Revisiting Binary Code Similarity Analysis using Interpretable Feature Engineering and Lessons Learned

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Abstract—Binary code similarity analysis (BCSA) is widely used for diverse security applications such as plagiarism detection, software license violation detection, and vulnerability discovery. Despite the surging research interest in BCSA, it is significantly challenging to perform new research in this field for several reasons. First, most existing approaches focus only on the end results, namely, increasing the success rate of BCSA, by adopting uninterpretable machine learning. Moreover, they utilize their own benchmark sharing neither the source code nor the entire dataset. Finally, researchers often use different terminologies or even use the same technique without citing the previous literature properly, which makes it difficult to reproduce or extend previous work. To address these problems, we take a step back from the mainstream and contemplate fundamental research questions for BCSA. Why does a certain technique or a feature show better results than the others? Specifically, we conduct the first systematic study on the basic features used in BCSA by leveraging interpretable feature engineering on a large-scale benchmark. Our study reveals various useful insights on BCSA. For example, we show that a simple interpretable model with a few basic features can achieve a comparable result to that of recent deep learning-based approaches. Furthermore, we show that the way we compile binaries or the correctness of underlying binary analysis tools can significantly affect the performance of BCSA. Lastly, we make all our source code and benchmark public and suggest future directions in this field to help further research.

Index Terms—Binary code similarity analysis, similarity measures, feature evaluation and selection, benchmark.

1 Introduction

PROGRAMMERS reuse existing code to build new software. It is a common practice for them to find the source code from another project and repurpose that code for their own needs [1]. Inexperienced developers even copy and paste code samples off of the Internet to ease the development process.

This trend has deep implications on software security and privacy. When a programmer takes a copy of a buggy function from an existing project, the bug will remain intact even after the original developer has fixed it. Furthermore, if a developer in a commercial software company inadvertently uses a library code from an open-source project, the company can be accused of violating an open-source license such as the GPL [2].

Unfortunately, however, detecting such problems from binary code using a similarity analysis is *not* straightforward, especially when the source code is not available. This is because binary code lacks high-level abstractions, such as data types and functions. For example, it is not obvious from binary code whether a memory cell represents an integer, a string, or another data type. Moreover, identifying precise function boundaries is radically challenging in the first place [3], [4].

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Therefore, measuring the similarity between binaries has been an essential research topic in many areas such as malware detection [5], [6], plagiarism detection [7], [8], authorship identification [9], and vulnerability discovery [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21].

However, despite the surging research interest in binary code similarity analysis (BCSA), we found that it is still significantly challenging to conduct new research on this field for several reasons.

First, most of the methods focus only on the end results without considering the precise reasoning behind their approaches. For instance, during our literature study in the field, we observed that there is a prominent research trend in applying BCSA techniques to cross-architecture and cross-compiler binaries of the same program [11], [12], [13], [15], [16], [19], [22]. Those approaches aim to measure the similarity between two or more seemingly distinct binaries generated from different compilers targeting different instruction sets. To achieve this, multiple approaches have devised complex analyses based on machine learning to extract the semantics of the binaries, assuming that their semantics should not change across compilers nor target architectures. However, none of the existing approaches clearly justifies the necessity of such complex semantics-based analyses. One may imagine that a compiler may generate structurally similar binaries for different architectures, even though they are syntactically different. Do compilers and architectures really matter for BCSA in this regard? Unfortunately, it is difficult to answer this question as most of the existing approaches leverage **uninterpretable** machine learning techniques [12], [13], [19], [20], [21], [23],

[24], [25], [26], [27], [28], [29]. Further, it is not even clear why a BCSA algorithm works only on some benchmarks and not on others.

Second, each and every existing paper on BCSA that we studied utilizes its own benchmark to evaluate the proposed technique, which makes it difficult to compare the approaches with one another. Moreover, reproducing the previous results is often infeasible because most researchers reveal neither their source code nor their dataset. Only 10 of the 39 papers that we studied fully released their source code, and *only two* of them opened their entire dataset.

Finally, researchers in this field do not use unified terminologies, and often miss out critical citations that appeared in top-tier venues of other fields. Some of them even mistakenly use the same technique without citing the previous literature properly. These observations motivate one of our research goals, which is to summarize and review widely adopted techniques in this field, particularly in terms of generating features.

To address these problems, we take a step back from the mainstream and contemplate fundamental research questions for BCSA. As the first step, we precisely define the terminologies and categorize the features used in the previous literature to unify terminologies and build knowledge bases for BCSA. We then construct a comprehensive and reproducible benchmark for BCSA to help researchers extend and evaluate their approaches easily. Lastly, we design an interpretable feature engineering model and conduct a series of experiments to investigate the influence of compilers, their options, and their target architectures on the syntactic and structural features of the resulting binaries.

Our benchmark, which we refer to as BinKit, encompasses various existing benchmarks. It is generated by using major compiler options and targets, which includes 8 architectures, 9 different compilers, 5 optimization levels, as well as various other compiler flags. BinKit contains 243,128 distinct binaries and 75,230,573 functions built for 1,352 different combinations of compiler options, on 51 real-world software packages. We also provide an automated script that helps extend BinKit to handle different architectures or compiler versions. We believe this is critical, because it is not easy to modify or extend previous benchmarks, despite us having their source codes. Cross-compiling software packages using various compiler options is challenging because of numerous environmental issues. To the best of our knowledge, BinKit is the first *reproducible* and *extensible* benchmark for BCSA.

With our benchmark, we perform a series of rigorous studies on how the way of compilation can affect the resulting binaries in terms of their syntactic and structural shapes. To this end, we design a simple *interpretable* BCSA model, which essentially computes relative differences between BCSA feature values. We then build a BCSA tool that we call TikNib, which employs our interpretable model. With TikNib, we found several misconceptions in the field of BCSA as well as novel insights for future research as follows.

First, the current research trend in BCSA is founded on a rather exaggerated assumption: binaries are radically different across architectures, compiler types, or compiler versions. However, our study shows that this is not necessarily the case. For example, we demonstrate that simple numeric features, such as the number of incoming/outgoing calls in a function, are largely similar between binaries compiled across different architectures. We also present other elementary features that are robust across compiler types, compiler versions, and even intra-procedural obfuscation. With these findings, we show that TikNib with those simple features can achieve a comparable accuracy to that of the state-of-the-art BCSA tools, such as VulSeeker, which relies on a complex deep learning-based model.

Second, most researchers focus on vectorizing features from binaries, but not on recovering abstract information, such as variable types, which is lost during the compilation. However, our experimental results suggest that focusing on the latter can be highly effective for BCSA. Specifically, we show that TikNib with recovered type information achieves an accuracy of over 99% on all our benchmarks, which was indeed the best result compared to all the existing tools we studied. This result highlights that recovering type information from binaries can be as critical as developing a novel machine learning algorithm for BCSA.

Finally, the interpretability of a tool not only helps deeply understand BCSA results but also helps advance the field. For example, we present several practical issues in the underlying binary analysis tool, i.e., IDA Pro, used by TikNib, and discuss how such errors can affect the performance of BCSA. Because our tool uses an interpretable model, we were able to easily pinpoint those fundamental issues, which can eventually benefit binary analysis tools and the entire field of binary analysis.

Contribution. In summary, our contributions are as follows:

- We study the features and benchmarks used in the past literature regarding BCSA and clarify underexplored research questions in this field.
- We propose BinKit[1], which is the first reproducible and extensible benchmark for BCSA. It consists of 243,128 binaries and 75,230,573 functions compiled for 1,352 combinations of compilers, their options, and their target architectures.
- We implement a BCSA tool, TikNib[2], which employs a simple interpretable model. We demonstrate that TikNib can achieve an accuracy comparable to that of a state-of-the-art deep learning-based tool. We believe this will serve as a baseline to evaluate future research in this field.
- We investigate the effectiveness of basic BCSA features with TikNib on our benchmark and unveil several misconceptions and novel insights.
- We make our source code, benchmark, and our experimental data public to support open science.

2 Binary Code Similarity Analysis

Binary Code Similarity Analysis (BCSA) is the process of identifying whether two given code snippets have similar semantics. Typically, it takes in two code snippets as input, and returns a similarity score ranging from 0 to 1, where 0 indicates the two snippets are completely different, and 1 means that they are equivalent. The input code snippet can be a function [11], [16], [19], [21], [24], [30], [31], [32], or

1. https://github.com/SoftSec-KAIST/binkit
2. https://github.com/SoftSec-KAIST/tiknib

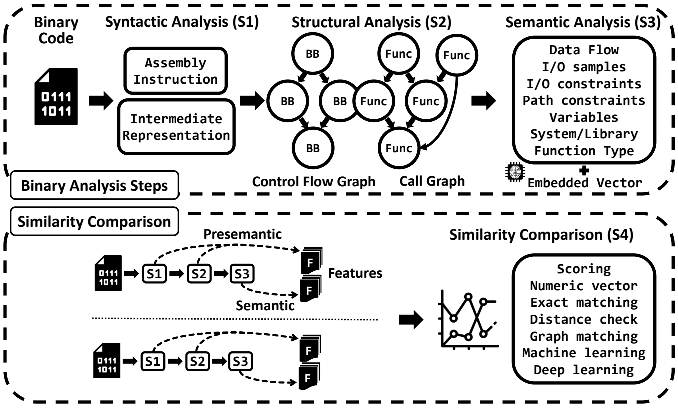


Fig. 1: Binary Code Similarity Analysis (BCSA) workflow.

even an entire binary image [7], [8]. Additionally, the actual comparison can be based on functions, even if the inputs are entire binary images [12], [13], [15], [23], [33], [34], [35].

At a high level, BCSA performs four major steps as described below:

(S1) Syntactic Analysis. Given a binary code snippet, one disassembles the code and represents its low-level semantics in a canonicalized form, which is often referred to as an intermediate representation (IR). If the code snippet is an entire binary file, s/he first parses it based on its file format and split it into sections before disassembling it.

(S2) Structural Analysis. Then, one analyzes the low-level meanings of the target binaries using IRs to identify functions and to analyze their control structures. This step involves recovering the control-flow graphs (CFGs) and call graphs (CGs) of the binaries [36], [37].

(S3) Semantic Analysis. After recovering the control structure of the binary code from the structural analysis phase, one can perform traditional program analyses, such as data-flow analysis and alias analysis, to figure out the high-level semantics. S/he can also post-process the features gathered from S1–S2 to obtain high-level features.

(S4) Vectorization and Comparison. The final step is to vectorize all the information gathered from S1–S3 to compute the similarity between the binaries. This step essentially results in a similarity score between 0 and 1.

Figure 1 depicts the four-step process. The first three steps determine the inputs to the comparison step (S4), which are often referred to as *features*. Some of the first three steps can be skipped depending on the underlying features being used. The actual comparison methodology in (S4) can also vary depending on the BCSA technique. For example, one may compute the Jaccard distance [38] between feature sets, calculate the graph edit distance [39] between CFGs, or even leverage deep learning algorithms [40], [41]. However, *as the success of any comparison algorithm significantly depends on the chosen features, this paper focuses on features used in previous studies rather than the comparison methodologies.*

In this section, we first describe the features used in the previous papers and their underlying assumptions (§2.1). We then discuss the benchmarks used in those papers and point out their problems (§2.2). Lastly, we present several research questions identified during our study (§2.3).

Our study focuses on recent papers that appeared in top-tier venues to keep the scope manageable. There are, of course, plentiful research papers in this field, all of which are invaluable. Nevertheless, our focus here is not to conduct a complete survey on them, but to introduce a prominent trend and the underlying research questions in this field, as well as answering these questions. Because of the space limit, we excluded papers [42], [43], [44], [45], [46], [47], [48], [49], [50], [51], [52] that were published before 2014 and those not regarding top-tier venues. We also excluded binary diffing tools [53], [54], [55] used in industry. However, we believe that the recent papers can cover the features used in the previous ones including those used in the industrial tools [43], [44]. Meanwhile, we discuss papers that present vital technical improvements in the text. Additionally, we also excluded papers that specifically aim to address a specific purpose such as malware detection, library function identification, or patch identification, and we discuss them further in §8. Lastly, we excluded papers that require source code.

2.1 Features Used in Prior Works

We categorize features into two groups based on when they are generated during BCSA. Particularly, we call features obtained before and after the semantic analysis step (S3) as *presemantic features* and *semantic features*, respectively. Presemantic features can be derived from either (S1) or (S2), and semantic features can be derived from (S3). We summarize both features used in the recent literature in Table 1.

