Identifying Software Defects Using Neural Graph Classifiers

By

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A thesis submitted to the
Faculty of Graduate and Postdoctoral Affairs
in partial fulfilment of the requirements for the degree of

Master in Computer Science

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Abstract

Static analysis tools are commonly used to assist with program verification. Most existing tools, however, identify defects using a predefined repertoire of defect specifications. These repertoires are rarely extended by users due to the effort and complexity involved in producing new specifications.

I propose a supervised approach for learning defective code patterns directly from coarsely labelled examples, allowing users to produce new defect classifiers with minimal effort. This approach represents a program as a directed multi-graph modelling operations and their dependencies, and aims to identify defects caused by incorrect, or missing, dependencies between operations. Given this representation, the task of identifying these defects can be seen as identifying specific partial subgraphs.

The proposed approach is evaluated against several open source projects and test suites targeting the Java virtual machine (JVM). The proposed approach performs well against an adapted subset of the Juliet [60] test suite, and demonstrates a modest ability to transfer to unseen natural code.

Acknowledgements

I wish to thank Dr. Guo, and everyone else whom I pestered for feedback and review, for their infinite patience and support.

For my mother, Ann.

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Abbreviations

AP	average precision
API	application programming interface
AST	abstract syntax tree
AUC	area under curve
BPTT	backpropagation through time
CBOW	continuous bag of words
CFG	control-flow graph
CFR	chaos-free recurrence
CWE	Common Weakness Enumeration
DFG	data-flow graph
DSL	domain specific language
FC LAYER	fully-connected layer
FDR	false discovery rate
FPR	false positive rate
GRU	Gated Recurrent Unit
IPA	interprocedural analysis
IR	intermediate representation
JVM	Java virtual machine
LSTM	Long Short-Term Memory
MLP	multi-layer perceptron
OOV	out-of-vocabulary
RHS	right-hand-side expression
RNN	recurrent neural network
ROC	receiver operating characteristics
SGD	stochastic gradient descent
SQL	Structured Query Language
SRNN	simple recurrent neural network
SSA	single static assignment
TPR	true positive rate

UTF-8 Unicode Text Format 8-bits

CHAPTER 1

Introduction

Static analysis tools are frequently used to assist with the verification of software. However, their capabilities are limited by the fact that almost all programs lack a complete machine-verifiable specification against which they can be verified. This is unfortunate since the defectiveness of a behaviour can depend on the program’s functional requirements. As a result, most static analysis tools verify programs against specifications derived from the programming language’s own specification, assuming one exists, or a set of ad-hoc specifications covering common application-agnostic defects. This set of specifications constitutes an analyzer’s repertoire of known defects.

While some tools support customization of their repertoire of specifications, adding or refining specifications often requires specialist knowledge orthogonal to that required to identify and characterize the defect under consideration. This dissuades users from customizing a specifications reporting false positives for their program, or adding new specifications to cover a false negative.

1.1 Problem Statement

The objective of this work is to explore the feasibility of applying machine learning techniques to learn defect detectors from examples. Users should be able to label examples by simply specifying the lines of code which induce the defect, while the classifiers produced from this data should be capable of issuing predictions with sub-function level granularity.

This per-line approach is intended to reduce the effort required by a user to label a positive sample. In exchange, we accept that the labels provided will be coarse; they may only partially intersect with the true set of operations which induce the defect in question.

1.2 Contributions

I propose a new supervised approach for identifying application defects caused by incorrect, or missing, dependencies between operations. This is accomplished by learning to identify partial subgraphs within a graphical representation of a program’s operation dependencies using learned inductive representations for each operation. These learned representations are produced using a graph neural network. By specifically considering dependencies between operations (such as subroutine invocations), the proposed approach is well suited for identifying defects caused by improper application programming interfaces (APIs) usage.

I demonstrate that this approach is effective against an adapted subset of the Juliet test suite [60], and that it can weakly transfer to unseen natural code.

1.3 Organization

We begin with a brief review of relevant background material in chapter 2, covering program representations and common neural models. Chapter 3 discusses related works for graph embedding, graphical neural models, and program modelling. The proposed approach is presented in chapter 4, and experimental results are presented in chapter 5, including ablative studies. Chapter 6 presents my conclusions, and outlines avenues for future work.

CHAPTER 2

Background

This chapter provides background information on neural network models, program representations, and a brief discussion on handling structured inputs. The intent of this chapter is to establish a basic context for this work, as well as works discussed in chapter 3.

2.1 Program Representations

A program can be expressed using different representations, each specialized for specific use cases. For example, programs are typically written in a human-friendly notation (source code) and then mechanically translated into a form interpretable by a computer (machine code). A typical pipeline for this process is depicted in fig. 2.1. These two representations are quite dissimilar: the former is a sequence of characters, while the latter is a sequence of data and instructions. The translation from one to the other requires significant prior knowledge regarding both representations.

This prior knowledge requirement makes it difficult to reliably infer program properties from the source code or compiled form. However, a well-defined program¹ has precise semantics which can be mechanically evaluated. Instead of inferring the syntax or low level semantics from source code, one can obtain them directly using a compiler’s machinery and representations. These representations can be classified as either syntactic or semantic.

Syntactic Representations. Syntactic representations are used by compilers to verify the encoding of unstructured source code text and translate it into a structured form. This is typically accomplished in two phases:

1. Lexical analysis

¹For some language-defined notion of ‘well-defined.’

Fig. 2.1: A typical compiler pipeline for translating source code into executable code. In this example, a toy language is compiled to a stack machine. The majority of a compiler's complexity lies within the intermediate representations (IRs), where semantic analyses and transformations occur.

2. Grammatical analysis

Lexical analysis (lexing) transforms the source code from a sequence of characters into a sequence of lexemes. Grammatical analysis (parsing) transforms the sequence of lexemes into an abstract syntax tree (AST) for the language in question.

Semantic Representations. Semantic representations, or **IRs**, are data structures used to reason about a program's meaning, prove properties, and justify various transformations and optimizations. It is common to use multiple **IRs**, each modelling some specific aspect of the program, and most can be naturally expressed as directed graphs. Three particularly important **IRs**, control-flow graphs (CFGs), data-flow graphs (DFGs), and single static assignment (SSA), are introduced below.

2.1.1 Control & Data Flow Graphs

Practically all program analyses depend upon reasoning about possible paths of execution through a program, and how values are computed or consumed. This information can be obtained through various control flow analyses (CFA) and data flow analyses (DFA), the results of which are directed graphs describing the control or data dependencies in question. (See fig. 2.2.)

A **CFG** is a directed graph describing the possible paths of execution through a program. Vertices in a **CFG** represent **basic blocks**, sequences of operations which may only be entered at the head of the block and which may only transfer control at its end. Consequently, if a basic block is entered then all operations within it must be completed prior to control leaving the block. The use of basic blocks instead of single operations for vertices simplifies the **CFG**; only the potential control branches must be explicitly represented.

While **CFGs** model the control flows between basic blocks, **DFGs** model the data flows between operations. Specifically, they model the data dependencies between operations where a directed edge $a \rightarrow b$ designates that b consumes the value computed by a .

CFGs and **DFGs** are often used by other analyses and transformations, such as reachability

Fig. 2.2: A program, its CFG, and its non-SSA DFG.

analysis or converting the program into SSA form.

2.1.2 Single Static Assignment

Precise data-flow analysis is complicated by situations where a variable, a named store for a value, has more than one assignment. One solution is to convert the program into SSA form where variable is assigned exactly once. This is done by introducing a fresh variable at every assignment, and adding ϕ -nodes to disambiguate situations where the choice of fresh variable is dependent upon the executed control flow of the program [15, 21, 70]. Figure 2.3 provides an illustration of this conversion.

2.2 Type Systems

Many languages offer a type system for verifying a program's data-flow. Broadly speaking, in a typed language program terms are annotated with a type designating a set of permitted values. The program can then be verified (type checked) against these annotations to ensure

(a) An example program without control-dependent data flow.

(b) An example program containing a control-dependent data flow. $a := \phi(a_1, a_2)$ is inserted to select the correct variable depending on the control flow.

Fig. 2.3: Two programs containing multiple assignments to a variable. While `a` can be trivially transformed to use two independent variables, `b` cannot and requires the use of a ϕ -node.

it does not violate the type system's rules.

While type systems vary in terms of expressiveness and capabilities, the majority guarantee² that a program which successfully type-checks contains no operations using values which are incompatible with the operation's declared type. Type-checking can occur either prior to execution (static) or during execution (dynamic). The details depend heavily on the type system in question, and any guarantees are often contingent upon the program being otherwise well-defined according to the language.

2.2.1 JVM Type System

The Java virtual machine (JVM) uses a dynamic type-system designed to map closely onto Java's original static type system [1, 2].³ Specifically, the JVM's type system is an example of a *nominal subtyping* system, where two types are considered identical if and only if they have the same fully qualified name, and types may be declared to be a subtype of one

²Very few type-systems are formally and comprehensively verified. As a result, it is not uncommon to find type systems or implementations which are unsound. e.g. Java and Scala are both unsound due to an interaction between generics and the bottom value `null` [7], while TypeScript is deliberately unsound to allow for idioms inherited from JavaScript.

³Java's type system was later extended to support parametric polymorphism but this was implemented using type erasure and runtime conversion checks in order to avoid changes to the JVM.

another. The notion of a subtype allows defining non-disjoint sets of values: If **A** is a subtype of **B** (formally written as $A <: B$) then the set of values encompassed by **A** is subset of values encompassed by its supertype **B**. Note that the JVM type system permits a type to have multiple supertypes.

2.3 Neural Networks

Artificial neural networks (neural networks from this point forward) are a class of parameterized functions inspired by biological neural networks. The objective was to create a system capable of learning from experience much like biological brains. This was accomplished by crudely mimicking the interconnections and non-linear behaviour of biological neurons using scalar weights, and simple non-linear activation functions to approximate the complex stimulus-response behaviour of biological neurons. Neural networks were later proven capable of approximating arbitrary functions [27, 42, 43, 53, 61].

A neural network can be factored into two components: [11]

- **Architecture:** Network parameters which are defined prior to fitting the network against a dataset, such as the choice of activation function(s), network size, and network connectivity.
- **Weights:** Network parameters which are obtained while fitting the network against a dataset.

Some architectural parameters (also referred to as hyper-parameters) are chosen by a human, such as the general connectivity structure of the network, while others are tuned to a specific task or dataset using an automated search.

