Constraint Solving with Deep Learning for Symbolic Execution

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ABSTRACT
Symbolic execution is a powerful systematic software analysis technique, but suffers from the high cost of constraint solving, which is the key supporting technology that affects the effectiveness of symbolic execution. Techniques like Green and GreenTrie reuse constraint solutions to speed up constraint solving for symbolic execution; however, these reuse techniques require syntactic/semantic equivalence or implication relationship between constraints. This paper introduces DeepSolver, a novel approach to constraint solving with deep learning for symbolic execution. Our key insight is to utilize the collective knowledge of a set of constraint solutions to train a deep neural network, which is then used to classify path conditions for their satisfiability during symbolic execution. Experimental evaluation shows DeepSolver is highly accurate in classifying path conditions, is more efficient than state-of-the-art constraint solving and constraint solution reuse techniques, and can well support symbolic execution tasks.

KEYWORDS
symbolic execution, constraint solving, deep learning, neural networks

1 INTRODUCTION
Forward symbolic execution [13, 16, 20, 30, 39, 44] is a powerful technique for systematic exploration of program behaviors, and provides a basis for various software testing and verification techniques, such as program equivalence checking, regression analysis, and continuous testing [37, 45, 51]. Symbolic execution executes a program with symbolic values instead of concrete values, and enumerates the program paths up to a given bound. For each path it explores, symbolic execution builds a path condition, i.e., constraints on the symbolic inputs to follow the corresponding path. During symbolic execution, off-the-shelf constraint solvers [6, 11] are used to check the satisfiability of path conditions whenever they are updated. If a path condition becomes unsatisfiable, the corresponding path becomes infeasible and is discarded in symbolic execution.

As the most time-consuming task in symbolic execution, constraint solving is the key supporting technology that affects the effectiveness of symbolic execution. The advances in constraint solving techniques, for example, by leveraging multiple decision procedures in synergy [18], have enabled symbolic execution to be applicable to larger programs. However, despite these technological advances, symbolic execution still suffers from the high cost of constraint solving. Several techniques have been developed to speed up constraint solving for symbolic execution by reusing previous solving results [25, 27, 34, 50, 55]. Various forms of results caching are utilized, so that solutions of path conditions encountered in previous analysis can be reused without calling a constraint solver. As a result, the total number of solver calls as well as the corresponding time cost is reduced. For example, Green [50] uses an in-memory database Redis [4] to store path conditions and their constraint solutions as key-value pairs, in which key is a path condition string and value is a Boolean value showing whether the corresponding path condition is satisfiable or not, and reuses constraint solutions based on string matching. GreenTrie [27] further improves the reuse rate of previous constraint solutions by applying logical reduction and logical subset and superset querying for given constraints. However, such reuse techniques require syntactic/semantic equivalence or implication relationship between constraints. If the equivalence or implication relationship is not satisfied, these reuse techniques are able to reuse previous constraint solutions.

In this paper, we introduce DeepSolver, a novel approach to constraint solving with deep learning for symbolic execution. Our key insight is to utilize the collective knowledge of a set of constraint solutions to train a deep neural network, which is then used to classify path conditions for
their satisfiability during symbolic execution. Deep learning is a popular technique which has found many applications recently [32, 35, 46, 49]. It uses an existing dataset to train a system, similar to the learning process of a biological neural network, so that the system can process complex data inputs without being programmed in detail with the task-specific rules. It has been proved to be effective and efficient for difficult classification problems such as image recognition[23]. Rather than reusing each individual constraint solution, DeepSolver uses the whole set of constraint solutions to train a deep neural network, and then uses the deep neural network to classify newly encountered path conditions as "satisfiable" or "unsatisfiable". Thus, DeepSolver can classify path conditions during symbolic execution without calling a constraint solver which is potentially expensive.

Using nine Java programs that have all previously been studied in the symbolic execution literature, we evaluate DeepSolver’s accuracy and efficiency in classifying path conditions, compared to Z3 and GreenTrie, the state-of-the-art constraint solving and constraint solution reuse techniques. We also evaluate how DeepSolver supports symbolic execution compared to GreenTrie.

We make the following contributions in this paper:

- We introduce the idea of constraint solving with deep learning for symbolic execution. To the best of our knowledge, this is the first work on using deep learning for speeding up constraint solving in symbolic execution.
- We design an algorithm for vectorizing a path condition to a matrix that enables training of deep neural networks for classifying path conditions in symbolic execution.
- We design an algorithm for symbolic execution with DeepSolver for constraint solving, which addresses the misclassification errors introduced by deep learning and makes DeepSolver useful in practice.
- We present an experimental evaluation of DeepSolver on nine Java subjects, which shows that DeepSolver is highly accurate in classifying path conditions for their satisfiability, is more efficient than state-of-the-art constraint solving and constraint solution reuse techniques, and can well support symbolic execution tasks.

2 BACKGROUND

This section introduces the background on symbolic execution and deep neural networks.

```java
int example(int x, int y)
{
    if (x > y)
    {
        if (y > 0)
            x = y + x;
        else
            x = y - x;
    }
    else
    {
        if (x > 0)
            y = x + y;
        else
            y = x - y;
    }
}
```

Figure 1: Example program.