2.1.1 Presemantic Features

Presemantic features denote direct or indirect outcomes of the syntactic (S1) and structural (S2) analyses. Therefore, we refer to any attribute of binary code, which can be derived without a semantic analysis, as a presemantic feature. We can further categorize presemantic features used in previous literature based on whether the feature represents a number or not. We refer to features representing a number as *numeric presemantic features*, and others as *non-numeric presemantic features*. The first half of Table 1 summarizes them.

Numeric presemantic features. Counting the appearance of a program's properties is common in BCSA as it can be directly used as a numeric vector in the similarity comparison (S4). We categorize numeric presemantic features into three groups based on the granularity of the information required for extracting them.

First, many researchers extract numeric features from each basic block of a target code snippet. One may measure the frequency of raw opcodes (mnemonics) [17] or grouped instructions based on their functionality [11], [28]. This numeric form can also be post-processed through machine learning [12], [13], [23], [28], as we further discuss in §2.1.2.

Similarly, numeric features can be extracted from a CFG as well. CFG-level numeric features can also reflect structural information that underlies a CFG. For example, a function can be encoded into a numeric vector, which consists of the number of nodes and edges as well as grouped instructions in its CFG [11], [28], [60]. One may extend such numeric vectors by adding extra features such as the number of child nodes and the betweenness centrality of a CFG [12], [23], [28]. The concept of 3D-CFG [70], which places each node in a CFG into a 3D space, can be utilized

TABLE 1: Features used in the recent literature.

		2014						2015	2016							2017									2018										2019						2020				
		TEDEM	Tracy	CoP	LoPD	BLEX	BinClone	Multi-k-MH	discovRE	Genius	Esh	BinGo	MockingBird	Kam1n0	BinDNN	BinSign	Xmatch	Gemini	GitZ	BinSim	BinSequence	IMF-sim	CACompare	ASE17	BinArm	SANER18	BinGo-E	WSB	BinMatch	MASES18	Zeek	FirmUp	αDiff	VulSeeker	InnerEye	Asm2Vec	SAFE	BAR19i	BAR19ii	FuncNet	DeepBinDiff	ImOpt	ACCESS20	Patchecko	BinKit
		[10]	[56]	[7]	[8]	[30]	[57]	[22]	[11]	[23]	[58]	[15]	[33]	[32]	[59]	[60]	[16]	[12]	[61]	[62]	[34]	[31]	[35]	[63]	[17]	[64]	[18]	[65]	[66]	[25]	[67]	[14]	[19]	[13]	[24]	[20]	[21]	[26]	[29]	[68]	[27]	[69]	[52]	[28]	★
Presemantic	BB-level Numbers	·	·	·	·	·	·	·	○	◑	·	·	·	·	·	·	·	◑	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	◑	·	·	·	·	·	◑	·	·	·	◑	○
	CFG-level Numbers	·	·	·	·	·	○	·	○	◑	·	·	·	·	·	○	·	◑	·	·	○	·	·	·	○	○	○	·	·	·	·	·	·	◑	·	·	·	·	·	◑	·	·	·	◑	○
	CG-level Numbers	·	·	·	·	·	·	·	○	·	·	○	·	·	·	○	·	·	·	·	·	·	·	·	○	○	○	·	·	·	·	·	○	·	·	◑	·	·	·	·	·	·	·	◑	○
	Raw Bytes	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	◑	·	·	◑	·	·	·	·	·	·	·	·	·	○	·	·
	Instructions	○	○	·	·	·	○	·	·	·	·	○	·	○	○	·	·	·	·	·	○	·	·	·	·	·	○	·	·	·	·	·	·	·	◑	◑	◑	◑	◑	·	◑	◑	·	·	·
	Functions	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·
Semantic	Symbolic Constraints	·	·	○	○	·	·	·	·	·	○	·	·	·	·	·	○	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·
	I/O Samples	·	·	·	○	·	·	○	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·
	Runtime Behavior	·	·	·	·	○	·	·	·	·	·	·	○	·	·	·	·	·	·	○	·	○	○	○	·	·	○	○	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	◑	·
	Manual Annotation	·	·	·	·	·	·	·	·	·	·	○	·	·	·	○	·	·	·	○	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·
	Program Slices, PDG	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	○	○	·	◑	·	·	·	·	·	·	·	·	·	·	·
	Recovered Variables	·	·	·	·	·	·	·	○	◑	·	·	·	·	·	○	·	◑	·	·	·	·	·	·	○	○	○	·	·	·	·	·	·	·	·	·	·	·	·	◑	·	·	·	◑	·
	Embedded Vector	·	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	○	·	·	·	·	·	·	·	·	·	·	·	○	·	·	○	○	○	○	○	○	○	○	○	○	·	○	·

◑ This mark represents a feature which is not directly used for similarity comparison, but is necessary to extract other features in post-processing.

as well. Here, the distances among the centroids of two 3D-CFGs can represent their similarity score [18]. Other numeric features can be the graph energy, skewness, or cyclomatic complexity of a CFG [17], [28]. Even loops in a CFG can be converted into numeric features by counting the number of loop headers and tails as well as the number of forward/backward edges [64].

Finally, past approaches considering numeric features from a CG mostly measure the number of callers and callees [11], [17], [19], [23], [28], [64], [71]. When extracting these features, one can selectively apply an inter-procedural analysis using the ratio of the in-/out- degrees of the internal callees in the same binary and the external callees of imported libraries [15], [18], [20], [28] This is similar to the coupling concept [72], which analyzes the inter-dependence between software modules. The extracted features can also be post-processed using machine learning [19].

Non-numeric presemantic features. Program properties can also be directly used as a feature. The most straightforward approach involves directly comparing the raw bytes of binaries [6], [52], [73]. However, people tend to not consider this approach because byte-level matching is not robust compared to simple code modifications. For example, anti-malware applications typically make use of manually written signatures using regular expressions to capture similar, but syntactically different malware instances [74]. Recent approaches have attempted to extract semantic meanings from raw binary code utilizing a deep neural network (DNN) to build a feature vector representation [19], [25].

Another straightforward approach involves considering the opcodes and operands of assembly instructions [18], [75]. Researchers often normalize operands [32], [34], [56] because their actual values can significantly vary across different compiler options. Recent approaches [61], [69] have also applied re-optimization techniques [76] for the same reason. To compute a similarity score, one can measure the number of matched elements or the Jaccard distance [15] between matched groups, within a comparison unit such as a sliding window [57], basic block [34], or tracelet [56]; a tracelet is essentially a series of basic blocks. Although these approaches take different comparison units, one may adjust their results to compare two procedures, or to find the longest common subsequence [32], [34] within procedures. If one converts assembly instructions to a static single assignment (SSA) form, s/he can compute the tree edit distance between the SSA expression trees as a similarity score [10]. Recent approaches have proposed applying popular techniques in natural language processing (NLP) to represent an assembly instruction or a basic block as an embedded vector, reflecting their underlying semantics [20], [21], [24], [26], [27], [29].

Finally, there are features that can be directly extracted from functions. Such features may include the names of imported functions, and the intersection of two inputs can show their similarity [19], [60]. Note that these features can collaborate with other features as well.

2.1.2 Semantic Features

We call features that we can obtain from the semantic analysis phase (S3) *semantic features*. To obtain semantic features, a complex analysis, such as symbolic execution [7], [8], [15], [18], [62], dynamic evaluation of code snippets [8], [30], [31], [33], [35], [62], [63], [65], [66], or machine learning-based embedding [12], [13], [19], [20], [21], [23], [24], [25], [26], [27], [28], [29] is necessary. There are mainly seven distinct semantic features used in the previous literature, as listed in Table 1. It is common to use multiple semantic features together or combine them with presemantic features.

First, one straightforward method to represent the semantics of a given code snippet is to use symbolic constraints. The symbolic constraints could express the output variables or states of a basic block [7], a program slice [16], [58], [62], or a path [8], [77], [78]. Therefore, after extracting the symbolic constraints from a target comparison unit, one can compare them using an SMT solver.

Second, one may represent code semantics using I/O samples [8], [15], [18], [22]. The key intuition here is that two identical code snippets produce consistent I/O samples, and directly comparing them would be time-efficient. One can generate I/O samples by providing random inputs [8], [22] to a code snippet, or by applying an SMT solver to the symbolic constraints of the code snippet [15], [18]. One can also adopt inter-procedural analysis to precisely model I/O samples, if the target code includes a function call [15], [18].

Third, the runtime behavior of a code snippet can directly express its semantics, as presented by traditional malware analysis [79]. By executing two target functions with the same execution environment, one can directly compare the executed instruction sequences [63] or visited CFG edges of the target functions [65]. For comparison, one may focus on specific behaviors observed during the execution [18], [28], [30], [31], [35], [66], [80]: the read/write values of stack and heap memory, return values from function calls, and invoked system/library function calls during the executions. Moreover, one can further check the call names, parameters, or call sequences for system calls [18], [33], [35], [62], [66].

The next category is to manually annotate the high-level semantics of a program or function. One may categorize library functions by their high-level functionality, such as whether the function manipulates strings or whether it handles heap memory [15], [18], [60]. Annotating cryptographic functions in a target code snippet [81] is also helpful because its complex operations hinders analyzing the symbolic constraints or behavior of the code [62].

The fifth category is extracting features from a program slice [82], because they can represent its data-flow semantics in an abstract form. Specifically, one can slice a program into a set of strands [14], [61]; a strand is a series of instructions within the same data-flow. Next, these strands can be canonicalized, normalized, or re-optimized for precise comparison [14], [61]. Additionally, one may hash strands for quick comparison [67] or extract symbolic constraints from the strands [58]. One may also extract features from a program dependence graph (PDG) [83], which is essentially a combination of a data-flow graph and CFG, to represent convoluted semantics of the target code, including its structural information [13].

Recovered program variables can also be semantic features. For example, one can compare the similarity of string literals referenced in code snippets [11], [12], [17], [23], [28], [60], [64]. One can also utilize the size of local variables, function parameters, or the return type of functions [11], [28], [60], [68]. One can further check registers or local variables that store the return values of functions [18].

Recently, several approaches have been utilizing embedding vectors, adopting various machine learning techniques. After building an attributed control-flow graph (ACFG) [23], which is a CFG containing numeric presemantic features in its basic blocks, one can apply spectral clustering [84] to group multiple ACFGs or popular encoding methods [85], [86], [87] to embed them into a vector [12]. The same technique can also be applied to PDGs [13]. Meanwhile, recent NLP techniques, such as Word2Vec [88] or convolutional neural network models [89], can be utilized for embedding raw bytes or assembly instructions into numeric vectors [19], [20], [21], [24], [25], [26], [27], [29]. For this embedding, one can also consider a higher-level granularity [20], [24] by applying other NLP techniques, such as sentence embedding [90] or paragraph embedding [91]. Note that one may apply machine learning to compare embedding vectors rather than generating them [59], [67], and Table 1 does *not* mark them to use embedded vectors.

2.1.3 Key Assumptions from the Past Research

During our literature study, we found that most of the approaches highly rely on semantic features extracted in (S3), assuming that they should not change across compilers nor target architectures. However, none of them clearly justifies the necessity of such complex semantics-based analyses. They focus only on the end results without considering the precise reasoning behind their approaches.

This is indeed the key motivation for our research. Although most existing approaches focus on complex analyses, there may exist elementary features that we have overlooked. For example, there may exist effective presemantic features, which can beat semantic features regardless of target architectures and compilers. It can be the case that those known features have not been thoroughly evaluated on the right benchmark as there has been no comprehensive study on it.

Furthermore, existing research assumes the correctness of the underlying binary analysis framework, such as IDA Pro [92], which is indeed the most popular tool used as shown in the rightmost column of Table 2. However, it is possible that CFGs derived from those tools may be inherently wrong. They may miss some important basic blocks, for instance, which can directly affect the precision of BCSA features.

Indeed, both (S1) and (S2) are challenging research problems per se: there are abundant research efforts to improve the precision of both analyses. For example, disassembling binary code itself is an undecidable problem [93], and writing an efficient and accurate binary lifter is significantly challenging in practice [94], [95]. Identifying functions from binaries [3], [4], [93], [96], [97], [98] and recovering control-flow edges [99] for indirect branches are still an active research field. All these observations lead us to research questions in §2.3.

