Neuro-Symbolic Execution: The Feasibility of an Inductive Approach to Symbolic Execution

Shiqi Shen   Soundarya Ramesh   Shweta Shinde
Abhik Roychoudhury   Prateek Saxena
National University of Singapore
{shiqi04, soundary, shweta24, abhik, prateeks}@comp.nus.edu.sg

ABSTRACT
Symbolic execution is a powerful technique for program analysis. However, it has many limitations in practical applicability: the path explosion problem encumbers scalability, the need for language-specific implementation, the inability to handle complex dependencies, and the limited expressiveness of theories supported by underlying satisfiability checkers. Often, relationships between variables of interest are not expressible directly as purely symbolic constraints. To this end, we present a new approach — neuro-symbolic execution — which learns an approximation of the relationship as a neural net. It features a constraint solver that can solve mixed constraints, involving both symbolic expressions and neural network representation. To do so, we envision such constraint solving as a procedure combining SMT solving and gradient-based optimization. We demonstrate the utility of neuro-symbolic execution in constructing exploits for buffer overflows. We report success on 13/14 programs which have difficult constraints, known to require specialized extensions to symbolic execution. In addition, our technique solves 100% of the given neuro-symbolic constraints in 73 programs from standard verification and invariant synthesis benchmarks.

1 INTRODUCTION
Symbolic execution is a code analysis technique which reasons about sets of input values that drive the program to a specified state [52]. Certain inputs are marked as symbolic and the analysis gathers symbolic constraints on these values, by analyzing the operations along a path of a program. Satisfying solutions to these constraints are concrete values that cause the program to execute the analyzed path leading to a particular state of interest. Manipulating these constraints allows one to reason about the reachability of different paths and states, thereby serving to guide search in the execution space efficiently. Symbolic execution, especially its mixed-dynamic variant, has been widely used in computer security. Its prime application over the last decade has been in white-box fuzzing, with the goal of discovering software vulnerabilities [42, 43, 82]. More broadly, it has been used for patching [30, 74], invariant discovery [46], and verification to prove the absence of vulnerabilities [24, 48]. Off-the-shelf symbolic execution tools targeting languages such as C/C++ [86], JavaScript [1, 58], Python [2, 20], and executable binary code [23] are available.

Symbolic analysis is a powerful technique; however, it has a number of limitations in practical applicability. First, symbolic analysis is mostly designed as a deductive procedure classically, requiring complete modeling of the target language (e.g., C vs. x64). A set of logical rules specific to the target language describe how to construct symbolic constraints for operations in that language [49, 83]. As new languages emerge, such symbolic analysis needs to be re-implemented for each language. More importantly, if a certain functionality of a program is unavailable for analysis — either because it is implemented in a language different from the target language, or because it is accessible as a closed, proprietary service — then, such functionality cannot be analyzed.

Second, the reasoning about symbolic constraints is limited to the expressiveness of theories supported by underlying satisfiability checkers (e.g., SAT / SMT solvers) [10]. Symbolic analysis typically uses quantifier-free and decidable theories in first-order logic, and satisfiability solvers have well-known limits [4]. For instance, non-linear arithmetic over reals is not well supported in existing solvers, and string support is relatively new and still an area of active research [37, 95]. When program functionality does not fall within the supported theories, analysis either precludes such functionality altogether, or encodes it abstractly using supported theories (e.g., arrays, bit-vectors, or uninterpreted functions).

Third, symbolic analyses often enumeratively analyze multiple paths in a program. Complex control flows and looping structures are well-known to be missed by state-of-the-art implementations, which have attracted best-effort extensions to the basic technique and do not offer generality [84]. In particular, dynamic symbolic execution is known to suffer from scalability issues in long-running loops containing a large number of acyclic paths in the iterations, owing to loop unrolling and path explosion [19, 91].

1.1 Neuro-Symbolic Execution
In this paper, we aim to improve the expressiveness of symbolic execution to reason about parts of the code that are not expressible in the theories supported by the symbolic language (including its SMT theories), too complex, or simply unavailable in analyzable form. We present a technique called neuro-symbolic execution, which accumulates two types of constraints: standard symbolic constraints (derived deductively) and neural constraints (learned inductively). Neural constraints capture relations between program variables of code that are not expressible directly as purely symbolic constraints. The representation of these constraints is chosen to be a neural network (or neural net) in this work. The constraints including both symbolic and neural constraints are called neuro-symbolic.

Our procedure infers and manipulates neural constraints using only two generic interfaces, namely learn and check satisfaction. The first interface learns a neural network given concrete values of variables and an objective function to optimize. The second interface checks for satisfiability: given an output value for a neural network, finding whether an input evaluates to it. Both of these can be instantiated by many different procedures; we present a specific set of algorithms in this work for concreteness. We believe
the general framework can be extended to other machine learning models which can implement such interfaces.

Our choice of representation via neural networks is motivated by two observations. First, neural nets can approximate or represent a large category of functions, as implied by the universal approximation theorem [36, 47]; and in practice, an explosion of empirical results are showing that they are learnable for many practical functions [7, 44]. Although specialized training algorithms are continuously on the rise [53, 76], we expect that neural networks will prove effective in learning approximations to several useful functions we encounter in practice. Second, neural nets are a differentiable representation, often trained using optimization methods such as gradient descent [79]. This differentiability allows for efficient analytical techniques to check for satisfiability of neural constraints, and produce satisfying assignments of values to variables [45, 73] — analogous to the role of SMT solvers for purely symbolic constraints. One of the core technical contributions of this work is a procedure to solve neuro-symbolic constraints: checking satisfiability and finding assignments for variables involved in neural and symbolic constraints simultaneously, with good empirical accuracy on benchmarks tested.

Inductive synthesis of symbolic constraints usable in symbolic analyses has been attempted in prior work [35, 70, 71]. One notable difference is that our neural constraints are a form of unstructured learning, i.e. they approximate a large class of functions and do not aim to print out constraints in a symbolic form amenable to SMT reasoning. Prior constraint synthesis works pre-determine a fixed template or structure of symbolic constraints — for instance, octagonal inequalities [71], low-degree polynomial equalities over integers [35], and so on. Each such template-based learning comes with a specialized learning procedure and either resorts to standard SMT solvers for solving constraints, or has hand-crafted procedures specialized to each template type. As a result, these techniques have found limited applicability in widely used symbolic execution analyses. As a side note, when the code being approximated does not fall within chosen template structure in prior works, they resolve to brute-force enumeration of templates to fit the samples.

1.2 Applications & Results

Neuro-symbolic execution has the ability to reason about purely symbolic constraints, purely neural constraints, and mixed neuro-symbolic constraints. This approach has a number of possible future applications, including but not limited to: (a) analyzing protocol implementations without analyzable code [29]; (b) analyzing code with complex dependency structures [92]; and (c) analyzing systems that embed neural networks directly as sub-components [13].

To anchor our proposal, we focus on the core technique of neuro-symbolic execution through the lens of one application — finding exploits for buffer overflows. In this setting, we show that neuro-symbolic execution can be used to synthesize neural constraints from parts of a program, to which the analysis only has black-box executable access. The program logic can have complex dependencies and control structure, and the technique does not need to know the operational semantics of the target language. We show that for many real programs, our procedure can learn moderately accurate models, incorporate them with symbolic memory safety conditions, and solve them to uncover concrete exploits.

**Tool.** We build a prototype tool (called NeuEx) to perform neuro-symbolic execution of C programs, where the analyst specifies which parts of the code it wants to treat as a black-box, and a memory safety condition (symbolic) which captures an exploit. NeuEx uses standard training algorithms to learn a neural net which approximates the black-box functionality and conjoins it with other symbolic constraints. Next, NeuEx employs a new procedure to solve the symbolic and neural constraints simultaneously, yielding satisfying assignments with high probability. The tool is constructive, in that it produces concrete values for free variables in the constraints, which can be tested as candidate exploits.

