Learning Scalable and Precise Representation of Program Semantics

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Abstract

Neural program embedding has shown potential in aiding the analysis of large-scale, complicated software. Newly proposed deep neural architectures pride themselves on learning program semantics rather than superficial syntactic features. However, by considering the source code only, the vast majority of neural networks do not capture a deep, precise representation of program semantics. In this paper, we present DYPRO, a novel deep neural network that learns from program execution traces. Compared to the prior dynamic models, not only is DYPRO capable of generalizing across multiple executions for learning a program’s dynamic semantics in its entirety, but DYPRO is also more efficient when dealing with programs yielding long execution traces. For evaluation, we task DYPRO with semantics classification (i.e. categorizing programs based on their semantics) and compared it against two prominent static models: Gated Graph Neural Network, and TreeLSTM. We find that DYPRO achieves the highest prediction accuracy among all models. To further reveal the capacity of all aforementioned deep neural architectures, we examine if the models can learn to detect deeper semantic properties of a program. In particular given a task of recognizing loop invariants, we show DYPRO beats both static models by a wide margin.

1 Introduction

“Big Code” emerged as a major line of research in the past decade. The idea is reusing the knowledge distilled from existing code repositories in an attempt to simplify the future development of software. Early methods applied NLP techniques to discover textual patterns existed in the source code [1, 2, 3]; following approaches opted to learn the syntactic program embedding from the Abstract Syntax Trees (ASTs) [4, 5, 6]. Although these pioneering efforts manage to transform programs in an amenable form to deep learning models, they only capture shallow, syntactic features and therefore are limited in what they can do. For example, a model that recognizes the reoccurring syntactic patterns may be sufficient for a code completion task; to conquer more sophisticated and challenging problems in program synthesis or repair, thorough understanding and precise representations of program semantics can not be circumvented. Of late, a number of new deep learning architectures has been developed to specifically address this issue [7, 8, 9, 10]. Those works can be divided into two categories: dynamic and static. The former learns from the execution of programs such as separate variable traces or sequences of program states [7]. The latter dissects program semantics from source code. As an example, Allamanis et al. [9] constructed a graph out of a program’s AST with additional semantic edges. Subsequently they fed the graph to a Gated Graph Neural Network (GGNN) [11] for predicting the variable misuse bug in a method.

In this paper, we present a novel deep neural architecture, DYPRO, that is capable of learning program semantics from execution traces. DYPRO targets two major issues of the existing dynamic models.
First, how to learn the dynamic semantics of a program as a whole rather than individual executions; second how to handle long execution traces that tends to hurt the generalization of underlying models. For the first challenge, we apply random testing, a powerful technique in software testing, to run a program with a large number of inputs, each of which will trigger a separate execution trace. DYPRO then learns an embedding for each execution before compressing them into a vector that represents the semantics of the whole program. Regarding the second challenge, DYPRO employs a bi-directional RNN to scan through an entire execution trace for filtering out the steps that are less important to the trace. Our hope is DYPRO could still learn a precise semantic representation since the reduced traces can preserve the essence of the executions. More importantly, such reduction helps DYPRO to handle longer traces more efficiently.

We create a dataset to thoroughly evaluate how precise DYPRO can capture the deep and rigid program semantics. The dataset consists of almost eighty thousand programs each of which solves one of eleven coding problems. We pick the set of problems to cover a wide spectrum of difficulty levels ranging from entry-level programming exercises to challenging algorithmic questions frequently appearing on the coding interviews of major tech companies. The task is to classify programs in the dataset based on their semantics. For example, given a sorting routine, our goal is to test if models can differentiate among the algorithms that implements the sorting function (e.g. Bubble Sort and Insertion Sort shown in Figure 1), an instance that in fact tricks all static models in our experiment. All programs in the dataset have been manually inspected and labeled before hand. Results show DYPRO achieves significantly higher prediction accuracy than two prominent static models including GGNN, and TreeLSTM. We also found out that as the size of execution traces grows, DYPRO suffers a smaller drop in prediction accuracy than Dynamic State Trace Neural Network (DSTNN) [7].