2.2 Benchmarks Used in Prior Works

It is imperative to use the right benchmark to evaluate a BCSA technique. Therefore, we studied the benchmarks used in the past literature, as shown in Table 2. However, during the study, we established that it is difficult to properly evaluate a new BCSA technique using the previous benchmarks.

First, we could not find a single pair of papers that use the same benchmark. Some of them share packages such as GNU Coreutils [15], [30], [31], but the exact binaries, versions, and compiler options are not the same. Although there is no known standard for evaluating BCSA, it is surprising to observe that none of the papers uses the same dataset. We believe this is partly because of the difficulty in preparing the same benchmark. For example, even if we can download the same version of the source code used in a paper, it is extraordinarily difficult to cross-compile the program for various target architectures with varying compiler options; it requires significant effort to set up the environment. Note, however, *only two out of 39 papers we studied fully open their dataset*. Even in that case, it is hard to rebuild or extend the benchmark because of the absence of a public compilation script for the benchmark.

Second, the number of binaries used in each paper is limited and may not be enough for analytics. The *Source* column of Table 2 summarizes the number of benchmark programs obtained from each different source. Because a single package can contain multiple binaries, we manually extracted the packages used in each paper and counted the number of binaries in each package. We counted only the

TABLE 2: Summary of the dataset in the recent literature.

		Source*		Architecture*								Optimization*					Compiler†*													Extra				Info.		
Year	Tool [Paper]	Binaries	Firmware	x86	x64	arm	aarch64	mips	mips64	mipseb	mips64eb	O0	O1	O2	O3	Os	GCC 3	GCC 4	GCC 5	GCC 6	GCC 7	GCC 8	Clang 3	Clang 4	Clang 5	Clang 6	Clang 7	etc.	Total #	Noinline	PIE	LTO	Obfus.	Code	Dataset	IDA
2014	TEDEM [10]	14	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○
	Tracy [56]	(115)	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	○
	CoP [7]	(214)	·	·	·	·	·	·	·	·	·	○	○	○	○	○	·	1	·	·	·	·	·	·	·	·	·	1	2	·	·	·	○	·	·	○
	LoPD [8]	48	·	○	·	·	·	·	·	·	·	○	○	○	○	○	·	1	·	·	·	·	·	·	·	·	·	1	2	·	·	○	○	·	·	·
	BLEX [30]	1,140	·	·	○	·	·	·	·	·	·	○	○	○	○	·	·	1	·	·	·	·	1	·	·	·	·	1	3	·	·	·	·	·	·	○
	BinClone [57]	90	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	○
2015	Multi-k-MH [22]	60	6	○	·	○	·	○	·	·	·	○	○	○	○	·	·	2	·	·	·	·	1	·	·	·	·	·	3	·	·	·	·	·	·	○
2016	discovRE [11]	593	3	○	·	○	·	○	·	·	·	○	○	○	○	○	·	1	·	·	·	·	1	·	·	·	·	2	4	○	·	·	·	○	◑	○
	Genius [23]	(7,848)	8,128	○	·	○	·	○	·	·	·	○	○	○	○	·	·	2	·	·	·	·	1	·	·	·	·	·	3	·	·	·	·	·	·	○
	Esh [58]	(833)	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	3	·	·	·	·	2	·	·	·	·	2	7	·	·	·	·	○	○	○
	BinGo [15]	(5,143)	·	○	○	○	·	·	·	·	·	○	○	○	○	·	·	3	·	·	·	·	1	·	·	·	·	1	5	·	·	·	·	·	·	○
	MockingBird [33]	80	·	○	·	○	·	○	·	·	·	○	·	○	○	·	·	1	·	·	·	·	1	·	·	·	·	·	2	·	·	·	·	·	·	○
	Kam1n0 [32]	96	·	○	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	○
	BinDNN [59]	2,064	·	○	○	○	·	·	·	·	·	○	○	○	○	·	·	1	·	·	·	·	·	·	·	·	·	1	2	·	·	·	·	·	·	○
2017	BinSign [60]	(31)	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	2	2	·	·	·	○	·	·	○
	Xmatch [16]	72	1	○	·	·	·	○	·	·	·	·	·	·	·	·	·	2	·	·	·	·	1	·	·	·	·	·	3	○	·	·	·	·	·	○
	Gemini [12]	18,269	8,128	○	·	○	·	○	·	·	·	○	○	○	○	·	·	·	1	·	·	·	·	·	·	·	·	·	1	·	·	·	·	·	·	○
	GitZ [61]	44	·	·	○	·	○	·	·	·	·	○	○	○	○	○	·	3	·	·	·	·	2	1	·	·	·	·	6	·	·	·	·	·	·	·
	BinSim [62]	1062	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	○
	BinSequence [34]	(1,718)	·	·	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○
	IMF-sim [31]	1,140	·	·	○	·	·	·	·	·	·	○	·	○	○	·	·	1	·	·	·	·	1	·	·	·	·	1	3	·	·	·	○	·	·	·
	CACompare [35]	72	·	○	·	○	·	○	·	·	·	○	·	○	○	·	·	1	·	·	·	·	1	·	·	·	·	·	2	·	·	·	·	·	·	○
	ASE17 [63]	55	·	○	○	·	·	·	·	·	·	○	·	○	○	·	·	1	·	·	·	·	1	·	·	·	·	·	2	·	·	·	○	·	·	·
2018	BinArm [17]	·	2,628	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○
	SANER18 [64]	7	·	○	○	·	·	·	·	·	·	·	·	·	·	·	·	1	1	1	·	·	1	·	·	·	·	1	5	·	·	·	·	·	·	○
	BinGo-E [18]	(5,145)	·	○	○	○	·	·	·	·	·	○	○	○	○	·	·	3	·	·	·	·	1	·	·	·	·	1	5	·	·	·	·	·	·	○
	WSB [65]	(173)	·	·	·	·	·	·	·	·	·	·	○	○	○	·	·	1	·	·	·	·	1	·	·	·	·	·	2	·	·	·	○	·	·	·
	BinMatch [66]	80	·	○	·	·	·	·	·	·	·	○	·	○	○	·	·	1	·	·	·	·	1	·	·	·	·	·	2	·	·	·	○	·	·	○
	MASES18 [25]	47	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○	·	·	·
	Zeek [67]	(20,680)	·	○	·	○	○	·	·	·	·	○	○	○	○	○	·	3	·	·	·	·	4	1	·	·	·	2	10	·	·	·	·	·	·	·
	FirmUp [14]	·	2,000	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○
	αDiff [19]	(69,989)	2	○	○	○	·	·	·	·	·	○	○	○	○	·	·	2	1	·	·	·	2	·	·	·	·	·	5	·	·	·	·	◑	◑	○
	VulSeeker [13]	(10,512)	4,643	○	○	○	○	○	○	·	·	○	○	○	○	·	·	1	1	·	·	·	·	·	·	·	·	·	2	·	·	·	·	○	·	○
2019	InnerEye [24]	(844)	·	·	○	○	·	·	·	·	·	·	○	○	○	·	·	·	·	·	·	·	·	·	·	1	·	·	1	·	·	·	·	◑	◑	·
	Asm2Vec [20]	68	·	·	○	·	·	·	·	·	·	○	○	○	○	·	·	1	1	·	·	·	2	·	·	·	·	·	4	·	·	·	○	○	·	○
	SAFE [21]	(5001)	·	·	○	○	·	·	·	·	·	○	○	○	○	·	1	3	1	1	1	·	2	1	1	1	·	·	12	·	·	·	·	○	◑	○
	BAR19i [26]	(804)	·	·	○	○	·	·	·	·	·	·	○	○	○	·	·	·	·	·	·	·	·	·	·	1	·	·	1	·	·	·	·	○	·	·
	BAR19ii [29]	(11244)	·	○	○	○	·	·	·	·	·	○	○	○	○	·	1	3	1	·	·	·	2	1	1	·	·	2	11	·	·	·	·	·	·	·
	FuncNet [68]	(180)	·	○	·	○	·	○	·	·	·	○	○	○	○	○	·	·	·	1	·	·	·	·	·	·	·	·	1	·	·	·	·	·	·	○
2020	DeepBinDiff [27]	2114	·	·	·	·	·	·	·	·	·	○	○	○	○	·	·	1	·	·	·	·	·	·	·	·	·	·	1	·	·	·	·	○	○	○
	ImOpt [69]	18	·	·	○	·	·	·	·	·	·	○	·	○	○	·	·	·	1	·	·	·	·	·	·	·	·	·	1	·	·	·	○	·	·	·
	ACCESS20 [52]	12,000	·	○	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·
	Patchecko [28]	2,108	2	○	○	○	○	·	·	·	·	○	○	○	○	○	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	·	○
	BinKit ★	243,128	·	○	○	○	○	○	○	○	○	○	○	○	○	○	·	1	1	1	1	1	·	1	1	1	1	·	9	○	○	○	○	○	○	○

* We did not mark items which have no ground truth from the paper and we use parentheses to mark over-approximated numbers.
† We focus on two major compilers: GCC and Clang for this table because other compilers can only target few architectures.
◑ This mark in the *Code* and *Dataset* columns indicates that only a part of them is available. For example, discovRE [11] discloses only their firmware images, and αDiff [19] opens transformed function images, but not the actual dataset.

binaries after a successful compilation, such that the object files that were generated during the compilation process were not counted. For the package versions that we could not obtain from the papers, we used the recent package versions and marked them with parentheses. Note that only 4 out of 39 papers have more than 10,000 binaries, and none reaches 100,000 binaries. Such a few binaries may not be sufficient to evaluate the proposed systems considering the numerous possible combinations of options. Firmware may include numerous binaries, but it cannot be directly used for BCSA because it does not have ground truth (see §3).

Finally, previous benchmarks only cover a few compilers, compiler options, and target architectures. Some papers do not even describe their tested compiler options or package versions. The *Compiler* column of the table presents the number of minor versions used for each major version of the compilers. Notably, all the benchmarks except one consider less than five different major compiler versions. The *Extra* column of the table shows the use of extra compiler options for each benchmark. Here, only a few of them consider function inlining and LTO. None of them deals with the PIE option, although, currently, it is widely used [100].

All these observations lead us to the research questions presented in the next subsection (§2.3) and eventually motivate us to create our own benchmark that we call BinKit, as shown in the last row of Table 2. We detail BinKit in §3.

2.3 Research Problems and Questions

We now summarize several key problems observed from the previous literature and address research questions. First, most papers use manually chosen ground truth data for their evaluation, which are easily error-prone. Second, none of the papers use the same benchmark for their evaluation, and the manner in which they evaluate their techniques differs significantly. Finally, only a few of the studies release their source code and data, which makes it radically difficult to reproduce or improve upon existing works. Furthermore, current state-of-the-art approaches in BCSA focus on extracting semantic features using complex analysis techniques (from §2.1.1 and §2.1.2). These observations naturally result in the research questions that we describe below, which will be discussed thoroughly in the rest of this paper. Note that some of the questions are indeed open-ended, and we only address them in part.

RQ1. How should we establish ground truth data?

To evaluate a BCSA algorithm on a benchmark, one needs to know which code snippets in the benchmark are the same. For a given function of a specific version of a program, suppose finding the semantically equivalent functions in other versions of the program. This is indeed a common problem setup for BCSA [13], [16], [19], [23]. In this case, knowing the ground truth of the function's equivalence is not evident, as two functions of the same name may have different semantics because they are from two distinct versions. Some researchers try to match a vulnerable function in a set of real-world binaries, e.g., firmware images [12], [13], [14], [17], [23]. However, this requires significant manual effort to set up the ground truth because we typically do not have source code for firmware images, and detected functions from BCSA are not guaranteed to be vulnerable unless they are manually verified. One may obtain the source code of commonly-used libraries for the Linux-based firmware. However, this cannot also guarantee the ground truth because actual binaries in firmware images may differ from the source code. In this paper, we address this challenge by presenting a script that can automatically build large-scale ground truth data from a given set of source packages (§3).

RQ2. Is the effectiveness of presemantic features limited to the target architectures and compiler options used?

We note that most previous studies assume that presemantic features are significantly less effective than semantic features as they can largely vary depending on the underlying architectures and compiler optimizations used. For example, compilers may perform target-specific optimization techniques for a specific architecture. Indeed, 32 out of the 39 papers ($\approx 82\%$) we studied focus on new semantic features in their analysis, as shown in Table 1. To determine whether this assumption is valid, we investigate it through a series of rigorous experimental studies. Although byte-level information significantly varies depending on the target and the optimization techniques, we found that some presemantic features, such as structural information obtained from CFGs, are broadly similar across different binaries of the same program. Additionally, we demonstrated that utilizing such presemantic features without a complex semantic analysis can achieve an accuracy that is comparable to that of recent deep learning-based approach with a semantic analysis (§5).

