BRIDGING THE GAP BETWEEN TESTING AND DEBUGGING THROUGH EXPLAINABLE DEEP ORACLES

BY

ALI REZA IBRAHIMZADA

THESIS

Submitted in partial fulfillment of the requirements
for the degree of Master of Science in Computer Science
in the Graduate College of the
University of Illinois Urbana-Champaign, 2024

Urbana, Illinois

Adviser:

Assistant Professor Reyhaneh Jabbarvand

ABSTRACT

Automation of test oracles is one of the most challenging facets of software testing, but remains comparatively less addressed compared to automated test input generation. Test oracles rely on a ground-truth that can distinguish between the correct and buggy behavior to determine whether a test fails (detects a bug) or passes. What makes the oracle problem challenging and undecidable is the assumption that the ground-truth should know the exact expected, correct, or buggy behavior. However, we argue that one can still build an accurate oracle without knowing the exact correct or buggy behavior, but how these two might differ. This research presents SEER, a learning-based approach that in the absence of test assertions or other types of oracle, can determine whether a unit test passes or fails on a given method under test (MUT). To build the ground-truth, SEER jointly embeds unit tests and the implementation of MUTs into a unified vector space, in such a way that the neural representation of tests are similar to that of MUTs they pass on them, but dissimilar to MUTs they fail on them. The classifier built on top of this vector representation serves as the oracle to generate "fail" labels, when test inputs detect a bug in MUT or "pass" labels, otherwise. Our extensive experiments on applying SEER to more than 5K unit tests from a diverse set of open-source Java projects show that the produced oracle is (1) *effective* in predicting the fail or pass labels, achieving an overall accuracy, precision, recall, and F1 measure of 93%, 86%, 94%, and 90%, (2) *generalizable*, predicting the labels for the unit test of projects that were not in training or validation set with negligible performance drop, and (3) *efficient*, detecting the existence of bugs in only 6.5 milliseconds on average. Moreover, by interpreting the neural model and looking at it beyond a closed-box solution, we confirm that the oracle is valid, i.e., it predicts the labels through learning relevant features.

ACKNOWLEDGMENTS

First and foremost, I would like to express my deepest gratitude to my adviser, Professor Reyhaneh Jabbarvand, whose expertise, understanding, and patience added considerably to my graduate experience. Her insightful guidance and unwavering support were instrumental in helping me navigate the complexities of my research and develop as a scholar. I started working in Software Engineering research without any background, I am grateful that she has given me a chance to participate in the University of Illinois Urbana-Champaign's research internship program in summer of 2021. She always believed in my abilities to become a successful researcher in the field.

I would like to particularly thank my academic mentor, Professor Darko Marinov. His diverse perspectives, expertise, and random arguments at Siebel Center for Computer Science has helped me a lot to understand the nature of my research, and think twice before making a conclusion. I will be always grateful to have a mentor like him.

I am forever indebted to my parents, my mom Freshta and my dad Abdul Hakim, for their unconditional love and support throughout my academic journey. My parents never formally attended university due to certain circumstances, but they always believed in my work, supporting me in every moment. I would like to thank my sister Yalda, and my brother Ferdows for their immense support as well.

I would like to thank Yiğit Varlı and Dilara Tekinoğlu for their valuable contributions in making this work possible. It was a great year working with them and publishing this work.

Finally, I would like to thank all my friends who have supported me throughout this journey, offering words of encouragement and much-needed distractions when the work seemed overwhelming. Special thanks to Bengü Süeda Şengül, Marc Edward Canby, Ahan Gupta, Kevin Johannes Ros and Louis Marek Schatzki for supporting me during my graduate studies. My time at the University of Illinois Urbana-Champaign would not have been pleasant if not for the presence of all my friends.

TABLE OF CONTENTS

CHAPTER 1: PROBLEM STATEMENT

1.1 MOTIVATION

A unit test similar to the example in Figure 1.1 consists of four main components: test input (`e1`, `e2`, and `e3`), MUT invocation (`obj.sort()`), test output, and test oracle (`assertEquals`). Given a ground-truth that knows the program's expected correct or buggy behavior for given inputs, oracles can determine test results, i.e., whether a test passes or fails. For example, the ground-truth in the example of Figure 1.1 identifies the sorted output for given inputs to be `e1, e2, e3`. Consequently, the assertion oracle checks if the produced output matches the expected one to generate the test result. Construction of the ground-truth can be a challenging task. Furthermore, the absence of automated ground-truths demands humans to decide whether the generated outputs are correct, demonstrating a significant bottleneck that inhibits absolute test automation [1].

```
@Test
public void testAdd() {
  ExampleObject obj = new ExampleObject();
  obj.add("e1");
  obj.add("e2");
  obj.add("e3");
  String output = obj.sort();
  Assert.assertEquals(output,"e1,e2,e3");
}
```

Figure 1.1: A simple JUnit test consists of four main components: input, MUT invocation, output, and assertion

1.2 RELATED WORK

State-of-the-art test oracle automation techniques can be divided into three main categories: *Implicit*, *Specified*, and *Derived* oracles.

1.2.1 Implicit Oracle

Implicit oracle relies on some implicit knowledge to identify whether a test passes or fails. Examples of such implicit knowledge are buffer overflow almost always yields an error, excessive CPU usage is a likely indicator of server disruptions, and unnecessary battery usage is evidence of energy defects in mobile apps. While quite effective and automated, implicit oracles can only determine the presence of limited categories of bugs. Implicit test oracle can be built on any procedure that detects anomalies such as abnormal termination due to a crash or an execution failure [2, 3]. This is because such anomalies are blatant faults; that is, no more information is required to ascertain whether the program behaved correctly or not.

1.2.2 Specified Oracle

Specified oracle determines the *expected* output of test execution and compares it with the actual output to decide whether a test passes or fails. To identify the expected output, these oracles require existence of formal specifications [4, 5, 6, 7, 8, 9] or contracts (pre-and post-conditions) [10, 11, 12, 13, 14] for the system under test. The performance and usability of such oracle highly depend on the availability, completeness, and quality of specifications. However, for many ever-changing software systems, specifications and contracts either do not exist or fall out of date. Even if automated techniques generate specifications, they are usually quite abstract, and inferring concrete test outputs from them is not guaranteed or is imprecise [1, 15]. State-of-the-art ML-enabled techniques alleviate such limitations by predicting meaningful specifications [16] or assert statements [17, 18, 19]. Compared to SEER, these techniques evaluate a limited set of properties related to program behavior only at a certain point the assertions [4].

1.2.3 Derived Oracle

Derived oracle decides the passing or failure of a test by distinguishing the system's correct from incorrect behavior rather than knowing the exact output. The correct and incorrect behavior can be (1) inferred from some meta-data such as *execution logs* [20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34]; (2) provided as properties of the intended functionality (metamorphic relations) [35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58]; or (3) checked against other versions of the software [59, 60, 61, 62, 63, 64]. Derived oracles are pragmatic, but are generally incomplete, i.e., can only identify test outputs for a subset of inputs. SEER, while considered as a derived oracle, alleviates this problem through a domain-specific embedding, i.e., semantically separating the buggy and correct code in the embedding space with respect to test results. Consequently, the neural model that serves as the oracle considers that *general* knowledge to predict a passing or failing verdicts.

1.3 HYPOTHESIS

To automatically build the ground-truth for test oracles, traditional and machine learning-based techniques rely on existing or derived formal specifications [4], assertions [17, 18, 19, 65, 66], program invariants [23, 67], and metamorphic relations [64, 68, 69, 70] for identifying the correct behavior. Some other techniques determine the patterns corresponding to specific types of bugs observed during test execution as an indicator of the buggy behavior [71, 72]. The commonality between these techniques is their emphasis on identifying the *exact* correct or buggy behavior to build the ground-truth. However, identifying the exact behavior and output is an undecidable problem; thereby, such techniques only partially validate the program. That is, the program can only be validated under a subset of test inputs with known expected outputs, or limited properties of the program determined by the invariants or metamorphic relations can be validated. While partial oracles enhance test automation to some degree, they may not guarantee the existence of a successful test driver.

The key insight in our research is that one can still create an accurate test oracle without knowing the *explicit relationship* between inputs and outputs under correct or buggy behavior. Instead, the ground-truth will determine how *different* the test inputs are *correlated* to outputs under the correct and buggy behavior. An oracle based on this ground-truth eliminates the need for assert statements and identifying the exact expected output in assertions, enhancing unit testing to a great extent [18].

In this research, we present SEER [1], an automated oracle to predict unit test results. Specifically, given a pair of $\langle t_i, m_i \rangle$, where t_i represents a unit test *without any assertions*, and m_i denotes the implementation of MUT, SEER automatically determines whether the test passes or fails on the MUT. To construct the ground-truth, SEER leverages joint embedding to distinguish between the neural representation of correct and buggy MUTs. A classifier on top of this embedding learns the correlation between inputs and outputs to predict test results.

[1] A person who can see what the future holds through supernatural insight.

1.4 SUMMARY OF FINDINGS

This work makes the following contributions:

- A novel domain-specific joint embedding of the unit tests and MUTs, which semantically separates MUTs' neural representations based on whether unit tests pass or fail on them.

- Design of an *interpretable* DL model that serves as a test oracle to generate passing or failing labels for unit tests without assertions. The interpretability enables us to go beyond the usage of DL as a closed-box technique and verify if the model predicts labels by looking at the relevant tokens in the implementation of MUTs. While it is out of the scope of this work, the relevant tokens involved in the model's decision can be further used by developers to localize the detected bugs.

- An extensive empirical evaluation on widely used open-source Java programs demonstrating that SEER is (1) *effective*—achieves an overall accuracy, precision, recall, and F1 measure of 93%, 86%, 94%, and 90%, (2) *generalizable*—predicting the labels for the unit test of projects that were not in training or validation set with negligible performance drop, and (3) *efficient*—once trained, it detects the existence of bugs in only 6.5 milliseconds on average. SEER's implementation and artifacts are publicly available [73].

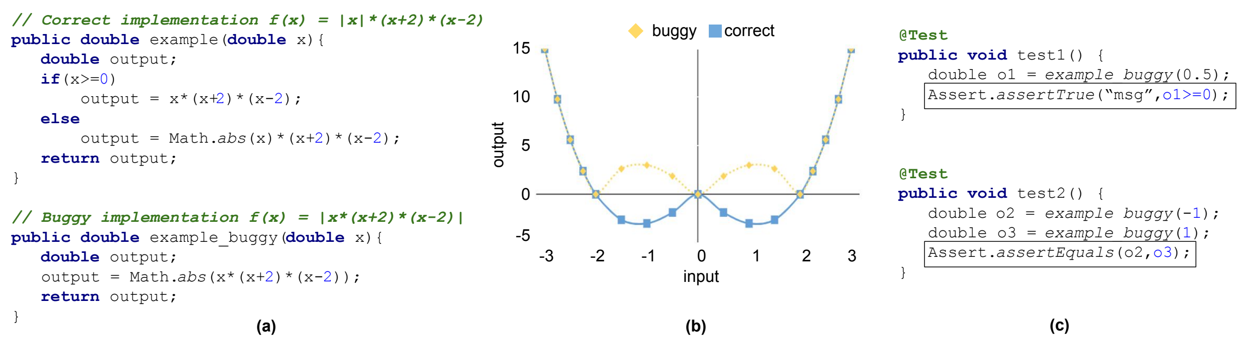
The remainder of this dissertation is organized as follows. Chapter 2 illustrates a motivating example. Chapter 3 provides an overview of SEER, while Chapter 4 describes details of the proposed technique. Finally, Chapter 5 presents the evaluation results.

CHAPTER 2: ILLUSTRATIVE EXAMPLE

To illustrate the limitations of prior work and explain the intuition behind our research, we use two code examples shown in Figure 2.1-a. The code snippet on the top is the *correct* implementation of a mathematical function that computes the output as $|x| \times (x+2) \times (x-2)$. The buggy version, on the other hand, computes the output as $|x \times (x+2) \times (x-2)|$ due to the displacement of a single parenthesis to the end of the assignment instead of after variable `x`.

