

# Improving Binary Code Similarity Transformer Models by Semantics-driven Instruction Deemphasis

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## ABSTRACT

Given a function in the binary executable form, binary code similarity analysis determines a set of similar functions from a large pool of candidate functions. These similar functions are usually compiled from the same source code with different compilation setups. Such analysis has a large number of applications, such as malware detection, code clone detection, and automatic software patching. The state-of-the-art methods utilize complex Deep Learning models such as Transformer models. We observe that these models suffer from undesirable instruction distribution biases caused by specific compiler conventions. We develop a novel technique to detect such biases and repair them by removing the corresponding instructions from the dataset and finetuning the models. This entails synergy between Deep Learning model analysis and program analysis. Our results show that we can substantially improve the state-of-the-art models' performance by up to 17% in the most challenging cases where test data may be out of the distributions of training data.

## KEYWORDS

binary similarity, deep learning model, program analysis

## 1 INTRODUCTION

Given a query function  $f$ , *code similarity analysis* [1, 6, 17, 29, 30] finds the functions from a pool  $P$  that are similar to  $f$ . Similarity analysis has a wide range of applications in automatic software patching [4, 37, 44, 53, 54, 64], software plagiarism detection [10, 34, 50, 58, 66], and 1-day vulnerability detection [16, 60]. For instance, a critical security vulnerability might be detected in a library. It is essential to detect whether an existing project contains the problematic function from that library. *Binary similarity analysis* is a special kind of code similarity analysis. It handles functions in the executable form, without source code or any symbolic information. In the context of binary similarity analysis, similar functions are usually compiled from the same source code with different compilers or compilation options. It is particularly useful in reverse engineering [22, 23, 42, 60] and malware analysis [7, 11, 19, 20, 25, 27, 65]. Traditionally, binary similarity analysis is achieved using classic program analysis such as control-flow differential analysis [8, 26], program dependence analysis [63], symbolic execution [14, 34], and trace analysis [14, 18, 23, 40, 60].

Recent research has shown that *Large Language Models* (LLMs), such as Transformer models, can achieve state-of-the-art results in binary similarity analysis, outperforming classic methods [42, 59]. For example, JTrans [59] uses Transformer models and achieves 62.5% accuracy, 30.5% better than the prior work. In JTrans, the

model first encodes  $f$  and every function in  $P$  to embeddings. It then computes the cosine similarity between the embedding of  $f$  and the embeddings of all functions in  $P$ . A high cosine similarity value between a pair of embeddings indicates that the model considers the related two functions similar. Functions in  $P$  are further ranked by the similarity values and the top- $k$  functions may be selected as similar functions. The model is trained on a large set of function pairs that are labeled as *similar* or *dissimilar*, using contrastive learning. In total, there are over 3 million function pairs used in training, much more than a few other similar methods [28, 38, 42].

However, as we will show in Section 2.2, the inherent compiler conventions (e.g., generating specific instruction sequences at function prologues) introduce instruction distribution biases, some of which are undesirably associated with specific similarity analysis results. For example, a particular instruction appearing in the prologue of a function but not in the other similar function may lead to a misclassification of dissimilarity. However, we cannot simply remove instruction distribution biases because many of them are not caused by compilers, but rather due to unique program semantics. In other words, they may be important to correct classification.

In this paper, we aim to identify and suppress undesirable biases to improve Transformer-based binary similarity analysis models. In particular, we first determine a set of instructions that are important to classification results (regarding all training samples). We then use program analysis to determine if these instructions indeed have semantics importance. If not, they are likely due to compiler introduced biases. We further propose to preclude these instructions by removing them from all the binary functions and finetuning the model with the updated dataset.

Our contributions are summarized as follows.

- We propose a novel instruction deemphasis technique that can effectively prevent a model from learning instruction distribution biases introduced by compilers, and improve the generalizability of models on out-of-distribution data.
- We devise a method to identify instructions from a binary function that may significantly affect the classification results of a binary similarity analysis model.
- We propose a novel metric that can measure the importance of a single instruction to the semantics of a binary function.
- We develop a prototype DiEMPH. We conduct experiments on 6 state-of-the-art models and evaluate the effectiveness of DiEMPH on 7 real-world projects widely-used for the binary similarity tasks. The results show that DiEMPH improves models' performance on out-of-distribution data by 4-17%. In the most practical application scenario, namely, using the most complex model trained on the largest dataset, DiEMPH achieves 17% accuracy improvement on out-of-distribution data, from 34% to 51%.

## 2 MOTIVATION

In this section, we use an example to discuss the limitation of existing methods and illustrate our method.

### 2.1 Motivating Example

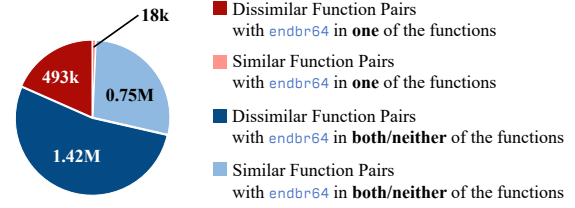
The example is simplified from the function `xrealloc()` in Coreutils [13]. It is shown in Fig. 2a. The function is used to change the sizes of an allocated memory region. It takes as input two parameters. The first one is a pointer to an allocated memory region, and the second is a new size. In common cases, the function returns a pointer with the new size (at line 13). If the second parameter is zero, `xrealloc` will free the region and return a null pointer (at line 7). The *if*-statement at line 12 handles exceptional cases: if the function `realloc` returns a null pointer, a non-return error processing function `xrealloc_die` will be invoked. The function emits an error message and terminates the execution.

We compile the function with the GCC compiler and the option `-O3`, and with the Clang compiler and the option `-O0`. The resulting control flow graphs (CFGs) are shown in Fig. 2b and Fig. 2c, respectively. We number the basic blocks and list the numbers in the red circle at the upper left corner of each basic block. Note that we label the corresponding basic blocks with the same numbers. At the beginning of both CFGs, the two parameters `p` and `n` are stored in registers `rdi` and `rsi`, respectively. The first basic blocks of both functions contain the function prologue (e.g., saving registers and allocating a stackframe). Basic blocks 2–3 contain the program logic for common cases: invoking `realloc` and returning its result. Basic blocks 4 (in both CFGs) free the pointer `p` when the new size `n` is zero. Basic blocks 5 process exceptional cases as shown at line 12 of Fig. 2a.

### 2.2 Limitations in State-of-the-Art Models

The CFGs in Fig. 2b and Fig. 2c have similar control structures and have many corresponding instructions. However, the state-of-the-art Transformer based method JTrans [59] produces a low similarity score (0.3) to this pair of CFGs. The majority of similar function pairs are expected to have a score larger than 0.5. Thus the model mistakenly concludes these two CFGs are not similar. We investigate the results and find that the model is undesirably sensitive to some special patterns in the function prologue, namely, these patterns are considered very important to classification results by the model. Some of the misclassification-inducing patterns are highlighted by the orange circles in Fig. 2b and Fig. 2c. Specifically, in the optimized version (Fig. 2b), the GCC compiler inserts an additional instruction `endbr64` at the beginning. The instruction is irrelevant to the program functionality. It is used to support *control flow integrity* [52], a security feature on recent processors. However, the model tends to consider a pair of functions likely dissimilar when one has the instruction and the other does not. By manually adding the `endbr64` instruction to the un-optimized version, we can increase the similarity score for this pair of binary functions to 0.60. Even removing the instruction from the optimized version allows us to improve it to 0.52.