2.1 Symbolic Execution

Symbolic execution [13, 16, 30, 39] is a powerful, systematic program analysis technique. In contrast to concrete execution which takes concrete values as input and executes only one program path, symbolic execution executes a program with symbolic values and systematically explores all program paths up to a given bound. For each path it explores, symbolic execution builds a path condition (\(PC\)), i.e., constraints on the symbolic inputs to follow the corresponding path. During symbolic execution, off-the-shelf constraint solvers [6, 11] are used to check the the satisfiability of path conditions whenever they are updated. If a path condition becomes unsatisfiable, the corresponding path becomes infeasible and is discarded in symbolic execution. The state of a symbolically executed program includes the (symbolic) values of program variables and a \(PC\). A symbolic execution tree characterizes all execution paths explored during symbolic execution. Each node represents a symbolic program state, and each arc represents a transition between two states.

Figure 2: Symbolic execution tree for the example program

We illustrate symbolic execution on a simple example program in Figure 1, which has two integer inputs: \(x\) and \(y\). For this example, symbolic execution explores four feasible paths shown in the symbolic execution tree in Figure 2. Initially, \(PC\)
is True and \( x \) and \( y \) have symbolic values \( X \) and \( Y \), respectively. At each branch point, all choices are examined with assumptions about the inputs to choose between alternative paths, while \( PC \) is updated accordingly. For example, after the execution of statement 2, both then and else alternatives of the if statement are checked, and \( PC \) is updated with different conditions as the condition is met or violated. Whenever \( PC \) is updated, a constraint solver [2, 6, 11] is called to check its satisfiability. When \( X > Y ∧ Y > 0 \) evaluates to true at line 3 in the source code, the expression \( Y + X \) is computed and stored as the value of \( x \); when \( X > Y ∧ (Y > 0) \) evaluates to true at line 3 in the source code, the expression \( Y − X \) is computed and stored as the value of \( x \).

Symbolic execution is a widely used technique for different software analysis purposes such as generating test cases, automatically checking programs against annotated properties, and detecting infeasible paths in a program [20, 21, 38, 44, 56]. However, it suffers from the high cost of constraint solving, which is the key supporting technology that affects the effectiveness of symbolic execution. \( PC \) accumulates the constraints on the inputs in order for an execution to follow the particular associated path, and becomes more and more complex as the path goes deeper in the symbolic execution tree. The complexity of \( PC \) increases when more constraints are accumulated, non-linear calculation are performed, or more symbolic variables are involved. The more complex a \( PC \) becomes, the more difficult it is for a constraint solver to check its satisfiability. Despite the recent advances in constraint solving [5, 17, 48] which have enabled symbolic execution to be applicable to larger programs, constraint solving remains a bottleneck of symbolic execution.

### 2.2 Deep Neural Networks

Deep neural networks (DNNs) have been widely used in many artificial intelligence areas, such as computer vision [32], natural language processing [46], and speech recognition [35]. In a deep learning model, many layers of information processing stages in hierarchical architectures are utilized for pattern classifications or feature learning purposes. DNNs use multiple layers to progressively extract higher level features from raw input.

One common usage of DNNs is as classifiers. Each input data to the DNN is assigned a pre-set label or class as an output. Each layer of a DNN is comprised of nodes, termed neurons, and the nodes refines and extracts information based on value sent from the previous layer, and then applies their own function to compute a value for the next layer. A typical DNN has one input layer which takes in the input data, one output layer which generates the final classification results, and several hidden layers to perform intermediate processing (e.g., feature extraction). Each neuron computes its output by applying an activation function (e.g., ReLu or sigmoid) to the weighted sum of its inputs according to a unique weight vector and a bias value.

### 3 DEEPSOLVER

In this section, we present DeepSolver, which consists of two stages: the first stage trains a DNN using existing constraint solutions (Section 3.1), and the second stage uses the trained DNN to classify path conditions for their satisfiability (Section 3.2).

#### 3.1 Training a DNN with Constraint Solutions

Figure 3 shows the overall process of training a DNN with existing constraint solutions in the form of \( PC \)-satisfiability pair where \( PC \) is the path condition and satisfiability is a Boolean value (i.e., True or False) indicating whether the \( PC \) is satisfiable or not. As DNNs require the input data to be in the form of a matrix. Thus, we first canonize and vectorize the PCs to matrices, and then use the matrices and satisfiability information to train a DNN. We currently only support linear integer arithmetic path conditions, and will support other types of path conditions in future work.

#### 3.1.1 Canonizing

Path conditions generated during symbolic execution do not have a common pattern by default. For instance, the name space of symbolic variables differs from subject to subject. Canonizing transforms a path condition into a unified format. Each constraint in the path condition is transformed into a normal form for linear integer arithmetic path conditions, specifically

\[
ax + by + cz + \ldots + k \cdot op \cdot 0, \quad \text{where } op \in \{=, \neq, \leq, \geq\}
\]

Other operators including \( >, < \) and \( \geq \) are transformed into the corresponding canonical forms with operators \( =, \neq, \leq \). Meanwhile, the constraints are sorted in a lexicographic order and then symbolic variables are renamed based on their appearances in the path condition in left-to-right order. For instance, both \( PC_1 : x + y < z ∧ x = z ∧ x − 10 > y \) and \( PC_2 : a + b < c ∧ a = c ∧ a − b > 10 \) will be canonized into a same shape as \( v_0 + v_1 − v_2 + 1 \leq 0 ∧ v_0 − v_2 = 0 ∧ −v_0 + v_1 − 9 ≤ 0 \). A unified name space of variables can help us vectorize path conditions into matrices, and eliminate the equivalent records in the training data set.