Formally speaking, the behavior of a code is a function $B : I \rightarrow O$ that maps inputs in I to corresponding outputs in O. In our example, the mapping functions representing the explicit behavior of correct and buggy implementations are depicted as blue and yellow graphs in Figure 2.1-b. If such a function is known, an oracle can use it as a ground truth to distinguish between buggy and correct behavior. However, in reality, MUTs take multiple complex inputs, e.g., arrays and user-defined objects, resulting in n-dimensional mappings between inputs and outputs that are infeasible to determine. Therefore, test oracles rely on partial ground-truths. No matter how we build the ground-truth, the oracle's decision for test inputs belonging to $(-2, 0) \cup (0, 2)$ should be *"fail"* due to different behavior of the correct and buggy implementations in this range.

Suppose that we have two JUnit tests shown in Figure 2.1-c to assess the correctness of the `example_buggy` method. The ground-truth for identifying the expected output in the assert statement of `test1` is based on dynamic invariant detection, while the ground-truth for the assert statement in `test2` is based on a metamorphic relation $f(x) = f(-x)$. Dynamic invariant detection techniques rely on the execution traces of the *existing code*. Since our MUT is buggy, the invariant only captures properties of the buggy behavior,



```
// Correct implementation f(x) = |x|*(x+2)*(x-2)
public double example(double x){
   double output;
   if(x>=0)
       output = x*(x+2)*(x-2);
   else
       output = Math.abs(x)*(x+2)*(x-2);
   return output;
}

// Buggy implementation f(x) = |x*(x+2)*(x-2)|
public double example_buggy(double x){
   double output;
   output = Math.abs(x*(x+2)*(x-2));
   return output;
}
```

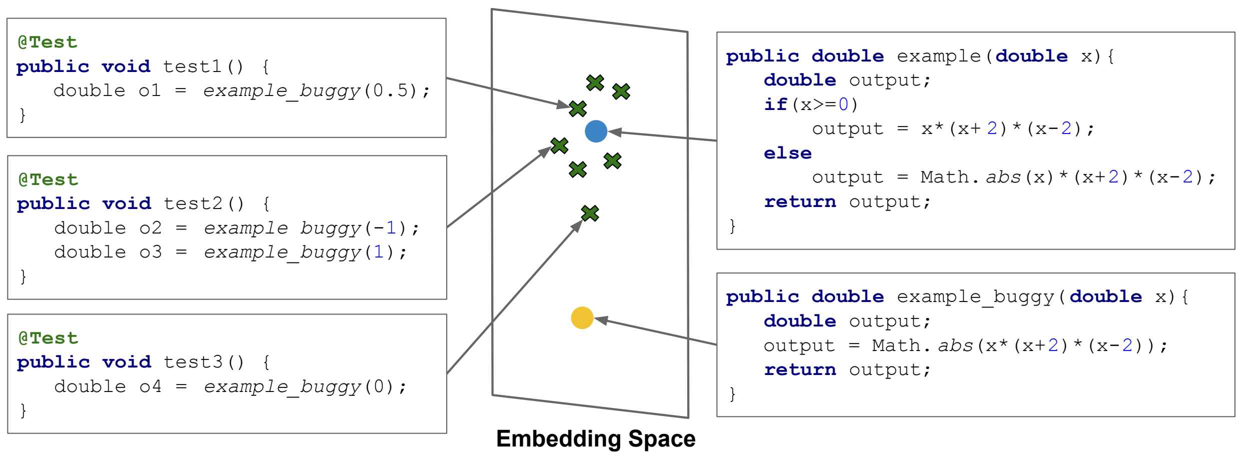
(a)

```
@Test
public void test1() {
   double o1 = example_buggy(0.5);
   Assert.assertTrue("msg",o1>=0);
}

@Test
public void test2() {
   double o2 = example_buggy(-1);
   double o3 = example_buggy(1);
   Assert.assertEquals(o2,o3);
}
```

(c)

Figure 2.1: (a) correct (top) and buggy (bottom) implementations of the mathematical function $f(x) = |x| \times (x+2) \times (x-2)$, (b) visualization of the correct and buggy implementations behavior, (c) JUnit tests with assertions to assess correctness of the buggy implementation



```java
@Test
public void test1() {
    double o1 = example_buggy(0.5);
}
```

```java
@Test
public void test2() {
    double o2 = example_buggy(-1);
    double o3 = example_buggy(1);
}
```

```java
@Test
public void test3() {
    double o4 = example_buggy(0);
}
```

```java
public double example(double x){
    double output;
    if(x>=0)
        output = x*(x+2)*(x-2);
    else
        output = Math.abs(x)*(x+2)*(x-2);
    return output;
}
```

```java
public double example_buggy(double x){
    double output;
    output = Math.abs(x*(x+2)*(x-2));
    return output;
}
```

Figure 2.2: The intuition behind the joint embedding of tests and MUTs with the goal of separating the representation of buggy and correct MUTs with respect to tests

i.e., *output* ≥ 0. By checking the generated invariant in the assertion, the test *passes* for $x = 0.5 \in (-2, 0) \cup (0, 2)$, while it should *fail* to demonstrate the bug. Similarly, the metamorphic relation of $f(x) = f(-x)$ holds for both correct and buggy implementations; thereby, the assertion wrongly decides the test inputs in the non-overlapping range as passed.

This example shows that identifying the explicit correct (or buggy) behavior to build a ground-truth, which has been the focus of prior work, has notable limitations. In this research, instead of realizing how the inputs are *explicitly related* to outputs under either correct or buggy behavior, we aim to learn how inputs are *differently correlated* to outputs for failing and passing pairs of $\langle t_i, m_i \rangle$. Here, t_i represents a unit test without any assertions, and m_i denotes the implementation of the MUT. To that end, SEER learns the vector representation of both MUT and test, so that the tests have a similar vector representation to the MUTs they pass on them, but dissimilar vector representation to MUTs they can reveal their bug, i.e., fail on them. Such joint embedding separates the representation of buggy and correct MUTs in the n-dimensional vector space.

Figure 2.2 shows the intuition behind the joint embedding in SEER. Here, since test inputs in `test1` and `test2` can reveal the bug in `example_buggy`, they are closer to the correct MUT and farther from the buggy MUT in the embedding space, i.e., they have a similar vector representation as correct MUT but dissimilar from buggy MUT. On the other hand, `test3` that cannot reveal the bug and should pass on both the buggy and correct MUTs, has the same distance from the correct and buggy MUTs in the embedding space. Compared to Figure 2.1-b, there is no explicit relationship between test inputs and outputs under correct or buggy behavior, but the embedding representation of correct and buggy MUTs are distinguished based on how the output they generate are correlated differently to the inputs of passing or failing tests.

In our research, we hypothesize that knowing the exact ground-truth is not necessary to construct an oracle. Instead, an automated oracle can decide the correct verdict on test execution if it can *correlate* tests, which represent inputs, and code, which transforms inputs to corresponding output, so that failure-inducing tests are *strongly* correlated with buggy code and *loosely* correlated with correct code.

SEER constructs oracles automatically in two distinct phases. In phase *one*, it learns the differences of correct and buggy code with respect to a test revealing the bug in high-dimensional space. Specifically, it uses contrastive learning to learn the similarity and dissimilarity between representations of buggy code, correct code, and test. Later, in phase *two*, SEER uses the learned representations from the previous phase and performs further training to predict test verdicts for a given code and test. That is, it predicts either a *"pass"* or *"fail"* outcome. The intuition here is that, when predicting a verdict during classification, the model will leverage the learned representations from phase *one*.

CHAPTER 3: OVERVIEW

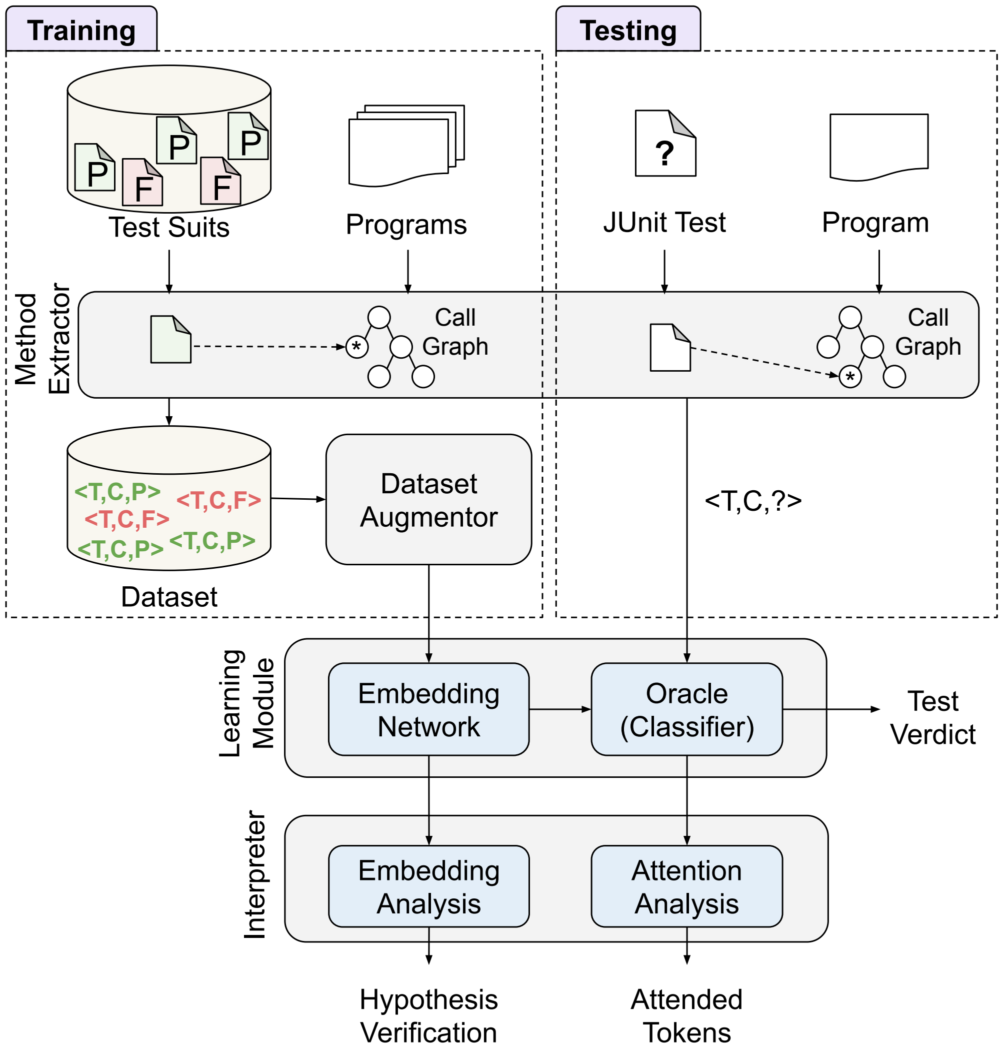


Figure 3.1: Overview of the SEER framework

Figure 3.1 provides an overview of SEER framework consisting of four major components: (1) *Method Extractor*, (2) *Dataset Augmentor*, (3) *Learning Module*, and (4) *Interpreter*. SEER requires a high-quality and large dataset of $\langle t_i, m_i \rangle$ instances to train the oracle. Given a set of programs and their corresponding test suites, the *Method Extractor* component builds such a dataset by extracting the implementation of MUT invocations in tests through a lightweight static analysis (details in §4.1). At the next step, *Method Extractor* creates labeled tuples in the form of $\langle t_i, m_i, l_i \rangle$, where t_i represents a unit test, m_i denotes the implementation of MUT, and l_i shows the test result outcome, which could be P (pass) or F (fail). *Dataset Augmentor* component then takes the generated dataset and augments it with additional instances to diversify the bugs and account for imbalanced labels (details in §4.3).

Once the training dataset is ready, SEER feeds it to the *Learning Module* to train the oracle through two phases. In the Phase 1 training, the *Learning Module* learns the vector representation of the test t_i and the MUT m_i through joint embedding by minimizing the distance among passing tuples $\langle t_i, m_i, P\rangle$, while maximizing the distance among failing tuples $\langle t_i, m_i, F\rangle$ (detail in §4.2). As a result, the vector representation of a test is similar to the MUTs it passes on them, but dissimilar to the MUTs it fails on. After learning the discriminative vector representations, *Learning Module* leverages transfer learning [74] and trains a classifier on top of the embedding network, which serves as our test oracle. To predict the label, SEER takes a unit test and the program under test as an input and extracts the implementation of invoked MUT(s). Given the produced pair of $\langle t_i, m_i\rangle$, the embedding network first computes their vector representations, and the classifier predicts the label, indicating whether a test passes on the given MUT or fails.