**Results.** Our main empirical results are two-fold. First, we select a benchmark which has difficult constraints, known to require specialized extensions to symbolic execution. We show that NeuEx finds exploits for 13/14 of programs in the benchmark. Our results are comparable to binary-level symbolic execution tools [84] with little knowledge of the semantics of the target code and the specific language. The second empirical experiment analyzes two benchmarks used in prior works in invariant synthesis for verification and program synthesis [70, 71]. They comprise 73 programs with 82 loops and 259 input variables in total. Given the neuro-symbolic constraints, NeuEx successfully solves 100% neuro-symbolic constraints for these benchmarks.

**Contributions.** We make the following contributions:

- **Neuro-Symbolic Constraints.** NeuEx represents the relationship between variables of code as a neural net without the knowledge of code semantics and language, and then conjoins it along with symbolic constraints.
- **Neuro-Symbolic Constraint Solving.** NeuEx envisions constraint solving as a search problem and encodes symbolic constraints as an objective function for optimization along with neural net to check their satisfiability.
- **Evaluation.** NeuEx successfully constructs exploits for 13 out of 14 vulnerable programs, which is comparable to binary-level symbolic execution [84]. In addition, NeuEx solves 100% of given neuro-symbolic constraints over 73 programs comprising of 259 input variables in total.

2 OVERVIEW

Symbolic execution provides a tool that is useful in a variety of security-related applications. In this work, we focus on the challenges within symbolic execution and present a solution that is general for various kinds of programs.

2.1 Motivation and Challenges

We outline a set of challenges posed to symbolic execution with the help of a real-world example from an HTTP server.

**Motivating Example.** Consider the simplified example of parsing the HTTP request shown in Figure 1. The code extracts the fields (e.g., uri and version) from the request and constructs the new message for further processing. Our goal is to check whether there exists any buffer overflow in this program. If so, we find the exploit that triggers the overflow. As shown in Figure 1, on Line 4-5,
void process_request(char * input){
    char URI[100], version[100], msgbuf[100];
    int ptr=0, uri_len=0, ver_len=0, i, j;
    if(strcmp(input, "GET \"", 4)!=0)
        fatal("Unsupported request!");
    while(input[ptr]!='\n'){
        if(uri_len>=88) URI[uri_len] = input[ptr];
        uri_len++, ptr++;
    }
    ptr++;
    while(input[ptr]!='\0'){
        if(ver_len==88) version[ver_len]=input[ptr];
        ver_len++, ptr++;
    }
    if(ver_len%8 || version[5]!=\"\")
        fatal("Unsupported protocol version");
    for(i=0,ptr=0, i<uri_len; i++,ptr++)
        msgbuf[ptr] = URI[i];
    while(input[ptr]!='\n'){
        if(uri_len<80) URI[uri_len] = input[ptr];
        ptr++;
        uri_len++; ptr++;
    }
    if(ptr!=\"\")
        fatal("Unsupported protocol version");
    for(j=0;j<ver_len;j++,ptr++)
        msgbuf[ptr]=version[j]; // buffer overflow
    msgbuf[ptr] = \"\0\"; // buffer overflow
    ... 
}

Figure 1: A simplified example that parses the HTTP request and constructs a new message.

the function process_request takes one input input and checks whether input starts with \"GET\". On Line 6-14, it finds the URI and version from input by searching for the delimiter \"\" and \'\n\' separately. Then, the function checks whether the program supports the request on Line 15-16 based on the version. Finally, it concatenates the version URI with the delimiter \"\" into a buffer msgbuf on Line 17-22. There exists a buffer overflow on Line 21-22, as the pointer ptr may exceed the boundary of msgbuf.

Challenge 1: Complex Dependency. To discover this buffer overflow via purely symbolic analysis, the technique has to reason about a complex dependency structure between the input and the variables of interest. Assume that the analyst has some knowledge of the input format, namely that the input has fields, URI and version, separated by \"\" and \'\n\' and knows the allocated size of the msgbuf (which is 100). By analyzing the program, the analyst knows the vulnerable condition of msgbuf is ptr>99, which leads to buffer overflows. Note that the path executed for reaching the vulnerability point on Line 21-22 involves updates to a number of variables (on Line 8 and 13) which do not have a direct dependency chain (rather a sequence of control dependencies) on the target variable ptr. Specifically, uri_len and ver_len are dependent on input, which in turn control ptr and the iterations of the vulnerable loop. Further, the relationship between uri_len, ver_len, and ptr involves reasoning over the conditional statements on Line 4 and 15, which may lead to the termination of function. Therefore, without specialized heuristics (e.g., loop-extension [84]), the state-of-the-art solvers resort to enumeration [17]. For example, KLEE enumerates characters on input over \"\" and \'\n\' until the input passes the checking on Line 15 and ver_len=uri_len+98.

The unavailability of source code is another challenge for capturing complex dependency between variables, especially when the functions are implemented as a remote call or a library call written in a different language. For example, a symbolic execution may abort for calls to native Java methods and unmanaged code in .NET, as the symbolic values flow outside the boundary of target code [6]. To handle this challenge, symbolic execution has to hard-code models for these unknown function calls, which requires considerable manual expertise. Even though symbolic execution tools often provide hand-crafted models for analyzing system calls, they do not precisely capture all the behaviors (e.g., the failure of system calls) [17]. Thus, the constraints generated by purely symbolic execution cannot capture the real behavior of functions, which leads to the failure in vulnerability detection.

Challenge 2: Lack of Expressiveness. Additional challenges can arise in such analysis due to the complexity of the constraint and the lack of back-end theorem for solving the constraint. As shown in Figure 1, the function is equivalent to a replacement based on regular expressions. It replaces the request of the form, "GET \"\" URI \", Version \"\"n\"\", to the message of the form, URI \", \"Version \"\"0\"\" on Line 4-22.¹ The complex relationship between the input and target buffer makes it infeasible for symbolic execution to capture it. Moreover, even if the regular expression is successfully extracted, the symbolic engine may not be able to solve it as the embedded SAT/SMT solver is not able to express certain theories (e.g., the string replacement and non-linear arithmetic). Although works have targeted these theories, current support for non-linear real and integer arithmetic is still in its infancy [4].

2.2 Our Approach

To address the above challenges, we propose a new approach with two main insights: (1) leveraging the high representation capability of neural nets to learn constraints when symbolic execution is infeasible; (2) encoding the symbolic constraints into neural constraint and leveraging the optimization algorithms to solve the neuro-symbolic constraints as a search problem.

NeuEx departs from the purist view that all variable dependencies and relations should be expressible precisely in a symbolic form. Instead, NeuEx treats the entire code from Line 4-22 as a black-box, and inductively learn a neural network — an approximate representation of the logic mapping the variables of interest to target variables. The constraint represented by the neural network is termed neural constraint. This neural constraint, say N, can represent relationships that may or may not be representable as symbolic constraints. Instead, our approach creates a neuro-symbolic constraint, which includes both symbolic and neural constraints. Such neural constraint learning addresses the preceding first challenge as it learns the constraints from test data rather than source code.

Revisiting the example in Figure 1, the neuro-symbolic constraints capturing the vulnerability at the last control location on Line 22 are as follows.

\[
\begin{align*}
\text{uri}_1\text{\_length} &= \text{strlen(input\_uri)} \quad (1) \\
\text{ver}_1\text{\_length} &= \text{strlen(input\_version)} \quad (2) \\
\text{ptr} &> 99 \quad (3) \\
N : (\text{uri}_1\text{\_length}, \text{ver}_1\text{\_length}) \mapsto \{\text{ptr}\} \quad (4)
\end{align*}
\]

where \text{uri}_1\text{\_length} is the length of uri field input\_uri and \text{ver}_1\text{\_length} is the length of version field input\_version in input.² The first

¹ \& matches as many characters as possible.
² input\_uri and input\_version are the content of the fields from input generated based on the knowledge of input, which is different from URI and version in Figure 1.
Variables
Symbolic
Target
Although this is a valid satisfiability result for the neural constraint, Table 1 presents the syntax of the neuro-symbolic constraint language supported by NeuEx.

| Neuro-Symbolic Constraint | NS | £ | N \land S |
|---------------------------|----|---|---|
| Neural constraint         | N  | £ | V_{in} \iff V_{on} |
| symbolic constraint       | S  | £ | e_1 \oplus e_2 | e |
| Variable                  | StrVar | £ | ConstStr | StrVar|StrVar |
|                           | NumVar | £ | ConstNum | NumVar|NumVar |
| Expression                | e   | £ | \text{contains(StrVar, StrVar)} | strtol(StrVar) | NumVar |
|                           |     |   | NumVar | NumVar |
| Logical                   | \ominus | £ | \lor | \land |
| Conditional               | \ominus | £ | \equiv | \geq | \prec | \leq |
| Arithmetic                | \ominus | £ | + | - | | * | / |

two constraints are symbolic constraints over the input fields, \texttt{ur1\_length} and \texttt{ver\_length}. The third symbolic constraint captures the vulnerable condition for \texttt{msgbuf}. The last constraint is a neural constraint capturing the relationship between the variable \texttt{ur1\_length} and \texttt{ver\_length} and the variable \texttt{ptr} accessing the vulnerable buffer \texttt{msgbuf}.