Since canonizing has been used in previous constraint solution re-use techniques [27, 50], this paper only briefly discusses vectorizing. Please refer to [50] for more details.

#### 3.1.2 Vectorizing

After canonizing, all path conditions have the same variable name space and are in a unified normal form. We then perform vectorizing to turn a path condition in plain text into a 2-dimensional matrix.
We have two important observations of path condition generated in symbolic execution:

**Observation 1.** A path condition is joined by multiple constraints. It is a typical conjunctive normal form (CNF) as it uses only AND logical operator between constraints.

**Observation 2.** In symbolic execution, all variables in a path condition are expressed by the symbolic input variables. Thus, each constraint can be represented as a multinomial formula on the symbolic input variables.

To further explain our technique, we give the following definitions, which will be used in the rest of this paper:

**Definition 1.** A path condition has a dimension of \((d, n, t)\), or it is a \((d, n)\) path condition, where \(d\) is the number of constraints, \(n\) is the highest degree of a term among all constraints, and \(t\) is the number of symbolic variables in the path condition.

**Definition 2.** A \((d, n, t)\) path condition is linear if \(n = 1\); otherwise, it is nonlinear.

For instance, \(x + y - z + 1 \leq 0 \land x - z = 0 \land -x + y - 9 \leq 0\) has a dimension of \((3, 1, 3)\) and it is a linear path condition. \(v_0^2 + v_0 \times v_1 + v_1^3 + 1 > 0\) is a nonlinear \((1, 3, 2)\) path condition.

After canonizing, a constraint is transformed into the form \(c_0 \times v_0 + c_1 \times v_1 + c_2 \times v_2 + \ldots + k \times op \times \mu\), where \(c_\mu\) is the coefficient of variable \(v_\mu\), \(k\) is the constant term, and \(op \in \{=, \neq, \leq, \geq\}\). Since the name space of symbolic variables is unified, a \((d, n, t)\) path condition joined by constraints in this format can be easily transformed into a 2-Dimensional matrix: each row of the matrix stands for a constraint, and the columns stand for the coefficient for one symbolic variable, the constant term, and an integer value used to represent \(op\). The size of the 2-Dimensional matrix is determined as follows:

The number of rows \(X\) is determined by the number of constraints in a path condition, each row representing one constraint. Since symbolic execution generates path conditions with different number of constraints, we can have two strategies: we can group path conditions based on the number of their constraints, and train a DNN for each group; or we can use padding to expand path conditions that have smaller number of constraints, until they have the same number of constraints with the path condition that has the largest number of constraints. Being a typical CNF, a path condition can be joined by any number of true conditions without changing its satisfiability. In our 2-Dimensional matrix model, we can simply add rows with all columns set to 0. By our design, such a row represents formula \(0 = 0\), which is identically True. Theoretically, any logic True formula can be used as padding. However, it may potentially impact the accuracy of the trained neural network. Thus, in this paper, we choose to use the first strategy and train multiple DNNs to handle path condition with different number of constraints. We leave the second strategy that trains one single neural network for all path conditions with different sizes for our future work.

For a linear path condition with \(t\) symbolic variables, the number of columns \(Y = t + 2\), where \(t\) means that we need \(t\) columns to represent the coefficients of \(t\) symbolic variables, while the constant value 2 means that we need 2 extra columns for the constant term and a number representing the operator. In our model, since we only have three different operators, we assign value 0 for =, 1 for ≠, and 2 for ≤, respectively.

Algorithm 1 shows how to vectorize a linear path condition into a matrix, after the path condition has been canonized. We first initialize the Matrix by the number of constraints and the largest index of symbolic variable in the path condition (Lines 1 − 3). The path condition is first split by “\(\land\)” into a list of constraints BCS (Line 4). Each constraint in BCS is checked to set up a row in Matrix (Lines 5 − 24). For each constraint, we first check its operator and set the corresponding item in the row as 0, 1 or 2 (Lines 7 − 13). Then the constraint is further broken down to a list of terms Terms by “\(+\)” after removing the equation operator \(op\) (Lines 14 − 15). As we go through each term in the Terms, if the term is in a shape of \(c_j \times v_j\), we set the \(j\)-th item in the row as \(c_j\) (Lines 17 − 18); otherwise, the term is a constant value \(k\), which is used as the value of the second last item in the row (Lines 20 − 21). After all constraints are processed, we return Matrix as the final vectorized result of the path condition (Line 25).