For this review we will be primarily focusing on supervised techniques, where a network is conditioned to emit response y given input x , i. e. $y = f_{\phi}(x)$ where ϕ is the network's weights. The process of conditioning a neural network's response to input is known as fitting or training, and is typically done by minimizing a function defining the model's prediction

error (loss). Minimizing the loss function is usually done by iteratively updating the weights using gradient descent along their partial derivatives with respect to the current loss. This approach is commonly referred to as backpropagation [75].

2.3.1 Activation Functions

All modern neural models feature a non-linear response to inputs. This is critical, as without non-linear responses increasing the network depth yields no increase in expressiveness. This can be easily proven by the following argument: Consider a trivial linear network of depth n with a single input vector and no biases where the layers are arranged in a single sequence. This network can be expressed as a series of weighed adjacency matrix multiplications, one for each layer, and can be simplified to a single matrix by multiplying the series. Any linear network can be expressed as the sum of such trivial networks, and are thus equivalent to some linear network of depth 1. Introducing a non-linear transformation between linear transformations solves this issue.

While any non-linear function can be used as an activation function, three are ubiquitous: sigmoid, tanh, and rectified linear (ReLU, rectified linear unit). These will be referred to as $\sigma(x)$, $\tau(x)$, and $\text{relu}(x)$, respectively. Figure 2.4 provides a visualization of their activation.

Tanh and ReLU are commonly used as primary activation functions, whilst sigmoid, due to its range of $(0, 1)$, is generally used in gating constructs (introduced below in section 2.3.3) and binary logistic regression. For other purposes, tanh and ReLU are generally preferred over sigmoid since sigmoid does not satisfy $0 = f(0)$. This property is desirable when using dropout [79] or bias regularization.

In turn, the choice between tanh and ReLU primarily depends on model depth and capacity relative to model size. ReLU is less susceptible to vanishing gradients than tanh, having a linear response for half of its domain, which is particularly desirable for deeper architectures where vanishing gradients often limit the effectiveness of backpropagation-based optimization. However, empirically they offer inferior capacity per hidden unit compared to tanh [32], do not offer a mean zero activation. In practice, the choice of activation matters less than the

Fig. 2.4: Common activation functions. The sigmoid activation function is defined by $\sigma(x) = \frac{1}{1+e^{-x}}$, and is notable for having a non-zero mean activation.

choice of architecture.

2.3.2 Feed-forward Networks

Neural network architectures can be broadly partitioned based on whether their connections form cycles. Those without cycles are termed feed-forward networks, and are generally applied to tasks whose inputs are independent of one another, such as image processing and general classification.

One of the earliest and simplest examples of a neural network is the perceptron (or linear perceptron) [71]. It is a binary classifier and uses a single fully-connected layer (FC LAYER) without any activation function:

$$f(\mathbf{x}) = 0 < \mathbf{W}\mathbf{x} + \mathbf{b}$$

The perceptron is only capable of modelling linear functions, and thus can only handle linearly separable datasets. These limitations were solved by the multi-layer perceptron (MLP), which used additional layers of neurons and non-linear activations [75]. The original **MLP** consists of two fully connected layers, each using a sigmoid activation function. It has been shown that a **MLP** with at least one hidden layer, i.e. 2 or more total layers, can

approximate any continuous function [43].

2.3.3 Recurrent Networks

Recurrent neural networks (RNNs) extend upon feed-forward networks by incorporating connection cycles, where an output signal is fed back as an input, endowing RNNs with a notion of state. This extension is sufficient to make RNNs Turing-complete [76]. RNNs are commonly used for tasks involving sequences, such as natural language translation and sentiment analysis [17, 81, 82, 93].

A simple recurrent neural network (SRNN) can be defined as:

$$h_{t+1} = \mathbf{W}[x_t, h_t] + b \quad (2.1)$$

where x_t and h_{t+1} are the inputs and outputs at step t of the sequence.

RNNs are usually fitted using a variant of backpropagation known as backpropagation through time (BPTT) [75]. In BPTT, backpropagation is performed on an ‘unrolled’ view of the network, allowing the recurrent network to be trained as if it were a feed-forward network with shared weights. In practice the network is only unrolled for a fixed number of steps, rather than the entire sequence. This approach is known as truncated BPTT.

While SRNNs are capable of approximating any dynamical system [27], they are difficult to train using BPTT when pitted against tasks involving long sequences [40, 41]. One popular mitigation is to introduce subnetworks which control how the RNN’s state is updated. Two examples of these are Long Short-Term Memory (LSTM) cells [33, 41] and Gated Recurrent Units (GRUs) [19]. Other solutions include using more exotic recurrence transform such as unitary and orthogonal recurrence networks [9, 87].

2.3.4 Graph Networks

Neural networks can also be applied to graphs [23, 26, 36, 55, 74, 81]. Common names for these include graphical neural networks, graph convolution networks, message-passing neural

Fig. 2.5: Information is propagated by repeatedly exchanging messages between adjacent vertices in an undirected graph. Displayed here are the first few update iterations. Note that V_0 and V_3 are part of $N^2(V_1)$, but not the edge (V_0, V_3) .

networks, and recursive networks (when operating on directed acyclic graphs with a single sink). Graph neural networks are also related to several techniques for learning unsupervised vertex embeddings [34, 63, 66, 95].

To avoid confusion between graph labels (data associated with a vertex or edge) and machine learning labels (ground truth or predicted values), graph labels will instead be referred to as *features*. Assume some graph $G = (V, E, \mathbf{X}, \mathbf{L})$ where V and E are the vertices and edges, and $\mathbf{X} \in \mathbb{R}^{|V| \times D}$ and $\mathbf{L} \in \mathbb{R}^{|E| \times D}$ are the features for the vertices and edges, respectively. Graph networks are generally of the form

$$\mathbf{h}_v^{i+1} = f_i(\mathbf{h}_{N(v)}^i, \mathbf{X}_{N(v)}, \mathbf{L}_{N(v)}) \quad (2.2)$$

where $v \in V$ and f_i is some parameterized function (possibly using shared parameters for all i) which updates vertex v 's state based on its closed neighbourhood $N(v)$. The inputs to f_i includes the features of incident edges, and the features and states of adjacent vertices. Information is thus diffused through the graph by iteratively updating vertices' states based on their immediate neighbourhood, as illustrated in fig. 2.5. Directional path information can be incorporated by using a non-commutative function for f . This process is sometimes referred to as message passing.

Most choices for f can be factored into two components: a message-generation function m

Table 2.1: Examples of previously proposed graph neural architectures, where f has been factored into a message-generation function m and a message-aggregation function g (eq. (2.3)). The choice of initialization for $\mathbf{h}_v^0$ generally depends on whether m makes use of $\mathbf{X}$. Note that some entries have been simplified for clarity of exposition.

$\mathbf{h}_v^0$	$m(\mathbf{h}_v, \mathbf{h}_u, \mathbf{X}_v, \mathbf{X}_u, \mathbf{L}_{u \rightarrow v})$	$g(\mathbf{h}_v, \mathbf{X}_v, \mathbf{M}_v)$	Used by
$\mathbf{0}$	$\text{MLP}(\mathbf{h}_u, \mathbf{X}_v, \mathbf{X}_u, \mathbf{L}_{u \rightarrow v})$	$\sum_{\mathbf{m} \in \mathbf{M}_v} \mathbf{m}$	[74]
$\mathbf{W}_{\text{init}} \mathbf{X}_v$	$\mathbf{h}_u$	$\text{GRU}(\mathbf{h}_v, \sum_{\mathbf{m} \in \mathbf{M}_v} \mathbf{m})$	[55]
$\mathbf{W}_{\text{init}} \mathbf{X}_v$	$\mathbf{W}_{\text{edges}}[\mathbf{h}_u, \mathbf{L}_{u \rightarrow v}]$	$\text{GRU}(\mathbf{h}_v, \sum_{\mathbf{m} \in \mathbf{M}_v} \mathbf{m})$	[6]
$\mathbf{W}_{\text{init}} \mathbf{X}_v$	$\mathbf{h}_u$	$\text{MLP}(\mathbf{h}_v, \frac{1}{ \mathbf{M}_v } \sum_{\mathbf{m} \in \mathbf{M}_v} \mathbf{m})$	[35]
$\mathbf{W}_{\text{init}} \mathbf{X}_v$	$\mathbf{h}_u$	$\text{MLP}(\mathbf{h}_v, \max_{\mathbf{m} \in \mathbf{M}_v} \mathbf{m})$	[35]

that operates on incident edges, and a message-aggregation function g . In other words:

$$\begin{aligned}
 \mathbf{h}_v^{i+1} &= f_i(\mathbf{h}_{N(v)}^i, \mathbf{X}_{N(v)}, \mathbf{L}_{N(v)}) \\
 &= g(\mathbf{h}_v^i, \mathbf{X}_v, \{ m(\mathbf{h}_v^i, \mathbf{h}_u^i, \mathbf{X}_v, \mathbf{X}_u, \mathbf{L}_{u \rightarrow v}) \mid \forall u \in N(v)/\{v\} \})
 \end{aligned} \tag{2.3}$$

Table 2.1 lists some examples used by existing work. Of these, the GRU-based architectures are the most closely related to the updated function used in this work (see section 4.2).

Graph networks for non-cyclic directed graphs (i.e. recursive networks) typically update each vertex exactly once. By contrast, networks for cyclic or undirected graphs are either run until convergence [74] or use a fixed number of updates [23, 35, 55]. Both have disadvantages. Convergence requires a contractive update function f , which excludes many useful architectures (e.g. gating or attention mechanisms), and imparts an exponential decay on the influence of one vertex on another based on their distance [55]. Using a fixed number of update, obviously, limits the maximum distance over which two vertices may interact, but allows for arbitrary neural architectures.

The per-vertex embeddings $\mathbf{h}$ can also be used to produce an embedding for the whole graph. Common techniques include simply aggregating (section 2.4) the embedding (e.g. $\frac{1}{|V|} \sum_v \mathbf{h}_v^i$) [46, 55], or designating a specific vertex to act as a representative of the entire graph [26, 55, 74].

2.4 Structured Representations

Representations can be broadly classified as either structured or unstructured. For this thesis, unstructured representations are defined as some embedding $\mathbf{x} \in \mathbb{R}^n$ while structured representations are defined as directed graphs whose vertices are labelled by unstructured representations. Undirected graphs, **multigraphs**, annotated edges, and vertices with structured annotations can all be encoded by introducing additional vertices and edges.