We conduct a second study to further examine if models can learn to detect deeper semantic properties of a program. Specifically we choose loop invariants to evaluate all the above-mentioned deep neural architectures. Our intuition is recognition of loop invariants poses significant challenges to the model capacity. An effective model, at a bare minimum, needs to capture a precise representation of the program semantics; in addition it may also estimate the program properties derived from its semantics. Note our goal is not to invent models for generating loop invariants [12] but detecting loop invariants from a set of given properties. We use the classification accuracy as a means to gauge how precise and deep models have learnt the program semantics. Results show DYPRO is far more accurate in predicting loop invariants than all static models. Our findings indicate DYPRO is the most precise deep neural network in learning representations of program semantics.

```c
static int Difference(int[] a)
{
    //step 1: bubble sort the input array
    int left = 0;
    int right = a.Length - 1;
    for (int i = left; i < right; i++) {
        if (a[i] > a[i + 1]) {
            int tmp = a[i];
            a[i] = a[i + 1];
            a[i + 1] = tmp;
        }
    }
    //step 2: compute the largest difference
    return a[a.Length-1] - a[0];
}
```

```c
static int Difference(int[] a)
{
    //step 1: insertion sort the input array
    int left = 0;
    int right = a.Length - 1;
    for (int i = left; i < right; i++) {
        for (int j = left; j < right; j++) {
            if (a[j] > a[j + 1]) {
                int tmp = a[j];
                a[j] = a[j + 1];
                a[j + 1] = tmp;
            }
        }
    }
    //step 2: same as the left
    return a[a.Length-1] - a[0];
}
```

Figure 1: Two functions both compute the largest difference between two elements in a given array. According to our evaluation, none of the static models recognizes the semantic differences between the two functions even though they apply distinct sorting routines: Bubble Sort and Insertion Sort. Code highlighted in shadow box are the only syntactic differences between the two functions.

We make the following contributions:

- We design DYPRO, a novel deep neural architecture capable of learning dynamic program semantics from execution traces.
- We evaluate DYPRO using a task of semantics classification. Results show DYPRO achieves the highest prediction accuracy among all competing models.
- We examine if models can learn to detect loop invariants. We find DYPRO is significantly more accurate than all static models.
2 Background

Execution Based Program Representation Neural program interpreter [13] is the first deep neural network that dealt with programs in the form of execution trace. The idea is to learn to synthesize a sequence of low-level primitive operations for solving a high-level task such as addition and sorting. Later Cai et al. propose an improvement [14] by addressing the NPI’s generalization issues. In particular they replaced loops with recursions that used to synthesize the low-level operations. Unlike the prior attempts which still rely on the syntactical representation of execution traces, Wang et al. [7] encodes each step of the execution trace as a snapshot of the memory. Their intuition is such processing, widely regarded as dynamic analysis in the field of program analysis, leads to a deeper and more precise representation of program semantics. As a result, models can directly work with the program semantics while totally detaching themselves from the program syntax. Furthermore, Wang et al. [7] deals with real world programs, albeit mostly entry-level programming exercises, whereas the others work with artificial programs written in low-level language.

In this paper, we choose to adopt the state trace encoding scheme, a more precise representation of program semantics than the variable trace encoding scheme. State trace encoding scheme also enables a far more efficient implementation in DSTNN that is almost as accurate as Dependency Enforcement Network according to Wang et al.’s evaluation [7]. We address two major weaknesses of DSTNN. First DSTNN learns semantic representations for individual executions rather than a entire program; second DSTNN has difficulty in handling programs yielding long execution traces.

Random Testing Random testing is a software testing technique where programs are tested by generating random, independent inputs. Results of the output are compared against software specifications to verify the test output is pass or fail. Alternatively, random testing can also be used to catch the exceptions of the language (i.e. crashes) which means if an exception arises during testing execution then it means there is a fault in the program.

Random testing is practical, effective that is shown to be able to achieve good coverage in a variety of testing domains [15][16]. As a result, it’s one of the most powerful and widely adopted testing technique in software testing.

3 The Model Architecture of DYPRO

In this section, we start with an overview of the overall architecture of DYPRO. Next we present a formalization of DYPRO’s workflow.