RQ3. Can debugging information help BCSA achieve a high accuracy rate?

We are not aware of any quantitative study on how much debugging information affects the accuracy of BCSA. Most prior works simply assume that debugging information is not available, but how much does it help? How would decompilation techniques affect the accuracy of BCSA? To answer this question, we extracted a list of function types from our benchmark and used them to perform BCSA on our dataset. Surprisingly, we were able to achieve a higher accuracy rate than any other existing works on BCSA without using any sophisticated method (§6).

RQ4. Can we benefit from analyzing failure cases of BCSA?

Most existing works do not analyze their failure cases as they rely on uninterpretable machine learning techniques. However, our goal is to use a simple and interpretable model to learn from failure and gain insights for future research. Therefore, we manually examined failure cases using our interpretable method, and observed three common causes for failure, which have been mostly overlooked by the previous literature. First, COTS binary analysis tools indeed return false results. Second, different compiler backends for the same architecture can be substantially different from each other. Third, there are architecture-specific code snippets for the same function. We believe that all these observations help in setting directions for future studies (§7).

3 Large-Scale BCSA Benchmark (RQ1)

Building a large-scale benchmark for BCSA and establishing its ground truth is not straightforward. One potential approach for generating the ground truth data involves manually identifying similar functions from existing binaries or firmware images [10], [56], [58]. However, this requires domain expertise of precisely analyzing raw binaries and firmware, which are often error-prone and time-consuming.

Another approach for obtaining the ground truth is to compile binaries from existing source code by changing compiler options and target architectures [13], [15], [16], [23]. Because the compiled binaries share the same source code, one can easily determine which functions in the binaries are from which source lines. Unfortunately, most existing works do not open their benchmarks nor compilation scripts used to produce them (Table 2). This trend makes it fundamentally difficult to reproduce or extend previous benchmarks with additional compiler options or target architectures.

Therefore, we present BinKit, which is a comprehensive benchmark for BCSA, along with automated compilation scripts that help reproduce and extend it for various research purposes. The rest of this section details BinKit and discusses how we establish the ground truth (RQ1).

3.1 BinKit

BinKit is a comprehensive BCSA benchmark that comprises 243,128 binaries compiled from 51 package source code with 1,352 distinct combinations of compilers, compilation options and compilation targets. Therefore, BinKit is a superset of the benchmarks used in existing approaches as shown in Table 2. BinKit includes binaries compiled for 8 different architectures. For example, we use both little- and big-endian binaries for MIPS to investigate the effect of endianness. It uses 9 different versions of compilers: GCC v{4.9.4, 5.5.0, 6.4.0, 7.3.0, 8.2.0} and Clang v{4.0, 5.0, 6.0, 7.0}. We also consider 5 optimization levels from `O0` to `O3` as well as `Os`, which is the code size optimization. Finally, we take PIE, LTO, and obfuscation options into account, which are less explored in BCSA.

We select GNU software packages [101] as our compilation target because of their popularity and accessibility: they are realistic applications that are used widely in Linux systems, and their source code is publicly available. We successfully compiled 51 packages for all our target architectures and compiler options.

To better support targeted comparisons, we divide BinKit into six datasets: Normal, SizeOpt, NoInline, Pie, Lto, and Obfuscation. The summary of each dataset is shown in Table 3. Each dataset contains binaries obtained

TABLE 3: Summary of BINKIT.

	Name	# of Pkgs	# of Binaries	# of Archs	# of Opts	# of Comps	# of Options	# of Functions
BINKIT	NORMAL	51	67,680	8	4	9	288	18,783,986
	SIZEOPT	51	16,920	8	1	9	72	4,425,792
	PIE	46	36,000	8	4	9	288	14,482,863
	NOINLINE	51	67,680	8	4	9	288	22,762,434
	LTO	29	24,768	8	4	9	288	5,966,790
	OBFUSCATION	51	30,080	8	4	4	128	8,808,708
	Total	51	243,128	8	5	13	1,352	75,230,573

by compiling the GNU packages with different combinations of compiler options and targets. There is *no* intersection among the datasets.

NORMAL includes binaries compiled for 8 different architectures with different compilers and optimization levels. We did not use other extra options such as PIE, LTO, and no-inline for this dataset.

SIZEOPT is the same as NORMAL except that it uses only the `Os` optimization option instead of `O0`–`O3`.

Similarly, PIE, NOINLINE, LTO, OBFUSCATION are no different from NORMAL except that they are generated by using an additional flag to enable PIE, to disable inline optimization, to enable Link-Time Optimization (LTO), and to enable compile-time obfuscation, respectively.

PIE makes memory references in binary relative in order to support ASLR. On some architectures, e.g., x86, compilers inject additional code snippets to achieve relative addressing. As a result, the compiled output can differ severely. Although PIE became the default on most Linux systems [100], it has not been well studied for BCSA. Note we were not able to compile all the 51 packages with the PIE option enabled. Therefore, we have fewer binaries in PIE than NORMAL.

Function inlining embeds callee functions into the body of the caller. This makes presemantic features largely vary. Therefore, we investigate the effect of function inlining on BCSA by explicitly turning off the inline optimization with the `fno-inline` option.

LTO is an optimization technique that operates at link time. It removes unnecessary code blocks, thereby reducing the number of presemantic features. However, it also has been less studied in BCSA. We were only able to successfully compile 29 packages when the LTO option is enabled.

Finally, the OBFUSCATION dataset uses Obfuscator-LLVM [102] to obfuscate the target binaries. We chose Obfuscator-LLVM from among various other tools previously used [102], [103], [104], [105], [106], [107] because it is the most commonly used [20], [31], [60], [66], [69], and we can directly compare the effect of obfuscation using the vanilla LLVM compiler. We use Obfuscator-LLVM's latest version with four obfuscation options: instruction substitution (SUB), bogus control flow (BCF), control flow flattening (FLA), and a combination of all the options. We regard each option as a distinct compiler, as shown in the *Comp* column of Table 3. One can obfuscate a single binary multiple times. However, we only applied it once. This is because obfuscating a binary multiple times could emit a significantly large binary, which becomes time-consuming for IDA Pro to preprocess it. For example, when we obfuscate `a2ps` twice with all three options, the compiled binary reaches over 30 MB, which is 30 times larger than the normal one.

The numbers of binaries and options are different for each dataset because some packages only compile with a specific set of compile options and targets. Some packages fail to compile because they have architecture-specific code, such as inline assemblies, or because they use compiler-specific grammars. For example, Clang does not support both the Link Time Optimization (LTO) option and the `Os` option to be turned on. There are also cases where packages have conflicting dependencies. We also excluded the ones that did not compile within 30 min because some packages require a considerable amount of time to compile. For instance, `smalltalk` took more than 10 h to compile with the obfuscation option enabled.

To summarize, BINKIT contains 243,128 binaries and 75,230,573 functions in total, which is indeed many orders of magnitude larger than the other benchmarks that appear in the previous literature. The *Source* column of Table 2 shows the difference clearly. BINKIT does not include firmware images because our goal is to automatically build a benchmark with the clear ground truth. One may extend our benchmark with firmware images. However, it would take significant manual effort to identify their ground truth. For additional details regarding each package, refer to Table 7 in the Appendix.

Our benchmark and compilation scripts are available on GitHub. Our compilation environment is based on Crosstool-NG [108], GNU Autoconf [109], and Linux Parallels [110]. Through this environment, we compiled the entire datasets of BINKIT in approximately 30 h on our server machine with 144 Intel Xeon E7-8867v4 cores.

3.2 Building Ground Truth

To build the ground truth, we performed the following steps. We first compiled all the binaries with debugging symbols. We then leveraged IDA Pro [92] to identify functions in the compiled binaries. Of course, IDA might have missed some functions [93]; hence, we only considered the identified ones. Next, we labeled each identified function with the corresponding package names, file names, and line numbers obtained from the debugging information. We only considered functions in `code` segments. For example, we disregarded functions in Procedure Linkage Table sections because they do not include function bodies. We also found that approximately 5% of the identified functions from IDA Pro did not have any corresponding source lines. Such functions are mostly created during compile time by the compiler. We disregarded them when counting functions. The last column of Table 3 reports the counting results.

4 BUILDING AN INTERPRETABLE MODEL

Previous BCSA techniques focused on achieving a higher accuracy by leveraging recent advances in deep learning techniques [12], [13], [19], [25]. This often requires building a complicated model, which is not straightforward to understand and hinders researchers from reasoning about the BCSA results and further answering the fundamental questions regarding BCSA. Therefore, we design an *interpretable* model for BCSA to answer the research questions and implement TIKNIB, which is a BCSA tool that employs the model. This section illustrates how we obtain such a model and how we set up our experimental environment.

4.1 TIKNIB Overview

At a high level, TIKNIB leverages a set of presemantic features widely used in the previous literature to reassess the effectiveness of presemantic features (RQ2). It evaluates each feature based on our similarity scoring metric (§4.3), which directly measures the difference between each feature value. In other words, it captures how much each feature differs across different compile options.

We do not here claim that TIKNIB is the best approach for addressing BCSA problems. However, we intentionally design a simple and interpretable model to answer the research questions presented in §2.3. Despite the simplicity of our approach, TIKNIB still produces a high accuracy rate that is comparable to state-of-the-art tools (§5.2).

TIKNIB focuses on function-level similarity analyses because functions are a fundamental unit of binary analysis. In other words, we extract features from each function to measure the similarity. Indeed, function-level BCSA is mostly widely used in the previous literature [11], [16], [19], [21], [24], [30], [31], [32]. However, it is straightforward enough to extend our scope to binary-level analyses similarly to the previous papers [7], [8].

4.2 Features Used in TIKNIB

From the RQ2, one of our goals is to reconsider the capability of presemantic features. Therefore, we focus on choosing various presemantic features used in the previous BCSA literature instead of inventing novel ones.

However, creating a comprehensive feature set is not straightforward because of two main reasons. First, there are numerous existing features, which are similar to one another, as discussed in §2. Second, some features require domain-specific knowledge, which is *not* publicly available. For example, several existing papers [11], [12], [13], [17], [18], [23], [60], [64] categorize instructions into semantic groups. However, grouping instructions is largely a subjective task, and there is no known standard for it. Furthermore, most existing works do not make their grouping algorithms public.

We address these challenges by (1) manually extracting representative presemantic features and (2) open-sourcing our feature extraction implementation. Specifically, we focus on numeric presemantic features. Because these features are represented as a number, the relationship among their values across different compile options can be easily observed.

Table 4 summarizes the selected features. Our feature set consists of CFG- and CG-level numeric features as they can effectively reveal structural changes in the target code. In particular, we extract features related to basic blocks, CFG edges, natural loops, and strongly connected components (SCCs) from CFGs. We also categorize instructions into several semantic groups based on our careful judgment by referring to the reference manuals [111], [112], [113] and leveraging Capstone [114]'s internal grouping. Next, we count the number of instructions in each semantic group per each function (i.e., CFG). Additionally, we extract six features from CGs. The number of callers and callees represents a unique number of outgoing and incoming edges from CGs, respectively. For extracting features, we leveraged IDA Pro [92], NetworkX [115], and Capstone [114].

TABLE 4: Numeric presemantic features used in TIKNIB.

Category	Features	Count
CFG	# of basic blocks, edges, loops, SCCs, and back edges # of all, arith, data transfer, cmp, and logic instrs. # of shift, bit-manipulating, float, misc instrs. # of arith + shift, and data transfer + misc instrs. # of all/unconditional/conditional control transfer instrs. Avg. # of edges per a basic block Avg./Sum of basic block, loop, and SCC sizes Avg. # of all, arith, data transfer, cmp, and logic instrs. Avg. # of shift, bit-manipulating, float, misc instrs. Avg. # of arith + shift, and data transfer + misc instrs. Avg. # of all/unconditional/conditional control transfer instrs.	41
CG	# of callers, callees, imported callees # of incoming/outgoing/imported calls	6
	Total	47

4.3 Scoring Metric

Our scoring metric is based on the computation of the relative difference [116] between feature values. Given two functions A and B, let us denote a value of feature f for each function as A_f and B_f, respectively. Recall that any feature in TIKNIB can be represented as a number. We can compute the relative difference δ of the two feature values, as follows:

$$\delta(A_f, B_f) = \frac{|A_f - B_f|}{|\max(A_f, B_f)|} \tag{1}$$

Let us suppose we have N distinct features $(f_1, f_2, \cdots, f_N)$ in our feature set. We can then define our similarity score s between two functions A and B by taking the average of relative differences for all the features, as follows:

$$s(A, B) = 1 - \frac{\left(\delta(A_{f_1}, B_{f_1}) + \cdots + \delta(A_{f_N}, B_{f_N})\right)}{N} \tag{2}$$

Although each numeric feature can have a different range of values, TIKNIB can effectively handle them using relative differences by representing the difference of each feature with a value between 0 and 1. Therefore, the score s is always within the range of 0 to 1.