SEER goes beyond the use of DL as a closed-box approach and interprets the learned model for two purposes: (1) to verify if the embedding does its job in separating the representation of MUTs based on whether a test passes or fails on them, and (2) to verify the validity of the model by checking if the code tokens that impacted the oracle's decision are relevant (§4.4). In the next section, we describe the details of SEER's components.

CHAPTER 4: SEER

This section will first explain how to prepare the inputs to the *Learning Module*, followed by the details about SEER's neural architecture, dataset curation, and model interpretation.

4.1 METHOD EXTRACTOR

SEER's *Learning Module* requires labeled pairs of $\langle t_i, m_i \rangle$ to realize the correlation between the inputs (provided by unit tests t_i) and outputs (produced by MUT m_i). Given a test suite $T = \{t_1, t_2, \ldots, t_n\}$ consists of n unit tests and the program under test $P = \{m_1, m_2, \ldots, m_k\}$ consists of k developer-written methods[2], *Method Extractor* extracts m_i, the implementation of a MUT directly called in the body of the unit test t_i.

Method extraction can be performed statically, i.e., extracting the whole body of the MUTs regardless of the statements covered by a given test, or dynamically, i.e., only considering the executed statements by a test. While the latter is more intuitive in helping the model focus on the executed lines for predicting test verdicts, recent studies have shown that neural models learn the semantics of the code and context more effectively if provided global information [75, 76]. Consequently, the *Model Extractor* performs a lightweight flow-sensitive analysis on a given unit test t_i, identifies the `MethodInvocation` that belongs to the program under test, and extracts the corresponding method signature and the body. If a test invokes multiple methods, *Model Extractor* concatenates the extracted information for the MUTs in the order of invocation. In the illustrative example of Figure 2.1, *Method Extractor* identifies `example_buggy` method as m_i and extracts the whole text of the method, including the method signature and body.

4.2 LEARNING MODULE

The neural architecture of SEER is shown in Figure 4.1. Learning the neural model that serves as an oracle happens in two phases. In Phase 1 training, SEER learns the vector representation of unit tests and MUTs, in such a way that the representation of buggy and correct MUTs are different. At the next step, the representation of $\langle t_i, m_i \rangle$ pairs will be fed into a classifier, helping SEER to learn the correlation between inputs provided by t_i and outputs produced by m_i. Since the produced representation of buggy and correct MUTs are

[2]We exclude third-party APIs as their code may not be available.

different, the oracle ultimately learns how differently the inputs are correlated to outputs under the correct and buggy behavior.

During the Phase 1 training, SEER learns the vector representation of unit tests and MUTs through joint embedding [77]. Joint embedding, also known as multi-modal embedding, has been widely used to embed heterogeneous data into a unified vector space so that semantically similar concepts across the two modalities reside closer in the embedding space. For example, in computer vision, researchers have used Convolutional Neural Network (CNN) and Recurrent Neural Network (RNN) to jointly embed images and text into the same vector space for labeling images [78].

We adopt the concept of joint-embedding in our problem to semantically separate the representation of correct and buggy MUTs concerning the result of tests. Specifically, we hypothesize that by jointly embedding the unit tests and MUTs into a unified vector space, so that tests have similar vector representations to the MUTs they pass on them but are different from the MUTs they fail on them, the resulting embedding separates the representation of correct and buggy MUTs. The joint embedding of unit test, t_i, and implementation of MUT, m_i, can be formulated as follows:

$$m_i \xrightarrow{\phi} D_{m_i} \rightarrow J(D_{m_i}, D_{t_i}) \leftarrow D_{t_i} \xleftarrow{\psi} t_i \tag{4.1}$$

where ϕ is an embedding function to map m_i into a d-dimensional vector space D; ψ is an embedding function to map t_i into the same vector space D; and $J(,)$ is a similarity measure to score the matching degrees of D_{m_i} and D_{t_i} in order to put m_i and t_i closer or farther in the embedding space. SEER uses the cosine similarity metric to measure the similarity between the vector representations of t_i and m_i. A small cosine similarity means two vectors are closer together in d-dimensional embedding spaces, while a bigger cosine similarity means the vectors point to different angles, i.e., are farther from each other in the embedding space. To learn and semantically separate the representation of correct and buggy m_is with respects to the test results, SEER minimizes the ranking loss as follows:

$$\mathcal{L}(\theta) = \sum_{\langle t_i, m_i+, m_i- \rangle} max(cos(D_{t_i} - D_{m_i+}) - cos(D_{t_i} - D_{m_i-}) + \alpha, 0) \tag{4.2}$$

where D_{t_i} is the vector representation of t_i, D_{m_i+} is the vector representation of a MUT that t_i passes on it, and D_{m_i-} is the vector representation of a MUT that t_i fails on it. The θ and α represent model parameters and a constant margin value, respectively. Intuitively, by minimizing the margin ranking loss, SEER learns to minimize the distance between D_{t_i} and D_{m_i+}, while maximizing the distance between D_{t_i} and D_{m_i-}.

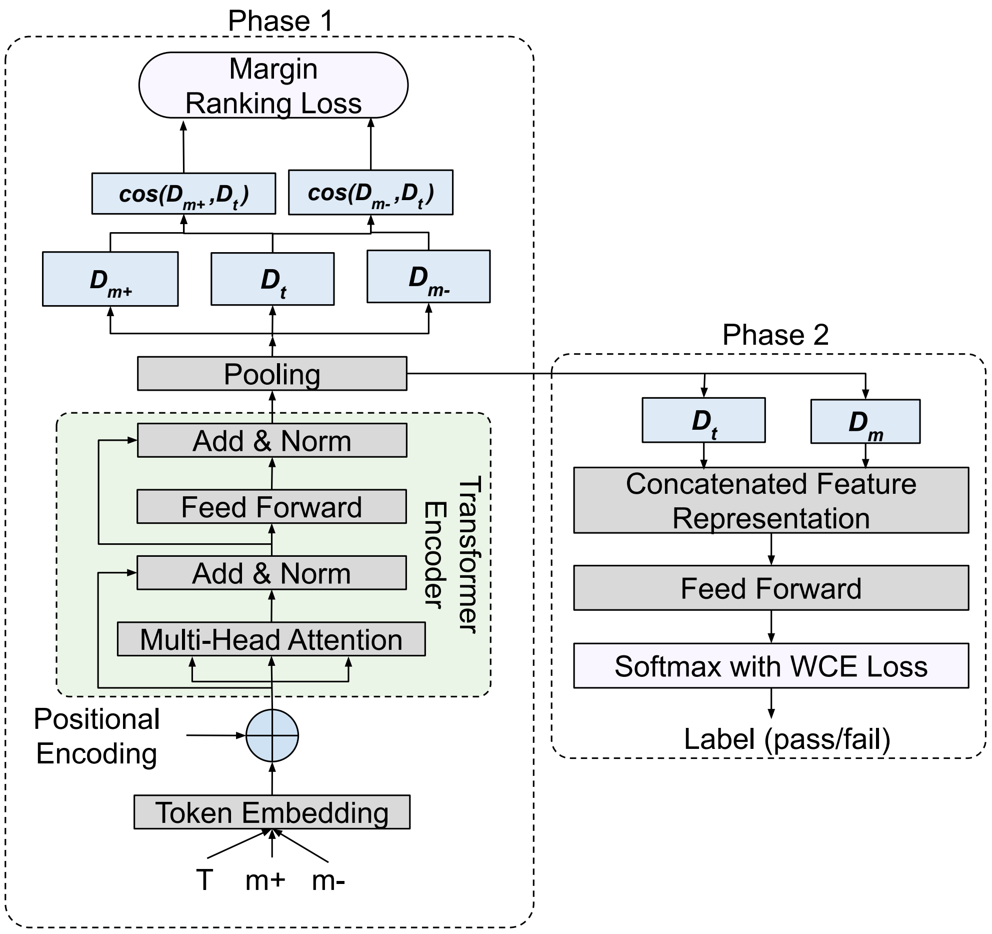


Figure 4.1: Overall architecture of SEER

After learning the vector representation of tests, D_{t_i}, and MUTs, D_{m_i}, in Phase 1, SEER concatenates them to create a single continuous feature representation for the $\langle t_i, m_i \rangle$ pair. The resulting combined feature vector is fed into a series of fully connected layers in Phase 2 training to decode the learned features into a specific target class, i.e., pass or fail.

4.3 DATASET CURATION

Training of SEER requires a large and high-quality dataset, i.e., a dataset consists of passing and failing $\langle t_i, c_i \rangle$ pairs representing a diverse set of bugs across different projects. To construct the dataset, we started with the Defects4J [79], which is a collection of reproducible bugs in large and widely-used Java projects. Each bug in this dataset is accompanied by the buggy and fixed versions of subject programs as well as developer-written passing and failing tests. Our rationales to build the dataset based on Defects4J are: (1) the bugs are isolated and reproducible, making it easier for the neural model to learn relevant features; and (2) it

Algorithm 4.1: Dataset Augmentation Algorithm

```
   Input: MUT, order
   Output: A Higher Order Mutant of MUT (HOM)
1  $Mutables \leftarrow$ getUniqueMutables ($MUT$)
2  $counter \leftarrow order$
3  $HOM \leftarrow MUT$
4  foreach $mutable \in Mutables$ do
5      $mutant \leftarrow$ mutate ($MUT, mutable.op, mutable.loc$)
6      if $counter > 0$ then
7          if $isCompilable(mutant)$ then
8              $HOM \leftarrow mutant$
9              $counter \leftarrow counter - 1$
10         else
11             return $HOM$
12     else
13         break
14 return $HOM$
```

contains failing developer-written tests, helping with the generation of a balanced dataset, since the automated generation of failure-triggering tests using Randoop [66] and EvoSuite [65] is not guaranteed.

A significant limitation of Defects4J dataset is the complexity of the bugs, i.e., the majority of bugs involve only one statement in the code. This issue can degrade the performance of Seer in two ways. First of all, the model may treat small changes in the code as noise and may not include them in learning, achieving a lower performance [80, 81]. More importantly, a model trained on simple bugs may not generalize to complex, more realistic bugs. Inspired by the power of mutation testing in curating high-quality training datasets [71] and the fact that higher-order mutants [82] are more representative of complex bugs, *Dataset Augmentor* component of Seer takes a passing $\langle t_i, m_i \rangle$ pair as input and mutates the MUT repeatedly at different locations to generate *higher-order* mutants.

Algorithm 4.1 explains our dataset augmentation process. The algorithm takes the MUT and *order*—the maximum number of times we mutate a given MUT—as an input and generates a higher-order mutant, HOM. To that end, it first identifies unique pairs of $Mutables = \langle op, loc \rangle$ that demonstrate the locations loc in MUT where a mutation operator op can be applied (Line 1). Next, it mutates the MUT once at a time using these pairs (Lines 4-5). After each mutation, the algorithm checks whether or not the generated mutant is compilable (Line 7). The algorithm continues the mutation using the next *mutable* (Lines

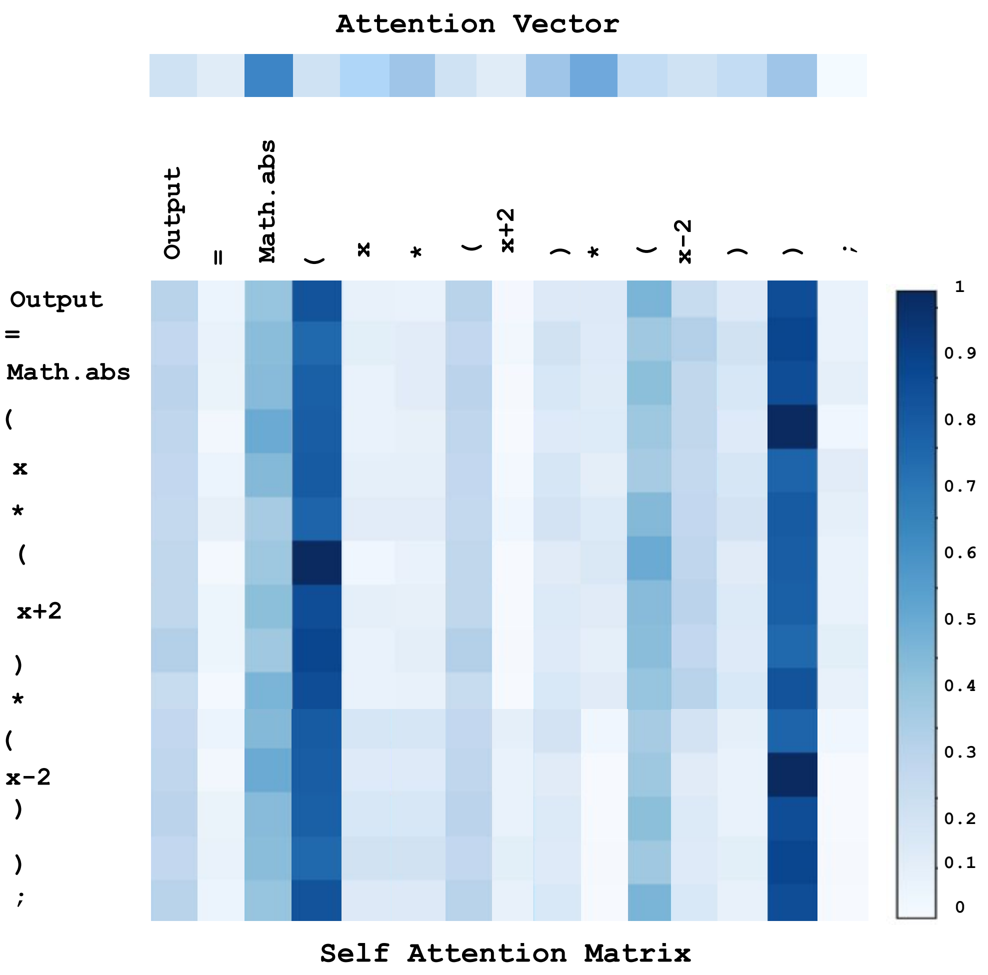


Figure 4.2: The importance of Self-Attention in the oracle problem

8-9) if the mutant is compilable. Otherwise, it reverts the mutation and terminates with the produced *HOM* (Lines 10-11). Mutation continues until the MUT is mutated *order* times or it has been mutated at all the mutable locations.

