforming the manual heuristics by >12%. For the 10 real-world programs (Figure 7(b)), LEARCH outperformed all manual heuristics except for *sgs* which found the same number of violations as LEARCH, even though LEARCH achieved higher coverage than *sgs*. This is likely because the parts of the programs explored by *sgs* contained more UBSan labels. We provide a manual analysis of the UBSan violations detected with LEARCH in Section 6.5.

6.4 Seeding for Fuzzing

Fuzzing has gained substantial interest recently [1, 27, 30, 31, 45, 72]. It is shown that fuzzing performance heavily depends on the choices of initial seeds [39, 45]. While the initial seeds used in prior works

are usually empty, randomly generated, or manually constructed [12, 26, 45, 71], symbolic execution can be used to automatically generate fuzzing seeds (see [29] for how initial seeds generated by KLEE compare to simple and expert seeds). In this work, we investigate if LEARCH can generate better fuzzing seeds than the manual heuristics.

We selected AFL (version 2.52b) [1] due to its popularity and ran it on the four largest programs in our real-world benchmarks whose input format supports AFL-style fuzzing: *objcopy*, *readelf*, *make*, and *sqlite*. For each program and each strategy, we constructed the initial seed set by selecting the top three tests from our previous experiment (i.e., Figure 6) based on the best coverage and ran AFL starting from the initial seeds for 8h. We selected only three initial seeds because using a small set of initial seeds is recommended by AFL and adopted by many fuzzing works [3, 7, 27, 45, 51]. Aware of the randomness in AFL, we repeated each run for 20 times and report the mean and standard deviation.

Discovering paths. AFL generates a test when a new path is triggered. Therefore, one of the most direct indicator of AFL's progress is path coverage, i.e., the number of discovered paths

```

1 static bool consider_arm_swap (struct predicate *p) {
2     ...
3     pr = &p->pred_right;
4     // findutils-4.7.0/find/tree.c: line 538
5     pl = &p->pred_left->pred_right;
6     ...

```

Figure 9: A null pointer dereference.

```

1 static char * find_map_unquote (...) {
2     ...
3     // make-4.3/src/read.c: line 2354
4     memmove (&p[i], &p[i/2],
5             (string_len - (p - string)) - (i/2) + 1);
6     ...
7 }

```

Figure 11: An overflow leading to wrong array accesses.

[30, 31, 42]. In Figure 8(a) to Figure 8(d), we show the number of paths discovered by AFL for the four programs, respectively. When using the initial seeds from LEARCH, AFL discovered the most number of paths for all four programs. With the initial seeds from `rss` and `rps`, AFL discovered very few paths for `readelf`, which is not surprising as `rss` and `rps` achieved very low coverage on `readelf` with KLEE.

Detecting security violations. We re-ran the tests generated by AFL with UBSan checkers turned on. The number of detected violations is shown in Figure 8(e) to Figure 8(h). Overall, with initial seeds from LEARCH, AFL found 128 violations in total, outperforming other heuristics (10 more than the best heuristic, `sgs`). We provide a manual analysis of the detected violations next.

6.5 Manual Analysis of Security Violations

Unlike standard crash bugs, UBSan violations may not crash the program but can indicate deeper, functional misbehaviors. Moreover, some UBSan violations may be benign. In this section, we performed a manual inspection of the violations found with LEARCH to understand the severity of the violations.

The vast majority of detected violations were overflows. We manually inspected 112 violations detected by running KLEE with LEARCH, as well as 152 violations discovered by AFL with initial seeds from LEARCH. From these violations, we identified 46 potential bugs (see column "Bug reports" in Table 5). These potential bugs can result in logical errors (e.g., setting a wrong value, moving a file cursor to a wrong position, wrong control flow, etc.) or out-of-bound reads/writes. The remaining violations were benign cases, mainly categorized as: (1) the programs already consider the violation and have specialized handlers; (2) the operations are used for hashing or generating random numbers so the overflows do not affect program logic; (3) the related variables are set to a new value or not used after the violations.