Furthermore, we can intuitively understand and interpret the BCSA results using our scoring metric. For example, suppose there are two functions A and B derived from the same source code with and without compiler option X, respectively. If the relative difference of the feature value f between the two functions is small, it implies that f is a robust feature against compiler option X.

In this paper, we focus only on simple relative difference, rather than exploring complex relationships among the features for interpretability. However, we believe that our approach could be a stepping-stone toward fabricating more improved interpretable models to understand such complex relationships.

4.4 Feature Selection

Based on our scoring metric, we perform lightweight preprocessing to select useful features for BCSA as some features may not help in making a distinction between functions. To measure the quality of a given feature set, we compute the area under the receiver operating characteristic (ROC) curve (i.e., the AUC) of generated models.

Suppose we are given a dataset in BINKIT, which is generated from source code containing N unique functions. In total, we have maximum $N \cdot M$ functions in our dataset, where M is the number of combinations of compiler options used to generate the dataset. The actual number of functions can be less than $N \cdot M$ due to function inlining. For each unique function λ, we randomly select two other functions with the following conditions. (1) A true positive (TP) function, λ^{TP}, is generated from the same source code as in λ, with different compiler options, and (2) a true negative (TN) function, λ^{TN}, is generated from source code that is different from the one used to generate λ, with the same compiler options as for λ^{TP}. We generate such pairs for each unique function, thereby acquiring around $2 \cdot N$ function pairs. We then compute the similarity scores for the functions in each pair and their AUC. The same methodology has been used in several previous works [12], [13].

Unfortunately, there is no efficient algorithm for selecting an optimal feature subset to use; it is indeed a well-known NP-hard problem [117]. Therefore, we leverage a hill climbing approach to greedily select features to use [118]. Starting from an empty set $\mathbb{F}$, we determine whether we can add a feature to $\mathbb{F}$ to increase its AUC. For every possible feature, we make a union with $\mathbb{F}$ and compute the corresponding AUC. We then select one that maximizes the AUC, and update $\mathbb{F}$ to include the selected feature. We repeat this process until the AUC does not increase further by adding a new feature. Although our approach does not guarantee finding an optimal solution, it still provides empirically meaningful results, as we describe in the following sections.

4.5 Experimental Setup

For all experiments in this study, we perform 10-fold cross validation on each test. When splitting a test dataset, we ensure functions of the same name are either in a training or testing set, but not in both. For each fold, during the learning phase, i.e., the feature selection phase, we select up to two million functions from a training set, which is around 10% of the largest dataset in BINKIT. In the validation phase, however, we test all the functions in a testing set without any sampling. Thus, after 10-fold validation, all the functions in the target dataset are tested at least once.

We ran all our experiments on a server equipped with four Intel Xeon E7-8867v4 2.40 GHz CPUs (total 144 cores), 896 GB DDR4 RAM, and 4 TB SSD. We setup Ubuntu 16.04 with IDA Pro v6.95 [92] and MongoDB [119] on the server. For feature selection and similarity comparison, we utilized Python scikit-learn [120] and SciPy [121].

5 PRESEMANTIC FEATURE ANALYSIS (RQ2)

We now present our experimental results using TIKNIB on the presemantic features (§4.2) to answer RQ2 (§2.3). With our comprehensive analysis on these features, we obtained several useful insights for future research. In this section, we discuss our findings and lessons learned.

5.1 Analysis Result

To analyze the effect of various compiler options and target architectures on BCSA, we conducted a total of 72 tests using TIKNIB. Table 5 describes the experimental results where each column corresponds to a test we performed. For additional results, refer to Table 8 in the Appendix. Note that we present only 26 out of 72 tests because of the space limit. Unless otherwise specified, all the tests were performed on the NORMAL dataset. As described in §4.4, we prepared 10-fold sets for each test. We divided the tests into seven groups according to their purposes as shown in the top row of the table. For example, the *Arch* group contains a set of tests to evaluate each feature against varying target architecture.

We also chose function pairs for each test based on the testing goal. For instance, we test the influence of varying the target architecture from x86 to ARM (*x86 vs. ARM* column of Table 5). For each function λ in the x86 binaries of our dataset, we select both λ^{TP} and λ^{TN} from the ARM binaries compiled with the same compiler option as in λ. In other words, we fix all the other options, except for the target architecture for choosing λ^{TP} and λ^{TN}, to focus on our testing goal. The same rule applies to other columns. For the *Rand.* columns, we alter all the compiler options in the group randomly to generate function pairs.

Each cell in the *Feature* row of Table 5 represents the average of $\delta(\lambda_f, \lambda_f^{\mathrm{TN}}) - \delta(\lambda_f, \lambda_f^{\mathrm{TP}})$ for feature f, which we call *TP-TN gap* of f. This TP-TN gap measures the similarity between λ^{TP} and λ, as well as the difference between λ^{TN} and λ, in terms of the target feature. Thus, when the gap of a feature is larger, its discriminative capability for BCSA is higher. As we conduct 10-fold validation for each test, we highlight the cells with gray when the corresponding feature is chosen in all the ten trials. Such features show relatively higher TP-TN gaps than the others do in each test. We summarize our observations as follows.

5.1.1 *Optimization is largely influential*

Many researchers have focused on designing a model for *cross-architecture* BCSA [11], [15], [18], [22], [33]. However, our experimental results show that architecture may not be the most critical factor for BCSA. Instead, optimization level was the most influential factor in terms of relative difference between presemantic features. In particular, we measured the average TP-TN gap of all the presemantic features for each test (*Avg. of TP-TN Gap* row of the table) and found that the average gap of the `O0` vs. `O3` test (0.26) is less than that of the x86 vs. ARM test (0.39) and the x86 vs. MIPS test (0.33). Furthermore, the optimization level random test (*Rand.* column of the *Opt Level* group) shows the lowest AUC (0.95) compared to that of the architecture and compiler group (0.98). These results confirm that compilers can produce largely distinct binaries depending on the optimization techniques used; hence, the variation among the binaries due to the optimization is considerably greater than that due to the target architecture on our dataset.

5.1.2 *Compiler version has a small impact*

Approximately one third of the previous benchmarks shown in Table 2 employ multiple versions of the same compiler. However, we found that even the major versions of the same compiler produce similar binaries. In other words, compiler versions do not heavily affect presemantic features. Although Table 5 does not include all the tests we performed because of the space constraints, it is apparent from the *Compiler* column that the two tests between two different versions of the same compiler, i.e., GCC v4 vs. GCC v8 and Clang v4 vs. Clang v7, have much higher TP-TN gaps than other tests, and their AUCs are close to 1.0.

TABLE 5: In-depth analysis result with BINKIT.

Feature		Opt Level			Compiler				Arch						vs. SizeOpt†			vs. Extra†			vs. Obfus.†				Bad‡	
	Rand.	O0 vs. O3	O2 vs. O3	Rand.	GCC v4 vs. GCC v8	Clang v4 vs. Clang v7	GCC vs. Clang	Rand.	x86 vs. ARM	x86 vs. MIPS	ARM vs. MIPS	32 vs. 64	LE vs. BE	Rand.	O0 vs. Os	O1 vs. Os	O3 vs. Os	PIE	NoInline	LTO	BCF	FLA	SUB	All	Norm.	Norm. vs. Obfus.†
CFG Avg. # of edges	0.33	0.26	0.42	0.34	0.44	0.46	0.37	0.41	0.43	0.37	0.37	0.43	0.47	0.41	0.34	0.42	0.36	0.45	0.44	0.40	0.26	0.34	0.47	0.22	0.32	0.19
CFG # of backedges	0.39	0.33	0.44	0.39	0.46	0.45	0.41	0.43	0.47	0.45	0.45	0.46	0.48	0.46	0.39	0.42	0.38	0.50	0.40	0.46	0.23	0.08	0.47	0.05	0.32	0.03
CFG # of edges	0.47	0.37	0.63	0.48	0.66	0.69	0.52	0.60	0.65	0.57	0.57	0.65	0.72	0.61	0.46	0.59	0.52	0.71	0.61	0.64	0.25	0.23	0.72	0.10	0.42	0.06
CFG # of loops	0.40	0.34	0.44	0.40	0.46	0.46	0.41	0.44	0.47	0.45	0.45	0.46	0.47	0.46	0.40	0.42	0.39	0.50	0.40	0.46	0.23	0.13	0.47	0.10	0.33	0.08
CFG # of basic blocks	0.41	0.36	0.59	0.46	0.62	0.65	0.48	0.56	0.44	0.55	0.39	0.62	0.69	0.52	0.43	0.56	0.50	0.67	0.57	0.60	0.26	0.23	0.67	0.10	0.26	0.00
CG # of callees	0.50	0.43	0.59	0.52	0.62	0.63	0.52	0.58	0.63	0.54	0.55	0.57	0.64	0.57	0.50	0.59	0.53	0.60	0.57	0.57	0.60	0.59	0.64	0.56	0.46	0.47
CG # of callers	0.45	0.40	0.54	0.48	0.59	0.58	0.49	0.54	0.53	0.41	0.45	0.54	0.60	0.50	0.50	0.57	0.50	0.56	0.54	0.52	0.54	0.54	0.58	0.52	0.37	0.41
CG # of imported callees	0.44	0.39	0.54	0.47	0.58	0.56	0.48	0.52	0.59	0.44	0.45	0.55	0.55	0.50	0.46	0.53	0.48	0.55	0.50	0.52	0.53	0.53	0.56	0.50	0.36	0.43
CG # of imported calls	0.45	0.38	0.56	0.48	0.60	0.58	0.48	0.54	0.61	0.45	0.47	0.57	0.57	0.52	0.46	0.54	0.48	0.57	0.52	0.54	0.49	0.54	0.59	0.46	0.37	0.40
CG # of incoming calls	0.46	0.41	0.56	0.50	0.61	0.60	0.50	0.56	0.55	0.42	0.46	0.56	0.62	0.52	0.52	0.58	0.50	0.58	0.57	0.55	0.50	0.56	0.60	0.47	0.37	0.38
CG # of outgoing calls	0.52	0.44	0.62	0.54	0.66	0.66	0.54	0.60	0.67	0.57	0.58	0.61	0.68	0.60	0.52	0.61	0.55	0.64	0.60	0.61	0.53	0.62	0.67	0.50	0.48	0.44
Inst Avg. # of arith+shift	0.17	0.16	0.51	0.30	0.50	0.50	0.27	0.39	0.21	0.08	0.10	0.29	0.52	0.21	0.19	0.43	0.41	0.49	0.50	0.43	0.28	0.22	0.46	0.17	0.07	0.12
Inst Avg. # of ctransfer	0.17	0.15	0.28	0.20	0.28	0.30	0.20	0.25	0.26	0.19	0.21	0.25	0.32	0.22	0.19	0.24	0.22	0.30	0.27	0.27	0.19	0.18	0.31	0.12	0.12	0.07
Inst Avg. # of dtransfer+misc	0.17	0.08	0.44	0.22	0.42	0.46	0.27	0.36	0.30	0.15	0.17	0.31	0.49	0.25	0.09	0.36	0.35	0.45	0.44	0.36	0.28	0.26	0.45	0.17	0.12	0.08
Inst Avg. # of dtransfer	0.19	0.10	0.45	0.23	0.43	0.48	0.28	0.37	0.30	0.20	0.22	0.32	0.53	0.28	0.11	0.38	0.36	0.46	0.46	0.38	0.28	0.27	0.47	0.18	0.10	0.08
Inst Avg. # of instrs.	0.17	0.11	0.38	0.21	0.37	0.41	0.25	0.33	0.30	0.15	0.15	0.28	0.45	0.24	0.12	0.32	0.31	0.40	0.38	0.33	0.26	0.25	0.37	0.17	0.14	0.10
Inst Avg. # of logic	0.24	0.23	0.51	0.34	0.45	0.56	0.27	0.39	0.22	0.21	0.25	0.40	0.54	0.31	0.25	0.40	0.42	0.56	0.48	0.54	0.23	0.22	0.40	0.12	0.24	0.05
Inst # of arith+shift	0.24	0.26	0.59	0.40	0.59	0.60	0.38	0.49	0.28	0.11	0.12	0.37	0.61	0.27	0.28	0.52	0.48	0.58	0.56	0.53	0.26	0.41	0.55	0.14	0.13	0.02
Inst # of ctransfer	0.42	0.35	0.56	0.43	0.57	0.62	0.43	0.51	0.57	0.51	0.54	0.56	0.64	0.54	0.38	0.51	0.46	0.62	0.54	0.57	0.25	0.23	0.64	0.10	0.32	0.03
Inst # of dtransfer+misc	0.27	0.15	0.58	0.30	0.58	0.60	0.43	0.51	0.46	0.26	0.29	0.46	0.63	0.38	0.11	0.52	0.47	0.60	0.57	0.51	0.28	0.22	0.59	0.09	0.25	0.01
Inst # of arith	0.24	0.26	0.59	0.39	0.59	0.60	0.38	0.49	0.27	0.12	0.13	0.38	0.61	0.27	0.28	0.52	0.48	0.57	0.57	0.53	0.25	0.41	0.55	0.14	0.12	0.01
Inst # of bit-manipulating	0.09	0.12	0.34	0.21	0.31	0.23	0.18	0.24	0.07	0.04	0.06	0.22	0.20	0.10	0.14	0.31	0.28	0.36	0.32	0.34	0.17	0.16	0.20	0.05	0.05	0.01
Inst # of compare	0.47	0.42	0.62	0.53	0.67	0.68	0.55	0.62	0.39	0.58	0.32	0.61	0.72	0.55	0.54	0.61	0.52	0.71	0.60	0.64	0.23	0.25	0.68	0.09	0.40	0.06
Inst # of cond ctransfer	0.53	0.42	0.62	0.54	0.67	0.70	0.58	0.63	0.67	0.65	0.65	0.68	0.72	0.66	0.55	0.62	0.51	0.72	0.60	0.65	0.23	0.23	0.71	0.10	0.42	0.06
Inst # of dtransfer	0.28	0.16	0.58	0.31	0.58	0.60	0.43	0.51	0.45	0.29	0.35	0.46	0.63	0.41	0.13	0.53	0.48	0.60	0.57	0.52	0.31	0.22	0.59	0.09	0.23	0.03
Inst # of float instrs.	0.09	0.09	0.27	0.16	0.16	0.28	0.12	0.17	0.09	0.10	0.08	0.17	0.32	0.11	0.09	0.22	0.23	0.27	0.23	0.17	0.24	0.12	0.30	0.08	0.00	0.00
Inst # instrs.	0.31	0.21	0.57	0.34	0.58	0.60	0.45	0.52	0.52	0.29	0.30	0.48	0.62	0.42	0.18	0.52	0.47	0.60	0.55	0.52	0.26	0.22	0.56	0.08	0.30	0.02
Inst # of misc	0.10	0.04	0.47	0.17	0.40	0.46	0.20	0.32	0.06	0.11	0.02	0.36	0.67	0.19	0.04	0.29	0.27	0.47	0.44	0.37	0.16	0.19	0.49	0.09	0.00	0.00
Inst # of shift	0.22	0.23	0.42	0.30	0.42	0.39	0.27	0.34	0.22	0.20	0.19	0.31	0.54	0.26	0.24	0.35	0.34	0.48	0.37	0.41	0.40	0.34	0.42	0.31	0.19	0.23
Avg. TP-TN Gap	0.31	0.26	0.49	0.35	0.49	0.51	0.36	0.43	0.39	0.33	0.32	0.43	0.54	0.38	0.30	0.44	0.40	0.52	0.47	0.47	0.28	0.26	0.50	0.17	0.24	0.11
Avg. of Grey	0.43	0.34	0.42	0.48	0.57	0.59	0.49	0.50	0.55	0.44	0.49	0.57	0.61	0.52	0.46	0.56	0.45	0.55	0.57	0.51	0.44	0.47	0.55	0.41	0.33	0.33
ROC AUC	0.94	0.90	0.97	0.95	0.99	1.00	0.96	0.98	0.99	0.98	0.98	0.99	1.00	0.98	0.96	0.98	0.95	1.00	0.97	0.98	0.98	0.98	1.00	0.95	0.91	0.91
Std. of ROC AUC	0.01	0.01	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.01