4.4 INTERPRETATION

Without interpretation, one cannot trust the performance of ML, and specifically DL models, as their learning depends on millions of parameters. Specifically, such intelligent models can create unrealistically good predictions, but based on learning from irrelevant features due to the noise in the dataset or data leakage problem [83]. To ensure the trustworthiness of Seer, we validate the following two hypotheses by interpreting the *Learning Module*: *Hypothesis 1.* The oracle looks at relevant tokens in the MUT to predict a test result; and (2) *Hypothesis 2.* The embedding network separates buggy and correct MUTs in the embedding space by distinguishing their vector representations. We will discuss the details of *Attention Analysis* and *Embedding Analysis* to investigate the correctness of *Hypothesis 1* and *Hypothesis 2*, respectively.

4.4.1 Attention Analysis

Attention mechanism [84], which was initially proposed to overcome the *long sequence problem* in Recurrent Neural Networks (RNNs), is a method for helping DL models to identify the importance of single features in a feature sequence as they perform their tasks. Attention mechanism serves two purposes in neural architectures; first, it helps with the model's performance. More importantly, it has been extensively used to resolve the interpretability of deep neural models. The initial implementations of the Attention mechanism were neural layers between the encoder and decoder components in the neural architecture, producing attention weight vectors, $\overrightarrow{AT} = \{w_0, \ldots, w_n\}$, as an output. In the context of neural code analysis, w_i is the probability that given a statement with n tokens, how important is the token at location i in the statement when predicting a label. The higher the Attention weight for a feature, the more the model attends to it when making a prediction.

Seer uses Multi-Head Attention [84, 85], also known as Self Attention, to consider the relative importance of a token in the statement when learning. The output of a Self Attention layer is an $n \times n$ matrix $SA = [[w_{0_0}, \ldots, w_{0_n}], \ldots, [w_{n_0}, \ldots, w_{n_n}]]$, where w_{i_j} represents the how important is the token at location i given a specific token at location j. Figure 4.2 shows the difference between these two Attention mechanisms for the buggy statement in our illustrative example (for the sake of space and readability, Figure 4.2 shows only a subset of SA corresponding to the buggy statement). (Figure 2.1-a). As shown in this figure, Self Attention is more successful at capturing the importance of closing parenthesis with respect to open ones compared to the traditional Attention mechanism. Algorithm 4.2 presents Seer's approach for Attention analysis, i.e., analyzing the SA matrix to identify which tokens and statements attended the most in the MUT to predict the test result.

For a given pair of $\langle t_i, m_i \rangle$, Algorithm 4.2 takes MUT's tokens, $\{c_0, \ldots, c_n\}$, Self Attention matrix, $SA = [[w_{0_0}, \ldots, w_{0_n}], \ldots, [w_{n_0}, \ldots, w_{n_n}]]$, and Attention threshold value, k, as an input to identify the set of attended tokens, $ATkn$ and attended statements $ASmt$, as outputs. To that end, the Algorithm traverses SA matrix row by row (Lines 3-7), identifies the top k% most attended tokens—top k tokens with the highest Attention weight value (Line 4), and merges the attended tokens per each row for the entire matrix along with their corresponding indices (Lines 5-7). The outcome of merge is the set of attended tokens, $ATkn$. When merging, considering the indices is specifically important, as similar tokens at different indices

Algorithm 4.2: Attention Analysis

```
   Input: MUT's tokens $\overrightarrow{Tkn} = \{c_0, \ldots, c_n\}$
   Input: MUT's statements $\overrightarrow{Smt} = \{s_0, \ldots, s_m\}$
   Input: $SA = [[w_{0_0}, \ldots, w_{0_n}], \ldots, [w_{n_0}, \ldots, w_{n_n}]]$
   Input: Attention threshold $k$
   Output: Attended tokens $ATkn$, Attended statements $ASmt$
 1 $ATkn \leftarrow \emptyset$ $ASmt \leftarrow \emptyset$
 2 foreach $row = [w_{i_0}, \ldots, w_{i_n}] \in SA$ do
       // $localATkn = \{\langle c_i, ind_i \rangle | \; ind_i$ is index of $c_i$ in $\overrightarrow{Tkn}\}$
 3     $localATkn \leftarrow getMostAttended(row, Tkn, k)$ foreach $\langle c_i, ind_i \rangle \in localATkn$ do
 4         if $\neg ATkn.contains(\langle c_i, ind_i \rangle)$ then
 5             $ATkn \leftarrow ATkn \cup c_i$
 6 foreach $s_i \in Smt$ do
 7     if $|s_i \cap ATkn| > k$ then
 8         $ASmt \leftarrow ASmt \cup s_i$
```

might be attended differently. In the example of Figure 4.2, while the token "(" appears multiple times in SA at different indices, its highest attention is in the last index.

Finally, the Algorithm iterates over MUT's statements, $\{s_0, \ldots, s_m\}$, and determines the statements that k% of their tokens overlap with the attended tokens in $ATkn$ (Lines 8-10). Such statements indicate the buggy statements in cases that the predicted label for a $\langle t_i, m_i \rangle$ pair is "fail". The intuition here is that since the number of buggy lines is limited, according to the *Generalized Pigeonhole Principle* [86], there is at least one statement with more than k% tokens among attended tokens $ATkn$.

4.4.2 Embedding Analysis

Seer relies on visualization techniques to validate the separation of the buggy and correct MUT representations in the embedding space. Given the high dimensionality of embedding vectors, however, the first step in the embedding analysis is reducing the dimension of representations. Dimensionality reduction algorithms such as PCA [87], LDA [88], and tSNE [89] concentrate on placing dissimilar data points far apart in a lower dimension representation.

Among the most popular dimensionality reduction algorithms, Seer uses Linear Discriminant Analysis (LDA), as it recognizes the class labels and maximizes the separation between classes during the dimensionality reduction. Figure 4.3 shows the intuition behind how LDA

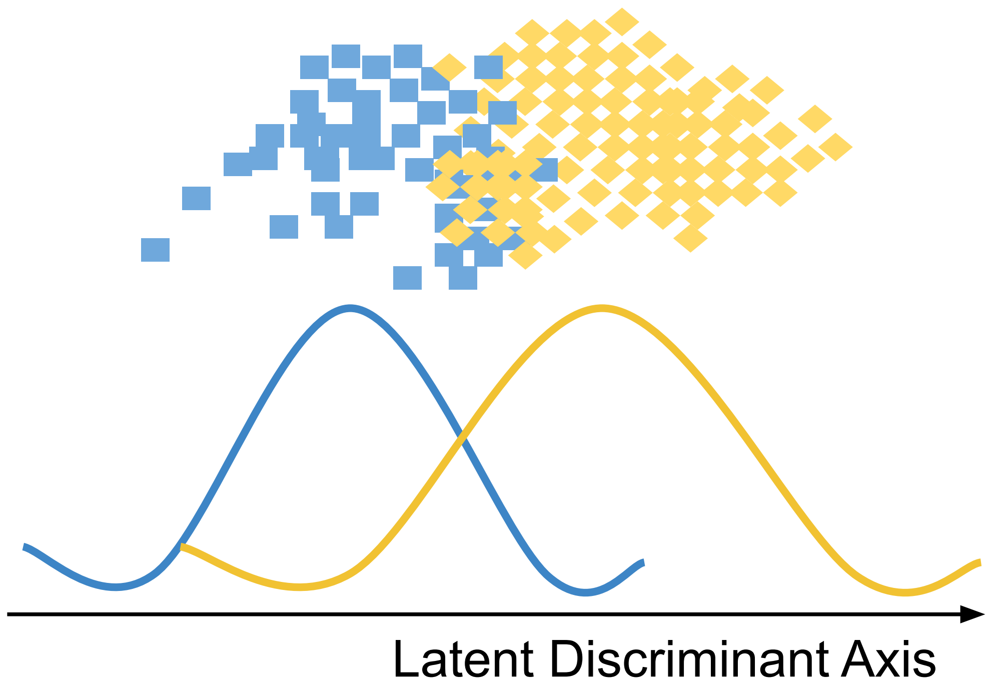


Figure 4.3: The intuition behind LDA dimensionality reduction

performs high-dimensionality reduction. The scattered plots represent the distribution of buggy (yellow) and correct (blue) MUTs in high-dimensional embedding space, and the curves represent that of in the lower dimension. As demonstrated by Figure 4.3, if the distributions of reduced-dimension instances of two classes overlap, they are not separated correctly in the higher dimension. Otherwise, the instances of buggy and correct classes are separated in the high-dimensional embedding space.

CHAPTER 5: EVALUATION

To evaluate effectiveness of Seer, we investigate the following research questions:
RQ1: *Effectiveness*. How effective are the proposed techniques in predicting accurate passing or failing test labels? What type of bugs the proposed oracle can detect, and what bugs are harder for the oracle to detect?
RQ2: *Generalization*. To what extent the proposed technique can predict test labels for the Java projects it has not been trained on?
RQ3: *Interpretation*. Can embedding truly distinguish between the representation of MUTs for passing and failing ⟨test,MUT⟩ pairs? What features impact the oracle's decision?
RQ4: *Performance*. What are the performance characteristics of the proposed technique?

5.1 EXPERIMENT SETUP

We will explain the details of our experimental setup for the sake of reproducibility. Morever, we have made all artifacts of Seer publicly available on GitHub [73].

5.1.1 Dataset:

Table 5.1 shows details about the properties of the dataset used for training, validation, and testing of Seer. Our dataset is built on top of Defects4J [79], which consists of 835 bugs in 17 widely-used Java projects. In addition to the data collected from Defects4J, we also augmented the dataset with higher-order mutants and automatically generated Randoop [66] tests. The former helps diversify the bugs in the dataset, and the latter generates tests that either pass or fail on the newly added bugs. Finally, we removed all the assert statements from the developer-written and automatically generated tests to avoid bias in learning from them.

For generating our syntactic faults, we use mutation testing tool Major [90]. There are two main reasons to prefer Major tool in our research: (1) Defects4J already supports Major, and its CLI has commands to mutate (`defects4j mutation`) a specific bug using Major, and (2) Major allows us to export source codes of generated mutants. We apply mutation to 15 projects of Defects4J. Collections and Mockito projects are not mutable as this is stated in the issue tracker of Defects4J repository on GitHub. For mutable bugs of 15 projects, we first find mutation operators applicable to buggy version and fixed version of each changed method separately. To ensure that our mutants are representative of real bugs, we use higher order mutation (up to 5th order). After mutation step is completed, we choose at most 4 random-compilable higher order mutants for a found method (for buggy and fixed version separately). Then we run both developer-written tests and Randoop tests on these chosen mutants.