With this algorithm, any path condition can be transformed into a 2-Dimensional matrix and expanded to a larger equivalent matrix if needed. For instance, the previous example path condition \(x + y - z + 1 \leq 0 \land x - z = 0 \land -x + y - 9 \leq 0\)
Algorithm 1 Algorithm for vectorizing canonized linear PC to a corresponding matrix

Require:Canonized path condition $PC$, which is linear and in shape of $BC_0 \land BC_1 \land \ldots \land BC_m$, where $BC_m$ is in shape of $c_0 \times c_0 + c_1 \times v_1 + \ldots + c_n \times v_n + k \cdot op \cdot 0 \ (op \in \{\cdot, +, \leq\})$

1: $X \leftarrow m+1$;
2: $Y \leftarrow n+3$;
3: $\text{Array}[X][Y] \text{ Matrix} \leftarrow \text{empty}$;
4: $\text{List BCS} \leftarrow \text{PC split by "$\land$"}$;
5: $i \leftarrow 0$;
6: while $i < X$ do
7:   if $op$ in $BCS[i]$ is $"=\"$ then
8:      Matrix[i][Y-1] $\leftarrow$ 0;
9:   else if $op$ in $BCS[i]$ is $"\neq\"$ then
10:      Matrix[i][Y-1] $\leftarrow$ 1;
11:   else if $op$ in $BCS[i]$ is $"\leq\"$ then
12:      Matrix[i][Y-1] $\leftarrow$ 2;
13: end if
14: $BCS[i] \leftarrow BCS[i]$ remove $op$;
15: List Terms $\leftarrow BCS[i]$ split by "$+\"$;
16: for all $\text{term}$ in $\text{Terms}$ do
17:   if $\text{term}$ in shape of $c_j \times v_j$ then
18:      Matrix[i][j] $\leftarrow c_j$;
19:   else
20:      $\{\text{term is the constant term}\}$
21:      Matrix[i][Y-2] $\leftarrow k$;
22: end if
23: end for
24: end while
25: return Matrix;

3.2 Classifying Path Conditions Using a DNN

Figure 4 shows the steps involved to classify a path condition generated in symbolic execution using a DNN that have been trained with existing constraint solutions. The path condition also goes through the same canonizing and vectorizing as in the training stage, in order to get its corresponding matrix. The vectorized path condition in form of a matrix is then sent to a previously trained DNN based on its size (defined by the X and Y dimensions of the matrix) and the classification output (satisfiability of path condition) is then returned to symbolic execution to decide whether the corresponding path is feasible or not.

After training, we only require the DNNs and their corresponding vectorization algorithms to classify a path condition. As long as a path condition can be transformed into a matrix that is acceptable by one of the previously-trained DNNs, our approach is capable to classify the path condition for its satisfiability. Moreover, since DNNs are trained offline, i.e. they are totally separated from symbolic execution runs, users can train a different DNN while the classification with current DNNs is still in progress. This ensures that our framework can be updated and expanded with minimum extra work to check more complicated path conditions.

4 SYMBOLIC EXECUTION WITH DEEPSOLVER

Ideally, a DNN should be about to reach 100% accuracy in classification. However, in practice this goal is extremely difficult to achieve, and in most cases 100% accuracy indicates the possibility of over-fitting problem [14]. An over-fitting problem happens when a classifier is overly refined to a certain data set and thus cannot be applied on other inputs while keeping a high accuracy. As a result, DNNs are usually used with a high accuracy while tolerating potential misclassifications.

When DNNs are used for satisfiability checking of path conditions in symbolic execution, the misclassification problem can make symbolic execution unsound, and thus we need to address the problem. In particular, there are two types of misclassification errors: a satisfiable PC is classified
as unsatisfiable (Type I misclassification) or an unsatisfiable PC is classified as satisfiable (Type II misclassification). We discuss in the following how to deal with each of the two types of misclassification errors.

4.1 Type I Misclassification

When a satisfiable PC is classified as unsatisfiable, the corresponding path is incorrectly identified as infeasible. Since symbolic execution will not continue the exploration of a path when it becomes infeasible, this type of misclassification causes symbolic execution to explore fewer states and must be avoided. To address this problem, we propose to double-check the questionable classification result when a PC is classified as unsatisfiable by calling a conventional constraint solver. This extra constraint solving of course will introduce an overhead; however, this overhead is relatively small for two reasons. First, in most cases, the number of infeasible paths explored in symbolic execution is relatively small compared to the number of feasible paths. Second, assuming the DNN models are highly accurate, the chance of a Type I misclassification happening is low. Therefore, we do not have to frequently double-check the classification result, and thus the overhead introduced by calling a conventional constraint solver is small.

4.2 Type II Misclassification

On the other hand, when a unsatisfiable PC is classified as satisfiable, the corresponding path is incorrectly identified as feasible, and thus symbolic execution may continue exploring states that are in fact not feasible. For intermediate states, instead of double-checking "unsatisfiable" classification results to avoid Type I misclassification errors, we ignore the possible Type II misclassification errors based on the following two observations: First, it is safe to explore some infeasible states. Second, assuming the classification of our approach is highly accurate, it is very likely that symbolic execution based on DNNs will explore few such infeasible states and thus the extra cost is low. Consider an infeasible path with a condition PC as an example. If the classification accuracy of our approach is over 90%, the chance of Type II misclassification less than 10%. When such misclassification happens, symbolic execution will continue on this path and explore another infeasible path with the updated path condition PC′ = PC ∧ c, where c is the new constraint collected along the path. Assuming PC and PC′ are treated independent in DNN classification, the chance of misclassifying both of them is only 10% × 10% = 1%. Therefore, the chance of continuous misclassification drops significantly as the exploration goes deeper. In other words, even if an unsatisfiable PC is classified as satisfiable, it is very likely that the exploration will only explore very small number of extra states before a new PC is classified as unsatisfiable.