Unstructured representations are typically defined to be (or interpreted as) a sample drawn from some probability distribution. They can be used with practically all common models (support vector machines, graphical models, random forests, etc). By contrast, structured representations are more difficult to handle since a graph may contain an arbitrary number of interdependent unstructured representations. e.g. a sequence might have an unlimited length. Many machine learning models, however, can only handle unstructured inputs.

There are three approaches for dealing with structured representations: one can ignore the connectivity of the graph, one can require that the graph be comprised of uniform local regions, where a region is an induced subgraph of the structured representation; or one can use kernel methods to abstract away how the structure is considered.

The first approach, aggregation, uses the unstructured representations of the graph with no regard to connectivity. This approach is suitable when the input has a variable size and no notion of finite position for the vertices within it (e.g. a set, or unbound sequence). Examples of this class include bag of words, continuous bag of words, multi-instance learning techniques [8], and transformer networks [85].⁴

The second approach, convolution, considers the local structure of a region within the graph. Unlike aggregation, convolutional approaches consider both a vertex's features and its position within the region in question.⁵ Examples of this approach include convolutional neural networks and graph neural networks.

⁴Note that some transformer networks add a periodic feature clock to encode a vertex's position within sequence.

⁵A vertex might not have an unambiguous position relative to the entire structure, e.g. cyclic graphs with no sources or sinks.

The third class, kernel methods, entirely side-steps the issue of finding an unstructured reduction. Instead, a kernel function $k : X \times X \rightarrow \mathbb{R}$ provides a similarity score between two samples. This score can be used as a scalar product of some implicit embedding ψ :

$$k(X_i, X_j) = \langle \psi(X_i) \cdot \psi(X_j) \rangle$$

Kernel functions can replace scalar products of embeddings in any linear model, and are often used in conjunction with support vector machines (SVMs).

The main drawback of kernel methods for structured representations lies in the computational cost of evaluating the kernel function. Kernel functions based on random walks of vertices matched by sub-kernel functions have a complexity of $O(|V|^2)$, assuming sparse graphs ($|E| = O(|V|)$) [86]. For models which require a complete **Gram matrix** between training and test samples, this corresponds to a total complexity of $O(|V|^2 nm)$ for n training and m test samples, where $|V|$ is the largest graph. Faster graph kernels have been suggested, but these require a trade-off in terms of flexibility, such as support for discrete or continuous labels.

CHAPTER 3

Related Work

The approach proposed in this thesis is based on two ideas: using dependence graphs and graph neural networks to represent programs [6, 31, 46], and classifying (sub)graphs using neural networks [31, 74].

This chapter discusses existing works¹ applying machine learning to programs. This includes works related to defect detection using neural models, techniques for representing programs for neural models (graphical or otherwise), and works concerned with classifying programs or other graphical data.

The first section provides a sampling of various program representations used in recent works, with a focus on techniques suitable for modelling fine grain program properties. e.g. the name of a local variable, rather than the name of a function. The following three sections discuss machine learning based approaches for defect detection. This includes approaches based on supervised classification (section 3.2), detecting “unnatural” outliers (section 3.3), and inferring specifications for formal verification (section 3.4).

Note that many of the works discussed here use unsupervised techniques, and while vast amounts of open source code can be readily obtained, labelled datasets for programs or source code are less common [5, 45, 46, 49, 60, 65, 91]. Finally, the works discussed in this chapter represent a small subset of recent research on probabilistic models of programs and source code. A more general survey of these efforts is available [5].

3.1 Program Representations

As discussed in section 2.1, a program can have multiple representations. While that discussion was framed from a compiler’s or interpreter’s point of view, the same principles apply for

¹Including works concurrent or subsequent to the approach presented here (early 2018).

machine learning: the input representation should be tailored to the task at hand.

Syntactic representations are particularly appealing for machine learning because they are simple, mostly task agnostic, and easy to produce. Their only requirements are a lexer and a parser for the language in question, and that the source code is syntactically valid. In exchange, they offer the equivalents to part-of-speech tagging (**tokens**) and sentence structure (abstract syntax trees (ASTs)).

Semantic representations offer much more information than syntactic representations [37], but they are also more difficult to obtain. Producing these representations requires prior knowledge of the semantics of the language, and, depending on the semantic analysis in question, other ancillary information (e.g. library dependencies, build configurations, etc).

The most readily available representation, a sequence of **lexemes** or **tokens**, is generally a poor one for learning fine grain program properties (e.g. the name or type of a variable). Briefly, programming languages are sensitive to minor lexical changes, grammatically complex with deep and broad syntax trees; and riddled with nonce words. [5, 24, 37] Altering a single lexeme can drastically change the semantics of a program, and the distance between two lexemes in the source code might have little correlation with their distance within the syntax tree. This is further complicated by syntactic sugar (equivalent but distinct syntactic constructions), and the fact that references to a common entity, such as a variable, are often lexically and grammatically distant from one another. Finally, the name of an identifier generally has no effect on the semantics of a program or program element.

Despite all of this, natural source code (i.e. code written by humans) exhibits greater regularity than text drawn from a natural language [28, 39], and even simple lexical representations can be surprisingly effective when augmented with a small amount of semantic or grammatical information.

For example, Allamanis et al. [4] predicted the name of a function given its body using sub-lexemes and an n-gram-like log-bilinear neural model [58]. Their approach indirectly includes grammatical information by only using the lexemes which appear within the body of the function under consideration.

White et al. [92] approached the task of code clone detection using auto-encoder embeddings of lexical and grammatical contexts, and measuring similarity based on embedding distances.

Explicit combinations of syntactic and semantic representations have also been used. In Allamanis and Brockschmidt [3], variables were represented using an aggregation of their context vectors; a context vector being an embedding of the n-gram centered on the variable's lexeme. This aggregation was done using a recursive network upon the variable's data flow graph, providing the model with semantic information regarding the usage of each variable. Their model inferred which variable should be used for a given context.

A similar model was proposed by Bavishi et al. [13], who inferred the likely names for an identifier given an embedded aggregation of that identifier's n-gram token contexts. These contexts were embedded using a sequence auto-encoder. [22] Like Allamanis and Brockschmidt [3], Bavishi et al.'s approach implicitly included semantic knowledge of the language by recognizing which identifiers refer to the same entity (variable or local function), and aggregating the contexts surrounding these references.

This approach was generalized in Allamanis et al. [6], where programs were represented using a graph consisting of the union of their lexeme sequence, **AST**, and data-flow edges. This graph was processed using a gated graph sequence neural network[55] to produce embeddings for each node. The nodes' state were initialized using a concatenation of an embedding of their name and the type of value produced. As in Allamanis and Brockschmidt [3], they applied their model to inferring which variable was most likely used in a given context, and demonstrated a significant improvement over the n-gram lexeme context approach. They also evaluated the ability of the model to learn embeddings suitable for inferring the name of a variable given its usage contexts.

By contrast, Raychev et al. [68] proposed a non-neural approach using conditional random fields and a graphical model describing relationships between program properties. These relationships include data flow dependencies and other semantic information. Given a program for which a subset of properties are known, the remaining unknown properties are iteratively assigned their most likely candidate. They demonstrated their approach by

inferring the names and types of variables in **minified source code**.

A purely semantic representation was proposed in Henkel et al. [37], where a program is represented using its set of possible traces (execution paths). Each trace is in turn represented as a sequence of semantic events, where an event is some notable action (e.g. function invocation), or a relationship between two or more entities (e.g. two function invocations sharing a common argument). Each distinct event is handled as symbolic value and embedding using GloVe. [62] This approach eagerly decomposes a graphical structure into a set of sequences, simplifying later processing. However, the number of traces for a program can be exponential relative to the number of possible branch points, and nested branch points can induce many distinct traces sharing a common prefix, biasing the embeddings for symbols in the shared prefix.

3.2 Supervised Classification of Programs

The most direct approach for learning defect detection is to handle it as a supervised classification problem. Supervised modelling of programs, or structured data in general, is not a new idea, and has a history tracing back to heuristics for Checker playing programs [73] and theorem provers [25, 30, 80]. The main complication is dealing with the structured nature of programs. This requires both selecting an appropriate representation for the program (section 3.1), and a decision regarding the granularity of the classification: should the program be classified as a whole, or should each part of the program be assigned a classification? The latter is more general, but may be more expensive and difficult to train.

Several recent works on defect detection use unstructured representations and most use representations implicitly capturing structured information. Examples of these works include syntax-derived embeddings used to infer both very coarse (per class or file) classifications [54, 88], and fine grain (per token) classifications [65, 72]. These efforts are only cursorily mentioned here since using unstructured representations shifts the responsibility, and complexity, of handling the program’s structure from the model to the representation extraction (see section 3.1).

Early neural models for program classification made use of vertex auto-encoders and recursive networks [31, 78]. Toy benchmark used in these experiments involved classifying lambda calculus expressions based on the presence of specific sub-expressions. The core idea was to represent a program (e.g. a lambda expression) as a directed graph, and use its topology to define a graph neural network. [26, 31, 77, 78] Modern variants of this idea have been used to learn heuristics for selecting promising theorems [46], estimating the throughput of basic blocks [56], and learning the most likely return codes for function traces [37]. Lastly, neural networks have also been used for detecting specific sub-graph isomorphisms [74]. While not directly a program classification task, it bears mention as it is directly related approach proposed in this thesis.

3.3 Outlier-based Defect Detection

Given that natural source code is regular and repetitive [28, 39], and the (perhaps optimistic) assumption that the majority of code is non-defective, one approach for detecting defects is to simply identify “unnatural” code. Ray et al. [67] provide a direct example of such an approach. Using a lexeme n-gram based model, they show that examining lines of code ranked by perplexity can be cost-competitive with conventional static analyzers.

Henkel et al. [37] performed a similar exercise, where they trained a Long Short-Term Memory (LSTM) model to predict the most likely return code for a given trace. The fitted model was evaluated against real world defective traces, and in the majority of cases the defective return code was not within the top-3 predictions issued by the model.

Non-probabilistic models have also been applied to code anomaly detection. Wasylkowski et al. [89] data mined function invocation sequences and proposed a scoring method for quantifying a sequence’s abnormality. When applied to existing software, their approach identified several defects, ranking them among the top-10 most anomalous sequences. Monperrus and Mezini [59] proposed a related, but more specialized, approach focused on identifying erroneously omitted invocations.

3.4 Specification Inference

An alternative approach to defect detection is to infer a specification rather than directly attempt to rank or classify a sample as unnatural or defective. The inferred specifications can then be used to deterministically verify programs. These techniques overlap with other approaches based on identifying unnatural code, but the primary distinction between them lies in the explicability of their results: a specification is a white-box model and can be systematically analysed; by comparison, discerning why a given sample is highly perplexing for a black box model can itself be a rather perplexing exercise for the examiner [47].