After the above-mentioned steps are completed, we have the following source codes extracted for each modified method of each Defects4J bug:

- FC (fixed version of code)
- BC (buggy version of code)
- FC(M)s (set of mutants that are generated from fixed version)
- BC(M)s (set of mutants that are generated from buggy version)

We also have the information that whether a particular test of the bug is passed or failed on each of these source codes. By using this information, we construct triplets of form $\langle T, C+, C-\rangle$ where T stands for test code, $C+$ is code that passes T and $C-$ is code that fails on T. The examples below can better clarify our approach:

- If $FC(M)$ passes on T and $BC(M)$ fails on T, we extract the $\langle T, FC(M), BC(M)\rangle$ triplet.
- If FC passes on T and $FC(M)$ fails on T, we have $\langle T, FC, FC(M)\rangle$ triplet.
- If FC passes on T and BC fails on T, we have $\langle T, FC, BC\rangle$ triplet.

We also apply below constraints when generating our dataset:

- For each triplet, $C+$ and $C-$ must be different than empty string. If not, we remove the triplet from the dataset.
- There must not be any duplicates in the dataset. By checking the existence of duplicate triplets and removing them, we ensure that all instances of our dataset are unique triplet-wise.
- For each triplet, T must a covering test for modified method of $C+$ and $C-$. In other words, T must directly call the modified method in its body. If it does not, we remove the triplet from our dataset.

Table 5.1: Properties of the dataset.

Projects	# Bugs	# Mutants	#Tests	Dataset							
				Defects4J				Higher-order Mutants			
				Developer Tests		Randoop Tests		Developer Tests		Randoop Tests	
			#Pass, #Fail (Contrib %)	# Pass	# Fail	# Pass	# Fail	# Pass	# Fail	# Pass	# Fail
Compress	47	24,322	30,753 (30.26%)	1,214	22	2,965	2230	385	265	192	23,480
Lang	64	12,824	15,130 (14.89%)	702	59	1,249	296	397	509	1,124	10,794
Chart	26	4,313	14,901 (14.66%)	248	37	5,316	4987	154	109	229	3,821
Math	106	9,488	13,580 (13.36%)	1,685	91	1,584	732	732	814	546	7,396
Codec	18	8,973	10,210 (10.05%)	271	11	648	307	375	54	93	8,451
Closure	174	1,615	3,170 (3.12%)	1,431	8	113	3	768	76	49	722
JacksonDB	112	581	2,818 (2.77%)	2,133	27	77	0	410	94	42	35
Time	26	203	2,415 (2.38%)	1,765	39	255	153	84	70	18	31
Jsoup	93	677	2,134 (2.1%)	925	57	458	17	125	234	277	41
Cli	39	913	1,612 (1.59%)	348	10	292	49	106	75	371	361
Csv	16	1,166	1,582 (1.56%)	327	6	83	0	297	2	23	844
JacksonCore	26	941	1,420 (1.4%)	331	15	105	28	320	163	136	322
Gson	18	531	1,386 (1.36%)	678	15	93	69	295	92	144	0
JxPath	22	143	314 (0.31%)	93	1	74	3	0	1	105	37
Mockito	38	0	100 (0.1%)	56	39	5	0	0	0	0	0
JacksonXml	6	49	81 (0.08%)	19	1	9	3	28	12	2	7
Collections	4	0	7 (0.01%)	4	1	2	0	0	0	0	0
Total	835	66,739	101,613 (100%)	12,230	439	13,328	8,877	4,476	2,570	3,351	56,342

As shown in Table 5.1, the final augmented dataset consists of $33,385$ passing pairs and $68,228$ failing pairs of $\langle t_i, m_i \rangle$, making a total of $101,613$ $\langle t_i, m_i \rangle$ pairs in the dataset. For Phase 1 training, we construct $\langle t_i, m_i+, m_i- \rangle$ tuples by merging passing and failing $\langle t_i, m_i \rangle$ pairs for common tests. That is , for a given test t_i, we find all the m passing pairs and n failing pairs of $\langle t_i, m_i \rangle$. If m and n are non-zero, we get total $m \times n$ tuples of $\langle t_i, m_i+, m_i- \rangle$. This provides us with $20,759$ tuples of $\langle t_i, m_i+, m_i- \rangle$ for Phase 1 training, divided into 90% training, 5% validation, and 5% testing instances. For Phase 2 training, we similarly divided the original dataset with $101,613$ instances represented by Table 5.1.

5.1.2 Learning Module Configuration:

We implemented Seer's *Learning Module* using PyTorch [91] open-source library. Multiple factors can affect the neural models' learning process and final performance. For the loss function, which determines how well the algorithm approaches learning from the training data, we used Margin Ranking Loss (MRL) in Phase 1 training and Weighted Cross-Entropy Loss (WCEL) in Phase 2 training. MRL has been shown to outperform Cross-Entropy Loss in learning the embeddings and putting data instances of the same target class closer to each other than instances from other classes [92]. Since our embedding goal is similar, i.e., to put passing pairs of $\langle t_i, m_i \rangle$ closer to each other compared to failing ones, MRL was a reasonable loss function for learning the MUT and test embeddings.

For Phase 2 training, we chose Weighted Cross-Entropy Loss rather than Cross-Entropy

Loss, which is commonly used in classification problems, since our dataset has more failing pairs of $\langle t_i, m_i \rangle$ compared to passing pairs. To enhance the performance, we utilize AdamW optimizer [93], which has been shown to outperform Adam optimizer [94] to update the network weights and minimize this loss function iteratively.

The other factors that affect the model's performance are hyperparameters and overfitting. We followed a guided hyperparameter tuning to find a configuration for the model that results in the best performance on the validation data. One of the most important hyperparameters is the learning rate, which controls how much to change the model in response to the estimated error each time the model updates weights. Choosing the learning rate is challenging as a value too small may result in a long training process that could get stuck, whereas a larger value may result in an unstable training process. The learning rate of SEER's *Learning Module* for Phase 1 and Phase 2 training are $1.34e^{-4}$ and $1.34e^{-6}$, respectively. The difference in learning rates is because Phase 2 learning is incremental compared to Phase 1, and a similar learning rate results in large, i.e., NaN, loss function values. Furthermore, we used 10-fold cross-validation to avoid overfitting and implemented early-stopping criteria to terminate the training. That is, we repeated the training/validation for 10 times on different training and validation sets and chose the model that achieved the best performance. To automatically terminate the learning, our patience level was 5 epochs, i.e., if the validation loss of the model did not improve in 5 consecutive epochs, we assumed that learning had reached an optimum level.

5.2 RQ1: EFFECTIVENESS

For this research question, we divided $101,613$ pairs of $\langle T, C, F \rangle$ instances in our dataset into 90% training, 5% validation, and 5% testing instances. To that end, we downsampled such instances for each project by 90%, and used the remaining if possible. The only exception was the Collections project, which we included its few instances only in the training set. We select accuracy, precision, recall, and F1 score as metrics to measure the effectiveness of SEER in predicting correct labels. Table 5.2 shows the result for this experiment under "SEER with embedding" columns. These results are obtained through a 10-fold cross-validation, i.e., downsampling repeated 10 times.

Each row in Table 5.2 shows one of our subject projects and the percentage of instances they have correctly predicted for different versions of SEER. These results confirm **the original implementation of Seer illustrated in Figure 4.1 can effectively predict passing and failing labels for the test suite of each subject program, achieving** 93% **accuracy,** 86% **precision,** 94% **recall, and** 90% **F1 score**. Despite an overall good

Table 5.2: Effectiveness and Generalization of Seer in predicting test labels. TP, FP, TN, and FN stands for True Positive, False Positive, True Negative, and False Negative, respectively.

Subjects	Seer with embedding	
	# Pass	# Fail
	TP (%), FN (%)	TN (%), FP (%)
Compress	92.53%, 7.47%	98.18%, 1.82%
Lang	81.07%, 18.93%	92.6%, 7.4%
Chart	94.74%, 5.26%	88.03%, 11.97%
Math	93.83%, 6.17%	89.98%, 10.02%
Codec	79.12%, 20.88%	99.58%, 0.42%
Closure	98.36%, 1.64%	80.56%, 19.44%
JacksonDB*	100%, 0%	30.77%, 69.23%
Time*	100%, 0%	0%, 100%
Jsoup*	98.81%, 1.19%	0%, 100%
Cli	96.23%, 3.77%	60%, 40%
Csv	94.59%, 5.41%	98.21%, 1.79%
JacksonCore	97.06%, 2.94%	41.94%, 58.06%
Gson*	100%, 0%	66.67%, 33.33%
JxPath*	100%, 0%	25%, 75%
Mockito*	100%, 0%	0%, 100%
JacksonXml*	100%, 0%	0%, 100%
Collections*	N/A, N/A	N/A, N/A
Total	93.63%, 6.37%	92.77%, 7.23%

performance, Seer did not perform well on some projects (those marked by asterisks in Table 5.2. Our investigation showed that due to the low contribution of these projects to the dataset, the test data instances from them were either none, e.g., Collections project, or very few. Consequently, the effect size of classification was very large.

False Negatives are not big issues in our proposed technique, as Seer is interpretable and developers can quickly check the Attended tokens to verify the False Negative. To understand the reasons for False Positives, we compared the True Negative and False Positive instances from the following perspectives:

- *Test type.* The unit tests in our dataset are either developer-written tests or automatically generated by Randoop. Majority of t_is for True Negative instances belonged to Randoop. However, for False Positives, half of the t_is are developer-written tests while the other half are Randoop tests. As a result, there is no significant correlation between the False Positive instances and test type.

- *# Test Tokens.* The average number of test tokens for False Positive instances is 74 compared to 85 for True Negatives, which shows that Seer performs better when tests are longer. We believe that this is potentially because the representation of longer tests are unique compared to shorter tests, making it easier for the model to predict a correct label for them.

- *# MUT tokens.* The average number of MUT tokens for False Positive instances is 89 compared to 131 for True Negatives, which shows that SEER performs better when MUT's implementation has more tokens and statements. Similar to our argument about # test tokens, short MUT sequences carry less semantic information, making it harder for the model to predict test results.

- *Bug type.* SEER correctly predicts the test results for 95% of the higher order mutants. This ratio for the real bugs from the Defects4J dataset is 80%. Given that we found no significant correlation between the number of buggy lines in False Positive and True Negative instances, we believe this happens because real bugs are unique. That is, while higher-order mutation injects bugs at different locations and considers different combinations of mutation operators, the operators are limited, making it easier for SEER to learn the bugs that involve those operators. We argue that this is not a limitation of SEER, but the dataset, which can be resolved by including more real bugs in the training dataset.

Moreover, the average number of tokens for the MUTs in misclassified examples is 89, which is smaller than the average 131 tokens for instances that were correctly classified. This indicates the fact that short sequences carry less semantic information and are harder for the model to learn. In contrast, longer sequences make it easier for the model to predict them since they have more embedding vectors. (2) Randoop tests are much longer than developer-written tests. That is, the average length of Randoop tests is 108 tokens, while it is 40 for developer-written tests. (3) The average number of lines changed when fixing a bug in C- is significantly high in mutant MUTs. On average, there are roughly 3.61 lines changed when fixing a buggy mutant code, while it is 1.35 lines for buggy real fault code.

5.3 RQ2: GENERALIZATION

In the previous research question, we showed that SEER can effectively serve as an oracle on the unseen $\langle t_i, m_i \rangle$ pairs from the projects that were in the training dataset. In this research question, we go one step forward to investigate how SEER generalizes to predict test labels for $\langle t_i, m_i \rangle$ pairs, where m_i belongs to a project that was not in the training data. To that end, we computed the contribution of each project (column "# Tests" in Table 5.1) and divided the dataset into high-contribution projects with contribution values greater than 10%, and low-contribution projects. We used all the instances of the projects in the high-contribution dataset for training and validation. Then, we tested the trained model on the projects in the low-contribution dataset. For this research question, we only consider the precision and recall values to evaluate the performance of SEER, as the low-contribution dataset is highly imbalanced (passing $\langle t_i, m_i \rangle$ pairs are 3.5× more than failing pairs).

Compared to the original precision and recall values computed in RQ1 (86% and 93%), the value of SEER's performance metrics on unseen projects are 77% (9% ↓) and 82% (9% ↓). Given that unseen projects have different statistical distributions compared to the projects used for training, i.e., different tokens and hence vocabularies, the performance drop is expected due to the Out of Distribution (OOD) problem [95]. Our further investigation of the misclassified instances confirmed that the model's performance was better on unseen projects, whose vocabularies had a higher overlap with the vocabularies of the projects used for training SEER, compared to that of for projects with less overlap in vocabularies. These results demonstrate that **Seer can achieve comparable performance on unseen projects whose vocabularies overlap with the projects for training the oracle**.