3.1 Overview

In a general description, DYPRO consists of two recurrent neural networks (RNN) and another bi-directional RNN. Given the execution traces obtained from random testing, we encode each trace into a sequence of program states. Specifically, a program state is a tuple of values based on the
variable valuations (i.e. the state of the memory) upon the creation of the program state. A program state is created due to a memory update issued by a statement/instruction. By collecting the history of memory updates occurred during an execution, one can convert the trace into a sequence of program states. Upon receiving the inputs, DYPRO uses the first RNN (i.e. RNN1 in Figure 2) to encode each program state into a embedding vector. Next DYPRO employs a bi-directional RNN to scan through the entire sequence of state embeddings for picking the states that capture the essence of the execution. In other words, state embeddings that are not selected will be pruned away. After we feed the resulting state embeddings as a sequence to the second RNN (i.e. RNN2 in Figure 2), we extract its final state to represent an execution. Then we perform max pooling across embeddings that are learnt from executions of the same program to obtain the program embeddings. Finally, we add a one layer softmax regression to make the predictions.

3.2 Formalization

Given a program \( P \), and its variable set \( V \) \( (v_1, v_2, \ldots, v_n \in V) \), we represent an execution of \( P \) as a sequence of program states, each of which is a tuple of variable values. For example, we encode \( S_{t,e} \) the \( t \)-th program state in \( e \)-th execution of \( P \), to be \( (x_{t,e,v_1}, x_{t,e,v_2}, \ldots, x_{t,e,v_n}) \), where \( x_{t,e,v_n} \) is the value of variable \( v_n \) in \( S_{t,e} \). Using the notations, we explain DYPRO’s working pipeline.

**Embedding Program States** Each program state will be embedded by RNN1 into a vector. Take \( S_{t,e} \) for example, we feed the variable values (i.e. \( x_{t,e,v_1} \) to \( x_{t,e,v_n} \)) as a sequence to RNN1 and extract its final hidden state as the state embedding vector. Equation (1) defines \( h_{t,e} \), the embedding vector of \( S_{t,e} \), \( h_{t,e,v_1}, \ldots, h_{t,e} \in \mathbb{R}^{k_1} \) where \( k_1 \) denotes the size of the hidden layer of RNN1. Note that we do not assume the order in which variables values are encoded by RNN1 for each program state but rather maintain a consistent order throughout all states for a given trace.

\[
\begin{align*}
    h_{t,e,v_1} &= \text{RNN1}(h_{t,e,v_0}, x_{t,e,v_1}) \\
    h_{t,e,v_2} &= \text{RNN1}(h_{t,e,v_1}, x_{t,e,v_2}) \\
    &
\end{align*}
\] (1)

**Improving DYPRO’s Scalability** State reduction layer is dedicated to enhancing DYPRO’s resilience against programs yielding long execution trace. We describe its inner workings as follow. After obtaining all the state embeddings, we feed them into a bi-directional RNN which aims to filter out those that are less essential to the execution. Formally, let \( h_{1,e} \) to \( h_{m,e} \) denote the whole sequence of state embedding vectors for \( e \)-th execution of \( P \), we register the hidden vectors \( \hat{H}_{1,e} \) to \( \hat{H}_{m,e} \) of the forward one in the bi-directional RNN, denoted by FR in Equation (2). Similarly we also extract \( \hat{H}_{1,e} \) to \( \hat{H}_{m,e} \) out of the backward RNN, denoted by BR in Equation (3). Next for each program state, we define two context vectors to represent its prior and subsequent execution using \( \hat{H}_{1,e} \) to \( \hat{H}_{m,e} \) and \( \hat{H}_{1,e} \) to \( \hat{H}_{m,e} \). For example, given embedding vector \( h_{t,e} \) for program state \( S_{t,e} \), we define the two context vectors \( C_f(h_{t,e}) \) and \( C_b(h_{t,e}) \) in Equation (4). Finally we concatenate the context vectors with the state embedding vector to determine if a program state should be retained or discarded. Specifically we train a multi-layer perceptron (MLP) of one single sigmoid output neuron to produce a mask for each program state (Equation (5) where \( \odot \) denotes vector concatenation). Equation (6) applies the mask on the program states; \( \top \) denotes element-wise matrix multiplication assuming consistent broadcasting behavior. Our intention is to equip DYPRO with the capability of selecting program states that are most essential to the execution while discarding others that somewhat recoverable.