For leaf states, which represent complete paths or paths stopped due to errors, we call the underlying constraint solver to find input values to test the corresponding path or to trigger the detected errors, for the two most popular application of symbolic execution: test case generation and error detection.

4.3 Algorithm

Algorithm 2 Symbolic Execution with DeepSolver

Require: Trained DNN model collection M
1: Test Suit T ← ϕ;
2: init.state.PC ← True;
3: stack.push(init.state);
4: Boolean φ ← True;
5: while ~stack.empty() do
6: s ← stack.pop();
7: pc ← s.PC
8: φ ← check(pc, M);
9: if φ is False or pc is not supported by M then
10: φ ← solve(pc);
11: end if
12: if φ is True then
13: for each instruction inst do
14: if inst is if(c) then
15: [Let c be constraint for True branch]
16: s′.PC ← pc ∧ c;
17: stack.push(s);  
18: s′.PC ← pc ∧ ¬c;
19: stack.push(s');
20: break;
21: else if inst is abort or halt then
22: Test case t ← solve(pc);
23: T ← T ∪ {t};
24: break;
25: else
26: s ← execute(inst, s);
27: end if
28: end for
29: end if
30: end while
31: return T

We show our algorithm of symbolic execution with DeepSolver in Algorithm 2. It is similar to traditional forward symbolic execution that uses depth-first search to explore all feasible paths of a program, except for several key steps to address the aforementioned problems. In particular, instead of calling a constraint solver to check the satisfiability of a path condition pc, we first use DeepSolver to check its satisfiability, noted as check(pc, M) (Line 8). This represents the process described in Section 3.2, where the pc is canonized and vectorized to generate the corresponding matrix. If a DNN corresponding to the matrix size exists in M, a Boolean
value of will be returned. If there is no DNN in \( M \) that could handle the matrix, the underlying constraint solver will be called instead. Also, if the classification result shows the \( pc \) is not satisfiable, we double-check it with the constraint solver to avoid Type I misclassification as stated in Section 4.1 (Lines 9 – 11). In addition, constraint solver is called to generate input values for paths that are naturally completed or aborted due to errors (Lines 22 – 23).

5 EVALUATION

This section evaluates DeepSolver on its performance in classifying path conditions as well as in supporting symbolic execution. Our evaluation aims to answer the following four research questions:

- **RQ1:** How accurate is DeepSolver in path condition classification?
- **RQ2:** How efficient is DeepSolver in path condition classification compared to state-of-the-art constraint solving and constraint solution reuse techniques?
- **RQ3:** How do the DNN structure and the size of the training data impact DeepSolver’s accuracy and efficiency?
- **RQ4:** How well does DeepSolver support symbolic execution?

5.1 Implementation and Subjects

We train our DNNs with Keras [15], which is a high-level deep learning API written in Python and is capable of running on top of TensorFlow [7]. We implement canonizing and vectorizing modules, and symbolic execution with DeepSolver in Symbolic Pathfinder (SPF) [39], a widely used open-source symbolic execution framework for Java programs. Since Keras models cannot be directly run with Java framework, we convert the trained DNNs into TensorFlow’s format and run them with official TensorFlow Java library.

The subjects chosen for our evaluation are widely used as benchmarks before for evaluating symbolic execution techniques [9, 12, 26, 27, 37, 41, 42, 48, 54, 55].

**Traffic Anti-Collision Avoidance System (TCAS)** is a system to avoid air collisions. Its code in C together with 41 mutants are available at SIR repository [1]. We manually converted the code to Java and only used the original version for this case study.

**Wheel Brake System (WBS)** is a synchronous reactive component from the automotive domain. This method determines how much braking pressure to apply based on the environment. The Java model is based on a Simulink model derived from the WBS case example found in ARP 4761 [28, 43]. The Simulink model was translated to C using tools developed at Rockwell Collins and manually translated to Java.

**MerArbiter** is a component of the flight software for NASA JPL’s Mars Exploration Rovers (MER).

**Red-Black Tree Data Structure** is the code of data structure originally from Sun’s JDK 1.5.

**Dijkstra** is a benchmark developed by Jacob Burnim from University of California, Berkeley. It is an algorithm for finding the shortest paths between nodes in a graph, which may represent road networks for instance.

**TSP** is a benchmark solution for Traveling Salesman Problem. This subject is developed by Sudeep Juvekar and Jacob Burnim from California, Berkeley.

**Rational** is a case study for computing greatest common divisor and its related operations on rational numbers.

**BinTree** implements a binary search tree with element insertion, deletion.

**BinomialHeap** is a Java implementation of binomial heap.

5.2 DNN Training

As the structure of a DNN may affect its accuracy and efficiency, in this evaluation we compare two different structures of DNN based on the number of hidden layers and the number of neurons in each layer. One small structure has 5 hidden layers and 5 neurons in each layer (we refer to this size as \( 5 \times 5 \)), and one big structure has 10 hidden layers and 10 neurons in each layer (we refer to this size as \( 10 \times 10 \)). Both structures use dense connection with ReLu activation function [8].