5.4 RQ3: INTERPRETATION

Recall that the goal of SEER's interpretation is two-fold. First, we interpret the embedding network to verify if it has correctly learned to separate the representation of correct and buggy MUTs. More importantly, we interpret the oracle to identify which features, i.e., tokens in the MUT, and which statements were mostly attended when predicting a label. From this information, we can determine whether the attended features are relevant to the decision and whether the model's performance is valid.

5.4.1 Attention Analysis

Given a threshold number k, SEER's attention analysis algorithm (Algorithm 4.2) produces a set of top k% attended tokens and attended statements in the MUT. To confirm that SEER has attended to *relevant tokens* for predicting labels, we measured the percentage of the buggy statements that are among attended statements in the MUT. Specifically, we computed this metric for *true negative* test instances, i.e., $\langle t_i, m_i \rangle$ pairs for which the SEER correctly identified to fail. Figure 5.1 shows the percentage of buggy statements that were among the attended statements, and how this percentage changes in response to the change of threshold value. These results demonstrate that **Seer has indeed attended to relevant tokens to predict test labels, and even with a small threshold value of 5%, it**

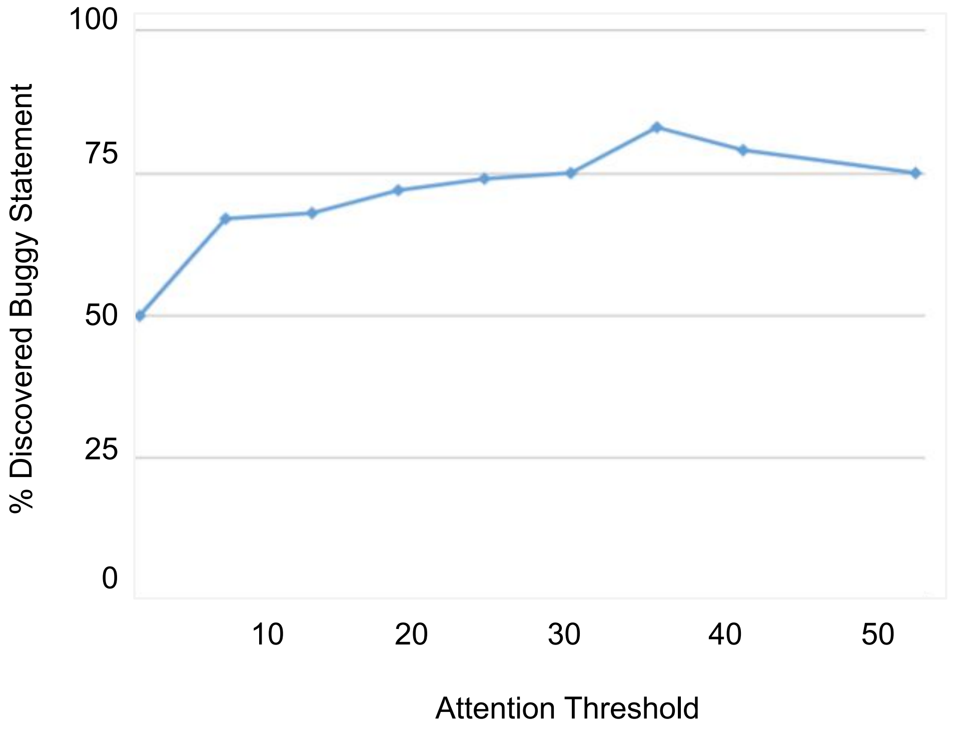
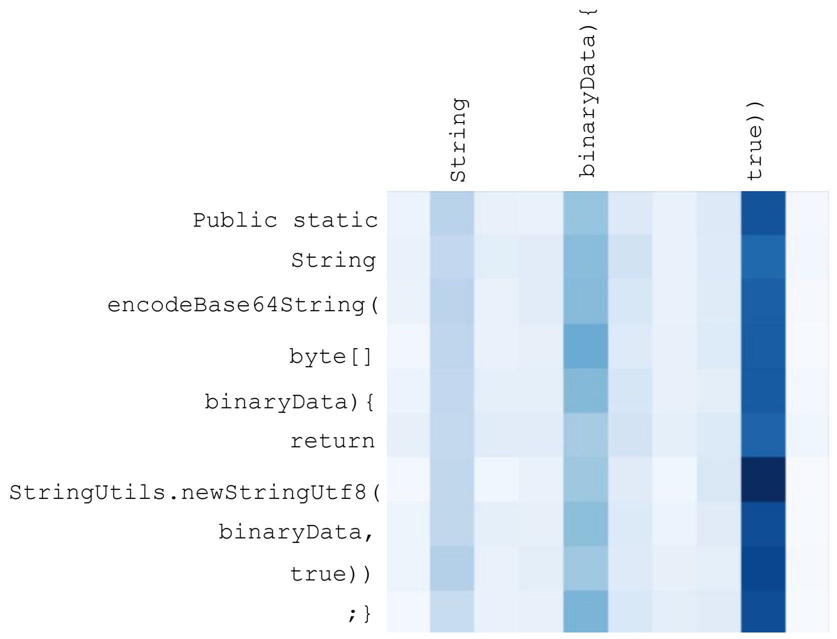


Figure 5.1: The percentage of attended buggy statements with respect to attention threshold

can correctly identify 50% **of the buggy statements in the subject MUTs.** One interesting observation here is that increasing the threshold may not result in better bug localization. For example, increasing the threshold to 40% or 50% results in non-buggy statements being among the attended statements, decreasing the contribution of buggy statements among attended statements.

We also manually investigated the heatmap visualization of the Self Attention matrix for the failing $\langle t_i, m_i \rangle$ pairs to qualitatively confirm if SEER has considered relevant tokens to predict labels. Figure 5.2 illustrates such case, where the buggy MUT is `encodeBase64String` of the Codec project. As shown in Figure 5.2, the bug is due to feeding an incorrect argument to `encodeBase64` method, i.e., "true" instead of "false". By looking at the heatmap visualization of the Self Attention matrix, we can see that SEER has paid the most attention to the buggy token when predicting the "fail" label for this test instance (for the sake of space and readability, we have merged some of the tokens and adjusted the weights in the heatmap visualization). As another example, where the bug is more complex and involves multiple tokens or statements, consider the buggy MUT and its corresponding heatmap [3] visualization of Self Attention in Figure 5.3. In this example, the return values of the two highlighted

[3]The tokens are merged in this heatmap and only the most attended tokens are labeled.



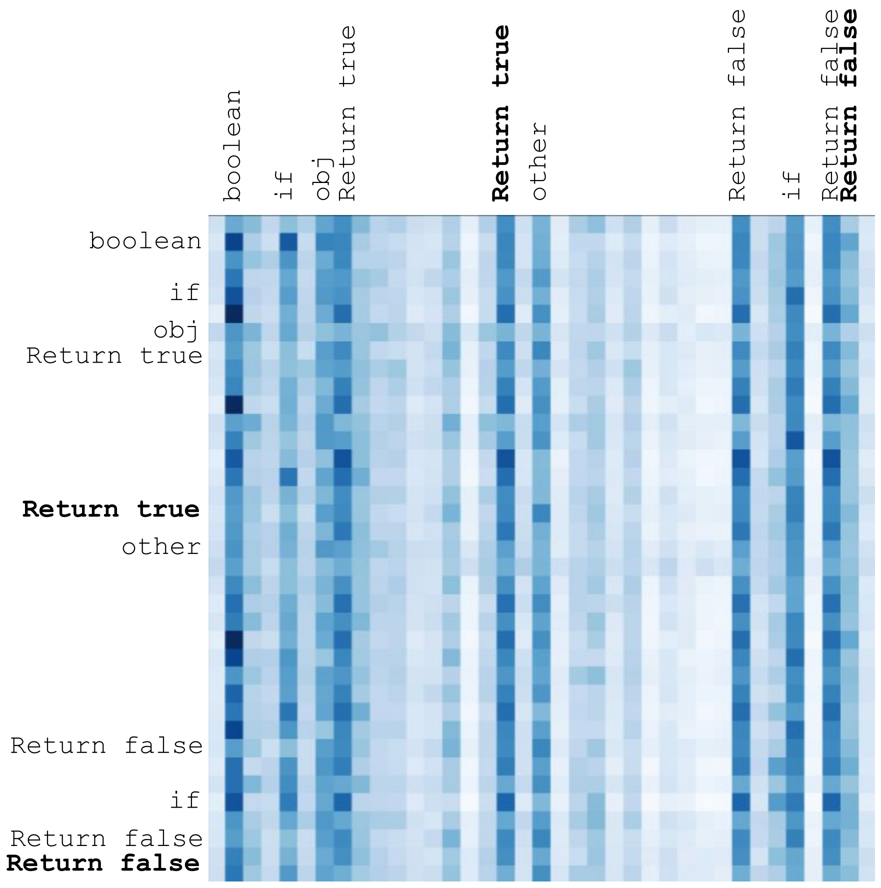
```
public static String encodeBase64String(byte[] binaryData){
   return StringUtils.newStringUtf8(
                encodeBase64(binaryData, true));
}
```

Figure 5.2: Visualization of the Self Attention for the method `encodeBase64String` in Codec project, demonstrating that SEER has paid the highest attention to the buggy token, i.e., "true"

return statements are incorrect. Looking at the heatmap, we can see that the tokens of these two statements are among the most attended tokens to predict the "fail" label.

5.4.2 Embedding Analysis

Figure 5.4 shows the result of embedding analysis as discussed in Section 4.4.2. The blue and yellow distributions show the distinction between the embeddings of correct and buggy MUTs, respectively, after LDA dimensionality reduction. As demonstrated by this figure, the distribution of correct and buggy MUTs are almost distinct in the low-dimension space, which confirms **Seer's ability to semantically distinguish the representation of buggy and correct MUTs in the embedding space.** There are some overlapping instances near $x = 0$ between the correct and buggy MUTs distributions. Such overlap indicates that the embeddings of a few buggy and correct MUTs are close to each other in the embedding space with 200 dimensions. By manually investigating those instances, we realized that they belong to $\langle t_i, m_i \rangle$ pairs that SEER failed to predict a correct label.



```
public boolean equals(Object obj){
   if (this == obj)
       return true;
   if (obj == null || getClass() != obj.getClass())
       return true;
   ZipArchiveEntry other = (ZipArchiveEntry) obj;
   if (name == null) {
       if (other.name != null)
           return false;
   } else if (!name.equals(other.name))
       return false;
   return false;
}
```

Figure 5.3: Visualization of the Self Attention for the method `equals`, demonstrating that SEER has attended to buggy tokens at multiple locations

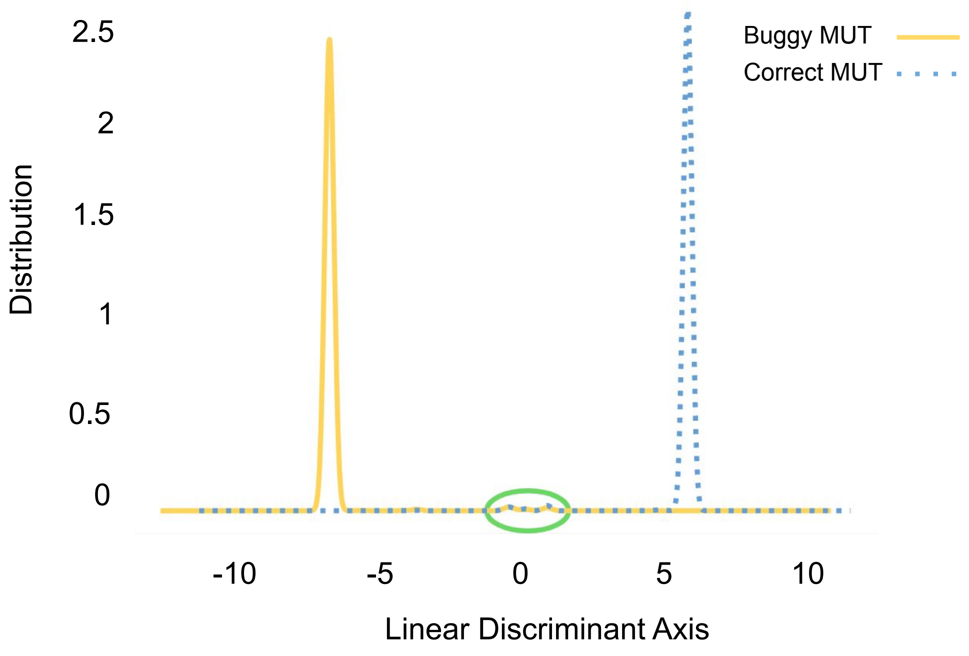


Figure 5.4: Linear Discriminant Analysis (LDA) results. The yellow graph represents the distribution of buggy MUTs and the dashed blue graph represents the distribution of correct MUTs in the reduced dimension