\[
\begin{align*}
    \hat{H}_{1,e} &= \text{FR}(\hat{H}_{0,e}, h_{1,e}) \\
    \hat{H}_{2,e} &= \text{FR}(\hat{H}_{1,e}, h_{2,e}) \\
    &
\end{align*}
\] \( \text{(2)} \)

\[
\begin{align*}
    \hat{H}_{1,e} &= \text{BR}(\hat{H}_{0,e}, h_{m,e}) \\
    \hat{H}_{2,e} &= \text{BR}(\hat{H}_{1,e}, h_{m-1,e}) \\
    &
\end{align*}
\] \( \text{(3)} \)

\[
\begin{align*}
    C_f(h_{t,e}) &= \text{pooling}(\hat{H}_{1,e}, \hat{H}_{2,e}, \ldots, \hat{H}_{t-1,e}) \\
    C_b(h_{t,e}) &= \text{pooling}(\hat{H}_{1,e}, \hat{H}_{2,e}, \ldots, \hat{H}_{m-t,e}) \\
\end{align*}
\] \( \text{(4)} \)

\[
M(h_{t,e}) = \text{MLP}(C_f(h_{t,e}) \odot C_b(h_{t,e}) \odot h_{t,e}) \\
\] \( \text{(5)} \)

\[
[h_{1,e}; h_{2,e}; \ldots; h_{m,e}] = [h_{1,e}; h_{2,e}; \ldots; h_{m,e}] \odot [M(h_{1,e}); M(h_{2,e}); \ldots; M(h_{m,e})] \\
\] \( \text{(6)} \)
Embedding Executions  Given \( h_{1,e}', h_{2,e}', \ldots, h_{m,e}' \), the state embeddings preserved by the previous layer. Equation (7) computes \( h_{e}'' \), the embedding vector that represents the whole execution. \( h_{1,e}'', h_{2,e}'', \ldots, h_{e}'', \in \mathbb{R}^{k_2} \) where \( k_2 \) denotes the size of the hidden layer of RNN2.

\[
\begin{align*}
  h_{1,e}'' &= \text{RNN2}(h_{0,e}'', h_{1,e}') \\
  h_{2,e}'' &= \text{RNN2}(h_{1,e}'', h_{2,e}') \\
  &\quad \ldots \\
  h_{e}'' &= \text{RNN2}(h_{m-1,e}'', h_{m,e}') \\
  h_P &= \max\text{pooling}(h_{1}'', h_{2}'', \ldots, h_{e}'') \\
  L &= H + \sum_{e=1}^{m} \sum_{t=1}^{M} M(h_{t,e})
\end{align*}
\]

Embedding Programs  Pooling layer is solely responsible for distilling the program representation among all execution embeddings. Let \( h_{1}'', h_{2}'', \ldots, h_{e}'' \) denote the embedding vectors for all executions of \( P \). Equation (8) computes the embedding vector of program \( P \). \( h_P \in \mathbb{R}^{k_2} \).

Loss Function  The network is trained to minimize the cross-entropy loss on a softmax over the semantic labels (denoted by \( H \) in Equation (9)) along with the sum of \( M(h_{t,e}) \) w.r.t. all program states among all executions of \( P \). In other words we force DYPRO to cut as many states from each trace as possible provided that it can still maintain a high prediction accuracy.

4 Evaluation

We present the evaluation of DYPRO which begins with semantics classification followed by the detection of loop invariants.

4.1 Semantics Classification

Dataset  The dataset consists of 96,853 programs in total. They are obtained from a popular online coding platform. Programs were written in several different languages: Java, C# and Python. All programs solve a particular coding problem. We hand picked the problems to ensure the diversity of the programs in the dataset. Specifically it contains introductory programming exercises for beginners, coding puzzles that exhibit considerable algorithmic complexity and challenging problems frequently appearing on coding interviews. The dataset was manually analyzed and labeled. The work was done by fourteen PhD students and exchange scholars at University of California, Davis. To reduce the labeling error, we distributed programs solving the same coding problem mostly to a single person and had them cross check the results for validation. The whole process took more than three months to complete. Participants came from different research backgrounds such as programming language, database, security, graphics, machine learning, etc. All of them were interviewed and tested for their knowledge on program semantics. The labeling is on the basis of operational semantics. We allow certain kind of variations to keep the total number of labels manageable. Readers are invited to consult the supplemental material for the descriptions of all coding problems and the list of all labels.