Another important factor in deep learning techniques is the training data. Generally speaking, a dataset of thousands of records is enough to train an applicable DNN. A training dataset for image or video processing with deep learning usually has thousands of records. For example, UCF-101 [47] has 13K videos, and HMDB-51 [33] has 6.8K videos. In our evaluation, we use two different training datasets: a small dataset and a large dataset. The small dataset consists of constraint solutions from running symbolic execution with Z3 [6] on TCAS, WBS and MerArbiter. The large dataset consists of all the constraint solutions in the small dataset plus additional constraint solutions from running symbolic execution with Z3 on the mutants of the three subjects. Meanwhile, we noticed that due to different computation orders used in different subjects, there are logically equivalent records in the data sets even after canonization. For instance, \(((2 \times x) + (3 \times y)) − (4 \times z)) + 1 \leq 0\) and \(((2 \times x) + (3 \times y) − (4 \times z)) + 1 \leq 0\) are treated as two records in the datasets although they are identical after being vectorized in to the Matrix. We removed all logically equivalent path conditions from the training datasets, for duplicate records can interfere with our training process and lead to potential over-fitting problem. Finally, the small dataset has 514, 230 records, while the large dataset has 1, 417, 691 records.
We group path conditions based on the number of constraints involved in the path conditions, and train a DNN for each group. The path conditions in our training data have at most 28 constraints involved. Therefore, the size of matrix used in our evaluation ranges from $22 \times 11$ to $22 \times 28$, which represent path conditions with 11-28 constraints and 20 different symbolic variables (20 columns for the 20 symbolic variables and 1 column for the constant term, and 1 column for the operator mark). Table 2 shows the number of records we have for each group of path conditions to train a DNN. Specifically, we have at least 3,584 records (using the small dataset) to train a DNN (for PCs with 11 constraints), and we have at most 150,212 records (using the large dataset) to train a DNN (for PCs with 20 constraints). We did not train DNNs for path conditions that have 10 or fewer constraints since the number of constraint solutions in our dataset for such path conditions is too small to train DNNs.

5.3 Results and Analysis
For the six subjects that are not used for training DNNs, we first run symbolic execution with Z3 [6], a state-of-the-art constraint solving technique, and collect all path conditions with 11 – 28 constraints (as DeepSolver does not support other path conditions). Then, we classify them using a state-of-the-art constraint solution reuse technique GreenTrie and our approach DeepSolver, respectively, and collect data from all three groups of approaches (including Z3) for evaluation.

For DeepSolver, we cross-match two DNN structures and two training datasets. We perform the experiments on the Lonestar 5 cluster at the Texas Advanced Computing Center (TACC) [3]. The computing nodes of Lonestar 5 use Xeon E5-2690 v3 (Haswell) CPU and 64 GB DDR4-2133 memory.

Table 1 shows the results of the experiments. We report the number of path conditions from each subject (# PCs) and the total time cost of solving them with Z3. For GreenTrie, we calculate the total time consumption related to constraint solving including pre-processing the PC, visit and retrieving data from the database, calling and solving the constraint when a cache miss happens. We also report the reuse rate of GreenTrie as the percentage of cache hit to the total invocations. For DeepSolver, we report the time cost as the sum of using deep neural networks to classify PCss as well as the accuracy of classification results. In addition, Table 2 groups the PCs from these six subjects according to the number of constraints involved (11 – 28), and reports the results of each individual DNN of DeepSolver in classifying each group of PCs.

RQ1: How accurate is DeepSolver in path condition classification?
According to the results in the Table 1, the overall accuracy of DeepSolver is high across different subjects. In particular, it always achieves over 97.5% accuracy for classifying PCs across different subjects. We further look into the performance of each individual DNN according to Table 2, and find that each DNN also achieves over 97.5% accuracy.

RQ2: How efficient is DeepSolver in path condition classification compared to conventional constraint solvers and state-of-the-art constraint solution reuse techniques?
We observe in Table 1 that DeepSolver outperforms GreenTrie for all subjects while both DeepSolver and GreenTrie are faster than conventional constraint solvers as expected. The overall speedup range of DeepSolver towards GreenTrie is 2.8X (with $10 \times 10$ DNN structure trained on large database on subject TSP) to 26.8X (with $5 \times 5$ DNN structure trained on small database on subject BinomialHeap), while the speedup range of DeepSolver towards Z3 is 13.6X (with $10 \times 10$ DNN structure trained on small database on subject BinomialHeap) to 28.5X (with $5 \times 5$ DNN structure trained on small database on subject Rational). A more intuitive comparison between the three groups of technique is shown in Figure 5, where we compare the average time cost of satisfiability checking of a path condition. For GreenTrie, we list two different costs of running on small or large database for reuse, and for DeepSolver, we list the average time cost of classifying the path conditions on the 5 × 5 DNN trained on the small dataset. We find that DeepSolver is significantly faster than Z3 or GreenTrie, and moreover the cost of DeepSolver is consistently low across different subjects. The performance of GreenTrie highly depends on the reuse rate, as it still needs to call Z3 when there is no matching of record for reuse. In our evaluation, the overall reuse rate is
Table 1: Results of classifying PCs using DeepSolver compared to Z3 and GreenTrie.