Kremenek et al. [50] and Banerjee et al. [12] both used factor graphs [96] and a set of relationship constraints to infer semantic roles for each function in a program. In Kremenek et al. [50] these roles modelled resource ownership, and were used to identify resource ownership violations (e.g. leaks, or double-releases). In Banerjee et al. [12] these roles consisted of tainted (adversary controlled) data sources, sanitizer, and vulnerable sinks (data consumers). A source directly connected to a sink without an intermediary sanitizer is considered a defect.

More general kinds of specifications can also be produced, such as separation logic formulas for describing heap structures [69]. Brockschmidt et al. [16] produced separation formulas using hand crafted features describing a graph structure. These hand crafted features were replaced in Li et al. [55] by a graphical neural network, which achieved superior accuracy with minimal manual feature engineering.

CHAPTER 4

Model

The objective of this thesis is to develop a method for learning to identify defects from source-line annotated examples. The proposed approach is to learn which partial subgraphs in a program’s *dependence graph*, a directed graphical representation of the program’s computation dependencies, are correlated with a defect. By considering dependencies between operations (such as subroutine invocations), the proposed approach is particularly suited for identifying defects caused by improper application programming interfaces (APIs) usage. The scope of these graphs is limited to individual subroutines, rather than the entire program, in order to keep their size tractable.

The problem of identifying a specific subgraph is approached bottom-up. Given a vertex v from some graph, we wish to infer the likelihood that v is part of a defect-indicating subgraph based on its k -neighbourhood, $P(v \mid N^k(v))$, where k is a hyper-parameter and $0 \leq k$. The choice of k determines the computational cost of the model and the size of defect subgraphs the model is capable of precisely classifying. Namely, to precisely classify the vertices of a defect subgraph with diameter d , $d \leq k$ is necessary.

The proposed approach can be summarized as follows: Assume a dependence graph $G = (V, E, X, L)$, where X and L are the features for the vertices and edges, respectively. The vertex features X are used to initialize a graph neural network, and the network is updated for k steps to produce a latent embedding for each vertex incorporating information from connected vertices up to k steps away. These latent embeddings are used as embeddings of the vertices’ k -neighbourhoods. Finally, vertices are independently classified using the concatenation of their features with their final graph network state. A depiction of this model is provided in fig. 4.1.

The graphical representation and features are described in section 4.1, followed by the $N^k(v)$ embedding graph neural network in section 4.2, and the objective function for the model

Fig. 4.1: Overview of the proposed classifier. $\diamond$ designates concatenation of feature vectors, FC- n is a fully-connected layer with n outputs, and η_G is a hyper-parameter specifying the width of the $N^k(v)$ embeddings. Layers with a common background colour shared weights.

(section 4.3). For clarity of presentation, the exact values for hyper-parameters selected via hyper-parameter search are defined in the next chapter, in section 5.2.1.

4.1 Representation

In this work, a subroutine is represented by a *dependence graph*, a directed **multigraph** where the subroutine's operations are vertices, and the dependencies between these operations are edges. Vertices and edges are labelled with symbolic (categorical) features describing their actions and operands. Some have pre-determined vocabularies, while others have dataset-defined vocabularies where the vocabulary is specified during fitting. Table 4.2 provides a summary listing of these features.

These representations are primarily produced using Soot [84], a Java byte-code optimization library. It is used to parse Java virtual machine (JVM) byte-code, perform basic semantic analysis, and apply basic compiler optimizations. The representations are derived from their single static assignment (SSA) intermediate representation (IR), Shimple, and each operation generally corresponds to a Shimple instruction.

4.1.1 Dependence Graphs

A dependence graph is a directed **multigraph** where vertices represent operations performed by a program and edges designate dependencies between operations. In principle, these dependencies should include control dependencies for sequencing operations with side-effect. However, I make a simplifying assumption that all operations are **pure functions**. This allows us to ignore control dependencies, which significantly reduces the graph connectivity, incidental neighbourhood diversity, and potential for overfitting. However, this simplification does preclude learning precise discriminators for defects dependent on specific side effect sequences.

Dependence graphs are produced by loading the target program in Soot, applying several basic compiler optimizer with the goal of reducing the program size by eliminating simple redundancies (table 4.1), and extracting the **SSA** data-flow graph (DFG) of the optimized subroutines. No interprocedural analyses or optimizations are used. A second pass of ad-hoc transformations is then applied to the extracted graphs to remove some uninformative artifacts (see section 4.1.2).

An example of a dependence graph and its associated source code is displayed in fig. 4.2. In this example, two related defects have been identified and their inducing lines marked as defective. The first defect is an Structured Query Language (SQL) injection vulnerability, while the second involves reading from a source of potentially tainted data without sanitation.

4.1.2 Graph Simplification

The graphs produced from Soot contain a number of incidental artifacts which are uninformative to a discriminative model. Examples include certain instructions which are (almost) always produced in pairs, explicit ϕ -nodes, and the use of temporary variables for storing the results of sub-expressions, even in situations where there is a single consumer for the result.

Most of these artifacts can be eliminated by applying the following transformations:

Table 4.1: Optimizations performed using Soot, applied in order from top to bottom. None are esoteric and they represent the minimum one would expect from an optimizing compiler.

Soot Optimization Passes
1. Nop Elimination Removes no-op instructions
2. Constant Propagation Simplifies indirect references to constants (e.g. $a = 5$; $b = x \rightarrow a = 5$; $b = 5$)
3. Copy Propagation Simplifies indirect references to variables (e.g. $a = x$; $b = x \rightarrow a = x$; $b = x$)
4. Constant Folding Constant expressions are immediately evaluated (e.g. $1 + 1 \rightarrow 2$)
5. Common Sub-expression Elimination Common sub-expressions are evaluated once (e.g. $a = (x+1)*(x+1) \rightarrow b = x+1$; $a = b*b$;)
6. Dead Assignment Elimination Assignments which have no possible reads are removed
7. Unused Local Elimination Unused variables are removed
8. Unconditional Branch Folding Simplifies branches which always occur (e.g. <code>if (true) { ... }</code>)
9. Unreachable Code Elimination Removes code which could never execute (e.g. <code>if (false) { ... }</code>)

```

public class CWE89_SQL_Injection__listen_tcp_executeUpdate_13 extends AbstractTestCase {
/* ... */
public void bad() throws Throwable {
    String data;
    if (IO.STATIC_FINAL_FIVE==5) {
        /* ... */
        listener      = new ServerSocket(39543);
        socket        = listener.accept();
        /* read input from socket */
        readerInputStream = new InputStreamReader(socket.getInputStream(), "UTF-8");
        readerBuffered    = new BufferedReader(readerInputStream);
        /* POTENTIAL FLAW: Read data using a listening tcp connection */
        data              = readerBuffered.readLine();
        /* ... */
        dbConnection      = IO.getDBConnection();
        sqlStatement       = dbConnection.createStatement();
        /* POTENTIAL FLAW: data concatenated into SQL statement used in executeUpdate(), which
        ↪ could result in SQL Injection */
        int rowCount       = sqlStatement.executeUpdate("insert into users (status) values
        ↪ ('updated') where name='"+data+"'");
        /* ... */
    }
}
/* ... */
}

```

(a) Source code excerpt from a Juliet test case (section 5.1.1). Ancillary lines are omitted.

(b) Subgraph induced by all vertices adjacent to a vertex with a positive label. Defect-labelled vertices are outlined in red.

- i. Fold statement place-holders into their hosted expression. (e.g. `invoke-statement`.)
- ii. Fold local variables onto their right-hand-side expression (RHS) expressions. Since Shimple is an SSA representation, all variable have exactly one RHS expression.
- iii. Replace dependencies onto a ϕ -node by dependencies onto the ϕ -node's transitive dependencies. Any duplicate dependencies are discarded, and all ϕ -nodes are erased.
- iv. Remove null-literal arguments for parameter 0 of non-static functions; such invocations can never succeed at runtime. This is a common artifact caused by a ϕ -fold referencing a null-initialization. If the ϕ -node was transitively dependent on a pre-SSA variable that was reused between otherwise independent sections of code then this can result in significant and spurious connectivity between those sections' connected components within the dependence graph.

An example of a fictional graph being simplified using transformations ii. and iii. is provided in fig. 4.3.

It is important to note that these simplifications generally do not introduce or remove information from the graph. The erased vertices and edges provide no information since their features can be precisely and unambiguously inferred from neighbouring vertices. By removing these uninformative vertices the graphs become less computationally expensive and larger neighbourhoods can be covered for the same number of message passing iterations.

On the Juliet dataset (section 5.1.1) these simplifications reduce the mean vertices per sample from 236.84(145.33) to 29.94(46.5), while on the natural-negative dataset (section 5.1.2) it reduces the mean vertices per sample from 40.09(282.97) to 19.36(144.05).

4.1.3 Vertex & Edge Features

Individual operations and dependencies are described using the features listed in table 4.2. The following subsections describe each feature's purpose and how they are embedded. Not all features necessarily apply to a given operation or dependence, and some features are

Fig. 4.3: Examples of **RHS** and ϕ -dependence simplification (items ii. and iii.). Edge labels denote the operand indices, if applicable. Note the multiple edges in iii..

Table 4.2: List of operation and dependence features.

Host	Feature	Type	Description
Operation	Instruction	Categorical	Action performed by operation.
Operation	Member	Categorical	Any referenced member.
Operation	Result Type	Set of Categorical	The operation result's type .
Operation	Const. Value	Sequence of Categorical	Any referenced constant value.
Dependence	Dep. Type	Categorical	The type of dependence.
Dependence	Operand Index	$\{x \mid x \in \mathbb{Z}, 0 \leq x\}$	Operand's argument index.

conditional upon others. A special non-applicable symbol is used whenever a specific feature does not apply. Note that this symbol is distinct from the out-of-vocabulary (OOV) symbol.

4.1.3.1 Operation Features

An operation v is described by the tuple $X_v = (X_v^{(I)}, X_v^{(M)}, X_v^{(T)}, X_v^{(C)})$, whose components are the operation's *instruction*, *member reference*, *result type*, and *constant value*, respectively. $X^{(I)}$ and $X^{(T)}$ are defined for all operations. $X^{(M)}$ and $X^{(C)}$, however, are only defined for operations with certain instructions. e.g. an operation with a numeric literal instruction must also have a constant value and cannot reference any members.