Moreover, SEER's embedding analysis relies on Linear Discriminant Analysis (LDA) [96] for reducing the embedding dimension from 200-d into a single one. There exist a number of dimensionality reduction algorithms like Principle Component Analysis (PCA) [97] which is not suitable in our context. That is, the PCA algorithm conserves the *representation* of data when reducing the dimensionality. However, in our problem domain, we are interested in showing the distinction between the learned embeddings of fixed code and buggy code in high dimensions. In contrast, the LDA aims to reduce the dimensionality of embeddings while maximizing the separation between classes (i.e., FC, BC). In a binary class setting, the cost function which LDA tries to maximize is shown in Equation 5.1. In this equation, m_1 and m_2 correspond to the mean, while s_1^2 and s_2^2 correspond to the within-class variance of projected distributions.

$$J(w) = \frac{|m_1 - m_2|^2}{s_1^2 + s_2^2} \tag{5.1}$$

5.5 RQ4: PERFORMANCE

To answer this research question, we evaluated the time required for Phase 1 and Phase 2 training, as well as the time for testing the oracle. We ran the experiments on a Tesla T4 GPU with 16GB GDDR6 memory. For a batch size of 16 $\langle t_i, m_i \rangle$ pairs, a single epoch took 447 and $1,745$ seconds on average for training Phase 1 and Phase 2, respectively. With the patience level of five epochs for the early termination criteria, Phase 1 and Phase 2 training took 22 and 30 epochs to complete, respectively, resulting in a total of 14 hours of training. Given that the SEER is generalizable, the one-time training of the model is reasonable. After training, it takes SEER only 6.5 milliseconds on average to predict the passing or failing label for a given pair of $\langle t_i, m_i \rangle$.

CHAPTER 6: CONCLUSION

Test oracle automation has been one of the most challenging problems in the software engineering community, yet it has received less attention compared to test input generation. This work proposed Seer, a novel DL-enabled technique to move one step forward in advancing automated test oracle constructions. Seer predicts a passing or failing verdict for a given pair of $\langle t_i, m_i \rangle$ by learning the semantic correlation between inputs and outputs from a high-quality and diverse dataset. Our experimental results show that the learned oracle is accurate and efficient in predicting test results, and generalizable to the projects it has not seen during training.

Currently, we are considering several directions for future work. Based on the promising results of our produced domain-specific representations for code and tests, we will explore its application in other software analysis tasks such as vulnerability detection, bug localization, and program repair. Also, we are planning to expand Seer to system tests. System tests are more complex and bigger than unit tests, which may entail changing the Seer's architecture to Graph Neural Networks (GNN) to better capture the code semantics and representations.

REFERENCES

[1] E. T. Barr, M. Harman, P. McMinn, M. Shahbaz, and S. Yoo, "The oracle problem in software testing: A survey," *IEEE transactions on software engineering*, vol. 41, no. 5, pp. 507–525, 2014.

[2] K. Shrestha and M. J. Rutherford, "An empirical evaluation of assertions as oracles," in *2011 Fourth IEEE International Conference on Software Testing, Verification and Validation*, 2011, pp. 110–119.

[3] C. Cadar, V. Ganesh, P. M. Pawlowski, D. L. Dill, and D. R. Engler, "Exe: Automatically generating inputs of death," *ACM Trans. Inf. Syst. Secur.*, vol. 12, no. 2, Dec. 2008. [Online]. Available: https://doi.org/10.1145/1455518.1455522

[4] D. Coppit and J. M. Haddox-Schatz, "On the use of specification-based assertions as test oracles," in *29th Annual IEEE/NASA Software Engineering Workshop.* IEEE, 2005, pp. 305–314.

[5] X. Feng, D. L. Parnas, T. Tse, and T. O'Callaghan, "A comparison of tabular expression-based testing strategies," *IEEE Transactions on Software Engineering*, vol. 37, no. 5, pp. 616–634, 2011.

[6] G. Gay, S. Rayadurgam, and M. P. Heimdahl, "Improving the accuracy of oracle verdicts through automated model steering," in *Proceedings of the 29th ACM/IEEE international conference on Automated software engineering*, 2014, pp. 527–538.

[7] D. Jackson, *Software Abstractions: logic, language, and analysis.* MIT press, 2012.

[8] Y. Jin and D. L. Parnas, "Defining the meaning of tabular mathematical expressions," *Science of Computer Programming*, vol. 75, no. 11, pp. 980–1000, 2010.

[9] D. K. Peters and D. L. Parnas, "Requirements-based monitors for real-time systems," *IEEE Transactions on Software Engineering*, vol. 28, no. 2, pp. 146–158, 2002.

[10] Y. Wei, C. A. Furia, N. Kazmin, and B. Meyer, "Inferring better contracts," in *Proceedings of the 33rd International Conference on Software Engineering*, 2011, pp. 191–200.

[11] W. Araujo, L. C. Briand, and Y. Labiche, "Enabling the runtime assertion checking of concurrent contracts for the java modeling language," in *2011 33rd International Conference on Software Engineering (ICSE).* IEEE, 2011, pp. 786–795.

[12] L. C. Briand, Y. Labiche, and H. Sun, "Investigating the use of analysis contracts to improve the testability of object-oriented code," *Software: Practice and Experience*, vol. 33, no. 7, pp. 637–672, 2003.

[13] Y. Cheon, "Abstraction in assertion-based test oracles," in *Seventh International Conference on Quality Software (QSIC 2007)*. IEEE, 2007, pp. 410–414.

[14] Y. Cheon and G. T. Leavens, "A simple and practical approach to unit testing: The jml and junit way," in *European Conference on Object-Oriented Programming*. Springer, 2002, pp. 231–255.

[15] M.-C. Gaudel, "Testing from formal specifications, a generic approach," in *International Conference on Reliable Software Technologies*. Springer, 2001, pp. 35–48.

[16] F. Molina, M. d'Amorim, and N. Aguirre, "Fuzzing class specifications," *arXiv preprint arXiv:2201.10874*, 2022.

[17] R. White and J. Krinke, "Reassert: Deep learning for assert generation," *arXiv preprint arXiv:2011.09784*, 2020.

[18] C. Watson, M. Tufano, K. Moran, G. Bavota, and D. Poshyvanyk, "On learning meaningful assert statements for unit test cases," in *Proceedings of the ACM/IEEE 42nd International Conference on Software Engineering*, 2020, pp. 1398–1409.

[19] M. Tufano, D. Drain, A. Svyatkovskiy, and N. Sundaresan, "Generating accurate assert statements for unit test cases using pretrained transformers," *arXiv preprint arXiv:2009.05634*, 2020.

[20] S. A. M. D. E. Adam and K. C. P. J. H. Perkins, "Finding the needles in the haystack: Generating legal test inputs for object-oriented programs," *and Object-Oriented Systems*, p. 27, 2006.

[21] A. Bertolino, P. Inverardi, P. Pelliccione, and M. Tivoli, "Automatic synthesis of behavior protocols for composable web-services," in *Proceedings of the 7th joint meeting of the European software engineering conference and the ACM SIGSOFT symposium on The foundations of software engineering*, 2009, pp. 141–150.

[22] D. Beyer, T. A. Henzinger, R. Jhala, and R. Majumdar, "Checking memory safety with blast," in *International Conference on Fundamental Approaches to Software Engineering*. Springer, 2005, pp. 2–18.

[23] M. D. Ernst, J. H. Perkins, P. J. Guo, S. McCamant, C. Pacheco, M. S. Tschantz, and C. Xiao, "The daikon system for dynamic detection of likely invariants," *Science of computer programming*, vol. 69, no. 1-3, pp. 35–45, 2007.

[24] M. D. Ernst, J. Cockrell, W. G. Griswold, and D. Notkin, "Dynamically discovering likely program invariants to support program evolution," *IEEE transactions on software engineering*, vol. 27, no. 2, pp. 99–123, 2001.

[25] K. Frounchi, L. C. Briand, L. Grady, Y. Labiche, and R. Subramanyan, "Automating image segmentation verification and validation by learning test oracles," *Information and Software Technology*, vol. 53, no. 12, pp. 1337–1348, 2011.

[26] R. Groz, K. Li, A. Petrenko, and M. Shahbaz, "Modular system verification by inference, testing and reachability analysis," in *Testing of software and communicating systems.* Springer, 2008, pp. 216–233.

[27] K. Li, R. Groz, and M. Shahbaz, "Integration testing of components guided by incremental state machine learning," in *Testing: Academic & Industrial Conference-Practice And Research Techniques (TAIC PART'06).* IEEE, 2006, pp. 59–70.

[28] C. Pacheco and M. D. Ernst, "Eclat: Automatic generation and classification of test inputs," in *European Conference on Object-Oriented Programming.* Springer, 2005, pp. 504–527.

[29] M. Merten, F. Howar, B. Steffen, P. Pellicione, and M. Tivoli, "Automated inference of models for black box systems based on interface descriptions," in *International Symposium On Leveraging Applications of Formal Methods, Verification and Validation.* Springer, 2012, pp. 79–96.

[30] S. Ratcliff, D. R. White, and J. A. Clark, "Searching for invariants using genetic programming and mutation testing," in *Proceedings of the 13th annual conference on Genetic and evolutionary computation*, 2011, pp. 1907–1914.

[31] S. R. Shahamiri, W. M. Wan-Kadir, S. Ibrahim, and S. Z. M. Hashim, "Artificial neural networks as multi-networks automated test oracle," *Automated Software Engineering*, vol. 19, no. 3, pp. 303–334, 2012.

[32] R. Singh, D. Giannakopoulou, and C. Păsăreanu, "Learning component interfaces with may and must abstractions," in *International Conference on Computer Aided Verification.* Springer, 2010, pp. 527–542.

[33] M. Staats, S. Hong, M. Kim, and G. Rothermel, "Understanding user understanding: determining correctness of generated program invariants," in *Proceedings of the 2012 International Symposium on Software Testing and Analysis*, 2012, pp. 188–198.

[34] N. Walkinshaw and K. Bogdanov, "Inferring finite-state models with temporal constraints," in *2008 23rd IEEE/ACM International Conference on Automated Software Engineering.* IEEE, 2008, pp. 248–257.

[35] S. Segura, G. Fraser, A. B. Sanchez, and A. Ruiz-Cortés, "A survey on metamorphic testing," *IEEE Transactions on software engineering*, vol. 42, no. 9, pp. 805–824, 2016.

[36] T. Y. Chen, F.-C. Kuo, H. Liu, P.-L. Poon, D. Towey, T. Tse, and Z. Q. Zhou, "Metamorphic testing: A review of challenges and opportunities," *ACM Computing Surveys (CSUR)*, vol. 51, no. 1, pp. 1–27, 2018.

[37] X. Xie, J. W. Ho, C. Murphy, G. Kaiser, B. Xu, and T. Y. Chen, "Testing and validating machine learning classifiers by metamorphic testing," *Journal of Systems and Software*, vol. 84, no. 4, pp. 544–558, 2011.

[38] C. Murphy, G. E. Kaiser, and L. Hu, "Properties of machine learning applications for use in metamorphic testing," 2008.

[39] S. Segura, D. Towey, Z. Q. Zhou, and T. Y. Chen, "Metamorphic testing: Testing the untestable," *IEEE Software*, vol. 37, no. 3, pp. 46–53, 2018.

[40] Z. Q. Zhou and L. Sun, "Metamorphic testing of driverless cars," *Communications of the ACM*, vol. 62, no. 3, pp. 61–67, 2019.

[41] T. Y. Chen, F.-C. Kuo, W. Ma, W. Susilo, D. Towey, J. Voas, and Z. Q. Zhou, "Metamorphic testing for cybersecurity," *Computer*, vol. 49, no. 6, pp. 48–55, 2016.