| Subjects      | # PCs | 5X5 DNN | 10X10 DNN |
|---------------|-------|---------|-----------|
|               |       | Small   | Large     | Small   | Large   | Small   | Large   |
|               |       | Time Cost (s) | Accuracy | Time Cost (s) | Accuracy |
| Red-Black Tree| 4907  | 86.83   | 98.2%     | 98.8%     |
| Dijkstra      | 8490  | 88.46   | 99.0%     | 99.5%     |
| TSP           | 11,108| 87.27   | 98.5%     | 99.0%     |
| Rational      | 716   | 87.58   | 98.7%     | 99.2%     |
| BinTree       | 2301  | 3,741   | 92.1%     | 96.0%     |
| BinomialHeap  | 21,156| 5,536   | 92.2%     | 96.3%     |
| Dijkstra      | 10,582| 1,149.55| 98.5%     | 99.0%     |
| TSP           | 11,108| 1,052.69| 98.8%     | 99.3%     |
| Rational      | 716   | 49.27   | 98.6%     | 99.1%     |
| BinTree       | 3,013 | 377.90  | 97.7%     | 98.2%     |
| BinomialHeap  | 23,156| 2,600.19| 98.4%     | 98.9%     |

Table 2: Individual DNN’s accuracy for classifying PCs with 11-28 constraints.

| # Constraints in a PC | # Records in Training Data | # New PCs | 5X5 DNN | 10X10 DNN |
|-----------------------|----------------------------|-----------|---------|-----------|
| 11                    | 12,386                     | 21,397    | 348     | 98.3%     |
| 12                    | 7,507                      | 29,174    | 634     | 98.2%     |
| 13                    | 10,596                     | 27,282    | 915     | 98.0%     |
| 14                    | 14,684                     | 39,805    | 1,421   | 97.9%     |
| 15                    | 19,043                     | 60,723    | 2,380   | 97.3%     |
| 16                    | 25,594                     | 86,656    | 3,907   | 97.0%     |
| 17                    | 34,119                     | 112,415   | 4,547   | 97.0%     |
| 18                    | 43,082                     | 132,410   | 5,306   | 96.8%     |
| 19                    | 51,273                     | 145,182   | 5,955   | 96.6%     |
| 20                    | 57,062                     | 150,212   | 7,877   | 96.4%     |
| 21                    | 59,464                     | 153,509   | 2,624   | 96.0%     |
| 22                    | 61,396                     | 157,405   | 3,159   | 95.9%     |
| 23                    | 64,396                     | 162,405   | 3,159   | 95.9%     |
| 24                    | 66,876                     | 164,421   | 3,163   | 95.8%     |
| 25                    | 74,768                     | 166,667   | 2,018   | 95.9%     |
| 26                    | 82,000                     | 168,421   | 3,129   | 95.8%     |
| 27                    | 91,216                     | 173,764   | 2,827   | 95.7%     |
| 28                    | 93,843                     | 178,386   | 295     | 95.0%     |

5.4 Threats to Validity

For external threats to validity, our results may not generalize to other subjects. Our study was performed on subjects that were used in previous studies of symbolic execution techniques, and only limited subjects and versions are suitable for data collection, training and classification purposes. To mitigate this threat we trained and selected multiple models, and carefully selected the results that can be potentially generalized, but it should be noticed that in deep learning the reuse rate is challenging for constraint reuse techniques. In contrast, for DeepSolver, we are still capable of training a powerful DNN using a relatively small dataset.

RQ4: How well does DeepSolver support symbolic execution?

We implemented the Algorithm 2 in Symbolic Pathfinder (SPF) to use DeepSolver to support symbolic execution. Table 3 shows the results of running SPF with DeepSolver using 5 x 5 DNN structure trained with large dataset compared to running SPF with GreenTrie using the same dataset. When a path condition is not supported by DeepSolver, we use Z3 to solve it. For each approach, we report the number of solved/classified PCs, the number of states, and the total time cost. For SPF with DeepSolver we also report the number of misclassification errors as well as the number of leaf states.

According to the results in the table, we find that due to the high accuracy of DeepSolver, the number of each type of misclassification errors are very small compared to the total PCs. Since we ignored Type II misclassification errors, DeepSolver checked more PCs and explored more states than GreenTrie. In the meantime, Type I misclassification happened in 4 out of 6 subjects. Despite the overhead introduced in addressing both of the two types of classification errors, the overall time cost of symbolic execution with DeepSolver is still much smaller than symbolic execution with GreenTrie (e.g., 2.80X speedup on BinomialHeap). This result demonstrates that the highly accurate and efficient PC classification in DeepSolver can greatly improve the efficiency of symbolic execution.
we used, including Keras, TensorFlow and SPF. To mitigate
the over-fitting problem with our DNNs, we mitigate this thread by introducing the large training dataset, as the mutations of subjects contributes a number of unsatisfiable path conditions which makes the large dataset more balanced than the small dataset. Based on the evaluation results, our DNNs can achieve more than 70% accuracy in classifying unsatisfiable path conditions.

For internal threats to validity, although we have carefully checked our implementation, it is possible that there are errors we did not notice. There are also potential threats related to correctness of the techniques and frameworks we used, including Keras, TensorFlow and SPF. To mitigate these threats, we treat them as black-box to ensure that we only made the necessary change to the original SPF implementation. Meanwhile, over-fitting is a common problem when training a DNN. To control this threat, we used different techniques including purifying and shuffling the data, changing the ratio of training/testing data, using different DNN structures and applying k-fold validation technique. The evaluation results show that all DNNs have a stable and high accuracy on different datasets, and there is no trace of over-fitting problem with our DNNs.