We further investigate the training dataset and find that the `endbr64` instruction has an undesirable bias in distribution. The training data of JTrans [59] contains over 3 million binary functions with different functionalities. For each pair of binary functions in



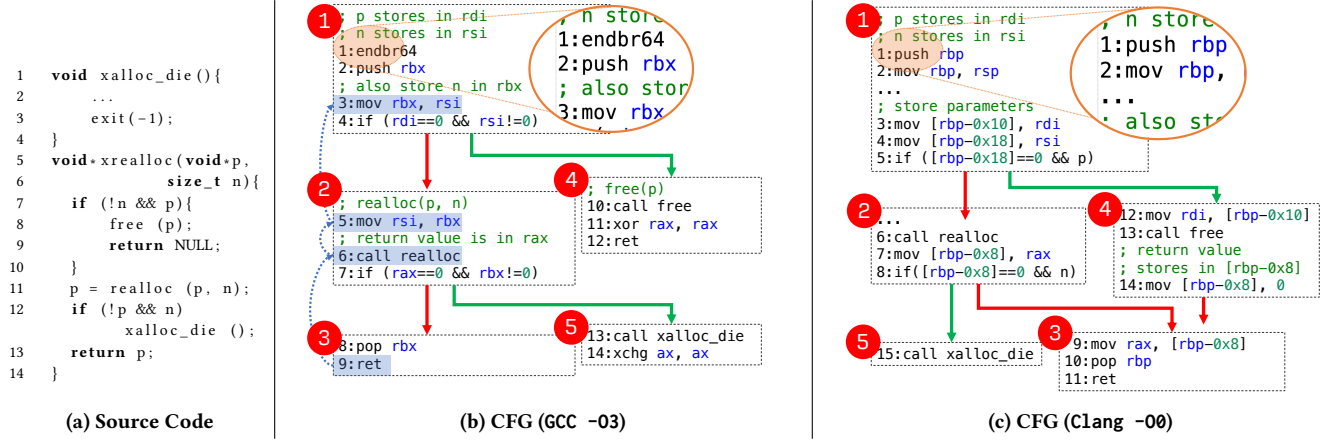
**Figure 1: Undesirable bias in the distribution of training dataset. We divide samples in the training dataset of JTrans into four categories. The pie chart depicts the number of samples in each category.**

the training dataset, there are two possible labels, i.e., *similar* and *dissimilar*, whose ratio is 1:2. Following the same ratio, we randomly select 0.9 million pairs of similar functions and 1.8 million pairs of dissimilar functions and study the distribution of the `endbr64` instruction in these two kinds of function pairs. The results are shown in Fig. 1. Observe that when only one of the function has the instruction, the numbers of similar and dissimilar function pairs have the ratio of 1:27, substantially deviated from the 1:2 ratio. Hence the trained model undesirably associates the inconsistency of `endbr64`'s presence with the conclusion of dissimilarity. Note that not all distribution biases are problematic. It is quite common that certain instructions (or sequences) are representative for specific functionalities. Therefore, a simple idea of removing all biases can hardly work.

### 2.3 Our Technique

Existing techniques suffer from biased distributions of certain instructions. These biases are caused by compilers whose inherent behaviors may not strictly follow a normal distribution due to their deterministic nature. The overarching idea of our technique is to deemphasize instructions that do not denote essential program semantics, such as the aforementioned `endbr64` instruction added to support control-flow-integrity.

We determine instructions that are important to classification results over the entire training set. The importance of an instruction *i* is determined by embedding changes of all functions involving *i* when we remove *i* from the function (Section 3.1). It is also called the *classification importance*. For an instruction *i* of top-*k* classification importance, we use program analysis to determine *i*'s *semantics importance*. Specifically, given a function, if *i* is in the backward slice of any *stable variable*, (e.g., a heap variable, or a return variable) in the function, *i* is considered semantically important to the function. A variable is unstable if it is likely changed by compiler optimization. A local variable of a primitive type (e.g., `int`) is unstable because it may be placed on stack in one version and in a register in another (optimized) version. Stable variables tend to have consistent representations in similar functions. Intuitively, an instruction is considered important if it directly or transitively contributes to the computation of some stable variables. We say *i* is semantically important regarding a dataset if it is important for at least a certain number of functions in the dataset. Additional challenges need to be addressed in the backward slicing as certain dependences need to be precluded (Section 3.2). If an instruction



**Figure 2: Motivating example.** The two control flow graphs (CFGs) are the compilation results of Fig. 2a. Green and red edges in the CFGs denote the control flow that the related branch is taken, or not taken, respectively. Red edges also denote the default control flow. We number the basic blocks and show the numbers in red circles.

has top classification importance but not semantics importance, it is removed from all the functions in the training dataset. We then finetune the model using the reduced dataset to repair the undesirable biases.

In our example, the `endbr64` at the beginning of Fig. 2b has a relatively high classification importance of 0.1, while the instruction `call realloc` has an importance of only 0.05. That is, the model considers `endbr64` even more important than the `call` instruction. Although `endbr64` has classification importance, it is not semantically important. In particular, we identify all the stable variables in the function and then determine the important instructions. For instance, the `ret` instruction (at line 9 in block 3) implicitly returns the value in `rax` to the caller<sup>1</sup>. Thus `rax@9` (meaning `rax` at line 9) is a stable variable. We highlight all the instructions that affect `rax@9` with blue shadow (i.e., its backward slice). The blue dashed arrows denote the dependences. First, `rax@9` is (implicitly) defined by the function call `realloc` at line 6 through its return. And the result of the function call is affected by its parameters. The first parameter (`rdi`) is defined at the function entry, and the second one (`rsi`) is defined at line 5. The instruction `mov rsi, rbx` means that copying the value in register `rbx` to `rsi`. The variable `rsi@5` hence depends on `rbx@5`, which is defined at line 3. The variable `rbx@3` is in turn defined by `rsi` from the function entry. Thus our analysis identifies that instructions at lines 3, 5, 6 affect the variable `rax@9` and consider them important. The `endbr64` instruction is considered semantically unimportant.

Removing `endbr64` and a few more instructions of similar nature from all functions in the dataset and fine-tuning the model allows us to improve JTrans’s accuracy from 34% to 51%.

### 3 DESIGN

The overall workflow of DiEMPH is shown in Fig. 3. At the top we show a typical training pipeline of Transformer model. The model is first pretrained. The pretraining usually consumes tremendous time and computing resources. Thus developers for downstream tasks

do not need to repeat the pretraining process. Instead, they directly finetune a pretrained model on a domain-specific dataset (e.g., a binary similarity dataset in our scenario), which takes significantly less effort.