Note that the symbol vocabularies for $X^{(\Gamma)}$ and $X^{(M)}$ are dataset-defined and are not known prior to fitting.

Instruction ($X^{(I)}$): Specifies the fundamental action performed by an operation. e. g. branch, invocation, addition. This particular implementation uses Shimple’s instruction set. Note that unlike **JVM** byte-code instructions, Shimple instructions are polymorphic, e. g. there is a single instruction for addition for all argument types, and do not use special instructions for common constant values.

This feature uses a predefined-defined symbol vocabulary, and is embedded using a one-hot vector.

Member ($X^{(M)}$): Specifies which, if any, member is referenced by an operation. A member is either a function or a field of an aggregate type. Member symbols consist of their fully qualified name at their point of *initial* declaration.

For fields, this makes no difference (they can only be declared once), but for methods this distinction is important, as dynamic dispatch is equivalent to invoking functions stored as values within fields. For example, consider some defect which only occurs given the invocation of a specific override of an abstract method. Given a program where the abstract method is invoked using dynamic dispatch, it is impossible to know which override should be invoked without knowing the object’s precise type. While this information is available at runtime, it cannot always be precisely determined using static analyses. In a dependence graph, the $X^{(\Gamma)}$ feature of a dynamic dispatch’s first argument (i. e. the dispatching object) can be used to infer a lower bound on the set of overrides which could be invoked.

This feature uses a dataset-defined symbol vocabulary, and uses learned embeddings of width η_E .

Type ($X^{(\Gamma)}$): Specifies the **type** of produced by an operation. The type **void** is used for operations which have no result value. Type symbols consist of their type’s fully qualified name.

Subtyping relationships are modelled using the approach proposed in Allamanis et al. [6],

where a type t is represented by a set of all its supertypes:

$$\Gamma_t = \begin{cases} t & t \in \Gamma \\ \text{OOV} & \text{otherwise} \end{cases} \quad (4.1)$$

$$S(t) = \{ \Gamma_u \mid \forall u. t <: u \} \quad (4.2)$$

where Γ is the model’s type vocabulary. Unlike Allamanis et al. [6], the type arguments of type constructor is not include in this set, as the **JVM**’s type system does not support type constructors.¹

One advantage of using a set-of-supertypes representation is that novel types encountered during testing need only be partially **OOV** if any of its supertypes were seen during fitting. Similarly, it is possible for an **OOV** member to have a (partially) known type, e. g. an **OOV** subroutine which returns a hash map (or some other common type).

This feature uses a dataset-defined symbol vocabulary, and each type in Γ uses a learned embedding of width η_E . This feature itself, however, is a set of supertypes. To capture the notion of set membership each supertype is embedded and the set is reduced by taking the element-wise maximum of its members [6].

During training, a modified variant of dropout is applied where members are randomly dropped from the set, ensuring that each member embedding has the chance to receive some measure of fitting [6, 44]. The technique is similar to regular dropout [79], except that the entire member is removed from the set, rather than setting a random subset of the member’s features to zero. The dropout probability is a tuned hyper-parameter, see section 5.2.1.

Note that this naive dropout approach can result in sets describing absurd type hierarchies. Namely, the presence of some type t does not guarantee that all of t ’s supertypes are also present. This is not a major concern in practice, but a proper approach would ensure that all subtypes of a dropped type are themselves dropped in turn.

¹Languages supporting type constructors use type erasure and dynamic type casts at the use-sites when targeting the **JVM**.

Table 4.3: List of string representations for numeric constants. Rational numbers are represented using whichever format is shortest.

Numeric Constant	Representation Formatting
Integral	Decimal
Rational	Decimal or exponential
Infinite	" +inf ", " -inf "
NaN	"NaN"

Constant Value ($X^{(C)}$): Specifies which, if any, constant value is used by an operation.

Constant values are limited to scalars and string literals.

All constants are represented as sequences of Unicode Text Format 8-bits (UTF-8) symbols; numeric constants are formatted as specified in table 4.3.

Constant values are reduced to an embedding $\mathbf{x} \in \mathbb{R}^{\eta_E}$ using a stack of convolution layers, rather than a recurrent network. This is primarily motivated by speed and simplicity concerns [14, 48, 82, 94].² The sequence of characters is first truncated or null-padded to a fix length 2^n , and each character projected using a learned embedding of width η_E . The sequence of dense embeddings is then reduced using a stack of n 1d convolutions, where each convolution uses a window and stride of 2, halving the the sequences at each layer. This encoder network is admittedly ad-hoc, but fast and efficient.

For the datasets used in chapter 4 (section 5.1), $n = 7$ is more than sufficient since as the mean length for a literal is 23.4(15.5) elements.³

4.1.3.2 Dependence features

A dependence $e = a \rightarrow b$ is described by $L_e = (L_e^{(Q)}, L_e^{(O)})$, where $L_e^{(Q)}, L_e^{(O)}$ are e 's *dependence type* and *operand index*, respectively.

Dependence Type ($L^{(Q)}$): Specifies the type of dependence between two operations. A listing of all dependence types is provided in table 4.4. This is a symbolic feature with a

²A bidirectional Long Short-Term Memory (LSTM) was initially used, but later abandoned as the computational overhead was unacceptable.

³This excludes the 100 largest outliers ($\approx 0.01\%$) as these are abnormally large, ranging in length from 470 to 48548. These outliers include command line help strings, documentation, and encoded binary blobs (lexer and parser tables, public keys, etc).

Table 4.4: List of dependence types.

Dependence Type	Operand Index
Assignment	
Index Base	
Index Expression	
Operand	✓

predefined dictionary of length 4. It is embedded as a one-hot vector.

Operand Index ($L^{(O)}$): Designates to which parameter an argument is applied. The index is zero based, and the ‘self’ argument of a method invocation uses index 0 by convention.

This feature is embedded as a one-hot vector of length 16. Operand indices above 15 are clamped to 15. While its domain is, in principle, unbound, in practice there are extremely few functions use more than a dozen parameters. The choice of 16 is arbitrary but is more than sufficient for non-contrived functions.⁴

4.2 Neighbourhood Embedding

The embedding $\mathbf{h}_v^k$ of operation v ’s k -neighbourhood $N^k(v)$ is generated using a graph neural network with a gated update function similar to a Gated Recurrent Unit (GRU). Assume a multi-digraph $G = (V, E, X, L)$ consisting of the set of vertices V , the directed edges E , and the vertex and edge features X and L . The update equations for this network are

$$\mathbf{m}_{e_{ij} \in E}^t = \tau(\mathbf{W}_m[L_e, \mathbf{h}_i^t] + \mathbf{b}_m) \quad (4.3a) \quad \mathbf{z}_v^t = \tau\left(\mathbf{W}_z \sum_{e_{iv} \in E} \mathbf{m}_{e_{iv}}^t + \mathbf{b}_z\right) \quad (4.3b)$$

$$\mathbf{u}_v^t = \sigma(\mathbf{W}_u[\mathbf{h}_v^t, \mathbf{z}_v^t] + \mathbf{b}_u) \quad (4.3c) \quad \mathbf{h}_v^0 = \mathbf{W}_{\text{init}} X_v \quad (4.3d)$$

$$\mathbf{r}_v^t = \sigma(\mathbf{W}_r[\mathbf{h}_v^t, \mathbf{z}_v^t] + \mathbf{b}_r) \quad (4.3e) \quad \mathbf{h}_v^{t+1} = (1 - \mathbf{u}_v^t) \odot \mathbf{h}_v^t + \mathbf{u}_v^t \odot (\mathbf{z}_v^t + \mathbf{r}_v^t \odot \mathbf{h}_v^t) \quad (4.3f)$$

Equation set 4.3: Update equations for $N^k(v)$ embedding network.

where $\mathbf{h}_{v \in V} \in \mathbb{R}^{k \times \eta_G}$, and both k and η_G are hyper-parameters.

⁴For the primary dataset defined in section 5.1, the mean operand index for operand dependencies is 0.722 (0.95) and the max index is 22.

The initial state of a vertex v , $\mathbf{h}_v^0$, is initialized based upon its features X_v . The learned projection $\mathbf{W}_i$ allows varying the symbol embedding width η_E and the N^k embedding width η_G independently of one another. If the choice of hyper-parameters results in $X \in \mathcal{R}^{|V| \times N}$ and $N \leq \eta_G$ then X is simply zero padded to $\mathcal{R}^{|V| \times G}$. Message passing is performed for k steps to produce the sequence $(\mathbf{h}_v^0, \mathbf{h}_v^1, \dots, \mathbf{h}_v^k)$. The final step, $\mathbf{h}_v^k$, is concatenated with X_v and feed through a multi-layer perceptron (MLP) for classification.

Note that information only flows along the directed edges of the graph. Consider an acyclic graph G and its sources $V_{\text{src}} = \{v \mid v \in V, \forall x \in V. (v \rightarrow x) \notin E\}$. If one were to assemble $N^i(v)$ based on outbound edges then $\forall v \in V_{\text{src}}, 0 \leq i. N^0(v) = N^i(v)$. The same general problem extends to non-source vertices. G is therefore augmented with its reversed-dependence edges in order to include the dependants of v in $\mathbf{h}_v$. These reversed edges are marked as such by using reversed variants for their Dependence Type feature. e. g. An **operand** edge $a \rightarrow b$ induces a **reverse-operand** edge $b \rightarrow a$. Reverse-dependence edges are excluded from all figures in the interests of visual clarity.

Messages are aggregated by summation eq. (4.3b), although it would be preferable to aggregate them using their element wise maximum. While counting aggregation (summation) subsumes presence aggregation (max), our task only requires the latter as defects are generally dependent only on the presence of specific symbol paths. Preliminary experiments showed that max-aggregation provides a modest improvement over summation, though in exchange for a substantial increase in memory and computation during training.

This architecture differs from a classic **GRU** in that it handles the recurrence term as a gated residual-like connection. The recurrence term $\mathbf{h}_v^i$ is not projected, and it is used in eq. (4.3f) rather than as an input to the activation function. Moving $\mathbf{h}_v^i$ outside of saturating activation avoids hidden unit saturation (typically mitigated in **GRUs** by the projection), which in turn reduces gradient attenuation for earlier states. The resulting design bears notable similarity to chaos-free recurrence cells [51], though it inherits an activation bias and double-gated resets from **GRUs**.