6 RELATED WORK
6.1 Machine Learning for Constraint Satisfaction Problems
Researches have been dedicated to applying machine learning techniques to constraint satisfaction problems with different models and techniques including support vector machines [10], linear regression [53], decision tree learning [19, 22], clustering [29, 40], k-nearest neighbors [36], and so on [31]. Xu et. al [24] successfully applied deep learning to predict the satisfiability of Boolean binary constraint satisfaction problems with high prediction accuracy. Different from our approach, this approach uses randomly generated constraint satisfaction problems as training data and applied a convolutional neural network (CNN) as the deep learning model, while we take the existing constraint solutions as a training data set and use a simpler DNN structure. Moreover, this approach only aims to predict the satisfiability of Boolean binary constraints, while our approach classify the satisfiability of path conditions that may have multiple symbolic variables. Meanwhile, our study is the first to evaluate DNN based path condition classification in terms of accuracy and efficiency compared to regular constraint solving and constraint solution reuse techniques.

6.2 Reuse of Constraint Solutions
Many techniques have been developed to speed up symbolic execution by reusing previous constraint solutions. For example, KLEE [13] optimizes constraint solving by an approach named counterexample caching. With the cached constraint solving results, KLEE can quickly check satisfiability of a path condition if it is a similar query to one of the stored records: If a path condition has a subset that is already known as unsatisfiable, it is unsatisfiable as well. Similarly, if a path condition has an already known satisfiable superset in the cache, it is satisfiable.

Green [50] applies Redis in-memory database to maintain the constraint solutions, and uses slicing and canonizing to path conditions in order to increase the reusing rate. To further improve Green, GreenTrie [27] stores constraints and solutions into L-Trie, which is indexed by an implication partial order graph of constraints and is able to carry out logical reduction and logical subset and superset querying for given constraints. GreenTrie provides more flexibility to conventional Green framework and expands the number of path conditions that can reuse previous constraint solutions. Compared to Green and GreenTrie, our approach reuse the collective knowledge of previous constraint solutions: once the DNN was trained offline, we do not need to use individual constraint solutions and can quickly classify the satisfiability of a path condition as long as it can be transformed into the required form of matrix.

Unlike techniques that store path conditions and their satisfiability information, memoized symbolic execution [55, 56] stores positions and choices taken during symbolic execution

| Subjects SPF with GreenTrie (Large Data Set) | SPF with DeepSolver (5X5 DNN Trained with Large Data Set) |
|---------------------------------------------|----------------------------------------------------------|
| # PCs | # States | Time Cost (s) | # PCs | Type I Misclassification | Type II Misclassification | # States | # Leaf States | Time Cost (s) |
|------|-------|-------------|------|----------------|-----------------|-------|-------------|-------------|
| Red-Black Tree | 1,329 | 1,330 | 395 | 1,331 | 0 | 2 | 1,332 | 15 | 182 |
| Dijkstra | 10,646 | 10,647 | 2,784 | 10,649 | 2 | 3 | 10,650 | 73 | 1,582 |
| TMF | 13,212 | 13,213 | 2,418 | 13,215 | 2 | 3 | 13,216 | 50 | 1,189 |
| Rational | 744 | 745 | 146 | 748 | 0 | 7 | 749 | 16 | 115 |
| BinTree | 3,467 | 3,468 | 907 | 3,579 | 1 | 12 | 3,580 | 37 | 362 |
| BinomialHeap | 23,216 | 23,217 | 7,651 | 23,230 | 5 | 14 | 23,231 | 385 | 2,713 |
in a trie [52] – an efficient tree-based data structure. When applied to regression analysis, the trie guided symbolic execution would potentially skip exploration of portions of program paths, whereas symbolic execution using our approach would only skip calls to the underlying constraint solver. Our approach could work together with memoized symbolic execution to provide a fast classification of path conditions whenever program paths cannot be skipped by memoized symbolic execution.

Some techniques take advantage of test suites to reduce expensive constraint solving calls typically in regression testing. For instance, Makhdoum et al. [34] use the test suite of a previous program version to check whether a new path condition is satisfiable or not. Hossain et al. [25] reuse constraint values by comparing the variables’ definitions and uses between program versions. If the definitions and uses for a certain variable have not changed on a certain path, constraint values for the variable in the old version can be reused in the new version. While these approaches reuse existing test cases for the purpose of maintaining an effective test suite for regression testing, our technique is designed to reuse constraint solving results for the purpose of efficiently classifying path conditions encountered in symbolic execution of different programs.

7 CONCLUSION AND FUTURE WORK

Symbolic execution is a powerful software engineering analysis technique, but suffers from the high cost of constraint solving. In this paper we introduced DeepSolver, a novel approach to solve constraints based on deep learning, which leverages existing constraint solutions for training DNNs to classify path conditions for their satisfiability during symbolic execution. To the best of our knowledge, this is the first work that results in a fully functional and applicable solution to use deep learning on constraint solution reuse for symbolic execution. Our evaluation shows that DeepSolver is highly applicable with a high accuracy, more efficient than conventional constraint solving and multiple existing constraint solution reuse frameworks in classifying path conditions for satisfiability, and can well support overall symbolic execution task. For future work, we plan to further evaluate our approach on more real-world artifacts, and compare our solution with other constraint solution reuse techniques. We also plan to investigate the use of different DNNs for our approach, e.g., exploring the best DNN structures for path conditions with different features, and building a universal DNN for all path conditions.

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