† We compare a function from the NORMAL to the function in each corresponding target dataset.
‡ We match functions whose compiler options are largely distant to test bad cases. Please see §5.1.8 for the details.

5.1.3 GCC and Clang have diverse characteristics

Conversely, the GCC vs. Clang test resulted in the lowest TP-TN gap and AUC among the tests in the *Compiler* group. This can be because each compiler employs a different backend, thereby producing different binaries. Another potential problem is that the techniques inside each optimization level can vary depending on the compiler. We detail this in §7.2.

5.1.4 ARM binaries are closer to x86 binaries than MIPS

The tests in the *Arch* group measure the influence of target architectures with the NORMAL dataset. Overall, the target architecture did not have much of an effect on the accuracy rate. The AUCs were over 0.98 in all the cases. Surprisingly, the x86 vs. ARM test had the highest AUC (0.99), indicating that the presemantic features of the x86 and ARM binaries are similar to each other, despite being distinct architectures. However, the ARM vs. MIPS test showed the lowest TP-TN gap although both of them are RISC architectures. Additionally, the effect of the word size and endianness was relatively small. Nevertheless, we cannot rule out the possibility that our feature extraction for MIPS binaries is erroneous. We further discuss this issue in §7.1.

5.1.5 Closer optimization levels show similar results

We also measured the effect of size optimization (`Os`) by matching function λ in the NORMAL dataset with a function (λ^{TP} and λ^{TN}) in the SIZEOPT dataset. Subsequently, the binaries compiled with the `Os` option were similar to the ones compiled with the `O1` and `O2` option. This is not surprising because `Os` enables most of the `O2` techniques in both GCC and Clang [122], [123]. Furthermore, we observe that the `O1` and `O2` options produce similar binaries, although it is not shown in Table 5 due to the space limit.

5.1.6 Extra options have less effect

To assess the influence of the PIE, no-inline, and LTO option, we compared functions in the NORMAL dataset with those in the PIE, NOINLINE, and LTO dataset, respectively. For the no-inline test, we limit the optimization level from `O1` to `O3` as function inlining is applied from `O1`. It was observed that the influence of such extra options is not significant. Binaries with and without the PIE option were similar to each other because it only changes the instructions to use relative addresses; hence, it does not affect our presemantic features. Function inlining also does not affect several features, such as the number of incoming calls, which results in the high AUC (0.98). LTO does not exhibit any notable effect either.

However, by analyzing each test case, we found that some options affect the AUC more than others. For example, in the no-inline test, the AUC largely decreases as the optimization level increases: `O1` (0.99), `O2` (0.97), and `O3` (0.94). This is because as more optimization techniques are applied, more functions are inlined and transformed. Similarly, in the LTO test, the AUC increases as the version of Clang increases: v4 (0.95), v5 (0.97), v6 (0.98), and v7 (0.98). In contrast, GCC shows stable AUCs across all versions, and all the AUCs are higher than those of Clang. This result indicates that varying multiple options would significantly affect the success rate, which we describe below.

5.1.7 Obfuscator-LLVM does not affect CG features

Many previous studies [20], [31], [60], [66], [69] chose Obfuscator-LLVM [102] for their obfuscation tests as it significantly vary the binary code [20]. However, applying all of its three obfuscation options shows an AUC of 0.95 on our dataset, which is relatively higher than that of the optimization level tests. In fact, obfuscation severely decreases the average TP-TN gaps except CG features. This is because Obfuscator-LLVM applies intra-procedural obfuscation. The `SUB` obfuscation substitutes arithmetic instructions, while preserving the semantics; the `BCF` obfuscation notably affects CFG features by adding bogus control flows; and the `FLA` obfuscation changes the predicates of control structures [124]. However, none of them conducts inter-procedural obfuscation, which modifies the function call relationship. Thus, we encourage future studies to use other obfuscators, such as Themida [125] or VMProtect [104], for evaluating their techniques against inter-procedural obfuscation.

5.1.8 Comparison target option does matter

Based on the experimental results thus far, we perform extra tests to understand the influence of comparing multiple compiler options by intentionally selecting λ^{TP} and λ^{TN} from binaries that could provide the lowest TP-TN gap. In this study, we present two of them because of the space limit. Specifically, for the first test, we selected functions from 32-bit ARM binaries compiled using GCC v4 with the `O0` option, and the corresponding λ^{TP} and λ^{TN} functions from 64-bit MIPS big-endian binaries compiled using Clang v7 with the `O3` option. For the second test, we changed the Clang compiler to the Obfuscator-LLVM with all three obfuscation options turned on. The *Bad* column of the table summarizes the results. In both cases, the AUC was approximately 0.91, and the average TP-TN gaps were significantly lower than those in the other tests. This signifies the importance of choosing the comparison targets for evaluating BCSA techniques. Existing BCSA research compares functions for all possible targets in a dataset, as shown in the *Rand.* tests in this study. However, our results suggest that researchers should carefully choose evaluation targets to avoid overlooking the influence of bad cases.

5.2 Comparison Against State-of-the-Art Techniques

From our experiments in §5.1, we show that using only presemantic features with a simple linear model, i.e., TIKNIB, is enough to obtain high AUC values. Next, we compare TIKNIB with the state-of-the-art techniques.

To accomplish this, we chose one of the latest approaches, VulSeeker [13], as our target because it utilizes both presemantic and semantic features in a numeric form by leveraging neural network-based post processing. Thus, we can directly evaluate our simple model using numeric presemantic features. Note that *our goal is not to claim that our approach is better, but demonstrate that the proper engineering of presemantic features can achieve results that are comparable to those of state-of-the-art techniques*.

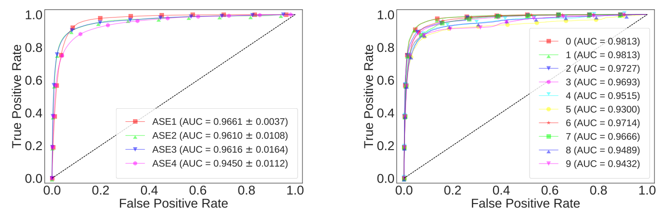
For this experiment, we prepared the datasets of VulSeeker, along with the additional ones as listed in Table 6, and we refer to them as ASE1 through ASE4. The ASE1 and ASE3 are the same datasets used in VulSeeker, and ASE2 and ASE4 are the extra ones with more packages, target architectures, and compilers. We intentionally omitted firmware images that do not provide solid ground truth.

Figure 2 depicts the results. Figure 2a shows that the AUCs of TIKNIB on ASE1 and ASE3 are 0.9661 and 0.9616, respectively. However, those of VulSeeker were 0.99 and 0.8849 as reported by the authors [13]. Figure 2b illustrates that the AUC of each fold in ASE3 ranged from 0.9300 to 0.9813 which is higher than that of VulSeeker (0.8849). Therefore, TIKNIB was more robust than VulSeeker in terms of the size and compile options in the dataset. TIKNIB also exhibits stable results even for ASE2 and ASE4.

From these results, we conclude that presemantic features with proper feature engineering can achieve results that are comparable to those of state-of-the-art BCSA techniques. Although our current focus is on comparing feature values, it is possible to extend our work to analyze the complex relationships among the features by utilizing advanced machine learning techniques [12], [13], [19], [20], [21], [23], [24], [25], [26], [27], [28], [29].

TABLE 6: Details of ASE datasets.

Name	Package	Architecture	Compiler	Train	Test
ASE 1	OpenSSL v1.0.1{f,u}	{x86,arm,mips} 32 bits	gcc v5.5.0	227K	25K
ASE 2	OpenSSL v1.0.1{f,u} BusyBox v1.21 Coreutils v6.{5,7}	″	″	593K	66K
ASE 3	″	{x86,arm,mips} 32 bits {x86,arm,mips} 64 bits	gcc v4.9.4 gcc v5.5.0	2339K	260K
ASE 4	″	Same as Normal options		13931K	1548K



(a) ROC of all ASE datasets. (b) ROC of 10-fold in ASE3.