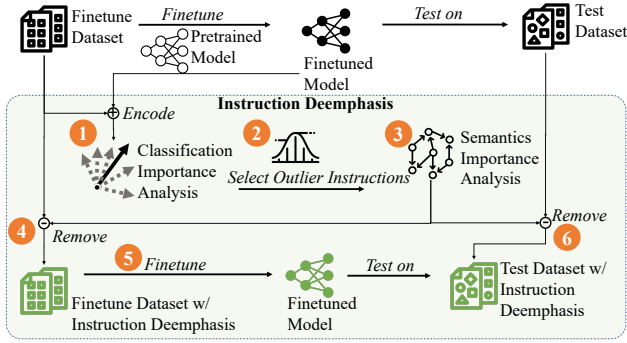
DiEMPH takes as input a finetuned binary similarity model and the dataset for finetuning. It aims to produce a new model with better performance via removing certain instructions from the dataset and rerunning the finetune process. Specifically, the technique samples 100 functions from the finetune dataset, and analyzes classification importance for all instructions in these 100 functions (Step 1). After that, it selects the instructions with exceptionally large classification importance (Step 2) and uses program analysis to determine whether these instructions are semantically important (Step 3). For instructions that have high classification importance but are not semantically important, we remove them from the finetune dataset (Step 4) and rerun the finetune process (Step 5). Finally, these problematic instructions will also be removed from the model input at inference time (Step 6) to ensure input space consistency in finetuning and testing.

This section is organized as follows. In Section 3.1, we introduce how classification importance of an instruction is computed. In Section 3.2, we illustrate the challenges and our solutions when analyzing the semantics importance of an instruction.

#### 3.1 Classification Importance

In the first step, we determine a set of instructions that are important to model classification results. As mentioned before, this is achieved by sampling 100 functions from the finetune/training dataset and studying function embedding changes caused by removing individual instructions. There are other alternatives to infer input importance in the literature of Deep Learning, e.g., by analyzing gradients [5, 45, 51] and attentions [12, 32, 57]. However, Transformer models have a discrete tokenization step which makes back-propagating gradients to the input space challenging. In addition, there are usually many attention heads, each yielding different importance results. We hence consider the model as a black box and observe how embeddings are changed by instruction removal.

<sup>1</sup>At the binary level, function return value is in `rax` by default.



**Figure 3: Workflow of DiEMPH.** At the top is a typical training pipeline of Transformer model. Our technique is shown in the light green box. Major steps are marked in orange circles.

Note that if after removing an instruction, function embeddings drastically change, similarity query results likely have significant changes as well. The removed instruction is hence important to the classification results.

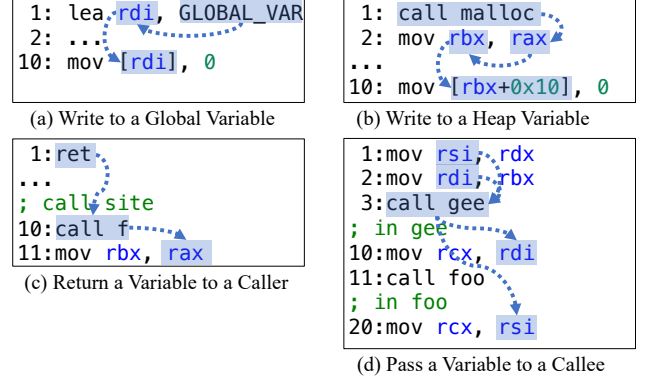
Formally, given an instruction  $i$  in a function  $f$ , the classification importance of  $i$  regarding the function, noted as  $\mathcal{I}_c$ , is defined as follows.

$$\mathcal{I}_c = 1 - \cos(\text{emb}(f), \text{emb}(f \setminus \{i\})) \quad (1)$$

In the above equation,  $\cos$  denotes the cosine similarity between two embeddings.  $\text{emb}(f)$  and  $\text{emb}(f \setminus \{i\})$  denote the embedding for  $f$  and the embedding for the resulting function after removing  $i$  from  $f$ , respectively.

The overall classification importance is then derived from the 100 sampled functions leveraging the above per-function classification importance equation. The process is formally described by Algorithm 1. The algorithm takes as input a model and 100 functions sampled from the finetune dataset, and produces a list of instructions of top- $k$  classification importance regarding the whole dataset. It first selects the most important instructions in each function (lines 3–10). The variable `importantInstr` defined at line 2 is a counter. It counts how many times an instruction is selected as one of the most important instructions (regarding a function) in lines 8–10. This is achieved by an outlier analysis explained later. Then the counter is sorted, and the most frequent  $K$  instructions are returned (line 11).

To select in a function the instructions with an exceptionally large classification importance, the algorithm uses the Kernel Density Estimation (KDE) (line 8) that finds outliers from a distribution. KDE fits a continuous probabilistic distribution given a list of discrete data points. Then it detects outliers by computing the probabilities that the corresponding importance values appear. Specifically, given an instruction  $i$ , it computes  $P(X < \mathcal{I}_c(i))$ , where  $X$  is a random variable following the fitted distribution, and  $P$  denotes probability that  $X$  is less than the classification importance of  $i$ . If  $P(X < \mathcal{I}_c(i))$  is close to 1, it means that the classification importance of  $i$  is significantly larger than other instructions.



**Figure 4: Examples about how DiEMPH identifies stable variables.** Dashed blue lines indicate data flows in the code snippets.

#### Algorithm 1: Selecting Instructions with High Classification Importance

```

1 Function select(model, functions)
    // importantInstr is a map from instructions to integers.
    // It counts how many times an instruction is considered
    // important. Initially, all instructions are mapped to 0.
2     importantInstr = {}
3     for f ∈ functions do
4         allInstrs = []
5         for i ∈ f do
6              $\mathcal{I}_c(i) = \cos(\text{model}(f), \text{model}(f \setminus \{i\}))$ 
7             allInstrs.append(i,  $\mathcal{I}_c(i)$ )
8         outliers = KDE(allInstrs)
9         for i_ ∈ outliers do
10             importantInstr[i_] += 1
11 return largestK(importantInstr)
    
```

## 3.2 Semantics Importance

After deciding a set of instructions that have classification importance, the next step is to identify their semantics importance. This is achieved by identifying the stable variables in the 100 sampled functions, computing the backward program slices of these variables through a specially designed algorithm, and calculating the frequencies of instructions in the slices. That is, if an instruction frequently occurs in the backward slices of stable variables, it is considered to have semantics importance (regarding the whole dataset).

**3.2.1 Detection of Stable Variables.** In our setting, stable variables include global, heap, return variables, and variables passed as function actual arguments. Stable variables are not sensitive to compiler and compilation option changes. For example, a heap variable tends to stay as a heap variable with compilation changes. Since we directly deal with binary executables, variable symbolic information is not available. We hence perform the following analysis to recognize the stable variables.