These alterations from a classic **GRU** are motivated by two factors. Firstly, updating a vertex

v with an $N^k(v) = \{v\}$ should, intuitively, be an idempotent action. Formally, I define this to mean that the sequence $(\mathbf{h}_v^0, \mathbf{h}_v^1, \dots)$ should be element-wise monotonic. Secondly, delayed recurrence-like connections are implicitly formed by the addition of reverse-dependence edges. Note that removing the input recurrence from eq. (4.3b) is technically insufficient for idempotent updates of edgeless vertices due to possible interactions between $\mathbf{b}_z$ and the recurrence connections in $\mathbf{u}_v^t$ and $\mathbf{r}_v^t$ (an example is provided in eq. (A.1)). In practice the fitted cells exhibit consistent $\mathbf{h}_v$ sequences when driven with null inputs, despite this potential interaction. Further information on this topic, including $\mathbf{h}_v$ transition plots, is provided in Appendix A.

4.3 Objective Function

The model is fitted by minimizing the vertices' cross-entropy. Assume a labelled dataset $\mathcal{D}$ where $(x, \mathbf{y}) \in \mathcal{D}$, $x = (V, E, X, L)$, and $\mathbf{y} \in \{0, 1\}^{|V|}$. Let the model prediction be $\hat{\mathbf{y}}$. The objective function is

$$\mathcal{L}(\theta, \phi) = \sum_{((V, E, X, L), \mathbf{y}) \in \mathcal{D}} \sum_{v \in V} H(\mathbf{y}_v, \hat{\mathbf{y}}_v) + \lambda \mathcal{R}(X_v, \theta) + \lambda \|\phi\|_2 \quad (4.4)$$

$$\mathcal{R}(X_v, \theta) = \sum_{X_v^{(\Gamma)} <: u} \|\theta_u^{(\Gamma)}\|_2^2 + \|\theta_{X_v^{(M)}}^{(M)}\|_2^2 \quad (4.5)$$

$$\hat{\mathbf{y}}_v = \text{MLP}(\mathbf{h}_v^k, X_v) \quad (4.6)$$

where $H(y, \hat{y})$ is the binary cross-entropy between a ground truth label y and a predicted label $\hat{y}$, $\theta_j^{(i)}$ is the learned embedding for symbol j of symbol vocabulary i (e.g. the Types symbol `boolean`), and ϕ consists of all other model parameters. The only unusual aspect of this loss function is the regularization term Equation (4.5), which imparts a term-frequency loss penalty on the learned embeddings for dataset-defined symbols.

Training and inference procedures for this model are effectively the same as those for a standard feed-forward network. Parameter optimization is done using stochastic gradient descent with RMSProp [83]. Since the number of message passing iterations, k , is a hyper-

parameter constant, the neighbourhood embedding network stack (the $N^k(v)$ block in fig. 4.1) can be implemented by simply unrolling the sequence.

CHAPTER 5

Experiments

The proposed approach is evaluated using various software projects and a number of test suits, as well as its ability to transfer to unseen projects.

Most experiments report two sets of metrics: vertex-level, and sample-level. These correspond to two different scoring methodologies. Vertex-level metrics represent the ability of the model to classify fine-grain details within a sample, and are applied to each vertex within a sample. Sample-level metrics represent the ability of the model to accurately classify a sample with no regards as to fine-grain accuracy. These metrics are applied to each sample as a whole, rather than its vertices. A sample’s ground truth and predicted likelihood is the maximum of its vertices’, i.e. it is defective if any of its vertices are defective. Sample-level metrics are expected to be much easier to learn, and offer a good proxy metric

Details regarding datasets are presented first, followed by model hyper-parameters and evaluation results. More information regarding the various metrics used in these experiments can be found in Appendix [C](#).

5.1 Datasets

To the best of my knowledge, there exists no standard benchmark dataset for identifying specific expressions within a realistic program. I therefore assembled a new using open source projects and static analysis test suites. These projects can be categorized as either synthetic, natural-negative, or natural-defective, depending on the nature of their code. The size and usage of these categories is listed in table [5.1](#). Projects belonging to the synthetic and natural-negative were combined to produce the primary dataset used for training and testing. This dataset was partitioned 0.6/0.1/0.3 for training, development, and evaluation, respectively. By contrast, projects in the natural-defective category were only used for

Table 5.1: Population and contents of sources used for the datasets. Despite its name the natural-defective dataset is expected to contain a mix of positive and negative samples.

Project	Category	# of Samples	Pos. Samples	Training	Eval.	Transfer	Eval.
	Synthetic	4081	✓	✓	✓		
	Natural (Negative)	155809		✓	✓		
	Natural (Defective)	6586	✓				✓

evaluating the fitted model’s ability to transfer to unseen natural code.

These categories are further described in the subsections below. Note that these datasets require some special handling, which is discussed in section 5.1.4.

5.1.1 Synthetic Projects

The synthetic category consists of Juliet [60], a test suite for evaluating static analyzers. It consists of several thousand test cases, the majority of which are synthetic variants of some base defect, and covers 74 Common Weakness Enumerations (CWEs).

Synthetic test cases are derived from examples using a template system and allows for the systematic evaluation of an analyzer’s ability to handle several variations of a defect. These variants can be classified into four categories: Base cases, control-flow dependent variants, intra-subroutine data-flow dependant variants, and interprocedural variants. Each subsequent variant increases the difficulty of the task. The first three generally only require reasoning about the contents of a single subroutine,¹ while the last extends the problem across several subroutines and requires interprocedural analysis (IPA) to solve precisely.

A specific subset of **CWEs** offered by Juliet is used for these experiments, a listing of which can be found in table 5.2. All variants were used, including the interprocedural data-flow variants.

The difficulty of identifying a specific partial subgraph depends in part on the size of the partial subgraph in question. Statistics regarding the radii of various classes of subgraphs within the dataset is available in table 5.3. A typical positive label induced subgraph consists

¹Some control flow variants do require reasoning about possible return values.

Table 5.2: Population statistics for the utilized subset of Juliet. A sample consists of a single subroutine, and is considered positive if, and only if, it contains a vertex with a positive label.

Common Weakness Enumeration	Kind	Per Sample			Per Vertex		
		Count	% Tot.	% Pos.	Count	% Tot.	% Pos.
HARD_CODE_KEY	Original	261	0.49	18.39	3370	0.16	7.29
	Simplified	65	1.59	43.07	1746	0.37	7.96
HTTP_RESPONSE_SPLITTING	Original	12012	22.82	21.67	319554	15.23	2.84
	Simplified	926	22.69	46.43	67176	14.39	3.02
LDAP_INJECTION	Original	3348	6.36	25.53	133958	6.38	4.52
	Simplified	176	4.31	78.40	22750	4.87	5.48
SQL_INJECTION_JDBC	Original	21250	40.38	23.81	1262116	60.18	2.40
	Simplified	1788	43.81	37.47	282164	60.48	2.10
UNVALIDATED_REDIRECT	Original	2349	4.46	22.09	45957	2.19	1.76
	Simplified	118	2.89	81.35	8325	1.78	2.34
XPATH_INJECTION	Original	4004	7.60	21.67	150110	7.15	4.40
	Simplified	404	9.89	33.16	41472	8.88	3.90
XSS	Original	9396	17.85	18.86	181920	8.67	7.35
	Simplified	604	14.80	69.53	42869	9.18	7.77
Total	Original	52620	100.0	22.28	2096985	100.0	3.17
	Simplified	4081	100.0	46.94	466502	100.0	3.11

Table 5.3: Subgraph radii for the connected components within the Juliet dataset.

Connected Component	Radius
Non-singleton	6.3 ± 11.8
Pos. label connected	51.4 ± 29.0
Pos. label adjacent	9.3 ± 5.8
Pos. label induced	6.7 ± 5.2

roughly of a fifth of its connected component ($\mu = 0.25$, $\sigma = 0.24$). Note that a sample may contain multiple connected components.

5.1.1.1 Labelling

The intended usage for Juliet is to evaluate an analyzer against each test case, where a given test case may span several subroutines or files. As such, it had to be adapted to fit the finer grain labelling scheme.

Special code comments in juliet were exploited to produce a dataset with per-vertex labels. These special comments annotate locations where a defect could manifest or where a defect mitigation occurs. Defects and mitigations are marked by code comments beginning with

the string `FLAW` or `POTENTIAL FLAW`, and `FIX`, respectively. Examples for both are shown in listing 5.1. Note that defect annotation comments are pessimistic and exist even if defect mitigation occurs within the same subroutine.

Algorithm 1 describes the algorithm used to extract labels from Juliet annotations for a single subroutine. The only notable complication has to do with a control flow test variant where a mitigation path exists but is triggered unpredictably. The mitigation in this test case variant is ignored as it is unreliable (line 4 of algorithm 1). Note that vertices may appear on multiple (non-contiguous) lines, e. g. subroutine parameters.

No interprocedural propagation of annotations was performed. As a result, samples derived from interprocedural variants were pessimistically labelled and thus imply that all subroutine parameters are potentially tainted.

Algorithm 1 Juliet label extraction algorithm

```

1: procedure LABEL(subroutine)
2:   label all vertices negative
3:   if subroutine name start with “bad”  $\vee$  no mitigation annotation in subroutine then
4:     for each defect annotation do
5:        $l \leftarrow$  nearest non-whitespace line
6:       mark all vertices appearing on line  $l$  as positive
7:     end for
8:   end if
9: end procedure

```

5.1.2 Natural-Negative Projects

The natural-negative category of projects consists of those which contain no defects of the kind modelled in Juliet. These served both as examples of natural code during training, contrasting with the synthetic nature of Juliet, and as a baseline for evaluating false positive rate of the fitted model. A complete listing of projects appearing in this category is provided in table B.1.

```

public void badSink(String dataArray[], /* ... */) {
    String    data = dataArray[2];
    /* ... */
    Statement s = dbConnection.createStatement();
    /* POTENTIAL FLAW: ... */
    Boolean   r = s.execute("insert into users (status) values ('updated') where
↪   name="+data+"'");
    if(r) { /* ... */ }
}

```

(a) Reduced example from test case (CWE89, `execute`, variant 66). Lines annotated as defective are highlighted in red. Note that any mitigation annotations in this subroutine would be ignored since the subroutine's name begins with “bad”.

```

public void hypotheticalGoodSink(String dataArray[], /* ... */) {
    /* FIX: use hardcoded string */
    dataArray[2] = "foo";
    String    data = dataArray[2];
    /* ... */
    Statement s = dbConnection.createStatement();
    /* POTENTIAL FLAW: ... */
    Boolean   r = s.execute("insert into users (status) values ('updated') where
↪   name='"+data+"'");
    if(r) { /* ... */ }
}

```

(b) Hypothetical fixed variant of [a](#). The mitigation annotation is highlighted in green, and the defect annotation is ignored.