Fig. 2: TIKNIB on ASE datasets.

6 BENEFIT OF TYPE INFORMATION (RQ3)

To evaluate the implication of debugging information on BCSA, we select type information as a case study on the presumption that they do not vary unless the source code is changed. Specifically, we extract three types of features per function: the number of arguments, types of arguments, and return type of a function. In fact, inferring the correct type information is challenging and is actively researched [126], [127]. In this context, we only consider basic types: `char`, `short`, `int`, `float`, `enum`, `struct`, `void`, and `void *`. To extract type information, we create a type map to handle custom types defined in each package by recursively following definitions using Ctags [128]. We then assign a unique prime number as an identifier to each type. To represent the argument types as a single number, we multiply their type identifiers.

As we conduct the same experiment described in §5, surprisingly, the AUC reached over 0.99 in all tests, and this is indeed the highest AUC compared to that of the existing state-of-the-art techniques. The TP-TN gaps of all tests also reached all over 0.50. Moreover, it shows a similar result when compared to VulSeeker datasets. For more information, please see Table 8 in the Appendix. This result confirms that debugging information indeed benefits BCSA in terms of the success rate, although recovering such information is a difficult task. Thus, we invite further research on BCSA to collaborate with type recovery and inference from binary code [126], [127], [129], [130], [131], [132].

7 FAILURE CASE INQUIRY (RQ4)

We carefully analyzed the failure cases in our experiments and found the causes. Note that this is possible because TIKNIB uses a simple and interpretable model. We first check the TP-TN gap of each feature for failure cases, and further analyze them using IDA Pro. We found that optimization is the main cause of the failure as described in §5.1. In this section, we discuss other failure causes and summarize the lessons learned. Consequently, we categorized the causes into three cases: (1) errors in binary analysis tools (§7.1), (2) differences in compiler back-ends (§7.2), and (3) architecture-specific code (§7.3).

7.1 Errors in Binary Analysis Tools

Most BCSA research heavily relies on COTS binary analysis tools such as IDA Pro [92]. However, we found that IDA Pro can yield false results. First, IDA Pro fails to analyze indirect branches, especially when handling MIPS binaries compiled with Clang using the position-independent code (PIC) option. The PIC option sets the compiler to generate machine code that can be placed in any address, and it is mainly used for compiling shared libraries or PIE binaries. Particularly, compilers use register-indirect branch instructions, such as `jalr`, to invoke functions in a position-independent manner. For example, when calling a function, GCC stores the base address of the Global Offset Table (GOT) in the `gp` register, and uses it to calculate the function addresses at runtime. In contrast, Clang uses the `s0` or `v0` register to store such base addresses. This subtle difference confuses IDA Pro and makes it fail to obtain the base address of the GOT, so that it cannot compute the target addresses of indirect branches.

Moreover, IDA Pro sometimes generates incomplete CFGs. When there is a *switch* statement, compilers often make a table that stores a list of jump target addresses. However, IDA Pro often failed to correctly identify the number of elements in the table, especially on ARM architecture, where switch tables can be placed in a code segment. Sometimes, switch tables are located in between basic blocks, and it is more difficult to distinguish them.

The problem worsens when handling MIPS binaries compiled for Clang with PIC, because switch tables are typically stored in a read-only data section, which can be referenced through a GOT. Therefore, if IDA Pro cannot fully analyze the base address of the GOT, it also fails to identify the jump targets of switch statements.

As we manually analyze the errors, we may have missed some. Systematically finding such errors is a difficult task because the internals of many disassembly tools are not fully disclosed, and they differ significantly. One may extend the previous study [93] to further analyze the errors of disassembly tools and extracted features, and we leave this for future studies.

7.2 Diversity of Compiler Back-ends

From §5.1, the characteristics of binaries largely vary depending on the underlying compiler back-end. Our study reveals that GCC and Clang emit significantly different binaries from the same source code.

First, GCC and Clang utilize different sets of instructions for code generation. For example, in the case of move instructions for ARM, GCC uses conditional instructions such as `MOVLE`, `MOVGT`, or `MOVNE`, unless the optimization level is zero (`O0`). In contrast, Clang utilizes regular move instructions along with branch instructions. This significantly affects the number of instructions as well as the number of basic blocks in the resulting binaries. Consequently, the functions compiled using GCC have a relatively smaller number of basic blocks compared to those compiled using Clang. However, Clang has twice as many basic blocks for binaries compiled with the `O0` option on ARM and MIPS. We figured out that Clang inserts dummy basic blocks, which have only one branch instruction to the next block, the details of which are described in the Appendix.

Moreover, on x86, GCC generates a special function, such as `__x86.get_pc_thunk.bx`, to load the current instruction pointer to a register, whereas Clang inlines this procedure inside the target function. This also largely affects the call-related features such as the number of control transfer instructions or outgoing calls.

Finally, compilers sometimes generate duplicate functions of the same code in the resulting binary to ensure that the distance between the caller and its callee is less than the page size [35]. In such cases, the duplicates may have a different body because different optimizations could be applied to their call site. We found cases in which the behaviors of GCC and Clang differ in applying such optimizations. For instance, for the `get_data` function of `binutils`, GCC yields three duplicates. However, Clang does not produce any duplicate. Such a subtle difference can make the resulting binaries divergent depending on the compiler back-ends used.

7.3 Architecture-Specific Code

When manually inspecting failures, we found that some packages have architecture-specific code snippets guarded with conditional macros such as `#if` and `#ifdef` directives. For example, various functions in `OpenSSL`, such as `mul_add` and `BN_UMULT_HIGH`, are written in architecture-specific inline assembly code to generate highly optimized binaries. This means that a function may correspond to two or more distinct source lines depending on the target architecture.

Therefore, instruction-level presemantic features can be significantly different across different architectures when the target programs have architecture-specific code snippets, and one should consider such code when designing cross-architecture BCSA techniques.

8 DISCUSSION

Our study identifies several future research directions in BCSA. First, many BCSA papers have focused on building a general model that can result in stable outcomes with any compiler options. However, one could train a model targeting a specific set of compiler options, as shown in our experiment, to enhance their BCSA techniques. It is evident from our experiment's results that one can easily increase the success rate of their technique by inferring the compiler options used to compile the target binaries. There exists such an inference technique [133], and combining it with existing BCSA methods is a promising research direction.

Second, there are only a few studies on utilizing decompilation techniques for BCSA. However, our study reveals the importance of such techniques, and thus, invites further research on leveraging them for BCSA. One could also conduct a comprehensive analysis on the implication of semantic features along with decompilation techniques.

Additionally, we investigated fundamental presemantic features in this study. However, the effectiveness of semantic features are not well-studied yet in this field. Therefore, we encourage further research on investigating the effectiveness of semantic features along with other presemantic features that are not covered in the study. In particular, as many recent studies have been adopting NLP techniques, inspecting their effectiveness would be another essential study.

Our scope is limited to a function-level analysis (§4.1). However, one may extend the scope to handle other BCSA scenarios to compare binaries [20], [27], [53] or a series of instructions [32], [34], [56]. Additionally, one can extend our approach for various purposes such as vulnerability discovery [11], [12], [20], [23], [28], [58], [134], malware detection [5], [6], [135], [136], [137], [138], [139], library function identification [81], [140], [141], [142], [143], [144], plagiarism/authorship detection [8], [80], [145], or patch identification [146], [147], [148]. However, extending our work to other BCSA tasks may not be directly applicable. This is because it requires additional domain knowledge to design an appropriate model that fits the purpose and careful consideration on the trade-offs. We believe that the reported insights in this study can help this process.

Recall from §2, we did not intend to completely survey the existing techniques, but instead, we focused on systematizing the fundamental features used in previous literature. Furthermore, our goal was on investigating underexplored research questions in the field by conducting a series of rigorous experiments. For a complete survey, we refer readers to the recent survey on BCSA [149].

Finally, because our focus is on comparing binaries without source code, we intentionally exclude similarity comparison techniques that require source code. Nevertheless, it is noteworthy that there has been plentiful literature on comparing two source code snippets [73], [150], [151], [152], [153], [154], [155], [156], [157], [158] or comparing source code snippets with binary code snippets [159], [160], [161].

9 CONCLUSION

We studied previous BCSA studies from the perspective of features and benchmarks. From this study, we realized that none of the previous BCSA studies uses the same benchmark for their evaluation, and some of them need to manually fabricate the ground truth for their benchmark. This observation led us to design BINKIT, the first large-scale public benchmark for BCSA, along with a set of automated build scripts. We also built a BCSA tool, TIKNIB, that employs an interpretable model. Using our benchmark and tool, we answered underexplored research questions regarding the syntactic and structural BCSA features. We found that several elementary features can be robust across different architectures, compiler types, compiler versions, or even intra-procedural obfuscation. We further proposed potential approaches to improve BCSA. We conclude by inviting further studies on BCSA using our findings and benchmark.

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APPENDIX A
IMPLICATION OF OPTIMIZATION LEVEL

One of the popular goals in BCSA is to identify similar functions compiled from the same source but with different architectures or compile options. However, as shown in §5.1, compiler optimization is a significant factor that affects the presemantic features of the resulting binary code. In this section, we further discuss their effects on BINKIT.

In Table 3, the number of functions in the NORMAL dataset is much smaller than that of the NOINLINE dataset. Here, we only consider the latest version of the compilers in BINKIT, which is GCC v8.2.0 and Clang v7.0, so that we can compare the numbers for GCC and Clang as well. To investigate the number of functions affected by function inlining for each optimization level, we counted the number of functions and basic blocks on these two datasets. Figure 3a illustrates the number of functions in the NORMAL dataset decreases according to the optimization levels. Meanwhile, the number of functions in the NOINLINE dataset remains the same as shown in Figure 3b.

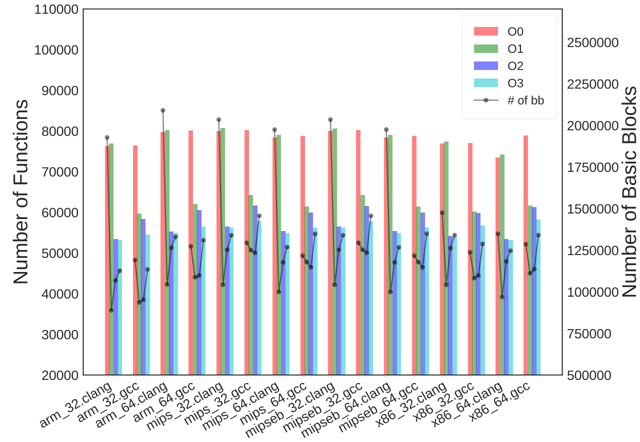
Conversely, the number of basic blocks slightly varies as the basic blocks survive in the target function although function inlining is applied. Note that the numbers of basic blocks in Figure 3a shows similar aspects to those in Figure 3b. Meanwhile, the number of basic blocks increases as the optimization level increases within the same dataset. We confirmed that one possible reason is loop unrolling, which unwinds the loops and generates multiple copies of instructions. Consequently, the number of basic blocks in `O3` reaches the highest. However, Clang produces twice as many basic blocks for binaries compiled with the `O0` option on ARM, MIPS, and MIPS big-endian. We figured out that Clang inserts dummy basic blocks which have only one branch instruction to the next block.

From these observations, we conclude that function inlining significantly varies the resulting binaries in terms of their presemantic features.

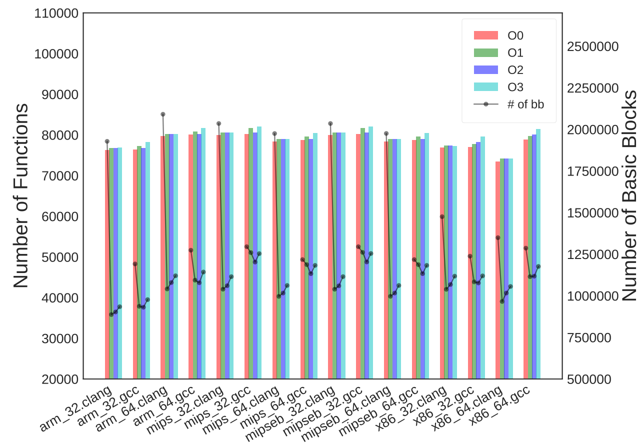
APPENDIX B
DETAILED INFORMATION ON BINKIT

As we described in §3.1, BINKIT consists of 75,230,573 functions of 243,128 binaries compiled from 51 GNU packages [101] with 1,352 distinct combinations. Table 7 lists their details in terms of the version of the package and the number of binaries and functions in the package for each dataset. Note that, for the PIE and LTO datasets, some packages failed to compile because they have architecture-specific code, such as inline assemblies, or because they use compiler-specific grammars. Moreover, some packages have conflicting dependencies.