To the best of our knowledge, our approach is the first to train a neural net as a constraint and solve both symbolic and neural constraint together. In our approach, we design an intermediate language, termed as neuro-symbolic constraint language. Table 1 presents the syntax of the neuro-symbolic constraint language supported by NeuEx, which is expressive enough to model various constraints specified in many real applications such as string and arithmetic constraints.

Given the learned neuro-symbolic constraints, we seek the values of variables of interest that satisfy all the constraints within it. There exist multiple approaches to solve neuro-symbolic constraints. One naive way is to solve the neural and symbolic constraints separately. For example, consider the neuro-symbolic constraints in Equation 1-4. We first solve the three symbolic constraints by SAT/SMT solvers and then discover a \textit{input\_uri} where \texttt{ur1\_length}=10, a \textit{input\_version} where \texttt{ver\_length}=20 and a \texttt{ptr} whose value is 100. Then, we feed the values of \texttt{ur1\_length}, \texttt{ver\_length} and \texttt{ptr} to the neural constraint to check whether it satisfies the learned relationship. For the above case, the neural constraint produces the output such as 32 for the \texttt{ptr} when \texttt{ur1\_length}=10 and \texttt{ver\_length}=20. Although this is a valid satisfiability result for the neural constraint, \texttt{ptr}=100 is not satisfiable for the current \textit{input\_uri} and \textit{input\_version}. This discrepancy arises because we solve these two types of constraints individually without considering the inter-dependency of variables within these constraints. Alternatively, one could resort to enumeration over values of these three variables as a solution. However, it will require a lot of time for discovering the exploit.

This inspires our design of neuro-symbolic constraint solving. NeuEx’s solving precedence is purely symbolic, purely neural and mixed constraints, in that order. Solving pure constraints is straightforward [33, 79]. The main technical novelty in our design is that NeuEx treats the mixed constraint solving as a search problem and utilizes the optimization algorithm to search for the satisfying solutions. To solve the mixed constraints simultaneously, NeuEx converts symbolic constraints to a loss function (or objective function) which is then used to guide the optimization of the loss function, thereby enabling conjunction of symbolic and neural constraints.

3 DESIGN
NeuEx is the first tool to solve neuro-symbolic constraints. We first explain the NeuEx setup and the building blocks we use in our approach. Then, we present the core constraint solver of NeuEx along with various optimization strategies.

3.1 Overview
Symbolic execution is a generic technique to automatically construct inputs required to drive the program’s execution to a specific program point in the code. To this end, a typical symbolic execution framework takes in a program and a vulnerable condition for which we want to test the program. The analyst using the framework also needs to mark the variables of interest as symbolic. Typically, all the input variables are marked symbolic irrespective of its type. Further, environment variables, implicit inputs, user events, storage devices can also be marked as symbolic based on the use-case [17, 18, 83]. Then the framework generates a set of test inputs to execute an execution path in the program. The analyst can aid this process by providing hints about input grammar and so on, which they know beforehand.

At each branch in the execution, the framework logs the symbolic constraints collected so far as the path conditions required to reach this code point. Specifically, a logical conjunction of all the symbolic constraints gives us the path constraints that have to be satisfied by the input to reach this code point. Solving the symbolic path constraints gives us the concrete input value which can lead us to this execution point in the program, by invoking a constraint solver to produce concrete values. The framework may also negate the symbolic constraints to explore other paths in the program or introduce a feedback loop which uses the concrete input.
Thus, whenever the symbolic engine’s default constraint solver is not able to find a solution and reaches its timeout, the framework can pause its execution and automatically trigger an alternative mechanism. This is where a neural constraint solver comes into play. If the framework is armed with a neural constraint solver such as NeuEx, it can model parts of the program as a black-box and invoke the neural counterpart to solve the constraints. Specifically, the framework can dispatch all the symbolic constraints it has collected so far along with the piece of code it wants to treat as a black box. NeuEx in turn first adds all the symbolic constraints to the symbolic execution tool to provide two interfaces: one for outputting the symbolic constraints and the other for querying the SAT/SMT solvers as shown in Figure 2. Table 1 shows the grammar that NeuEx’s constraint solver can reason about. For our example in Figure 1, we want to infer the vulnerable buffer msgbuf relations between input HTTP request and variable index accessing the vulnerable buffer msgbuf. So the symbolic framework will pass the following constraints to NeuEx:

\[
\text{uri\_length} = \text{strlen}([\text{input\_uri}]) \land \\
\text{ver\_length} = \text{strlen}([\text{input\_version}]) \land \\
\text{ptr} > 99 \land \\
N : \{\text{uri\_length}, \text{ver\_length}\} \rightarrow \{\text{ptr}\}
\] (5)

### 3.2 Building Blocks

NeuEx’s core engine solves the neuro-symbolic constraints such as in Equation 5 using its custom constraint solver detailed in Section 3.3. It relies on two existing techniques: SAT/SMT solver and gradient-based neural solver. These solvers referred to as SymSolv and NeuSolv respectively form the basic building blocks of NeuEx.

**SymSolv.** NeuEx’s symbolic constraint solver takes in first-order quantifier-free formulas over multiple theories (e.g., empty theory, the theory of linear arithmetic and strings) and returns UNSAT or concrete values as output. It internally employs Z3 Theorem Prover [33] as an SMT solver to solve both arithmetic and string symbolic constraints.

**NeuSolv.** For solving purely neural constraints, NeuSolv takes in the neural net and the associated loss function to generate the expected values that the output variables should have. NeuEx considers the neural constraint solving as a search problem and uses a gradient-based search algorithm to search for the satisfiable results. Gradient-based search algorithm searches for the minimum of a given loss function \( L(X) \) where \( X \) is a n-dimensional vector [79]. The loss function can be any differentiable function that monitors the error between the objective and current predictions. Consider the example in Figure 1. The objective of NeuEx is to check whether the index \( \text{ptr} \) overruns the boundary of \( \text{msgbuf} \). Hence, the error is the distance between the value of \( \text{ptr} \) leading to the buffer overflow and the value of \( \text{ptr} \) on Line 22 given by the function \( \text{process\_request} \) with current input. By minimizing the error, NeuEx can discover the input closest to the exploit. To minimize the error, gradient-based search algorithm first starts with a random input \( X_0 \) which is the initial state of NeuSolv. For every enumeration \( i \), it computes the derivative \( \nabla_{X_i} L(X_i) \) of \( L(X_i) \) given the input \( X_i \) and then update \( X_i \) according to \( \nabla_{X_i} L(X_i) \). This is based on the observation that the derivative of a function always points to a local nearest valley. The updated input \( X_{i+1} \) is defined as:

\[
X_{i+1} = X_i - \epsilon \nabla_{X_i} L(X_i)
\] (6)

where \( \epsilon \) is the learning rate that controls how much is going to be updated. Gradient-based search algorithm keeps updating the input until it reaches the local minima. To avoid the non-termination case, we set the maximum number of enumerations to be \( M_e \). If it exceed \( M_e \), NeuSolv stops and returns current updated result. Note that gradient-based search algorithm can only find the local minima since it stops when the error increases. If the loss function is a non-convex function with multiple local minima, the found local minima may not be the global minima. Moreover, it may find different local minima when the initial state is different. Thus, NeuEx executes the search algorithm multiple times with different initial states in order to find the global minima of \( L(X) \).
3.3 Constraint Solver

We propose a constraint solver to solve the neuro-symbolic constraints with the help of SymSolv and NeuSolv. If the solver returns SAT, then the neuro-symbolic constraints guarantee to be satisfiable. It is not guaranteed to decide all satisfiability results with a timeout. Algorithm 1 shows the algorithm for neuro-symbolic constraint solver. Interested readers can refer to Algorithm 1 for the precise algorithm.