Listing 5.1: Reduced example of a Juliet test case.

Table 5.4: Population statistics for natural-defective projects.

Project	Samples			Vertices	
	Count	% Tot.	% Pos.	Count	% Tot.
Facebroke	469	7.12	Unk.	18805	4.78
JavaVulnerableLabs	470	7.13	Unk.	22027	5.60
OWASP Benchmark*	2740	41.60	51.6%	280843	71.47
STONESOUP-INJ-1	1837	27.89	Unk.	56830	14.46
Vuln-WebApps-Piggybank	38	0.57	Unk.	355	0.09
WebGOAT	1032	15.66	Unk.	14054	3.57
Total	6586	100.0	Unk.	392914	100.0

* All subroutines from a given test case are merged into a single sample.

5.1.3 Natural-Defective Projects

The natural-defective category of projects consists of those which deliberately contain defects. These defects span several **CWEs**, including ones not present within the synthetic set. These projects were used to evaluate the ability of the model to transfer to natural code. A complete listing of projects appearing in this category is provided in table 5.4.

Most of these projects do not contain negative counterparts to positive samples, nor have they annotations or labels of any kind, making them unsuitable for inclusion in training set given a purely supervised approach. The OWASP Benchmark project is a partial exception as it possesses both a mix of positive and negative test cases for various **CWEs**, in addition to sample-level labels. However, the OWASP Benchmark also makes extensive use of test cases spanning multiple subroutines, in addition to storing tainted and untainted data within the same data structures.² The former is of particular note as it runs counter to the simplifying intra-subroutine-scope assumption and the pessimistic labelling specified for Juliet in section 5.1.1. This project should therefore be considered a particularly challenging unseen dataset.

²I have doubts regarding the representativeness of test cases mixing tainted and untainted information in data structures solely to complicate analysis. e. g. test cases which require reasoning about key-value pairs within the same map structure. These seem somewhat unrealistic.

5.1.4 Dataset Extraction & Handling

These datasets have a number of quirks which merit mention. These are enumerated below, along with any applied mitigations. All of these issues are related to various kinds of data imbalance.

5.1.4.1 Vertex-Label Imbalance

The most obvious imbalance is ratio of vertex-level class labels, with only 3.11% of vertices labelled as positive (defective).

The usual approaches for dealing with unbalanced classes involve either weighing the objective function such that expected loss for each class is equal, or altering the proportions of each class within the training set such that the classes are no longer imbalanced. The latter can be accomplished by resampling the minority classes or subsampling the majority classes.

However, none of these standard approaches are clearly applicable to this dataset. Subsampling and resampling can only be done at the sample level, which is already relatively balanced (46.94% of Juliet samples are positive). Weighing the objective function is also undesirable as each class has sufficient distinct feature distributions (see below, section 5.1.4.3) to roughly discriminate between them. This can be show by noting the vertex level receiver operating characteristics (ROC) area under curve (AUC) of the $k = 0$ model is near perfect (0.98, see table 5.7).

Given the above, no changes were applied to the dataset nor the objective function. However, care was taken to ensure all partitioning is done using stratified sampling based upon both class and **CWE** (see below).

5.1.4.2 Test Case Imbalance

The number of samples and, indirectly, test cases, for a given **CWE** varies wildly in Juliet ($\mu = 583$, $\sigma = 613$). Subsampling is not feasible, due to some **CWEs** having very few samples, e. g. **HARD_CODE_KEY**, and super-sampling would result in grossly exaggerated importance

on the smallest minority classes. Loss reweighing is, again, unhelpful as the active symbol vocabularies can vary significantly between **CWEs**.

This is partially mitigated by using stratified sampling when partitioning the datasets.

5.1.4.3 Symbol Vocabulary

A common approach for modelling a large vocabulary of symbols with a non-uniform usage distribution is keep the most frequently occurring symbols and substitute the remainder with a single out-of-vocabulary (OOV) marker. This approach is not well suited for our task, as a given defect may require the presence of some specific, but rarely-occurring, symbol.

On the other hand, using a vocabulary consisting of every symbol encountered during training greatly increases the likelihood of learning a spurious relationship relating an incidental symbol and a defect. Such spurious relations are not limited to infrequently occurring symbols. An example of this can be seen in listing 5.2. A related problem concerns extremely rare symbols, whose occurrence can be used to trivially memorize the training set. A prototypical example of this is show in listing 5.3.

One solution is to select the vocabulary based on the intersection of symbols appearing both in Juliet and in either the natural-negative dataset or the standard Java libraries:

$$\mathbb{S}_{\text{Active}} = \mathbb{S}_{\text{Juliet}} \cap (\mathbb{S}_{\text{NatNeg}} \cup \mathbb{S}_{\text{Java}})$$

Where $\mathbb{S}_{\text{Juliet}}$, $\mathbb{S}_{\text{NatNeg}}$ and $\mathbb{S}_{\text{Java}}$ are the vocabularies used by Juliet, the natural-negative projects, and the Java standard libraries, respectively.

This avoids introducing symbols which appear only in negative contexts, eliminates incidental symbols unique to Juliet, and preserves rarely occurring, but non Juliet specific, symbols.

5.1.4.4 Duplicate Samples

Subroutine duplicates are not uncommon within most programs. These typically arise either due to inlined copies of a library, copy and pasted code, or as artefacts of the compiler's

```

k = " \"constant\" ";
c = testcasesupport.IO.getDBConnection();
s = c.createStatement().execute("select ... where name = " + k);

```

Listing 5.2: The symbol `testcasesupport.IO.getDBConnection` is relatively common within Juliet but never appears in other projects, allowing one to infer which project produced this sample. Note that the symbol `SqlStatement::execute`, used on line 3, occurs less frequent than `testcasesupport.IO.getDBConnection` within the Juliet corpus.

```

class DefectTestCase1 {
    String data;
    void foo()
    { /* defective code using `DefectTestCase1::data` */ }
}

```

Listing 5.3: If the symbol `DefectTestCase1::data` is extremely rare, one can effectively memorize `DefectTestCase1::foo` based upon the symbol’s presence. The same issue can also occur through the type attribute of the implicit parameter `this`. Both cases require the defect subgraph to be connected to rare-symbol vertex, or that the model performs some sort of sample aggregation, e.g. continuous bag of words.

code generation. Roughly 3% to 5% of samples drawn from the projects were found to be duplicates and were discarded to avoid biasing the evaluation. Duplicates were identified by keying on the SHAKE-256 of their decompiled source code representation using fully qualified types. This deduplication pass served mainly as a quick a filter for removing trivial duplicates from the dataset.

A second deduplication pass was performed after graph simplification (section 4.1.2) and vocabulary handling (section 5.1.4.3), as both of these processes can cause previously distinct graphs to become equivalent. In this second pass, duplicates were identified and discarded using a graph isomorphism test [20]. Samples in the second pass were considered duplicates if, and only if, their graphs were isomorphic and they had identical labels. The consideration of the labels is necessary as many of the applied transformations are not injective. A single instance is kept for each distinct graph and label pair.

Table 5.5: Initializers for model parameters.

Parameter Type		Initialization
Symbol Embeddings	Uniform Random	$\in [-1, 1]$
Recurrence Parameters ³	Identity Matrix	[52]
Others	Glorot Uniform	[29]

5.2 Training Protocol

All models, including baseline variants, were fitted using the same protocol. Parameters are initialized as per table 5.5 and optimized using RMSProp [83] without momentum. Training continued until the average vertex cross-entropy on the development set failed to decrease by at least 0.5% over 10 epochs, or 500 epochs elapsed. Samples were aggregated into mini-batches of 15k vertices (≈ 575 samples) and shuffled each epoch.

5.2.1 Hyper-parameters

Hyper-parameters not specified in chapter 4 were selected by a grid-search using the training and development subsets. All hyper-parameter values, including those chosen manually, are enumerated in table 5.6.

Hyper-parameters were chosen in groups, designated by the partitioning in table 5.6, in order to limit the overall search domain. For example, while selecting regularization and network width, the learning rate was held at 10^{-4} . Parameters were chosen based on lowest cross-entropy on the development set after twenty epochs.

5.3 Primary Results

The proposed model is evaluated using neighbourhood sizes $k \in [0, 10]$. In addition to these, a continuous bag of words (CBOW) like model variant is also evaluated, where the $N^k(v)$

³Recurrence parameters are only used by the classic GRU variant in Appendix A. The proposed model has a recurrence connection, but does not (directly) project it.

Table 5.6: List of hyper-parameters. This table also include hyper-parameters which are chosen manually. Parameters sharing the a common background colour were selected jointly using a grid search over their listed domains.

Hyper-parameter	Value	Domain
Learning Rate	10^{-4}	$10^{[-5, -3]}$
Supertype Drop Rate	0.2	0, 0.05, 0.1, 0.2, 0.3
L2 Regularization (λ)	10^{-1}	$0, 10^{[-3, 0]}$
N^k Embedding Width (η_G)	128	$2^{[5, 7]}$
Symbol Embedding Width (η_E)	32	$2^{[4, 6]}$
Max Const. Val. Length	2^7	<i>Manual</i>
Max Operand Index	16	<i>Manual</i>
Batch Size	15k Vertices	<i>Manual</i>
RMSProp Decay	0.9	<i>Manual</i>

embedding $\mathbf{h}_v^k$ was replaced with:

$$h_v^{\text{CBOW}} = \tau(\mathbf{W} \sum_{v \in V} X_v + |V|\mathbf{b}) \quad (5.1)$$

The $k = 0$ and **CBOW** models serve as baselines. Neither made use of dependence features nor the graphs’ connectivity structure. Each experiment used a 5-fold evaluation with different random initialization for each fold, and the variance between folds reported. Each model used the same k-fold splits.

The results are tabulated in table 5.7 and fig. 5.1, and a breakdown of the $k = 10$ model per **CWE** and test case variant is provided in table 5.8. Figure 5.2 compares the models’ performance against FindSecBugs [10], an open source static analyzer for security defects. Unlike the proposed models, FindSecBugs makes use of interprocedural analyses, and often reports incidental defects or suggestions. In order to make a fair(er) comparison between FindSecBugs and the proposed approach, the following scoring protocol was used: A FindSecBugs prediction was considered correct if reported the correct **CWE**⁴ for the test case, and the report mentioned either the vulnerable sink method (“bad sink”) or the entry point for the test case (the “bad method”). If no predictions involved a given test case’s “bad method”, then it was considered a false negative.