**Identifying Global and Heap Variables.** Global and heap variables are recognized by identifying whether a memory access instruction accesses a global or heap address. This is achieved by performing backward slicing on the address operand, typically a register, and checking if it is based on a global address, which is reflected by a constant address value in the global memory region, or on the return value of a heap allocation function. For example, in Fig. 4a, the register `rdi` at line 10 is used to compute a memory address. By tracing back the data flow, DiEMPH finds that `rdi@10` is defined at line 1. The `lea` instruction at line 1 copies the address of a global variable (`GLOBAL_VAR`) to `rdi@1`<sup>2</sup>. Similarly, DiEMPH uses the same backward slicing technique to identify accesses to heap variables. Take Fig. 4b as an example. The memory address at line 10 is computed by `rbp+0x10`. `Rbx@10` is defined at line 2 by `rax@2`. `Rax@2` is the return value of the call (at line 1) to function `malloc`, which allocates a piece of heap memory. Thus `rbx@10` denotes a heap variable.

**Identifying Function Return Variables.** Return variables are considered stable variables since they denote function outputs. In x86 binary, an `ret` instruction does not have any operand. If there is a return value, it is by default stored in register `rax` (by instructions preceding the return instruction). The challenge lies in that a function that does not have an explicit return variable also uses `ret` to exit its execution. It is hence challenging to decide if a function has any return variable. Note that a simple method that searches for any write to `rax` before `ret` can hardly work as `rax` is a commonly used register in regular computation. Thus, when DiEMPH analyzes an `ret` instruction in a function, it further analyzes invocations to this function (in other functions) and checks whether `rax` is being used right after the invocations. The intuition is that if the function has a return value, the value tends to be used after the function call (e.g., assigning to some variable). Particularly, for each invocation, if the register `rax` is used after the call without a new definition, DiEMPH marks that the (invoked) function has a return value. For example, as shown in Fig. 4c, DiEMPH tries to analyze whether the return instruction at line 1 in function `f` returns a value to the caller. Suppose it finds an invocation of `f` at line 10. After the call to `f`, at line 11, `rax` is used without re-definition. This indicates the variable denoted by `rax` is returned from the function `f`. Note that if DiEMPH cannot find an invocation for the function, it conservatively assumes that the function has a return variable.

**Identifying Function Actual Arguments.** If a variable is being passed as an actual argument to some function, it is considered stable. However, without symbolic information, function signature is not available and variables passed as actual arguments are not explicit. We leverage the compiler convention that the first six actual arguments are passed from a caller to a callee using registers. This convention is true for all mainstream compilers as far as we know. As such, by checking data flow through registers across function call boundary allows us to identify variables that are passed as function arguments. For example, in Fig. 4d, the program calls to `gee` at line 3. DiEMPH steps into the function `gee`, and finds that `rdi@10` is used before definition. That indicates `rdi` is a parameter of `gee`. As

<sup>2</sup>Here, `GLOBAL_VAR` is a token introduced by our preprocessor that considers any constant value in address loading instructions like `lea` as a global variable.

## Algorithm 2: Computing Semantics Importance

```

1 Function getSemanticsImportance(function, stableVars)
  // instructionToCounter maps instructions to integers.
  // It counts how many stable variables an instruction may
  // affect. Initially, all instructions are mapped to 0.
2  instructionToCounter = {}
3  for v ∈ stableVars do
4    backSlice = backwardSlicing(function, v)
5    for i ∈ function do
6      if i ∈ backSlice then
7        instructionToCounter[i] += 1
8  semanticsImportance = {}
9  for i ∈ function do
10   semanticsImportance[i] = instructionToCounter[i] /
    len(importantVars)
11 return semanticsImportance

```

such, `rdi@2` is a stable variable. In some cases, the use of parameter-passing registers may not always be directly visible in the callee. For instance, in Fig. 4d, the register `rsi` is not used inside `gee`. However, function `gee` calls another function `foo` (line 11), and the parameters of `foo` are the same with `gee`. In this case, the compiler does not repeat the code for parameter passing. Instead, the variables in `rsi@10` and `rdi@10` are implicitly passed to `foo`. Note that at line 20, the register `rsi` is used before definition, indicating `rsi@20` is an argument. To handle such cases, DiEMPH recursively traverses the call graph of a binary project and detects direct and transitive parameter passing.

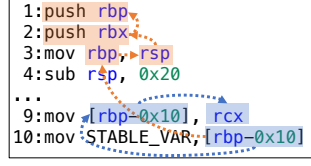
**3.2.2 Semantics Importance via Binary Slicing.** After identifying all stable variables, DiEMPH measures the semantics importance of each instruction based on the backward slices of these stable variables (within the 100 sampled functions). The procedure is defined in Algorithm 2. The algorithm takes as input a binary function and a set of stable variables. It computes and returns the semantics importance for each instruction. It maintains a counter (line 2) for each instruction, and increases the counter by 1 every time the instruction is found in the slice of a stable variable (line 6). Finally, the importance for each instruction is computed as the ratio between the number of stable variables it may affect and the number of all stable variables.

A prominent challenge in slicing a binary program is to handle memory accesses. Different from source code, a binary program accesses most variables by their addresses. Therefore, statically determining if a memory read is dependent on a memory write entails precisely determining the set of addresses these accesses may refer to. This is a hard problem, especially at the binary level. Existing methods such as *value set analysis* [3] and *stochastic analysis* [67] are either imprecise or unsound. DiEMPH resorts to a conservative solution and considers that any read to a global or a heap region is potentially dependent on any write to the same region, without disambiguating the addresses within the region. In contrast, for accesses to stack memory, which usually denote local variable or function argument accesses, we precisely determine their symbolic

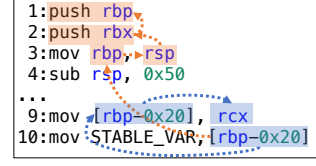
```

1  int g;
2  int foo() {
3      int x;
4      ...
5      g = x;
6  }
    
```

(a) Source Code of foo()



(b) Optimized Version



(c) Un-optimized Version

**Figure 5: Example for stack variable accesses in binary programs.** (a) shows a code snippet for function foo(). (b) and (c) are two possible resulting binary programs after compilation. (b) is an optimized version with fewer variables on stack. The variable *x* is located at [rbp-0x10]. (c) is an un-optimized version with more variables on stack, and *x* is located at [rbp-0x20].

addresses and compute precise dependences. The rationale of having an over-approximate solution for global and heap accesses is that we are collecting the slices for all global and heap variables anyway.