**Algorithm 1** Algorithm for neuro-symbolic constraint solving. $Sp$ is purely symbolic constraints; $Np$ is purely neural constraints; $Sm$ and $Nm$ are symbolic constraints and neural constraints in mixed components.

```
1: function NeuCL($S, N$) → $S$: Symbolic constraint list; $N$: Neural constraint list
2:   ($Sp$, $Np$, $Sm$, $Nm$) ← CheckDependency($N$, $S$);
3:   ($X$, assign1) ← SymSolv($Sp$, $\emptyset$);
4:   if $X = \text{UNSAT}$ then
5:     return (False, $\emptyset$);
6:   end if
7:   cnt ← 0;
8:   while cnt<MAX_TRIAL1 do
9:     ($X$, assign2) ← NeuSolv($Np$);
10:    if $X = \text{SAT}$ then
11:       go to 16
12:    end if
13:    cnt ← cnt+1;
14:   end while
15:   go to UNSAT
16:   assign ← Union(assign1, assign2);
17:   ConflictDB ← $\emptyset$; trial_cnt ← 0;
18:   while trial_cnt<MAX_TRIAL2 do
19:     ConflictConsts ← CreateConflictConsts(ConflictDB)
20:    ($X$, assign3) ← SymSolv($Sm$, ConflictConsts);
21:    if $X = \text{UNSAT}$ then
22:      go to SAT
23:    end if
24:    NeuralConsts ← PartialAssign($Nm$, assign3); cnt ← 0;
25:   while cnt<MAX_TRIAL1 do
26:     ($X$, assign4) ← NeuSolv(NeuralConsts);
27:     if $X = \text{SAT}$ then
28:       assign2 ← NeuSolv($F$);
29:       assign3 ← $X = \text{SAT}$;
30:     end if
31:     cnt ← cnt+1;
32:   end while
33:   trial_cnt ← trial_cnt+1;
34:   ConflictDB ← ConflictDB $\cup$ assign3;
35:   end while
36:   trial_cnt ← 0; $F$ ← Encode($Sm$, $Nm$);
37:   while trial_cnt<MAX_TRIAL1 do
38:     assign2 ← NeuSolv($F$);
39:     $X$ ← CheckSAT(assign2, $Sm$);
40:     if $X = \text{SAT}$ then
41:       go to SAT
42:     end if
43:     trial_cnt ← trial_cnt+1;
44: end while
45: UNSAT:
46:   return (False, $\emptyset$);
47: SAT:
48:   return (True, Union(assign, assign2))
```

DAG Generation. NeuEx takes the neuro-symbolic constraints and generates the directed acyclic graph (DAG) between constraints and its variables. Each vertex of the DAG represents a variable or constraint, and the edge shows that the variable is involved in the constraint. For example, Figure 3 shows the generated DAG for constraints $(V_1 \circ_{p_1} V_2) \land (V_5 \circ_{p_2} V_4) \land (V_5 \circ_{p_2} V_4) \land (V_6 \circ_{p_3} V_3 \circ_{p_4} V_6) \land (V_7 \circ_{p_5} V_6)$ where $p_i$ can be any operator.

Next, NeuEx partitions the DAG into connected components by breadth-first search [16]. Consider the example shown in Figure 3. There are 5 constraints that are partitioned into three connected components, $G_1$, $G_2$ and $G_3$. NeuEx topologically sorts the components based on the type of constraints to schedule the solving sequence. Specifically, it clusters the components with only one kind of constraints as pure components (e.g., $G_1$ and $G_2$) and the components including both constraints as mixed components (e.g., $G_3$). It further sub-categorizes pure components into purely symbolic (e.g., $G_1$) and purely neural constraints (e.g., $G_2$).

NeuEx assigns solving precedence to be pure and mixed constraints. NeuEx solves the mixed constraints in the end because the constraints have different representation and hence are time-consuming to solve. Thus, in our example, NeuEx first solves $S_1 \land N_1$ and then checks the satisfiability of $S_2 \land N_2 \land S_3$.

Pure Constraint Solving. In pure constraints, we first apply SymSolv to solve purely symbolic constraints on Line 3 and then handle purely neural constraints using NeuSolv on Line 9. Note that the order of these two kinds of constraints does not affect the result. We solve purely symbolic constraints first because the SymSolv is fast, while the search algorithm for neural constraints requires numerous iteration and may not terminate. So, if the SymSolv reports UNSAT for purely symbolic constraints, the whole pure-symbolic constraints is UNSAT, as all the constraints are conjunctive. Such an early UNSAT detection speeds up the satisfiability checking. If both solvers output SAT, NeuEx continues the process of solving the mixed constraints.

Mixed Constraint Solving I. NeuEx obtains the symbolic constraints from mixed components (e.g., $S_2$ and $S_3$) by cutting the edges between the neural constraints and its variables. Then, NeuEx invokes SymSolv to check their satisfiability on Line 20. If the solver returns UNSAT, NeuEx goes to UNSAT state; otherwise, NeuEx collects the concrete values of variables used in these symbolic constraints. Then, NeuEx plugs these concrete values into neural constraints on Line 24. For example, in Figure 3, if the satisfiability result of $S_2 \land S_3$ is $< t_5, t_6, t_7, t_8 >$ for the variables $< V_3, V_6, V_7, V_8 >$, NeuEx partially assigns $V_6$ and $V_8$ in $N_2$ to be $t_6$ and $t_8$ separately. Now, we have the partially assigned neural constraint $N_2'$ from $N_2$. All that remains is to search for the value of $V_7$ satisfying $N_2'$. 
To solve such a partially assigned neural constraint, NeuEx employs NeuSolv on Line 26. If the NeuSolv outputs SAT, NeuEx goes to SAT state. In SAT state, NeuEx terminates and returns SAT with the combination of the satisfiability results for all the constraints. If the NeuSolv outputs UNSAT, NeuEx considers the satisfiability result of symbolic constraints as a counterexample and derives a conflict clause on Line 19. Specifically in our example, NeuEx creates a new conflict clause \((V_3 \neq t_3) \lor (V_4 \neq t_4) \lor (V_5 \neq t_5) \lor (V_6 \neq t_6)\). Then NeuEx adds this clause (Line 34) and queries the SymSolv with these new symbolic constraints (Line 20). This method of adding conflict clauses is similar to the backtracking in DPLL algorithm [32]. Although the conflict clause learning approach used in NeuEx is simple, NeuEx is generic to adopt other advance strategies for constraint solving [60, 66, 87].

The above mixed constraint solving keeps executing the backtracking procedure until it does not find any new counterexample. Consider the example in Figure 1. NeuEx first finds the input whose \(w1\_length=10, \text{ver}\_length=30, \text{ptr}=100\). However, the result generated in this trial does not satisfy the neural constraint. Then, NeuEx transforms this counterexample into a conflict clause and goes to next trial to discover a new result. But this trail can be very expensive. For example, in Figure 3, mixed constraint solving takes more than 5000 trials in the worst case even after augmenting the constraints with additional information that the value of \(\text{ptr}\) is 100. To speed up mixed solving, NeuEx chooses to limit the number of trials to a threshold value.