| Benchmarks                  | Training | Validation | Testing |
|-----------------------------|----------|------------|---------|
| Print Chessboard            | 7,415    | 1,000      | 1,000   |
| Find Array Max Difference   | 5,821    | 1,000      | 1,000   |
| Check Matching Parenthesis  | 3,269    | 1,000      | 1,000   |
| Reverse a String            | 5,946    | 1,000      | 1,000   |
| Find Ugly Number            | 5,543    | 1,000      | 1,000   |
| Sum of Two Numbers          | 6,635    | 1,000      | 1,000   |
| Find Extra Character        | 5,020    | 1,000      | 1,000   |
| Maximal Square              | 4,836    | 1,000      | 1,000   |
| Maximal Product Subarray    | 5,174    | 1,000      | 1,000   |
| Longest Palindrome          | 3,273    | 1,000      | 1,000   |
| Trapping Rain Water         | 2,987    | 1,000      | 1,000   |
| Total                       | 57,919   | 11,000     | 11,000  |

Table 1: Dataset used in semantics classification.
Prediction Task

Similar to the image classification setting, models are required to predict the category a program falls into based on its semantics. In other words, not only do models need to classify which coding problem a program attempts to solve but also how the program solves it. We adopt prediction accuracy and F1 score as the evaluation metrics.

Evaluation Subjects

Apart from DYPRO, we select GGNN, arguably the state-of-the-art deep neural network for learning source code. We also include TreeLSTM [17], one of the mostly applied deep neural networks for learning data structure of trees, in our case the ASTs of programs.

Implementation

We use Roslyn, IronPython, and Eclipse JDT for parsing programs written in C#, Python, and Java. To seek random inputs for generating the execution traces, we separate 100 programs for each coding problem to apply random testing. In particular, we first generate $N$ different inputs to execute each program and then select top $N$ (out of $100 \times N$) inputs that achieve the highest line coverage to be the test cases for all programs. We remove programs that fail to pass all the test cases (i.e. crashes or incorrect outputs) from the dataset. In the end, we are left with 79,919 programs which we split into a training set containing 57,919 programs, a validation set of 11,000 programs, and a test set of the remaining 11,000 programs (Table 1). All models are implemented in Tensorflow. Before training, we have unified as many hyperparameters as possible across all models such as the number of recurrent layers: 1; the number of hidden unit in the recurrent layer: 100; the embedding dimensions for each input token: 100; the optimizer: the Adam algorithm; the maximum value for normalizing the gradient when clipping: 0.9, etc. We use two Red Hat Linux servers each of which host two Tesla V100 GPUs (of 32GB GPU memory). Training DYPRO took the longest: approximately 48 hours in total while all other models finished within three hours.

Results

Figure 3a shows the prediction accuracy of all models. DYPRO leads the pack by almost 15%. TreeLSTM are barely above 60%. In terms of the F1 score, DYPRO also achieves better results than all others (Figure 3d). Regarding scalability, Figure 3b (resp. 3e) depicts how DYPRO’s prediction accuracy (resp. F1 score) vary with the size of execution traces. As a baseline for comparison, we re-implemented DYPRO without the state reduction layer. Results show as the number of program states exceed two hundred, DYPRO starts to outperform the baseline configuration. Specially the gap grows to be approximately 10% in accuracy (resp. 0.1 in F1 score) for traces of five hundred program states. To measure DYPRO’s capability of compressing execution traces, we find on average DYPRO discarded 27% (median=26%, sd=2%) of the program states for each execution trace among all testing programs. Finally we investigate the influence of code coverage on DYPRO’s performance. According to Figure 3c (or 3f), as the value of $N$ increases from ten to eighty (i.e. the number of test cases for each program in the dataset), DYPRO begins with on average 64% line coverage among all programs which keeps increasing until reaching 95% where more test inputs no longer improves the
code coverage. Note even at the lowest coverage point, DYPRO still outperforms all static models in both prediction accuracies and F1 score, albeit by a small margin. Overall we demonstrate random testing lays a good foundation for DYPRO.