**Precluding Stack Address Dependences.** A special feature of our slicing algorithm is that we preclude dependences induced by address computation if the address is on stack. Note that although local variables, usually allocated on stack, do not belong to stable variables, their accesses may be involved in the slices of stable variables, e.g., when a local loop variable *i* is used to index a global array *A*[*i*]. In fact, the slice of a stable variable usually includes a larger number of local variable accesses on stack. Although the inclusion of these accesses in the slice is completely correct, the compilation convention for such accesses may lead to substantial distribution biases. For example, while a local variable read is as simple as the presence of the variable in an expression, at the binary level, the read is broken down into multiple instructions such as computing the appropriate stack address and then performing the read. The stack address computation itself may include multiple instructions. Strictly following the standard slicing algorithm, these instructions should all be included in the slice and hence have semantics importance. However, they are in fact semantically unimportant as they are just stack access conventions. Depending on the stack memory layout optimizations, the compiler may place a variable in different stack locations and use different instruction patterns to compute the address before any access. Such differences shall be neutralized. Hence in DiEMPH, we use data-flow analysis to determine if an address involved in a memory access denotes a stack address. If so, we preclude the dependence through the address operand from the slice. In the following, we use an example to illustrate the problem and then explain the data-flow analysis.

*Example.* Fig. 5 shows a function foo() in 5a and two versions of its compiled code in 5b and 5c. In 5a, the program declares a local integer variable *x*. It also has a global variable *g*, which is a stable variable according to our definition. The local variable is used in the computation of *g* (line 5) and hence included in the slice of *g*. Lines 1-4 in 5b and 5c show a typical function prologue. At first, the current values of the stack base register *rbp* and a general register *rbx* are stored on the stack (lines 1–2). In x86, there are two stack registers: the stack base pointer *rbp* pointing to the start of the previous stack frame (the stack frame of the caller function) and the stack pointer *rsp* denoting the end of the stack frame. Hence the region between *rbp* and *rsp* denotes the whole stack frame. Note that stack allocation is from high address to low address such

that the value of *rsp* is smaller than that of *rbp*. A push instruction saves a value of a register to the memory location pointed to by the stack pointer *rsp* and automatically reduces *rsp* by 8 (assuming a 64bit machine). The saved values will be restored before returning from foo() such that the caller’s stack frame can be re-activated. After saving, the registers can be safely updated inside foo().

Take 5b as an example. Lines 3-4 set up a new stack frame for foo(). In particular, the base pointer is set to the end of the previous stack frame (line 3) and the end of the new stack frame is set to an address that is 32 smaller. As such, a 32-byte stack region delimited by the new *rbp* and *rsp* values is allocated. In lines 9 and 10, a stack address falling into the frame *rbp*-0x10 is accessed in the computation of *g*, which is normalized to a symbol *STABLE\_VAR* by our preprocessor. Observe that due to different stack layout strategies (for optimization purposes), the stack addresses of *x* are different in 5b and 5c, and the instruction encodings of the accesses are hence also different.

The arrows in 5b and 5c denote the program dependences. Blue arrows denote the dependences between two variables in the source code, and orange ones denotes the address dependences (induced by *rbp*). Note that there is dependence between instructions on line 2 and line 3 because line 2 implicitly subtracts *rsp*. If we included the orange dependences, lines 1-3 (those in the orange shade) would be included in the slice of *g*. In fact, all the stack accesses in foo() are transitively dependent on lines 1-3, leading to a conclusion that these were semantically very important instructions. However, they are just low-level artifacts that do not correspond to source-level semantics. Therefore, DiEMPH precludes all dependences through stack address operands. Our ablation study in Section 4.6 demonstrates the importance of such strategy. □

The technical challenge lies in recognizing all operands denoting stack addresses. We achieve this by a data-flow analysis. A naive algorithm that simply finds all uses of *rbp* and *rsp* and rules out their dependences does not generalize well. For example, in the newer versions of GCC, the register *rbp* might be used as a normal register [21]. In this case, removing all dependencies with *rbp* may skip important dependencies. On the other hand, a compiler may copy stack pointers to other locations [61, 62]. Details of our data-flow analysis algorithm can be found in Section A of the supplementary material.

## 4 EVALUATION

DiEMPH is implemented on IDA Pro [24] and PyTorch [46]. Our code is uploaded at [2] for review. We evaluate our technique via the following research questions (RQs):

**Table 1: Performance (PR@1) improvement on the out-of-distribution dataset. The first column lists the name of binary programs. The model setups are listed in the first row. Each model is denoted with its architecture and the finetune dataset, in the form of *ModelArch<sub>dataset</sub>*. *BC*, *BK*, and *HS* denote BinaryCorp-3M, Binkit, and How-solve, respectively. In the second row, for each model, Ori. means the PR@1 for the original model, DiEMPH means the PR@1 for the model improved by DiEMPH, and Impr. means the improvement achieved by applying DiEMPH to the model.**

Programs	<i>JTrans<sub>BC</sub></i>			<i>Trex<sub>BC</sub></i>			<i>JTrans<sub>BK</sub></i>			<i>Trex<sub>BK</sub></i>			<i>JTrans<sub>HS</sub></i>			<i>Trex<sub>HS</sub></i>		
	Ori.	DiEMPH	Impr.	Ori.	DiEMPH	Impr.	Ori.	DiEMPH	Impr.	Ori.	DiEMPH	Impr.	Ori.	DiEMPH	Impr.	Ori.	DiEMPH	Impr.
Curl	44.6	62.2	17.6	31.8	41.0	9.2	44.6	47.8	3.2	15.8	20.8	5.0	58.8	62.4	3.6	9.8	14.6	4.8
Binutils	36.0	51.2	15.2	34.8	37.4	2.6	45.2	46.0	0.8	18.4	21.8	3.4	51.0	55.6	4.6	10.6	14.6	4.0
Coreutils	30.0	40.8	10.8	34.6	39.6	5.0	30.4	36.0	5.6	16.4	20.4	4.0	36.8	41.8	5.0	12.6	16.0	3.4
ImageMagick	21.8	39.4	17.6	29.4	36.0	6.6	24.0	30.6	6.6	10.8	19.2	8.4	37.4	41.6	4.2	10.4	15.2	4.8
SQLite	38.8	57.6	18.8	50.2	54.2	4.0	35.2	39.8	4.6	23.8	24.2	0.4	49.8	52.0	2.2	18.6	23.2	4.6
OpenSSL	37.2	62.6	25.4	40.0	44.8	4.8	45.8	50.2	4.4	25.4	28.6	3.2	58.4	66.4	8.0	18.4	24.4	6.0
Putty	29.6	43.4	13.8	37.8	44.6	6.8	34.2	38.6	4.4	17.0	21.2	4.2	47.0	52.2	5.2	13.2	20.8	7.6
<b>Average</b>	<b>34.0</b>	<b>51.0</b>	<b>17.0</b>	<b>36.9</b>	<b>42.5</b>	<b>5.57</b>	<b>37.1</b>	<b>41.3</b>	<b>4.2</b>	<b>18.2</b>	<b>22.3</b>	<b>4.1</b>	<b>48.5</b>	<b>53.1</b>	<b>4.7</b>	<b>13.4</b>	<b>18.4</b>	<b>5.0</b>

**RQ1:** Can DiEMPH help binary similarity models achieve better performance when the compiler configurations of the test dataset are different from the training dataset? We say that the test data are *out-of-distribution*. It denotes a realistic and challenging use scenario for binary analysis tools.

**RQ2:** Is DiEMPH effective with different pool sizes of the candidate functions?

**RQ3:** How does DiEMPH affect performance of models when the compiler configurations of the test dataset align with those of the training dataset? In this case, we say the test data are *in-distribution*.