[42] M. Zhang, Y. Zhang, L. Zhang, C. Liu, and S. Khurshid, "Deeproad: Gan-based metamorphic testing and input validation framework for autonomous driving systems," in *2018 33rd IEEE/ACM International Conference on Automated Software Engineering (ASE).* IEEE, 2018, pp. 132–142.

[43] Z. Q. Zhou, S. Xiang, and T. Y. Chen, "Metamorphic testing for software quality assessment: A study of search engines," *IEEE Transactions on Software Engineering*, vol. 42, no. 3, pp. 264–284, 2015.

[44] L. Sun and Z. Q. Zhou, "Metamorphic testing for machine translations: Mt4mt," in *2018 25th Australasian Software Engineering Conference (ASWEC).* IEEE, 2018, pp. 96–100.

[45] J. Ding, X. Kang, and X.-H. Hu, "Validating a deep learning framework by metamorphic testing," in *2017 IEEE/ACM 2nd International Workshop on Metamorphic Testing (MET).* IEEE, 2017, pp. 28–34.

[46] Q. Tao, W. Wu, C. Zhao, and W. Shen, "An automatic testing approach for compiler based on metamorphic testing technique," in *2010 Asia Pacific Software Engineering Conference.* IEEE, 2010, pp. 270–279.

[47] A. Dwarakanath, M. Ahuja, S. Sikand, R. M. Rao, R. J. C. Bose, N. Dubash, and S. Podder, "Identifying implementation bugs in machine learning based image classifiers using metamorphic testing," in *Proceedings of the 27th ACM SIGSOFT International Symposium on Software Testing and Analysis*, 2018, pp. 118–128.

[48] S. Segura, R. M. Hierons, D. Benavides, and A. Ruiz-Cortés, "Automated metamorphic testing on the analyses of feature models," *Information and Software Technology*, vol. 53, no. 3, pp. 245–258, 2011.

[49] S. Segura, J. A. Parejo, J. Troya, and A. Ruiz-Cortés, "Metamorphic testing of restful web apis," *IEEE Transactions on Software Engineering*, vol. 44, no. 11, pp. 1083–1099, 2017.

[50] A. F. Donaldson and A. Lascu, "Metamorphic testing for (graphics) compilers," in *Proceedings of the 1st international workshop on metamorphic testing*, 2016, pp. 44–47.

[51] J. Ahlgren, M. E. Berezin, K. Bojarczuk, E. Dulskyte, I. Dvortsova, J. George, N. Gucevska, M. Harman, M. Lomeli, E. Meijer et al., "Testing web enabled simulation at scale using metamorphic testing," in *2021 IEEE/ACM 43rd International Conference on Software Engineering: Software Engineering in Practice (ICSE-SEIP)*. IEEE, 2021, pp. 140–149.

[52] S. Yoo, "Metamorphic testing of stochastic optimisation," in *2010 Third International Conference on Software Testing, Verification, and Validation Workshops*. IEEE, 2010, pp. 192–201.

[53] P. Ma, S. Wang, and J. Liu, "Metamorphic testing and certified mitigation of fairness violations in nlp models." in *IJCAI*, 2020, pp. 458–465.

[54] S. Tolksdorf, D. Lehmann, and M. Pradel, "Interactive metamorphic testing of debuggers," in *Proceedings of the 28th ACM SIGSOFT International Symposium on Software Testing and Analysis*, 2019, pp. 273–283.

[55] M. Usman, W. Wang, and S. Khurshid, "Testmc: testing model counters using differential and metamorphic testing," in *Proceedings of the 35th IEEE/ACM International Conference on Automated Software Engineering*, 2020, pp. 709–721.

[56] S. Segura, R. M. Hierons, D. Benavides, and A. Ruiz-Cortés, "Automated test data generation on the analyses of feature models: A metamorphic testing approach," in *2010 Third International Conference on Software Testing, Verification and Validation*. IEEE, 2010, pp. 35–44.

[57] X. Lin, M. Simon, and N. Niu, "Exploratory metamorphic testing for scientific software," *Computing in science & engineering*, vol. 22, no. 2, pp. 78–87, 2018.

[58] S. Segura, A. Durán, A. B. Sánchez, D. L. Berre, E. Lonca, and A. Ruiz-Cortés, "Automated metamorphic testing of variability analysis tools," *Software Testing, Verification and Reliability*, vol. 25, no. 2, pp. 138–163, 2015.

[59] A. Zeller and R. Hildebrandt, "Simplifying and isolating failure-inducing input," *IEEE Transactions on Software Engineering*, vol. 28, no. 2, pp. 183–200, 2002.

[60] T. Xie and D. Notkin, "Checking inside the black box: Regression testing by comparing value spectra," *IEEE Transactions on software Engineering*, vol. 31, no. 10, pp. 869–883, 2005.

[61] Z. Gu, E. T. Barr, D. J. Hamilton, and Z. Su, "Has the bug really been fixed?" in *2010 ACM/IEEE 32nd International Conference on Software Engineering*, vol. 1. IEEE, 2010, pp. 55–64.

[62] T. Xie, "Augmenting automatically generated unit-test suites with regression oracle checking," in *European Conference on Object-Oriented Programming*. Springer, 2006, pp. 380–403.

[63] C.-A. Sun, A. Fu, P.-L. Poon, X. Xie, H. Liu, and T. Y. Chen, " METRIC$^+$+: A Metamorphic Relation Identification Technique Based on Input Plus Output Domains ," *IEEE Transactions on Software Engineering*, vol. 47, no. 9, pp. 1764–1785, 2019.

[64] T. Y. Chen, P.-L. Poon, and X. Xie, "Metric: Metamorphic relation identification based on the category-choice framework," *Journal of Systems and Software*, vol. 116, pp. 177–190, 2016.

[65] G. Fraser and A. Arcuri, "Evosuite: automatic test suite generation for object-oriented software," in *Proceedings of the 19th ACM SIGSOFT symposium and the 13th European conference on Foundations of software engineering*, 2011, pp. 416–419.

[66] C. Pacheco and M. D. Ernst, "Randoop: feedback-directed random testing for java," in *Companion to the 22nd ACM SIGPLAN conference on Object-oriented programming systems and applications companion*, 2007, pp. 815–816.

[67] L. Zhang, G. Yang, N. Rungta, S. Person, and S. Khurshid, "Feedback-driven dynamic invariant discovery," in *Proceedings of the 2014 International Symposium on Software Testing and Analysis*, 2014, pp. 362–372.

[68] T. Y. Chen, F.-C. Kuo, T. Tse, and Z. Q. Zhou, "Metamorphic testing and beyond," in *Eleventh Annual International Workshop on Software Technology and Engineering Practice.* IEEE, 2003, pp. 94–100.

[69] J. Zhang, J. Chen, D. Hao, Y. Xiong, B. Xie, L. Zhang, and H. Mei, "Search-based inference of polynomial metamorphic relations," in *Proceedings of the 29th ACM/IEEE international conference on Automated software engineering*, 2014, pp. 701–712.

[70] P. Zhang, X. Zhou, P. Pelliccione, and H. Leung, "Rbf-mlmr: A multi-label metamorphic relation prediction approach using rbf neural network," *IEEE access*, vol. 5, pp. 21 791–21 805, 2017.

[71] R. Jabbarvand, F. Mehralian, and S. Malek, "Automated construction of energy test oracles for android," in *Proceedings of the 28th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering*, 2020, pp. 927–938.

[72] C. Ma, S. Liu, J. Fu, and T. Zhang, "Test oracle generation based on bpnn by using the values of variables at different breakpoints for programs," *International Journal of Software Engineering and Knowledge Engineering*, vol. 31, no. 10, pp. 1469–1494, 2021.

[73] "Seer artifacts," https://github.com/Intelligent-CAT-Lab/SEER, 2022.

[74] S. J. Pan and Q. Yang, "A survey on transfer learning," *IEEE Transactions on knowledge and data engineering*, vol. 22, no. 10, pp. 1345–1359, 2009.

[75] V. J. Hellendoorn, C. Sutton, R. Singh, P. Maniatis, and D. Bieber, "Global relational models of source code," in *International conference on learning representations*, 2019.

[76] Y. Wang, K. Wang, F. Gao, and L. Wang, "Learning semantic program embeddings with graph interval neural network," *Proceedings of the ACM on Programming Languages*, vol. 4, no. OOPSLA, pp. 1–27, 2020.

[77] R. Xu, C. Xiong, W. Chen, and J. Corso, "Jointly modeling deep video and compositional text to bridge vision and language in a unified framework," in *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 29, no. 1, 2015.

[78] A. Karpathy and L. Fei-Fei, "Deep visual-semantic alignments for generating image descriptions," in *Proceedings of the IEEE conference on computer vision and pattern recognition*, 2015, pp. 3128–3137.

[79] "Defects4j dataset," https://github.com/rjust/defects4j, 2021.

[80] G. M. Weiss and H. Hirsh, "A quantitative study of small disjuncts," *AAAI/IAAI*, vol. 2000, no. 665-670, p. 15, 2000.

[81] S. Gupta and A. Gupta, "Dealing with noise problem in machine learning data-sets: A systematic review," *Procedia Computer Science*, vol. 161, pp. 466–474, 2019.

[82] Y. Jia and M. Harman, "Constructing subtle faults using higher order mutation testing," in *2008 Eighth IEEE International Working Conference on Source Code Analysis and Manipulation*. IEEE, 2008, pp. 249–258.

[83] S. Kaufman, S. Rosset, C. Perlich, and O. Stitelman, "Leakage in data mining: Formulation, detection, and avoidance," *ACM Transactions on Knowledge Discovery from Data (TKDD)*, vol. 6, no. 4, pp. 1–21, 2012.

[84] J. Cheng, L. Dong, and M. Lapata, "Long short-term memory-networks for machine reading," *arXiv preprint arXiv:1601.06733*, 2016.

[85] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin, "Attention is all you need," in *Proceedings of the 31st International Conference on Neural Information Processing Systems*, ser. NIPS'17. Red Hook, NY, USA: Curran Associates Inc., 2017, p. 6000–6010.

[86] R. A. Brualdi, *Introductory combinatorics*. Pearson Education India, 1977.

[87] M. Partridge and R. A. Calvo, "Fast dimensionality reduction and simple pca," *Intelligent data analysis*, vol. 2, no. 3, pp. 203–214, 1998.

[88] M. M. Tatsuoka and D. V. Tiedeman, "Chapter iv: Discriminant analysis," *Review of Educational Research*, vol. 24, no. 5, pp. 402–420, 1954.

[89] A. Gisbrecht, A. Schulz, and B. Hammer, "Parametric nonlinear dimensionality reduction using kernel t-sne," *Neurocomputing*, vol. 147, pp. 71–82, 2015.

[90] "The major mutation framework," http://mutation-testing.org, 2021.

[91] A. Paszke, S. Gross, F. Massa, A. Lerer, J. Bradbury, G. Chanan, T. Killeen, Z. Lin, N. Gimelshein, L. Antiga, A. Desmaison, A. Kopf, E. Yang, Z. DeVito, M. Raison, A. Tejani, S. Chilamkurthy, B. Steiner, L. Fang, J. Bai, and S. Chintala, "Pytorch: An imperative style, high-performance deep learning library," in *Advances in Neural Information Processing Systems 32*, H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, Eds. Curran Associates, Inc., 2019, pp. 8024–8035. [Online]. Available: http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf

[92] R. Gomez, L. Gomez, J. Gibert, and D. Karatzas, "Self-supervised learning from web data for multimodal retrieval," in *Multimodal Scene Understanding*. Elsevier, 2019, pp. 279–306.

[93] I. Loshchilov and F. Hutter, "Decoupled weight decay regularization," *arXiv preprint arXiv:1711.05101*, 2017.

[94] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," *arXiv preprint arXiv:1412.6980*, 2014.

[95] Z. Shen, J. Liu, Y. He, X. Zhang, R. Xu, H. Yu, and P. Cui, "Towards out-of-distribution generalization: A survey," *arXiv preprint arXiv:2108.13624*, 2021.

[96] C. J. Huberty, "Discriminant analysis," *Review of Educational Research*, vol. 45, no. 4, pp. 543–598, 1975. [Online]. Available: https://doi.org/10.3102/00346543045004543

[97] A. Maćkiewicz and W. Ratajczak, "Principal components analysis (pca)," *Computers & Geosciences*, vol. 19, no. 3, pp. 303–342, 1993. [Online]. Available: https://www.sciencedirect.com/science/article/pii/009830049390090R