**Analysis** To investigate the cause of inaccuracies, we look into the misclassifications static models produced. In general, we see two common classes of errors. First as briefly mentioned in Section 1, when given syntactically similar programs in Figure 1, static models struggle to differentiate their semantic differences. This type of mistakes indicates the insufficiency of the underlying program representation w.r.t. the provided model capacity. Similarly, when programs are written in vastly different syntax like what’s depicted in Figure 4, all static models failed to recognize the same semantics two programs denote. Our findings indicate static models still largely generalize at the level of program syntax. Although certain semantic features can be learnt, their generalization will result in imprecise modeling of program semantics. In contrast, DYPRO correctly classified all programs in Figure 1 and 4, especially the syntactic variations that hindered static models are automatically canonicalized by the executions. However, DYPRO can also be inaccurate at times for the reasons below. Although state reduction benefits DYPRO overall, it also causes DYPRO to misclassify which it otherwise wouldn’t. By simply removing the state reduction layer, DYPRO remedies more than 14% of the misclassifications. On the other hand, 47% of the misclassifications are due to programs yielding long execution traces (i.e. more than eight hundred program states) indicating DYPRO still has difficulties in generalizing longer traces despite the state reduction mechanism. This phenomenon necessitates the split of the problem into smaller ones which can be solved with separate tactics. In particular, when given shorter traces to learn, DYPRO may chose to skip the state reduction layer and take the trace in its entirety to preserve the precision of the learning. On the contrary, for much longer traces, DYPRO can employ a more aggressive strategy in traces reduction since trading precision for scalability is generally worthwhile as shown in this experiment.

```csharp
static void Main()
{
    int i;
    char X = "X";
    char O = "O";
    for (i = 0; i < 8; i++) {
        for (j = 0; j < 8; j++) {
            if ((i + j) % 2 == 0)
                Console.Write(X);
            else
                Console.Write(O);
        }
        Console.WriteLine();
    }
}
```

```csharp
static void Main()
{
    for (int i = 0; i < 8; i++) {
        for (int j = 0; j < 8; j++) {
            if (i % 2 == 0) {
                if (j % 2 == 0)
                    Console.Write("X");
                else
                    Console.Write("O");
            } else {
                if (j % 2 == 0)
                    Console.Write("O");
                else
                    Console.Write("X");
        }
        Console.WriteLine();
    }
}
```

Figure 4: Programs that are syntactically different but semantically equivalent.

**4.2 Detection of Loop Invariants**

As a more challenging task, we evaluate if models can recognize loop invariants — properties of loops that are true before (and after) each iteration — from a set of program expressions. Worth noting in this paper we do not formally infer loop invariants which requires extra functionalities such as search and logic deduction. Instead, our rationale is given a deeper program property like loop invariants, a capable model not only would understand the program semantics, but may also “infer” the properties determined by the semantics. In other words, a model with high prediction accuracy is a testament to its capability of learning deep and precise representation of program semantics.

**Data Preparation** In order to reuse the dataset introduced in Section 4.1, we need to find the loop invariants as our training labels. Here is our methodology: for each program in the dataset, first we request Daikon [18] to propose the likely loop invariants in each loop. Since Daikon’s output forms a specification from the view of a client for each procedure, it does not produce invariants for local variables, neither does it within a procedure. To address the issue, we convert all the local variables within a loop to be members of the class; in addition we insert a dummy procedure both at the beginning and end of the loop that takes in all the variables. The dummy procedure’s pre- and post-conditions will be identical and will represent the potential loop invariants. To formally
static int CountParentheses(string s) {
    int depth = 0, globalDepth = 0;
    var _var_ = -1;
    foreach (char c in s) {
        if (c.Equals(')')) { depth ++;
            globalDepth = Math.Max(depth, globalDepth); }
        else if (c.Equals(')')) { depth --;
            if (depth < 1) return 0; }
        // loop invariant to be detected
        _var_ = globalDepth >= depth;
        // non loop invariant
        _var_ = globalDepth > depth;
    }
    if (countOpen == 0) return globalDepth;
    else return 0;
}

Figure 5: Generating (non) loop invariants.

| Models     | Accuracy | F1 Score |
|------------|----------|----------|
| GGNN       | 47.5%    | 0.46     |
| TreeLSTM   | 51.8%    | 0.50     |
| **DYPRO**  | **73.9%**| **0.71** |

Table 2: Results of loop invariants detection.

verify the validity of obtained loop invariants, we inject Contracts.Assert statements for each candidate invariant at the beginning and end of the loop. We then invoke the static checker provided by the Microsoft Code Contract Utility [19] to perform the formal verification (we made our best efforts to translate programs written in Java and Python to C#). Any loop invariant that can not be proved, albeit may still be legitimate, will be removed from the dataset. In order to integrate a loop invariant into a program for the prediction task, we add a statement at the bottom of the loop where the invariant is assigned to a new variable. Since the assignment involves the evaluation of a real invariant, the statement will be labeled positive. As for negative examples, we exhaustively mutate loop invariants at the token level and pick a mutant that is confirmed to be a non-invariant (via random testing) to generate another assignment. Take the program in Figure 5 for example, after globalDepth >= currentDepth is verified to be an loop invariant, we generate a positive example by evaluating globalDepth >= currentDepth to variable _var_. Furthermore, we find a non loop invariant, in this case, globalDepth > currentDepth) by mutating the binary operator. Due to the limited power of the static checker, we collected 14,412 formally verified loop invariants out of 9,663 loops. We split the data into a training set of 10,412, a validation set of 2,000 and a test set of the remaining 2,000.