**RQ4:** How much time does DiEMPH take to analyze functions in training datasets?

**RQ5:** How does each component of DiEMPH affect the performance? We also conduct a case study to demonstrate the effectiveness of DiEMPH on out-of-distribution test data.

## 4.1 Experiment Setup

We conduct the experiments on a server with a 24-core Intel(R) Xeon(R) 4214R CPU at 2.40GHz, 188G memory, and Ubuntu 18.04.

**Baseline Models.** We train two state-of-the-art Transformer similarity analysis models, i.e., JTrans [59] and Trex [42] on three well-known public datasets, resulting 6 baseline models in total. Although there are other binary code similarity methods, some based on Deep Learning models as well, it was shown that the Transformer based methods (i.e., our baselines) outperform these techniques [42, 59]. For each model, we use the model pretrained by its authors, and finetune the model on three different well-known public datasets for the binary similarity task. The first dataset is BinaryCorp-3M [59]. It contains around 3 million binary functions (which correspond to around 600k functions in source code). The dataset is compiled by GCC with 5 different optimization flags. The second dataset is BinKit [28]. It contains 51 GNU projects compiled with 9 different compilers  $\times$  4 different optimization flags. It has around 4.5 million binary functions (which correspond to around 126k source code functions). The third dataset is HowSolve [36]. It contains 7 projects compiled with 8 compilers  $\times$  5 optimization flags, which correspond to around 4.4 million binary functions (around 110k source code functions). Note that for the later two datasets, we only use the binary programs compiled for the x64 architecture.

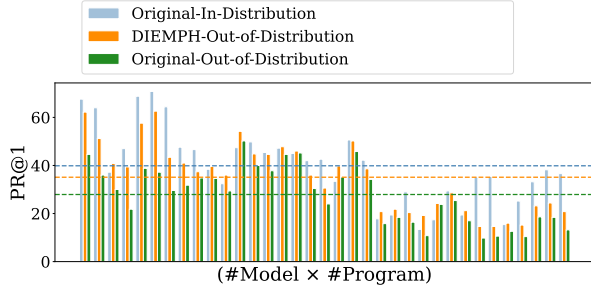
**Test Datasets.** We build two test datasets from 7 real-world projects commonly-used in binary similarity analysis [16, 22, 28, 36, 42]. They are Curl, Coreutils, Binutils, ImageMagick, SQLite, OpenSSL and Putty. Dataset-I: Binary programs in the first dataset are compiled by GCC-7.5 with -O0 and -O3 optimization flags. They are considered as test data within the distribution of the training dataset because (1) all training datasets contain binary programs compiled with GCC (2) all training datasets contain binary programs compiled by a compiler newer than GCC-7.5. That indicates all the optimizations/conventions by GCC-7.5 are very likely present in the training dataset. We obtain the binaries from [42]. Dataset-II: Binary programs in the second dataset are compiled by GCC-9.4 with -O3 flag and Clang-10 with -O0 flag. They are considered as test data with compiler configurations different to the training datasets because programs in the training dataset are compiled with older versions of compilers. The two new compilers introduce new optimizations and likely emit instructions with new patterns [21, 33]. For simplicity, we refer to Dataset-I as the *In-Distribution* dataset, and refer to Dataset-II as the *Out-of-Distribution* dataset. We want to point out that we exclude all projects in test sets from the training sets and make sure there are no overlapping libraries between the test sets and the training sets.

**Metrics.** We use precision at 1 (PR@1) as our metrics. Suppose that we iteratively query a set of binary functions from a pool of candidate functions. PR@1 measures in how many queries, the correct function (i.e., the function compiled from the same source code as the query function) is returned as the most similar function. Note that our experiments are conducted in a way that each function has only one similar function (more details later in the section).

## 4.2 RQ1: Performance Improvement on the Out-of-Distribution Dataset

In this section, we evaluate whether DiEMPH can help models achieve better performance on the out-of-distribution dataset. For each baseline model, DiEMPH takes as input the model and the training dataset, and outputs the instructions need to be de-emphasized. We remove these instructions from the training dataset, and rerun the finetune process, resulting an improved model. We then test the performance for both the baseline model and the improved model on the out-of-distribution dataset. For each binary program in our dataset, we randomly sample 500 functions from the O0 binary, and



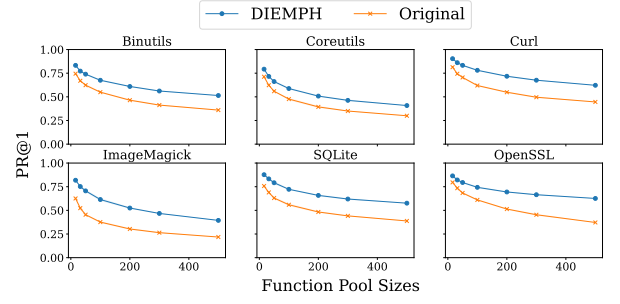


**Figure 6: DiEMPH helps models alleviate performance degradation.** Each bar in the figure shows the performance of one model on one test program. The  $y$  axis denotes PR@1. The blue bars show the performance of original models tested on the in-distribution dataset. The orange and green bars show the performance of original models and DiEMPH improved models tested on the out-of-distribution dataset, respectively. The dashed lines show the average performance.

query them one by one in a pool consisting of the corresponding 500 functions from the O3 binary. In other words, there is only one similar function in the pool for each query. Such a setup is consistent with the literature [23, 36, 60]. During testing, we also remove the de-emphasized instructions from the test inputs to the improved model for input space consistency.

The results are shown in Table 1. We can see that DiEMPH improves the PR@1 of models by 4.1-17.0%. Note that these improvements are considered significant for the binary similarity task due to its challenging nature. In the binary similarity literature, the improvement to the baseline method is usually 3-8% [16, 60]. We can see that the improvements are most prominent on the two models trained with the BinaryCorp-3M dataset. DiEMPH improves the JTrans and Trex model trained on it by 17% and 5.57%. In particular, the improved JTrans trained on the de-emphasized BinaryCorp-3M denotes the new state-of-the-art. Note that BinaryCorp-3M is significantly larger than the other datasets we use. The fact that we are able to achieve substantial improvement on the most complex model and the largest dataset indicates the value of instruction deemphasis in practice. The improvements are around 5% for the models trained on the How-Solve dataset. The performance for the original Trex models trained on this dataset is worse than the original JTrans because the dataset contains many functions with relatively complex control flow structure, and Trex does not precisely encode control flow information such that it may not learn control flow features well. The improvements on the models trained on the BinKit dataset are relatively low (around 4%). That is because BinKit contains only around 126k source code functions. Although each function is compiled with many different configurations, the limited program diversity leads to limited generalizability.