Specifically, if we do not have a SAT decision after mixed constraint solving \(\ell\) within \(k\) iterations\(^1\), NeuEx applies an alternative strategy where we combine the symbolic constraints with neural constraints together. There exist two possible strategies: transforming neural constraints to symbolic constraints or the other way around. However, collapsing neural constraints to symbolic constraints incurs massive encoding clauses. For example, merely encoding a small binarized neural network generates millions of variables and millions of clauses [67]. Thus, we transform the mixed constraints into purely neural constraints for solving them together.

**Mixed Constraint Solving II.** NeuEx collapses symbolic constraints to neural constraints by encoding the symbolic constraints to a loss function on Line 36. This ensures the symbolic and neural constraints are in the same form. For example, in Figure 3, NeuEx transforms the constraint \(S_2\) and \(S_3\) into a loss function of \(N_2\).

Once the symbolic constraints are encoded into neural constraints, NeuEx applies the NeuSolv to minimize the loss function on Line 38. The main intuition behind this approach is to guide the search with the help of encoded symbolic constraints. The loss function measures the distance between current result and the satisfiability result of symbolic constraints. The search algorithm gives us a candidate value for satisfiability checking of neural constraints. However, the candidate value generated by minimizing the distance may not always satisfy the symbolic constraints since the search algorithm only tries to minimize the loss, rather than exactly forces the satisfiability of symbolic constraints. To weed out such cases, NeuEx checks the satisfiability for the symbolic constraints by plugging in the candidate value and querying the SymSolv on Line 39. If the result is SAT, NeuEx goes to SAT state. Otherwise, NeuEx continues executing Approach II with a different initial state of the search algorithm. For example, in Figure 3, NeuEx changes the initial value of \(V_7\) for every iteration. Note that each iteration in Approach I has to execute sequentially because the addition of the conflict clause forces serialization. As opposed to this, each trial in Approach II is independent and thus embarrassingly parallelizable.

To avoid the non-termination case, NeuEx sets the maximum number of trials for mixed constraint solving II to be \(M_2\), which can be configured independently of our constraint solver. Empirically, we notice that the mixed constraint solving II is always able to find the satisfiability result for complex constraints before hitting the threshold of 10.

### 3.4 Encoding Mixed Constraints

NeuEx’s mixed constraints take up most of the time during solving. We reduce this overhead by transforming them to purely neural constraints. Specifically, NeuEx encodes the symbolic constraints \(S(X)\) as a loss function \(L(X)\) such as:

\[
S(X) = 5(\min_X(L(X)))
\]

Next, NeuEx uses this loss function along with neural constraints and applies NeuSolv to minimize the loss function of the entire mixed constraints. This encoding has two main advantages. First, it is straightforward to encode symbolic constraints into loss function. Second, there exists gradient-based search algorithm for minimizing the loss function, which speeds up constraint solving in NeuEx.

**Generic Encoding.** As long as we have a loss function for the symbolic constraints, we can apply NeuSolv to solve the mixed constraints. In this paper, given the grammar of symbolic constraints shown in Table 1, there exist six types of symbolic constraints and two kinds of combinations between two symbolic constraints based on its logical operators. Table 2 describes the loss function for all forms of symbolic constraints. Taking \(a = b\) as an example, the loss function \(L = \text{abs}(a - b)\) achieves the minimum value 0 when \(a = b\), where \(a\) and \(b\) can be arbitrary expressions. Thus, minimizing the loss function \(L\) is equivalent to solving the symbolic constraint. Similar logic is also useful to explain the equivalence between the other kinds of symbolic constraints and its loss function. These loss functions are not the only possible loss functions for these constraints. Any functions satisfying the Equation 7 can be used as loss functions and the same encoding mechanism can be applied to the other constraints. Note that there are three special requirements for the encoding mechanism.

**Non-Zero Gradient Until SAT.** The derivative of the loss function should not be zero until we find the satisfiability results. For example, when we encode \(a < b\), the derivative of the loss function should not be equal to zero when \(a = b\). Otherwise, the NeuSolv will stop searching and return an unsatisfiable result. To guarantee that, we add a small positive value \(\alpha\) and adapts the loss function to be \(L = \text{max}(a - b + \alpha, 0)\) for the constraint \(a < b\) and similarly for \(a > b\) and \(a \neq b\). Taking the motivation sample shown in Section 2 as an example, the loss function is \(L = \text{max}(99 - \text{ptr} + 0.5, 0)\) where \(\alpha = 0.5\).

\(^1\)Users can adapt \(k\) according to their applications.
Table 2: Transforming symbolic constraints into the corresponding loss function. $a$ and $b$ represent arbitrary expressions. $S_1$ and $S_2$ represent arbitrary symbolic constraints. $L$ represents the loss function used for neural constraint solving. $L_{S_1}$ and $L_{S_2}$ represents the loss function for symbolic constraints $S_1$ and $S_2$ respectively. $\alpha$ represents a small positive value. $\beta$ represents a small real value.

| Symbolic Constraint | Loss Function ($L$) |
|---------------------|---------------------|
| $S_1 \models a < b$ | $L = \max(a - b + a, 0)$ |
| $S_1 \models a > b$ | $L = \max(b - a + a, 0)$ |
| $S_1 \models a \geq b$ | $L = \max(b - a, 0)$ |
| $S_1 \models a = b$ | $L = \text{abs}(a - b)$ |
| $S_1 \models a \neq b$ | $L = \text{max}(-1, -\text{abs}(a - b + \beta))$ |
| $S_1 \land S_2$ | $L = L_{S_1} + L_{S_2}$ |
| $S_1 \lor S_2$ | $L = \text{min}(L_{S_1}, L_{S_2})$ |

Fixed Lower Bound on Loss Function. The loss function for each constraint needs a fixed lower bound to avoid only minimizing the loss function of one constraint within the conjunctive constraints. For instance, we should not encode $a \neq b$ to $L = -\text{abs}(a - b + \beta)$ as the loss function can be negative infinity, where $\beta$ is a small real value. If the constraint is $a \neq b \land c < d$ where $c$ and $d$ can be arbitrary expressions, NeuSolv may only minimize the loss function for $a \neq b$, because the loss function for $a \neq b \land c < d$ is the sum of the loss function for $a \neq b$ and $c < d$. Thus, it may not find the satisfiability result for both symbolic constraints. To avoid this, we add a lower bound and adjust the loss function to be $L = \max(-1, -\text{abs}(a - b + \beta))$. This lower bound ensures that the loss functions have a finite global minima.

Generality of Encoding. NeuSolv can only be applied to differentiable loss functions, because it requires computing the derivatives of the loss function. Thus, NeuEx need to transform the expression $a$ and $b$ in Table 2 to a differentiable function. The encoding mechanism of expressions is generic. As long as NeuEx can transform the expression into a differential function, any encoding mechanism can be plugged in NeuEx for neuro-symbolic constraint solving.

3.5 Optimizations

NeuEx applies five optimization strategies to reduce the computation time for neuro-symbolic constraint solving.

Single Variable Update. Given a set of input variables to neural constraint, NeuEx only updates one variable for each enumeration in NeuSolv. In order to select the variable, NeuEx computes the derivative values for each variable and sorts the absolute values of derivatives. The updated variable is the one with the largest absolute value of the derivative. This is because the derivative value for each element only computes the influence of changing the value of one variable towards the value of loss function, but does not measure the joint influence of multiple variables. Thus, updating them simultaneously may increase the loss value. Moreover, updating one variable per iteration allows the search engine to perform the minimum number of mutations on the initial input in order to prevent the input from being invalid.

Type-based Update. To ensure the input is valid, NeuEx adapts the update strategy according to the types of variables. If the variable is an integer, NeuEx first binarizes the value of derivatives and then updates the variables with the binarized value. If the variable is a float, NeuEx updates the variable with the actual derivatives.

Caching. NeuEx stores the updated results for each enumeration in NeuSolv. As the search algorithm is a deterministic approach, if we have the same input, neural constraints and the loss function, the final generated result is the same. Thus, to avoid unnecessary recomputation, NeuEx stores the update history and checks whether current input is cached in history. If yes, NeuEx reuses previous result; otherwise, NeuEx keeping searching for new input.