BINKIT is the first comprehensive benchmark including all the architectures and compiler options used in the previous literature with reproducibility and extensibility. As we release all our source code as well as the compiled binaries, we invite future research to utilize BINKIT to develop and evaluate their promising techniques.



(a) NORMAL dataset results



(b) NOINLINE dataset results

Fig. 3: Number of functions and basic blocks.

APPENDIX C
ADDITIONAL IN-DEPTH ANALYSIS RESULTS

We presented our experimental results of TIKNIB on BINKIT and discussed our findings in §5. Table 8 presents additional results omitted because of the space limit. The average number of the selected features for each test (first row of Table 8) shows that even a small number of presemantic features could achieve high AUCs. Additionally, the average precision of each test (second rows of the table) coincides with the high AUCs having small standard deviation.

The number of train and test pairs (third rows of Table 8) counts the number of function λ and its corresponding λ^{TP} and λ^{TN} function pairs for training and testing in each experiment. Therefore, for N functions, there exist $2 \cdot N$ functions pairs. Moreover, we present the time spent for training and testing in each test in the fourth rows of the table. Although we have not optimized our code, because we utilize a simple model without complex techniques, it took only a small amount of time. The average processing time for a single function took less than a millisecond. Note that this time excludes the time spent for loading the function data from the database as well as the time spent for preprocessing to extract features. In fact, it took roughly 3 milliseconds to preprocess a single function, which includes multiple steps: processing via IDA, fabricating the ground truth using source file and source line number, filtering functions, labeling type information, and extracting features. We believe that the processing time could be reduced if we optimize each step.

Finally, we also compare the results of only using the presemantic features to those of using the extra type features described in §6. The fifth rows of Table 8 show that the average TP-TN gap of the presemantic features in each test is much lower than that of the type features. The TP-TN gap of the type features in all tests reached over 0.50. Consequently, the AUC with type features reached over 0.99 in all tests (sixth rows of the table). This result shows that type information can indeed help BCSA, although recovering such information is a difficult task. Therefore, we invite future research on recovering debugging information and utilizing such information for BCSA.

TABLE 7: BINKIT Dataset

Package	Version	Normal		SizeOpt		PIE		NoInline		LTO		Obfuscation	
		Bins	Funcs	Bins	Funcs	Bins	Funcs	Bins	Funcs	Bins	Funcs	Bins	Funcs
a2ps	4.14	576	250,319	144	59,846	576	249,674	576	287,529	576	125,760	256	115,084
binutils	2.3	4,032	6,458,691	1,008	1,524,429	4,032	6,449,923	4,032	7,756,458	4,032	3,647,425	1,792	3,032,233
bool	0.2.2	288	14,576	72	3,530	288	14,519	288	16,190	288	10,154	128	6,723
ccd2cue	0.5	288	7,800	72	1,872	288	7,824	288	8,352	288	4,936	128	3,521
cflow	1.5	288	84,791	72	19,794	288	84,714	288	106,135	288	45,204	128	40,201
coreutils	8.29	30,240	3,833,379	7,560	875,715	-	-	30,240	4,919,319	1,728	58,139	13,440	1,821,531
cpio	2.12	576	125,990	144	30,980	576	125,952	576	158,898	576	66,398	256	59,822
cppi	1.18	288	22,733	72	6,202	288	22,729	288	27,291	288	7,465	128	10,727
dap	3.1	1,152	26,160	288	6,440	1,152	26,160	1,152	26,216	1,152	15,056	512	11,392
datamash	1.3	288	79,620	72	18,326	288	79,648	288	98,976	-	-	128	37,597
direvent	5.1	288	120,142	72	28,876	288	120,133	288	136,878	288	60,421	128	55,368
enscript	1.6.6	864	72,828	216	17,752	864	71,951	864	81,323	864	43,552	384	33,007
findutils	4.6.0	1,728	367,523	432	85,534	1,728	367,369	1,728	470,527	1,728	185,627	768	173,955
gawk	4.2.1	288	252,420	72	60,052	288	252,413	288	332,521	288	180,214	128	123,649
gcal	4.1	1,152	160,012	288	39,016	1,152	159,739	1,152	166,218	1,152	145,333	512	70,893
gdbm	1.15	1,152	112,553	288	26,821	1,152	112,565	1,152	126,604	-	-	512	52,037
glpk	4.65	576	399,334	144	96,280	576	399,334	576	445,544	-	-	256	183,966
gmp	6.1.2	288	181,250	72	43,850	288	181,250	288	198,221	-	-	128	82,560
gnu-pw-mgr	2.3.1	576	127,670	144	24,821	576	127,661	576	191,701	576	63,082	256	65,783
gnudos	1.11.4	576	82,777	144	20,393	576	81,958	576	83,074	-	-	256	36,168
grep	3.1	288	133,448	72	30,765	-	-	288	180,079	-	-	128	63,630
gsasl	1.8.0	288	83,740	72	20,321	288	83,740	288	89,802	-	-	128	38,468
gsl	2.5	1,152	1,693,985	288	412,421	1,152	1,693,985	1,152	1,850,896	-	-	512	770,498
gss	1.0.3	576	28,355	144	6,841	576	28,356	576	32,397	-	-	256	13,162
gzip	1.9	288	37,684	72	8,746	-	-	288	47,288	-	-	128	17,697
hello	2.1	288	19,575	72	5,634	288	19,569	288	22,061	288	5,879	128	9,000
inetutils	1.9.4	5,184	646,375	1,296	151,231	5,184	646,248	5,184	827,260	5,184	413,380	2,304	308,362
libiconv	1.15	864	89,764	216	21,569	864	89,764	864	101,087	-	-	384	41,934
libidn	2.0.5	288	22,571	72	5,234	288	22,574	288	30,504	-	-	128	12,250
libmicrohttpd	0.9.59	288	46,447	72	10,988	288	46,447	288	52,133	-	-	128	21,530
libtasn1	4.13	1,152	42,450	288	9,934	1,152	42,447	1,152	50,223	-	-	512	19,800
libtool	2.4.6	288	27,568	72	6,712	288	27,568	288	30,216	-	-	128	12,624
libunistring	0.9.10	288	180,208	72	41,464	288	180,208	288	214,861	-	-	128	86,062
lightning	2.1.2	288	100,610	72	21,826	288	100,610	288	143,611	-	-	128	48,009
macchanger	1.6.0	288	7,197	72	1,826	288	7,197	288	8,352	288	3,965	128	3,282
nettle	3.4	1,152	12,786	288	3,056	1,152	12,625	1,152	15,210	-	-	512	5,664
osip	5.0.0	576	188,032	144	46,443	576	188,032	576	195,522	-	-	256	84,639
patch	2.7.6	288	110,723	72	25,264	288	110,529	288	147,538	288	58,639	128	52,871
plotutils	2.6	864	43,128	216	10,626	864	43,124	864	44,624	864	24,364	384	19,227
readline	7	576	187,676	144	46,315	-	-	576	207,131	-	-	256	85,715
recutils	1.7	2,880	745,325	720	185,303	2,880	745,324	2,880	936,930	-	-	1,280	345,914
sed	4.5	288	95,136	72	22,185	-	-	288	129,583	-	-	128	45,383
sharutils	4.15.2	1,152	237,381	288	47,816	1,152	236,616	1,152	354,841	1,152	111,299	512	122,062
spell	1.1	288	3,412	72	864	288	3,412	288	3,788	288	2,492	128	1,508
tar	1.3	576	325,858	144	75,533	576	325,775	576	424,412	576	203,658	256	154,883
texinfo	6.5	288	47,114	72	10,955	288	47,147	288	63,650	288	26,963	128	22,064
time	1.9	288	6,190	72	1,292	288	6,190	288	8,000	288	2,949	128	2,964
units	2.16	288	37,023	72	9,289	288	37,019	288	37,012	288	24,824	128	16,507
wdiff	1.2.2	288	12,204	72	2,816	288	12,209	288	15,056	288	6,213	128	5,633
which	2.21	288	7,600	72	1,656	288	7,600	288	8,944	288	4,527	128	3,447
xorriso	1.4.8	288	783,853	72	190,338	288	783,032	288	851,448	288	418,872	128	357,702
Total		67,680	18,783,986	16,920	4,425,792	36,000	14,482,863	67,680	22,762,434	24,768	5,966,790	30,080	8,808,708

TABLE 8: Additional in-depth analysis result with BINKIT.

	Opt Level				Compiler				Arch						vs. SizeOpt†			vs. Extra†			vs. Obfus.†				Bad‡	
	Rand.	O0 vs. O3	O2 vs. O3	Rand.	GCC 4 vs. GCC 8	Clang 4 vs. Clang 7	GCC vs. Clang	Rand.	x86 vs. ARM	x86 vs. MIPS	ARM vs. MIPS	32 vs. 64	LE vs. BE	Rand.	O0 vs. Os	O1 vs. Os	O3 vs. Os	PIE	NoInline	LTO	BCF	FLA	SUB	All	Norm.	Norm. vs. Obfus.†
Avg. # of Selected Features	6.4	12.1	8.5	11.7	8.4	9.0	9.8	9.7	11.2	11.1	10.3	10.5	9.9	10.0	11.0	9.0	9.8	16.1	6.9	11.0	6.0	7.8	16.3	5.1	12.8	8.8
Average Precision (AP)	0.94	0.91	0.98	0.96	0.99	1.00	0.97	0.98	0.99	0.97	0.98	0.99	1.00	0.98	0.96	0.99	0.96	1.00	0.98	0.98	0.98	0.97	1.00	0.95	0.92	0.90
Std. of AP	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01
# of Train Pairs (10^6)	3.99	1.62	1.94	3.83	1.98	1.99	2.10	3.99	1.82	1.83	1.86	1.95	2.00	3.96	1.75	1.84	1.88	2.00	1.73	1.18	1.95	1.97	2.00	1.93	0.09	0.11
# of Test Pairs (10^6)	3.75	0.79	0.79	3.60	0.41	0.42	1.97	3.75	0.43	0.42	0.44	1.83	0.95	3.71	0.88	0.87	0.79	2.89	2.62	1.19	0.42	0.42	0.43	0.42	0.01	0.01
Train Time (10^3 sec)*	0.65	0.46	0.35	1.12	0.42	0.47	0.52	0.96	0.48	0.50	0.40	0.50	0.43	0.99	0.46	0.42	0.42	0.84	0.30	0.30	0.29	0.37	0.80	0.27	0.02	0.02
Test Time (sec)*	7.11	1.40	1.10	8.10	0.64	0.64	3.50	7.19	0.66	0.62	0.54	2.90	1.52	7.61	1.85	1.51	1.31	8.23	5.75	2.95	0.57	0.56	0.72	0.51	0.01	0.18
Avg. TP-TN Gap	0.31	0.26	0.49	0.35	0.49	0.51	0.36	0.43	0.39	0.33	0.32	0.43	0.54	0.38	0.30	0.44	0.40	0.52	0.47	0.47	0.28	0.26	0.50	0.17	0.24	0.11
Avg. TP-TN Gap with Type	0.53	0.54	0.55	0.54	0.54	0.54	0.54	0.54	0.53	0.53	0.54	0.53	0.54	0.53	0.54	0.54	0.54	0.54	0.54	0.51	0.54	0.54	0.55	0.54	0.54	0.54
ROC AUC	0.94	0.90	0.97	0.95	0.99	1.00	0.96	0.98	0.99	0.98	0.98	0.99	1.00	0.98	0.96	0.98	0.95	1.00	0.97	0.98	0.98	0.98	1.00	0.95	0.91	0.91
ROC AUC with Type	0.99	0.99	1.00	0.99	1.00	1.00	0.99	0.99	1.00	0.99	0.99	1.00	1.00	1.00	0.99	1.00	0.99	1.00	1.00	0.99	1.00	1.00	1.00	0.99	0.99	0.99

† We compare a function from the NORMAL to the function in each corresponding target dataset.
‡ We match functions whose compiler options are largely distant to test bad cases. Please see §5.1.8 for the details.
* The train and test time represent pure time excluding data loading.