To normalize the effectiveness of DiEMPH w.r.t. the differences introduced by model architectures and training datasets, we additionally run the baseline models on the in-distribution dataset, and show to what extent DiEMPH can help the model overcome the performance degradation caused by the distribution shift between testing and training data (i.e., different compiler configurations). The results are visualized in Fig. 6. We can see that on average, the performance of the original models degrades by 11.9% due to



**Figure 7: Effectiveness of DiEMPH (for  $JTrans_{BC}$ ) with different pool sizes.** Each figure shows the performance of two models on a program in the out-of-distribution dataset. The  $x$ -axis denotes the sizes of candidate function pool. The  $y$ -axis denotes PR@1. The orange and blue lines denote the performance of the original model and the performance of the model improved by DiEMPH, respectively.

distribution shift. DiEMPH can overcome 88% of the degradation, achieving performance close to the original models' performance on the in-distribution dataset (only 4.7% lower). That indicates DiEMPH makes these models generalize better.

### 4.3 RQ2: Effectiveness with Different Pool Sizes

The performance of a binary similarity model may vary when the size of candidate function pool is different [59]. Thus we validate whether DiEMPH can effectively improve model performance (on the out-of-distribution dataset) with different pool sizes. For each model, we test its performance on 7 function pools with different sizes from 16 to 500. We show in Fig. 7 the test results for the JTrans model trained on BinaryCorp-3M. The results for other models are shown in Fig. 9 of the supplementary material. The blue lines denote the performance of the model improved by DiEMPH. The orange lines denote the performance of the original model. We can see that DiEMPH can effectively improve the original model's performance on all different pool sizes. The improvement is more significant when the pool size is larger than 100. That is because the task of finding similar functions becomes harder when there are more candidate functions. It requires the model to more precisely distinguish functions based on instructions with important semantics. Note that we run each test for 10 times, and Fig. 7 shows the average results.

### 4.4 RQ3: Effects on In-Distribution Data

In this section, we study how DiEMPH affects the performance on the in-distribution dataset. Following the setup of RQ1, we run both the original model and the model improved by DiEMPH on the in-distribution dataset. The results are shown in Table 2. While DiEMPH can make the models generalize substantially better on the out-of-distribution dataset, we can see that in most cases, DiEMPH is also able to slightly improve models' performance on average on the in-distribution dataset. That is because DiEMPH removes from the training sets instructions with high classification importance but low semantics importance. This helps the models learn to represent a program based on the semantically important features. Compared with the improvement DiEMPH achieves on the out-of-distribution



**Table 2: Effects of DiEMPH on performance (PR@1) for the in-distribution dataset. The first column lists the binary programs. The model setups are listed in the first row in the form of  $ModelArch_{dataset}$ , where *BC* denotes BinaryCorp-3M, *BK* Binkit, and *HS* How-solve. In the second row, Ori. and DiEMPH mean the PR@1 of the original model and the model improved by DiEMPH, respectively. Diff. means the difference of performance between the two models.**

Programs	<i>JTrans<sub>BC</sub></i>			<i>Trex<sub>BC</sub></i>			<i>JTrans<sub>BK</sub></i>			<i>Trex<sub>BK</sub></i>			<i>JTrans<sub>HS</sub></i>			<i>Trex<sub>HS</sub></i>		
	Ori.	DiEMPH	Diff.	Ori.	DiEMPH	Diff.	Ori.	DiEMPH	Diff.	Ori.	DiEMPH	Diff.	Ori.	DiEMPH	Diff.	Ori.	DiEMPH	Diff.
Curl	67.6	71.4	3.8	47.6	49.2	1.6	47.2	50.2	3.0	17.8	16.6	-1.2	58.0	59.8	1.8	35.2	39.6	4.4
Binutils	64.0	72.0	8.0	46.6	46.8	0.2	45.0	49.0	4.0	19.4	18.8	-0.6	56.8	59.8	3.0	35.4	36.2	0.8
Coreutils	37.2	44.0	6.8	38.4	38.2	-0.2	42.0	46.2	4.2	29.0	29.6	0.6	53.6	53.0	-0.6	15.4	25.2	9.8
ImageMagick	47.0	51.2	4.2	32.4	34.8	2.4	42.6	43.4	0.8	13.4	18.4	5.0	51.8	52.4	0.6	25.2	28.6	3.4
SQLite	68.8	73.4	4.6	47.4	45.4	-2.0	33.4	38.0	4.6	17.4	17.6	0.2	55.4	59.2	3.8	33.2	37.0	3.8
OpenSSL	70.8	74.4	3.6	49.8	52.8	3.0	50.6	56.8	6.2	29.4	25.4	-4.0	64.4	65.6	1.2	38.2	40.2	2.0
Putty	64.4	66.0	1.6	45.4	47.6	2.2	42.2	47.2	5.0	19.4	17.8	-1.6	47.0	50.4	3.4	36.6	39.0	2.4
<b>Average</b>	<b>60.0</b>	<b>64.6</b>	<b>4.7</b>	<b>43.9</b>	<b>45.0</b>	<b>1.0</b>	<b>43.3</b>	<b>47.3</b>	<b>4.0</b>	<b>20.8</b>	<b>20.6</b>	<b>-0.2</b>	<b>55.3</b>	<b>57.2</b>	<b>1.9</b>	<b>31.3</b>	<b>35.1</b>	<b>3.8</b>

data, the improvement on in-distribution data is smaller. That is because the distribution of the testing set is similar to the training dataset. A baseline model may already achieve relatively good performance even if it represents programs based on semantically unimportant instructions. For the Trex model trained on the BinKit dataset, the performance slightly degrades after applying DiEMPH. As discussed before, that is because the dataset is relatively small and not diverse such that the semantically unimportant instructions may indeed be critical for achieving good performance.

#### 4.5 RQ4: Run Time Efficiency

We use DiEMPH to analyze the six models and test whether it is time efficient. Specifically, for each model, DiEMPH randomly samples 100 functions from the training data, computes the classification importance for each instruction, uses KDE to select outliers, and validates whether instructions with high classification importance are semantically important. We record the time for the overall run time and the most time-consuming parts. The results are shown in Table 3. The first column shows the models, in the form of  $ModelArch_{dataset}$ . The 2-4 columns show the time for KDE, then classification importance analysis, and the overall run time. All numbers are wall-clock time in seconds. We can see that on average, DiEMPH takes around 12 minutes to analyze one model with 100 sampled functions. Computing the classification importance for each instruction is most time-consuming, as the algorithm creates around 100 mutants of a given binary function and invokes the model to encode all the mutants. The time consumption of DiEMPH is acceptable since it is a one-time effort.

#### 4.6 RQ5: Ablation Study

We conduct an ablation study to show how each part of DiEMPH affects the performance. We alter our algorithms and generate three variants of DiEMPH, and use each variant to analyze the Trex model trained on the BinKit dataset, resulting in three improved models. For each model, we test its performance on both the in-distribution dataset and the out-of-distribution dataset. The results are shown in Table 4. The first column denotes the distribution of the test dataset. Columns 2-3 denote the performance of the original model and the performance of the model improved by DiEMPH with all components. Columns 4-6 denotes the performance of variants. The first row shows the performance on the out-of-distribution set, and the second row the in-distribution set.