SAT Checking Per Enumeration. To speed up the solving procedure, NeuEx verifies the satisfiability of the variables after each enumeration in NeuSolv. Once it satisfies the symbolic constraints, NeuSolv terminates and returns SAT to NeuEx. This is because not only the result achieving global minima can be the satisfiability result of symbolic constraint. For example, any result can be the satisfiability result of the constraint $a \neq b$ except for the result satisfying $a = b$. Hence, NeuEx does not wait for minimizing the loss function, but checks the updated result for every iteration.

Parallelization. NeuEx executes NeuSolv with different initial input in parallel since each loop for solving mixed constraints is independent. This parallelization reduces the time for finding the global minima of the loss function.

4 NEURAL CONSTRAINT LEARNING

We have described the constraint solver for neuro-symbolic constraint solving; now it remains to discuss how NeuEx obtains the neural constraints. In this section, we discuss the design of neural constraint learning engine in NeuEx.

Given a program, the selection of network architecture is the key for learning any neural constraint. In this paper, we use multilayer perceptron (MLP) architecture which consists of multiple layers of nodes and connects each node with all nodes in the previous layer [80]. Each node in the same layer does not share any connections with others. We select this architecture because it is a suitable choice for the fixed-length inputs. There are other more efficient architectures (e.g., CNN [55, 57] and RNN [63, 64]) for the data with special relationships, and NeuEx gives users the flexibility to add more network architectures in NeuEx.

The selection of activation function plays significant role for neural constraint inference as well. In this paper, we consider multiple activation functions (e.g., Sigmoid and Tanh) and finally select the rectifier function Relu as the activation function, because Relu obtains parse representation and reduces the likelihood of vanishing gradient [39, 61]. In other words, the neural network with Relu has higher chance to converge than other activation functions.

In addition, to ensure the generality of neural constraint, we implement an early-stopping mechanism which is a regularization approach to reduce over-fitting [91]. It stops the learning procedure when the current learned neural constraint behaves worse on unseen test executions than the previous constraint. As the unseen test executions are never used for learning the neural constraint, the performance of learned neural constraint on unseen test executions is a fair measure for the generality of learned neural constraints.
To show the effectiveness of neuro-symbolic constraint learning and solving, for each program, we mark the code from the beginning of the program to the location accessing buffers to be represented as neural constraints. Then, we mark all inputs and all buffer lengths in the program as symbolic by default. In cases where we know the input format, we provide it as additional information in form of program annotations (for e.g., specific input field values). In our example from Section 2, to analyze the program which takes HTTP requests as input, NeuEx marks the uri and version field as well as the length of all the buffers as symbolic. NeuEx randomly initializes the symbolic input arguments for each program, executes the program and collects the values of variables of interest. For our experiments, we collect up to 100000 samples of such executions. 80% of these samples are used for learning the neural constraints, while remaining 20% are used for evaluating the accuracy of learned neural constraints. To get the vulnerable conditions, we manually analyze the source code and set it as symbolic constraint.

Using the above steps, our experiments show that NeuEx is able to find the correct exploit for 13 out of 14 programs in the benchmark. Next, we compare the efficiency of NeuEx on buffer overflow exploit generation with an existing symbolic execution method called Loop-Extended Symbolic Execution (LESE) [84] which is a dynamic symbolic execution based tool. It is a heuristic-based approach which hard-codes the relationship between loop counts and inputs. We reproduce LESE’s machine configuration for fair comparison. Our experiments show that NeuEx requires maximum two hours to find the exploits on this setup. On the other hand, LESE requires more than five hours. Thus, NeuEx’s performance is comparable to LESE for exploit generation.

In addition, the time that NeuEx spends in exploit generation is not dependent on the complexity of the target code, as NeuEx is a black-box approach for neural constraint learning. For example, the time spent for analyzing the program Sendmail11 with one loop-dependent branch is as same as the time used for program Sendmail13 with 18 loop-dependent branches.

Table 3: NeuEx finds the exploits for 13 out of 14 programs in the buffer overflow benchmark. LD represents the number of branches of which the condition relies on loop counts but not input arguments, which indicates the complexity of the program for symbolic execution to analyze it.

| Program   | Vulnerable Condition | LD | Find Exploits? |
|-----------|----------------------|----|----------------|
| Bind1     | strlen(data) > 4140  | 16 | Yes            |
| Bind2     | strlen(data) > 4140  | 12 | Yes            |
| Bind3     | strlen(buffer) > 512 | 13 | Yes            |
| Sendmail1 | strlen(buffer) > 999 | 52 | Yes            |
| Sendmail2 | strlen(buffer) > 5   | 38 | Yes            |
| Sendmail3 | strlen(buffer) > 50  | 18 | Yes            |
| Sendmail4 | strlen(buffer) > 51  | 2  | Yes            |
| Sendmail5 | strlen(buffer) > 50  | 6  | Yes            |
| Sendmail6 | strlen(Tvec) > 100   | 11 | No             |
| Sendmail7 | strlen(r) = size     | 16 | Yes            |
| WuFTP1    | strlen(path) > 10    | 5  | Yes            |
| WuFTP2    | strlen(resolved) > 46| 29 | Yes            |
| WuFTP3    | strlen(curpath) > 46 | 7  | Yes            |

To evaluate the effectiveness of NeuEx in exploit generation, we select 14 vulnerable programs with buffer overflows from open-source network servers (e.g., BIND, Sendmail and WuFTP) [96]. We choose this benchmark because it comprises of multiple loops and various complex control and data dependencies which are challenging for symbolic execution to handle (discussed in Section 2). To measure the complexity of problems, we utilize the number of branches of which the condition is related to loop counts rather than input arguments in the vulnerable program. This metric is also used in [84]. Table 3 represents the complexity of each program along with the result of exploit generation.

5 EVALUATION

We implement NeuEx in Python and Google TensorFlow [3] with a total of 1808 lines of code for training the neural constraints and solving the neuro-symbolic constraints. Our evaluation highlights two features of NeuEx: (a) it generates the exploits for 13/14 vulnerable programs; (b) it solves 100% of the given neuro-symbolic constraints for each loop.

Experimental Setup. To evaluate NeuEx, we configure the maximum enumeration of NeuSolv Mn to be 10000 after which NeuSolv will terminate. (discussed in Section 3.1). The larger the maximum enumeration, the better the performance of NeuEx is on neural constraint solving. Our experiments are performed on a server with 40-core Intel Xeon 2.6GHz CPUs with 64 GB of RAM.

5.1 Effectiveness in Exploit Generation

To evaluate the effectiveness of NeuEx in exploit generation, we select 14 vulnerable programs with buffer overflows from open-source network servers (e.g., BIND, Sendmail and WuFTP) [96]. We choose this benchmark because it comprises of multiple loops and various complex control and data dependencies which are challenging for symbolic execution to handle (discussed in Section 2). To measure the complexity of problems, we utilize the number of branches of which the condition is related to loop counts rather than input arguments in the vulnerable program. This metric is also used in [84]. Table 3 represents the complexity of each program along with the result of exploit generation.

Finding 1: NeuEx is able to find the correct exploit for 13 out of 14 programs.
We ask three empirical questions with our micro-benchmarks:

1. How fast does NeuEx solve a given neuro-symbolic constraint?
2. What is the accuracy of neural constraints learned by NeuEx?
3. What is the influence of learning and solving on the overall efficiency of NeuEx?

For this, we use two benchmarks, namely HOLA and NLA, which comprise 73 programs with 82 loops and 259 input variables in total. These two benchmarks are widely used for invariant synthesis [46, 70, 71] which is useful for formal verification. We select these two benchmarks because they have various kinds of loop invariants and capturing them is known to be a challenge for symbolic execution. To this end, we evaluate NeuEx’s ability to reach the post-condition of the loops in these benchmarks. For each program, we mark the loop to be represented by neural constraints. In each loop, NeuEx needs to (1) learn the loop invariant \( N \), (2) get the symbolic invariant of loop guard \( S \) from the symbolic execution engine, and (3) solve \( N \land \neg S \). Consider the example in Figure 5. NeuEx first learns the neural constraint \( N : \{ a, b, cnt \} \mapsto \{ c, d \} \) representing the loop invariant on Line 5. Then, it gets the loop guard \( c > d \) on Line 3 from the symbolic execution engine. Finally, it solves the neuro-symbolic constraint \( N \land c \leq d \). For each loop in our benchmarks, we mark all the input arguments (e.g., \( a \) and \( b \)) as well as the loop count as symbolic. If the loop count is not an explicit variable, NeuEx adds an implicit count incremented each iteration to capture the number of iterations in the loop. Figure 4 shows the type distribution of the negative of loop guards in NLA and HOLA benchmarks which covers all kinds of constraints expressed in Table 2.