We reported the 46 potential bugs to the developers and 13 of them were confirmed as true bugs. The other potential bugs were recognized as false positives by the developers. Among the confirmed bugs, 11 bugs have been fixed or will be fixed, or the developers are discussing how to fix them. The number of confirmed and fixed bugs for each program is listed in Table 5.

```

1 const char * _bfd_coff_read_string_table (bfd *abfd) {
2     ...
3     // binutils-2.36/bfd/coffgen.c: line 1676
4     pos += obj_raw_syment_count (abfd)
5         * bfd_coff_symesz (abfd);
6     ...

```

Figure 10: Overflows leading to an incorrect file position.

```

1 # define ISDIGIT(c) (((unsigned int) (c) - '0' <= 9)
2     ...
3 // coreutils-8.31/lib/strncmp-in.h: line 224
4 for (log_a = 0; ISDIGIT (tmpa); ++log_a)
5     do { tmpa = *++a; }
6     while (tmpa == thousands_sep);
7     ...

```

Figure 12: A benign overflow.

Table 5: Our bug reports to the developers. The programs without any manually identified bugs are not listed.

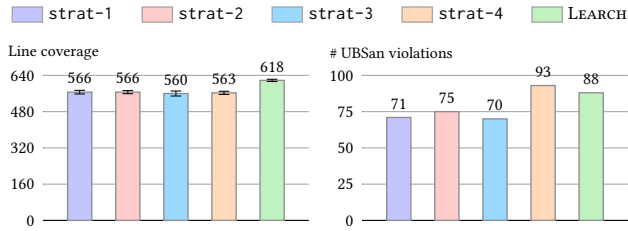
	Violations	Bug reports	Confirmed	Fixed/Will fix
coreutils	88	3	2	2
find	5	2	2	2
objcopy	73	29	3	3
readelf	57	5	1	1
make	26	3	3	3
sqlite	9	4	2	0
Total	258	46	13	11

Examples. We show four examples of UBSan violations detected with LEARCH. The first three are confirmed bugs and the last one is a benign case. In Figure 9, `&p->pred_left` is null pointer but the code tries to dereference it. This bug was detected by running KLEE with LEARCH on `find`. In Figure 10, the addition at Line 4 and the multiplication at Line 5 can overflow, affecting the value of `pos` and leading to a wrong file position when reading a binary executable file with `objcopy`. Figure 11 is taken from `make` and contains a subtract overflow at Line 5 which results in wrong or even out-of-bound array accesses. AFL detected Figures 10 and 11 using the initial seeds from LEARCH. Figure 12 shows a benign subtraction overflow detected by KLEE with LEARCH for the `coreutils` tool `sort`. The code computes the logarithm of a number stored in the unsigned char array `tmpa`. To decide if the current array element is a digit, the code uses the macro `ISDIGIT` which overflows when `c < '0'`. When this happens, `ISDIGIT` returns false, which is desired as `c` is not a digit. Therefore, the overflow case was already considered and handled.

6.6 Effectiveness of Design Choices

We investigate the usefulness of LEARCH's design choices. Due to space limit, we mainly present the results on `coreutils`. For the real-world programs, we observed the same phenomenon as `coreutils`.

Performance of individual strategies. As described in Section 6.1, LEARCH consists of four learned strategies. We ran each strategy for 1h on the `coreutils` test set and compare the results with LEARCH (a union of the four strategies each running for 15m) in



(a) Line coverage for the whole package. (b) Number of UBSan violations.

Figure 13: Results of learned strategies on coreutils test set.

Figure 13. The individual strategies already achieved more coverage (~20 lines) than the individual manual heuristics. Even though the absolute coverage numbers were similar, the four strategies covered different parts of the program. As a result, LEARCH, combined from the four strategies, was the most performant overall. This is the desired outcome of the iterative learning in Algorithm 4.

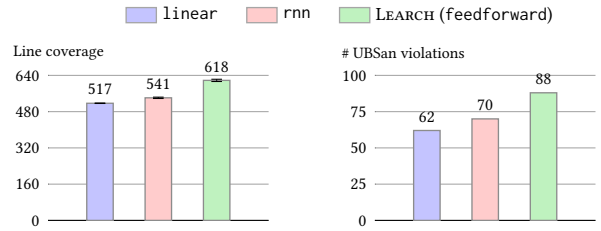
LEARCH also found more UBSan violations than strat-1, strat-2, and strat-3, as a result of the combination. LEARCH found 5 fewer violations than strat-4 because strat-4 found many violations after 15m. Therefore, to make LEARCH detect more violations, we can simply increase the time budget.