**Model Design** We adapt the existing models for detecting loop invariants. Specifically for GGNN (resp. TreeLSTM), we extract the final embeddings of the added assignments out of the program graph (resp. AST) and train with a new objective — hinge loss — to separate the two classes of examples. Customizing DYPRO for this task is slightly more involved. For starter, we need to explicitly encode the syntactic structure of loop invariants, especially the operator, into the program representation which are ignored by the state encoding scheme. Particularly we add a extra symbol $x_{t \_e \_v \_symbol}$ at the end of each program state $S_{t \_e}$ that takes the value of the index of UNK token except for the states that are created by the added assignment at which they are assigned the index of the operator. Next, to prevent DYPRO from cheating by picking assignments that evaluate to the same value in every loop iteration as the basis of the classification, we remove all program states that are created by the added assignments except those in the last loop iteration from the execution trace. Then we concatenate the state embedding of each added assignment with the execution embedding before perform max pooling to obtain the final representation of the (non) loop invariants. Similarly we train the network with the hinge loss function. The results are shown in Table 2. DYPRO significantly outperformed both GGNN and TreeLSTM indicating a far stronger capacity of learning deeper semantic properties. Static models’ struggle further confirms their limitations of learning simple, shallow semantic features.

**4.3 Remarks**

Through two experiments, we thoroughly demonstrated how DYPRO stacks up against the static models. To summarize, despite the considerable progress, static models are still limited in learning semantic representation of a program. It is evident their generalization mostly happens at the level of program syntax, manifested in their struggle of digging deeper semantic properties. On the other hand, DYPRO learns from executions, a more direct and concrete representation of program
semantics. To elevate the learning from the level of executions to programs, we adopt random testing which is shown to achieve good coverage. As a result, DYPRO can learn a representation for each execution before compressing them into a program representation. To cope with the issues of learning long-term dependencies, we equip DYPRO with the states reduction mechanism so it only generalizes from the key program states while discarding the peripherals. Also worth noting, even if we did not demonstrate the utility of DYPRO in specific problem settings, given its strong capability of learning scalable and precise representations of program semantics, DYPRO should be readily applicable to many downstream programming tasks such as bug prediction, patch generation, or program synthesis.

5 Related Work

Learning Program Representations Hindle et al. [1] pioneered the field of learning language models from source code. A significant finding of theirs is programs, similar to natural language, are highly repetitive and predictable. With the rapid development of deep learning techniques and the increasing accessibility of large scale open source code repository, many works begin to apply deep neural networks to learn syntactic program representations [2; 3; 4; 5; 6]. More recently, a new line of research emerges aiming to tackle the problem of learning semantic representation [7; 8; 9; 10]. In this paper we present DYPRO, a novel dynamic model that learns program semantics from execution traces. Our evaluation shows DYPRO is more accurate in understanding and analyzing program semantics than several prominent static models.

Learning from Execution Traces Learning from execution traces also shows promise in the domain of program synthesis. Neural program interpreter (NPI) [13] is the first to learn to execute programs given their execution traces. Cai et al. [14] further improves NPI's generalization capability via recursion. Shin et al. propose a new deep neural architecture to learn to synthesis programs [20]. A fundamental difference between DYPRO and those attempts is DYPRO learns from the sequence of program states created by the execution whereas they use execution trace in pure syntax.

6 Conclusion

In this paper, we propose DYPRO, a novel deep neural architecture that learns program semantics from execution trace. We thoroughly evaluated DYPRO in a couple of semantically related tasks including head-to-head comparisons against several prominent static models. Results show DYPRO is the most accurate in both tasks and more importantly demonstrates its ability of capturing deep semantic properties that static models have difficulty with. For future work, we expect DYPRO to be readily available to many downstream programming tasks. Due to its high efficiency and precision in understanding and analyzing program semantics, we expect DYPRO to be useful in the real problem settings too.
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