**Effectiveness of Neuro-Symbolic Constraint Solving.** Recall that NeuSolv randomly sets an initial state when it begins the gradient-based optimization of a loss function. If it fails to find a satisfiability result before the timeout, NeuEx needs to restart the search from a different initial state because the search is dependent on the initial state (discussed in Section 3.1). We call each search attempt from a new initial state as one **trial**. Thus, to evaluate how fast NeuEx solves a given neuro-symbolic constraint, we use the number of trials that NeuSolv takes as the metric. The lower the number of trials that NeuEx needs, the faster the neuro-symbolic constraint solving. \( T_{NS} \) column in Table 4 and Table 5 shows the number of trials NeuEx required to solve the given neuro-symbolic constraints for each loop in NLA and HOLA benchmarks. From these results, we find that NeuEx successfully solves 100% of the given neuro-symbolic constraints with a maximum of three trials. Among 82 loops, NeuEx solves 95% of neuro-symbolic constraints with only one trial. This result indicates that NeuEx can successfully solve various kinds of given neuro-symbolic constraints efficiently.

**Finding 3:** NeuEx is effective in neuro-symbolic constraint solving for 100% of constraints with a maximum of three trials.

NeuEx needs more than one trials for 4/82 loops because of two main reasons. First, our current timeout value is not enough for solving the constraints in two cases (program 14 and 40 in HOLA benchmark). To address this, we can either increase the timeout or restart the search with a new initial state. We experiment on both options and report that the latter can solve the constraints faster. For example, in program 40, NeuEx solves the given neuro-symbolic constraints within 2 trials, but it reaches timeout for one trial where the timeout is increased to three-folds. For the remaining two loops, NeuEx fails because of the inefficiency of gradient-based search in NeuSolv. For example, in program fermat2, NeuSolv gets stuck at the saddle point. To address this, we can apply trust region algorithm [88] or cubic regularization [68] which utilizes second-order derivative to find and avoid saddle points.

**Accuracy of Neural Constraint Learning.** To measure the effectiveness of neural constraint learning, we compute the learning accuracy \( Acc \) which is defined as: \( Acc = \frac{M_p}{M} \). where \( M_p \) is the number of (unseen) test executions where learned neural constraints predict the right outputs and \( M \) is the total tested executions. The higher the accuracy, the more precise the learned neural constraints. For 82 loops in our benchmarks, NeuEx achieves more than 80% accuracy for 66 neural constraints. For example, NeuEx achieves 97% accuracy for learning the second loop invariant in program hard which contains multiple multiplications with divisions.

---

**Figure 4:** Type distribution of the symbolic constraints in NLA and HOLA. T1 represents the constraints with \( \geq \) or \( \leq \) operator; T2 presents the constraints with \( > \) or \( < \) operator; \( \land \) or \( \lor \) operators. T3 represents the constraints with \( == \) or \( \neq \) operator; T4 represents the constraints with \( \land \) or \( \lor \) operators.

**Figure 5:** A simple function with one loop.

```
void func(int a, int b){
    int c,d,cnt; c = a; d = b; cnt=0;
    while(c>d){
        c = c+d+1; d = d+1; cnt++;
    }
}
```

---
Finding 4: NeuEx achieves more than 80% learning accuracy for 66/82 neural constraints.

Combined (Learning + Solving) Efficiency. There are two steps involved in solving a neuro-symbolic task (reaching the post-condition in this case) namely: infer the constraints and solve them. So far in our micro-benchmarks, we have evaluated these two steps independent of each other. For completeness, we now present our experimental analysis for understanding how these two steps affect the overall efficiency of NeuEx in performing a given task.

NeuEx successfully solves 71 out of 82 end-to-end tasks in total. Table 6 shows the contributions of each step in solving a neuro-symbolic task. When both steps are successful, NeuEx succeeds in solving 96.8% of tasks (in top left cell), However, when only NeuEx’s solving is unsuccessful (4 cases in bottom left cell), it always fails to complete the task. This shows that task solving is directly dependent on constraint solving, and justifies our focus on improving the neuro-symbolic constraint solving efficiency in our constraint solver. Ideally, NeuEx must always learn the constraints accurately as well as solve the constraints successfully in order to guarantee post-condition reachability. However, we notice that even when learning is inaccurate, NeuEx is still able to solve the 66.7% of the tasks (in top right cell). This is because NeuEx is at least able to learn the trend of certain variables involved in the constraints if not the precise constraints. Consider the example in Figure 5. If the neural constraint learns \( c = a + 4 \times cnt^2 \land d = b + cnt \), NeuEx finds the satisfiability result \( a = 2, b = 5, cnt = 1, c = 6 \) and \( d = 6 \). Even though the neural constraint does not capture

| P       | Type | TNS | TNE | P       | Type | TNS | TNE | P       | Type | TNS | TNE |
|---------|------|-----|-----|---------|------|-----|-----|---------|------|-----|-----|
| cohendiv| T2   | 1   | 1   | dijkstra_2 | T3   | 2   | -   | prodibr| T4   | 1   | 1   |
| divbin_1| T2   | 1   | 1   | freire1   | T1   | 1   | 1   | knuth  | T4   | 1   | 1   |
| divbin_2| T3   | 1   | 5   | freire2   | T1   | 1   | 1   | fermat1 | T3   | 1   | 1   |
| manaddiv| T2   | 1   | 1   | cohencu   | T2   | 1   | 1   | fermat2 | T3   | 3   | 5   |
| hard_1  | T2   | 1   | 1   | egcd      | T3   | 1   | 2   | lcm1    | T3   | 1   | 1   |
| hard_2  | T3   | 1   | 5   | egcd2     | T3   | 1   | 1   | lcm2    | T3   | 1   | 4   |
| sqrt1   | T1   | 1   | 1   | egcd3     | T3   | 1   | 5   | geo1    | T1   | 1   | 1   |
| dijkstra_1| T1 | 1   | 1   | prodbin   | T3   | 1   | 1   | geo2    | T1   | 1   | 1   |
|         |      |     |     |          |      |     |     |         |      |     |     |

Table 4: Evaluation results of NeuEx’s constraint solving on NLA benchmark. P represents the program name; Type shows the type of symbolic constraints; TNS shows the number of trials NeuSolv takes for solving the given neuro-symbolic constraints; TNE represents the number of trials NeuEx needs to reach the post-condition of the loop. ‘*’ represents that NeuEx reaches its timeout before reaching the post-condition.

| P       | Type | TNS | TNE | P       | Type | TNS | TNE | P       | Type | TNS | TNE |
|---------|------|-----|-----|---------|------|-----|-----|---------|------|-----|-----|
| 01      | T1   | 1   | 1   | 12_1    | T2   | 1   | 1   | 25      | T1   | 1   | 1   |
| 02      | T1   | 1   | 1   | 12_2    | T2   | 1   | 1   | 26      | T1   | 1   | 1   |
| 03      | T2   | 1   | 1   | 13      | T1   | 1   | 1   | 33      | T1   | 1   | 1   |
| 04      | T2   | 1   | 2   | 14      | T2   | 3   | 3   | 39      | T3   | 1   | 1   |
| 05      | T1   | 1   | 1   | 15      | T1   | 1   | 1   | 40      | T1   | 1   | 1   |
| 06      | T1   | 1   | 1   | 16      | T1   | 1   | 1   | 41      | T2   | 1   | 1   |
| 07      | T1   | 1   | 1   | 17      | T1   | 1   | 1   | 42      | T1   | 1   | 1   |
| 08      | T1   | 1   | 1   | 18      | T1   | 1   | 1   | 43      | T1   | 1   | 1   |
| 09_1    | T1   | 1   | 1   | 19      | T1   | 1   | 1   | 44      | T2   | 2   | 2   |
| 09_2    | T1   | 1   | 1   | 20      | T1   | 1   | 1   | 45      | T1   | 1   | 1   |
| 09_3    | T1   | 1   | 1   | 21      | T1   | 1   | 1   | 45      | T1   | 1   | 1   |
| 09_4    | T1   | 1   | 1   | 22      | T1   | 1   | 1   | 46      | T1   | 1   | 1   |
| 10      | T1   | 1   | 1   | 23      | T1   | 1   | 1   | 36_1    | T1   | 1   | 1   |
|         |      |     |     |         |      |     |     |         |      |     |     |