Different choices of machine learning model. Other than feedforward networks used in LEARCH, we considered simpler linear regression (*linear*) and more complicated recurrent neural networks (*rnn*). For *rnn*, we added a hidden state of dimension 64 between a state and its parent. We trained *linear* and *rnn* on the same supervised dataset as LEARCH, and ran them with the same configuration (i.e., four independent runs each taking a quarter of the time budget) as LEARCH on our test set. The results on the `coreutils` test set are shown in Figure 14, showing that LEARCH outperformed *linear* and *rnn*. The reason is likely that the complexity of feedforward networks is well-suited for our learning task.

7 RELATED WORK

We discuss works closely related to ours.

Symbolic execution. Symbolic execution based testing techniques have been developed for decades [18, 44], yielding a number of applications [23, 24, 27, 36, 53, 76] and systems [8, 16, 17, 22, 52, 68, 74]. The main challenges in symbolic execution include path explosion and expensive constraint solving [18]. A number of manual heuristics have been proposed for selecting promising paths [16, 48]. Our learning-based strategy LEARCH significantly outperforms those heuristics. Other orthogonal attempts for easing the path explosion problem include state merging [46], state pruning [13, 14, 21, 70], and code transformation [25]. A number of works focus on improving the performance of constraint solvers [9, 28, 32, 61]. Some works combine the constraint solving process with the symbolic execution framework by solving multiple path constraints once [77], leveraging pending path constraints [43], and introducing neural constraints [66]. While most of the above approaches aim to explore the whole program (same as our goal), directed symbolic execution aims to reach certain program parts or changes [50, 56, 73].



(a) Line coverage for the whole package. (b) Number of UBSan violations.

Figure 14: Results of different models on coreutils test set.

Concolic testing and fuzzing. Concolic testing and fuzzing are different approaches for program testing but can benefit from advances in symbolic execution because many of them use symbolic execution for triggering complex paths. Concolic testing [33, 57, 58, 62] concretely executes the program alongside symbolic execution and negates the path constraint of visited branches to produce new tests covering unvisited branches. Heuristics have been learned for selecting branches in concolic testing [19, 20]. Fuzzing is a technique that concretely executes the program and generates concrete inputs based on input specifications [11, 40, 47] or mutations from existing inputs [1, 7, 12, 26, 30, 31, 41, 42, 45, 65, 72]. Symbolic execution has been used for improving fuzzing [29, 54]. Hybrid testing [27, 69, 75] combines concolic testing and fuzzing in an alternative manner to benefit from the advantages of both.

Machine learning for program analysis and security. Machine learning has been extensively used for security tasks. Markov chain [12], feedforward networks [65], recurrent networks [35], imitation learning [37], reinforcement learning [72] have been used for improving test generation in fuzzing. The authors of [73] leverage reinforcement learning for directed symbolic execution. Many other tasks such as binary analysis [38], malware analysis [60], and taint analysis [64] have been solved by data-driven approaches.

8 CONCLUSION

In this work, we introduced LEARCH, a learning-based state selection strategy for symbolic execution. LEARCH works by estimating a reward for each state and selecting the state with the highest reward to maximize coverage while minimizing time cost. We construct LEARCH by applying off-the-shelf regression learning on a supervised dataset extracted from the tests generated by running symbolic execution on a set of training programs. The training process is iterative and constructs multiple strategies which produce more diverse tests than a single strategy. LEARCH benefits from existing heuristics by incorporating them in both training and feature extraction.

We instantiated LEARCH on KLEE [16] and evaluated it on the `coreutils` programs and ten real-world programs. The results demonstrated that LEARCH is effective and can produce higher-quality tests than existing manually designed heuristics, either individual ones or combined as portfolios: LEARCH’s tests yielded more code coverage, detected more security violations, and were better candidates as initial seeds for fuzzers like AFL.

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