**Table 3: Run time efficiency of DiEMPH (in seconds)**

Model	KDE	Class. Imp.	All
<i>JTrans<sub>BC</sub></i>	197	335	582
<i>JTrans<sub>BK</sub></i>	338	521	880
<i>JTrans<sub>HS</sub></i>	192	333	565
<i>Trex<sub>BC</sub></i>	91	396	535
<i>Trex<sub>BK</sub></i>	169	602	785
<i>Trex<sub>HS</sub></i>	176	726	934
<b>Average</b>	<b>193</b>	<b>485</b>	<b>713</b>

**Table 4: Ablation study.**

Test Dist.	Ori.	DiEMPH	No-Stack	No-Sem.	No-Class.
Out-of-Dist	18.23	22.31	20.20	20.37	20.31
In-Dist	20.83	20.60	20.74	19.51	20.31

For *No-Stack*, we do not trace the stack pointers and do not prune the dependencies introduced by stack operations. We can see that it still improves the baseline model’s performance on the out-of-distribution dataset, while the improvement is less significant than DiEMPH. That is because without pruning the stack dependencies, the variant is more conservative when computing the semantics importance of instructions. That is, fewer semantically unimportant (but classification-wise important) instructions are removed from the dataset. Although the removal helps the model learn to encode programs based on semantically important instructions, the resulting model may still learn some undesirable bias in the training data, thus it has worse generalization when tested on the out-of-distribution data. On the other hand, it more conservatively preserves some of the features that do not generalize well, which may help in-distribution performance.

For *No-Sem*, we do not analyze the semantics importance of instructions. Instead, we directly remove instructions with exceptionally high classification importance. We can see that the variant is still able to improve baseline model’s performance on the out-of-distribution dataset, although the improvement is less significant. That is because *No-Sem* removes instructions that substantially affect the embeddings generated by the original model, forcing the model to learn to represent a function differently. Moreover, *No-Sem* induces noticeable performance degradation on the in-distribution test. That is because *No-Sem* may undesirably remove some semantically important instructions (e.g., call instructions), breaking semantics and confusing the model.

For *No-Class.*, we do not analyze the classification importance of instructions, and directly remove instructions with low semantics importance. We can see that it slightly improves the out-of-distribution performance of the baseline model because removing semantically unimportant instructions from the training set guides the model to represent a program based on the semantically important parts. However, the improvement is less significant than DiEMPH because *No-Class* may miss removing some instructions that greatly affect the embeddings generated by the original model. In addition, it has some (less noticeable) negative effects on the in-distribution performance because the original model may depend on some semantically unimportant instructions that may be helpful for in-distribution performance.

## 4.7 Case Study

We conduct a case study with the JTrans model trained on the BinaryCorp-3M dataset to demonstrate how DiEMPH improves the performance of the model on the out-of-distribution dataset.

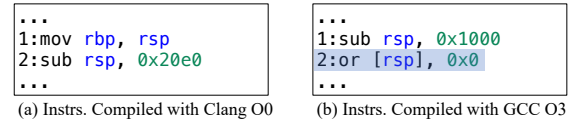
By analyzing the model and the training dataset, DiEMPH finds that an instruction “or [rsp], 0” has exceptionally high classification importance but low semantics importance in many functions. This instruction performs a bitwise-or operation between the variable stored in [rsp] and 0, and hence it does not modify the value of the variable. The instruction is inserted by an optimizing compiler to improve cache performance in modern processors.

We show in Fig. 8 an example in the test set that contains this instruction. The instruction is highlighted with the blue shade in Fig. 8b. In Fig. 8b, note that the variable stored in rsp at line 2 is not initialized (because the value of rsp is updated at line 1). And the inserted instruction does not modify the variable either. Thus the following instructions in the function are not likely to use the definition [rsp]@2. That is, the instruction is not semantically important in this function. Also note that this instruction is not in the function compiled (from the same source code) with Clang -O0, shown in Fig. 8a.

The original JTrans model generates a similarity score as low as 0.45 for this pair of functions due to the difference of the highlighted instruction. After we remove it from the optimized function (Fig. 8b), the similarity score increases to 0.52. On the other hand, the JTrans model improved by DiEMPH generates a similarity score as high as 0.69 for this pair of functions. That indicates DiEMPH indeed helps the model better represent a program based on semantically important instructions.

## 5 RELATED WORK

**Binary Similarity Analysis.** Binary similarity analysis has critical security applications. Thus the community has made significant efforts in this area, with various approaches proposed. For example, Pewny et al. [43] proposed a signature-based method for cross-architecture bug search; Blanket Execution [18] leverages a force-execution-based approach to collect runtime information; BinMatch [23] presents a hybrid approach that combines static and dynamic information; IMF [60] employs in-memory fuzzing to identify similar functions across binary executable files. Moreover, recent advances in Deep Learning techniques have led to



**Figure 8: Instructions in `head_lines()` of `Coreutils`. The two snippets of instructions are generated by `Clang -O0` and `GCC -O3`, respectively. The instruction highlighted in the blue box is inserted by GCC. It is used to optimize the cache performance in modern processors.**

unprecedented capabilities in many areas, including binary similarity [28, 36, 38] For instance, Asm2vec [15] and DeepBinDiff [16] adapt distributed word representation techniques [39] to generate vector representations for assembly code; *αDiff* [31] leverages CNN to detect cross-version similar binary code; ISRD [63] utilizes a multi-level birthmark model to uniquely represent program semantics. Furthermore, two Transformer-based methods [42, 59] have been proposed, demonstrating superior performance compared to previous work, leveraging the recent success of Transformers [9, 47, 48, 56] in the NLP domain. These techniques represent notable advances in binary similarity analysis and have the potential to aid in the identification and mitigation of security threats. Our work is an enhancement to these approaches, aiming to improve the generalizability of Transformer-based models.

**Model Debugging.** Although deep learning models achieve significant success in various domains, their opaque nature poses challenges in understanding the root cause of unexpected behaviors (e.g., low accuracy). As a result, many researchers focus on the area of *model debugging*, which treat deep learning models as traditional software and develop approaches to analyzing and debugging deep learning models [35, 41, 55]. However, these methods do not address the challenges in improving Transformer models for binary code analysis due to the complexity of the Transformer models and the domain-specific constraints of binary programs. Our approach focuses on such complex binary code models, leveraging domain knowledge about binary similarity analysis and binary program slicing. Our method can pinpoint the code patterns introducing biases to models and help models focus on semantically important instructions.

## 6 CONCLUSION

We develop a novel technique to improve the performance of Transformer-based binary code similarity analysis models. The technique detects instructions that have undesirably biased distributions in the training dataset because of compiler conventions. It features a (Deep Learning) model classification importance analysis that determines if an instruction is important for model output and a program analysis based semantics importance analysis that determines if an instruction denotes part of essential program semantics. Instructions that have classification importance but not semantics importance are removed from the dataset. Finetuning the model on the updated dataset yields substantially better performance than the original models.

## 7 DATA AVAILABILITY

Our experimental data and the source code is uploaded for review at [2].

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