Table 5: Evaluation results of NeuEx’s constraint solving on HOLA benchmark. P represents the program name; Type shows the type of symbolic constraints; TNS shows the number of trials NeuSolv takes for solving the given neuro-symbolic constraints; TNE represents the number of trials NeuEx needs to reach the post-condition of the loop.

| Learning | Solving | Success | Failure |
|----------|---------|---------|---------|
| Success  | 61/63   | 10/15   |
| Failure  | 0/3     | 0/1     |

Table 6: Effect of constraint learning and solving on NeuEx’s overall efficiency. We classify constraint learning to be a success when accuracy \( \geq 80\% \) and a failure otherwise. We classify constraint solving to be a success when NeuEx solves the given constraints with one trial and a failure otherwise. We classify task solving to be a success when the concrete values generated with 1 trial reaches the post-condition and a failure otherwise. The cell value represents the number of loops which succeed in task solving out of total loops under that category.
the precise loop invariant \( c = a + \text{cnt} \times \frac{2b+1+\text{cnt}}{2} \land d = b + \text{cnt}, \)
it at least knows that the value of \( c \) increases with the increase in \( \text{cnt}^2 \). This partial learning aids NeuEx to solve the task and find \( a = 2, b = 5 \) and \( \text{cnt} = 1 \). Thus, we conclude that although learning is important, it does not affect task solving as drastically as constraint solving. This highlights the importance of effectiveness in constraint solving.

**Finding 5:** Constraint solving affects NeuEx’s effectiveness more significantly than constraint learning.

### 6 RELATED WORK

NeuEx is a new design point in constraint synthesis and constraint solving. In this section, we discuss the problems of the existing symbolic execution tools to show how NeuEx can handle it and presents how NeuEx differs from existing constraint synthesis.

#### 6.1 Symbolic Execution

Symbolic execution [51] has been used for program verification [31], software testing [17, 51], and program repair via specification inference [69]. In the last decade, we have witnessed an increased adoption of dynamic symbolic execution [41] where symbolic execution is used to partition of the input space, with the goal of achieving increased behavioral coverage. The input partitions computed are often defined as program paths, all inputs tracing the same path belong to the same partition. Thus, the test generation achieved by dynamic symbolic execution suffers from the path explosion problem. The problem of path explosion can be exacerbated owing to the presence of complex control flows, including long-running loops (which may affect the scalability of dynamic symbolic execution since it involves loop unrolling) and external libraries. However, NeuEx does not suffer from the path explosion as it learns the constraints from test executions directly.

Tackling path explosion is a major challenge in symbolic execution. Boonstopel et al. suggest the pruning of redundant paths during the symbolic execution tree construction [14]. Veritesting alternates between dynamic symbolic execution and static symbolic execution to mitigate path explosion [9]. The other predominant way of tackling the path explosion problem is by summarizing the behavior of code fragments in a program [5, 8, 40, 56, 75, 85]. Simply speaking, a summarization technique provides an approximation of the behavior of certain fragments of a program to keep the scalability of symbolic execution manageable. Such an approximation of behaviors is also useful when certain code fragments, such as remote calls and libraries written in a different language, are not available for analysis.

Among the past approaches supporting approximation of behaviors of (parts of) a program, the use of function summaries have been studied by Godefroid [40]. Such function summaries can also be computed on-demand [5]. Kuznetsov et al. present a selective technique to merge dynamic states. It merges two dynamic symbolic execution runs based on an estimation of the difficulty in solving the resultant Satisfiability Modulo Theory (SMT) constraints [56]. Veritesting suggests supporting dynamic symbolic execution with static symbolic execution thereby alleviating path explosion due to factors such as loop unrolling [8]. The works of [75, 85] suggest grouping together paths based on similar symbolic expressions in variables, and use such symbolic expressions as dynamic summaries to group paths.

#### 6.2 Constraints Synthesis

To support the summarization of program behaviors, the other core technical primitive we can use is constraint synthesis. In our work, we propose a new constraint synthesis approach which utilizes neural networks to learn the constraints which are infeasible for symbolic execution. In comparison with previous solutions, the major difference is that NeuEx does not require any pre-defined templates of constraints and can learn any kind of relationships between variables.

Over the last decade, there are two lines of works in constraint synthesis: white-box and black-box approaches. White-box constraint inference relies on a combination of light-weight techniques such as abstract interpretation [11, 26–28, 65, 77, 78], interpolation [22, 50, 62] or model checking algorithm IC3 [15]. Although some white-box approaches can provide sound and complete constraints [25], it is dependent on the availability of source code and a human-specified semantics of the source language. Constructing these tools have required considerable manual expertise to achieve precision, and many of these techniques can be highly computationally intensive.

To handle the unavailability of source code, there also exist a rich class of works on reverse engineering from dynamic executions [35, 38, 46, 70–72, 81]. Such works can be used to generate summaries of observed behavior from test executions. These summaries are not guaranteed to be complete. On the other hand, such incomplete summaries can be obtained from tests, and hence the source code of the code fragment being summarized need not be available. Daikon [35] is one of the earlier works proposing synthesis of potential invariants from values observed in test executions. The invariants supported in Daikon are in the form of linear relations among program variables. DIG extends Daikon to enable dynamic discovery of non-linear polynomial invariants via a combination of techniques including equation solving and polyhedral reasoning [71]. Krishna et al. use the decision tree, a machine learning technique, to learn the inductive constraints from good and bad test executions [54].

NeuEx devises a new gradient-based constraint solver which is the first work to support the solving of the conjunction of neural and SMT constraints. A similar gradient-based approach is also used in Angora [21], albeit for a completely different usage. It treats the predicates of branches as a black-box function which is not differentiable. Then, it computes the changes on the predicates by directly mutating the values of each variable in order to find the direction for changing variables. Similarly, Li et al. utilize the number of satisfied primitive constraints in a path condition as the target function for optimization and applies RACOS algorithm [94] to optimize the non-differentiable function for complementing symbolic execution [59]. However, NeuEx learns a differentiable function to represent the behaviors of the program from the test cases, encodes the symbolic constraints into a differentiable function and embeds
it into neural constraints. It computes the values of derivatives for each variable for updating.

A recent work [12] suggests the combination of neural reasoning and symbolic reasoning, albeit for an entirely different purpose, automated repair of student programming assignments. In contrast, our proposed neuro-symbolic execution solves neural and symbolic constraints together, and can be seen as a general purpose testing and analysis engine for programs.

7 CONCLUSIONS

To our knowledge, NeuEx is the first work utilizing neural networks to learn the constraints from values observed in test executions without pre-defined templates. NeuEx offers a new design point to simultaneously solve both symbolic constraints and neural constraints effectively, which can be used for complementing symbolic execution. It achieves good performance in both neuro-symbolic constraint solving and exploit generation for buffer overflows.

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A APPENDIX

A.1 Neural Constraint Analysis

We analyze the learned neural constraints by observing the trained weights and bias of neural network. Given a set of variables as the input to the neural network, if the input variable is not related with the output variable, the weight between the input and output variable is zero; otherwise, it is larger than zero. For example, the length of vulnerable buffer in program Bind1 is controlled by dlen field which is the 43rd byte of DNS queries, because the weight for this input variable is 0.99 which has the largest absolute value compared with other fields.