⁴This need not be an exact match; there exists some overlap between **CWEs**. e.g. **CWE** 79, 80, 81, and 83 are all variants on XSS.

Except for $k = 0$ baseline, all models achieved excellent performances in terms of **ROC**, average precision (AP), and ϕ Coefficient. Performance generally improved as k increases, with rapid gains up to $k = 4$ followed by diminishing returns past $k = 6$. This inflection point is likely related to the typical radius for a non-singleton connected component or label-induced subgraph, see table 5.3 and the no-vertex-feature $k = 5$ variant in section 5.3.1.

The **CBOV** baseline proved to be a strong baseline despite having no access to the connectivity of the graph or edge features. It outperformed other models for most sample-level metrics, and was competitive on vertex-level metrics against models up to $k = 4$. However, it completely failed to transfer to unseen projects (see section 5.4).

5.3.1 Feature-set Ablation

As mentioned in section 4.1.3, while each feature does provide some information which cannot be inferred from others, none are completely independent: A member reference imparts an upper-bound on the result type of the operation. Similarly, a constant value affects the type due to the small number of constant value types, and the instruction determines whether a member or constant value is used.

In order to evaluate the utility of each operation feature for the primary dataset, a series of experiments was conducted using the **CBOV**, $k = 0$, and $k = 5$ models. Given the small number of operation features and their interdependencies this can be achieved with reasonable overhead by producing model variants fitted using various subsets of the vertex features. Edge features were not ablated in this experiment.

The results are tabulated in table 5.9. Note that the metrics reported in table 5.9 exclude samples from natural-negative projects. This was done to avoid saturating metrics sensitive to the relative size of the negative class. An equivalent listing considering all samples is provided in table D.1.

The results are generally as one would expect, with the member feature proving to be the most informative feature for all models, followed by the type or constant value, and the instruction as the least informative feature for this dataset. While baseline models are

Table 5.7: Results for various models against the Juliet + Natural-Negative dataset. Baseline models are **CBOW** and $k = 0$. The **ROC AUC** is saturated due to the size of the natural-negative dataset. A modestly clearer visualization of the **ROC** is available in fig. 5.1.

Model	Scope	Mean Cross-Entropy				Avg. Precision				Best ϕ Coefficient				ROC Area Under Curve			
		Train		Test		Train		Test		Train		Test		Train		Test	
		μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ	μ	σ
cbow	Sample	3 · 10 ⁻³	±508 · 10 ⁻⁶	1 · 10 ⁻³	±181 · 10 ⁻⁶	0.999	±160 · 10 ⁻⁶	0.996	±3 · 10 ⁻³	0.868	±3 · 10 ⁻³	0.989	±2 · 10 ⁻³	0.999 97	±8 · 10 ⁻⁶	0.999 92	±44 · 10 ⁻⁶
	Vertex	2 · 10 ⁻³	±72 · 10 ⁻⁶	2 · 10 ⁻³	±214 · 10 ⁻⁶	0.958	±1 · 10 ⁻³	0.964	±2 · 10 ⁻³	0.861	±2 · 10 ⁻³	0.874	±4 · 10 ⁻³	0.999 61	±19 · 10 ⁻⁶	0.999 68	±29 · 10 ⁻⁶
	Sample	25 · 10 ⁻³	±450 · 10 ⁻⁶	24 · 10 ⁻³	±1 · 10 ⁻³	0.701	±11 · 10 ⁻³	0.697	±7 · 10 ⁻³	0.667	±6 · 10 ⁻³	0.678	±5 · 10 ⁻³	0.984 76	±394 · 10 ⁻⁶	0.985 85	±175 · 10 ⁻⁶
k = 0	Vertex	16 · 10 ⁻³	±369 · 10 ⁻⁶	15 · 10 ⁻³	±516 · 10 ⁻⁶	0.378	±6 · 10 ⁻³	0.374	±7 · 10 ⁻³	0.416	±4 · 10 ⁻³	0.427	±7 · 10 ⁻³	0.976 39	±578 · 10 ⁻⁶	0.979 85	±1 · 10 ⁻³
k = 1	Sample	15 · 10 ⁻³	±662 · 10 ⁻⁶	14 · 10 ⁻³	±2 · 10 ⁻³	0.839	±12 · 10 ⁻³	0.854	±18 · 10 ⁻³	0.769	±17 · 10 ⁻³	0.805	±27 · 10 ⁻³	0.990 52	±891 · 10 ⁻⁶	0.992 15	±1 · 10 ⁻³
	Vertex	9 · 10 ⁻³	±199 · 10 ⁻⁶	9 · 10 ⁻³	±603 · 10 ⁻⁶	0.643	±3 · 10 ⁻³	0.654	±11 · 10 ⁻³	0.633	±3 · 10 ⁻³	0.651	±5 · 10 ⁻³	0.993 66	±221 · 10 ⁻⁶	0.993 99	±639 · 10 ⁻⁶
	Sample	6 · 10 ⁻³	±229 · 10 ⁻⁶	6 · 10 ⁻³	±832 · 10 ⁻⁶	0.952	±2 · 10 ⁻³	0.947	±7 · 10 ⁻³	0.855	±3 · 10 ⁻³	0.865	±12 · 10 ⁻³	0.996 69	±106 · 10 ⁻⁶	0.996 63	±645 · 10 ⁻⁶
k = 2	Vertex	5 · 10 ⁻³	±135 · 10 ⁻⁶	5 · 10 ⁻³	±323 · 10 ⁻⁶	0.845	±2 · 10 ⁻³	0.840	±5 · 10 ⁻³	0.768	±3 · 10 ⁻³	0.773	±5 · 10 ⁻³	0.998 29	±34 · 10 ⁻⁶	0.998 35	±119 · 10 ⁻⁶
	Sample	3 · 10 ⁻³	±325 · 10 ⁻⁶	3 · 10 ⁻³	±770 · 10 ⁻⁶	0.978	±2 · 10 ⁻³	0.979	±3 · 10 ⁻³	0.919	±8 · 10 ⁻³	0.936	±4 · 10 ⁻³	0.998 70	±141 · 10 ⁻⁶	0.998 76	±198 · 10 ⁻⁶
	Vertex	2 · 10 ⁻³	±146 · 10 ⁻⁶	2 · 10 ⁻³	±309 · 10 ⁻⁶	0.948	±4 · 10 ⁻³	0.952	±3 · 10 ⁻³	0.879	±6 · 10 ⁻³	0.887	±4 · 10 ⁻³	0.999 49	±52 · 10 ⁻⁶	0.999 52	±99 · 10 ⁻⁶
k = 3	Sample	2 · 10 ⁻³	±348 · 10 ⁻⁶	2 · 10 ⁻³	±222 · 10 ⁻⁶	0.991	±1 · 10 ⁻³	0.989	±2 · 10 ⁻³	0.940	±5 · 10 ⁻³	0.948	±7 · 10 ⁻³	0.999 52	±71 · 10 ⁻⁶	0.999 47	±71 · 10 ⁻⁶
	Vertex	1 · 10 ⁻³	±58 · 10 ⁻⁶	1 · 10 ⁻³	±75 · 10 ⁻⁶	0.983	±2 · 10 ⁻³	0.983	±2 · 10 ⁻³	0.931	±3 · 10 ⁻³	0.936	±3 · 10 ⁻³	0.999 81	±21 · 10 ⁻⁶	0.999 74	±75 · 10 ⁻⁶
	Sample	1 · 10 ⁻³	±429 · 10 ⁻⁶	2 · 10 ⁻³	±1 · 10 ⁻³	0.997	±1 · 10 ⁻³	0.995	±2 · 10 ⁻³	0.965	±8 · 10 ⁻³	0.975	±5 · 10 ⁻³	0.999 84	±64 · 10 ⁻⁶	0.999 84	±155 · 10 ⁻⁶
k = 4	Vertex	444 · 10 ⁻⁶	±85 · 10 ⁻⁶	483 · 10 ⁻⁶	±121 · 10 ⁻⁶	0.998	±886 · 10 ⁻⁶	0.997	±699 · 10 ⁻⁶	0.978	±5 · 10 ⁻³	0.979	±6 · 10 ⁻³	0.999 96	±20 · 10 ⁻⁶	0.999 84	±155 · 10 ⁻⁶
	Sample	1 · 10 ⁻³	±544 · 10 ⁻⁶	2 · 10 ⁻³	±576 · 10 ⁻⁶	0.999	±613 · 10 ⁻⁶	0.997	±2 · 10 ⁻³	0.988	±6 · 10 ⁻³	0.985	±6 · 10 ⁻³	0.999 94	±31 · 10 ⁻⁶	0.999 78	±167 · 10 ⁻⁶
	Vertex	319 · 10 ⁻⁶	±77 · 10 ⁻⁶	260 · 10 ⁻⁶	±73 · 10 ⁻⁶	0.999	±342 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.988	±5 · 10 ⁻³	0.991	±4 · 10 ⁻³	0.999 98	±7 · 10 ⁻⁶	0.999 77	±312 · 10 ⁻⁶
k = 5	Sample	1 · 10 ⁻³	±302 · 10 ⁻⁶	2 · 10 ⁻³	±557 · 10 ⁻⁶	0.999	±210 · 10 ⁻⁶	0.997	±851 · 10 ⁻⁶	0.986	±3 · 10 ⁻³	0.984	±6 · 10 ⁻³	0.999 97	±10 · 10 ⁻⁶	0.999 83	±104 · 10 ⁻⁶
	Vertex	242 · 10 ⁻⁶	±37 · 10 ⁻⁶	2 · 10 ⁻³	±103 · 10 ⁻⁶	0.999	±240 · 10 ⁻⁶	0.998	±836 · 10 ⁻⁶	0.990	±3 · 10 ⁻³	0.991	±6 · 10 ⁻³	0.999 97	±21 · 10 ⁻⁶	0.999 90	±99 · 10 ⁻⁶
	Sample	748 · 10 ⁻⁶	±384 · 10 ⁻⁶	2 · 10 ⁻³	±981 · 10 ⁻⁶	0.999	±451 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.989	±4 · 10 ⁻³	0.989	±3 · 10 ⁻³	0.999 96	±44 · 10 ⁻⁶	0.999 83	±151 · 10 ⁻⁶
k = 6	Vertex	198 · 10 ⁻⁶	±20 · 10 ⁻⁶	296 · 10 ⁻⁶	±620 · 10 ⁻⁶	0.999	±149 · 10 ⁻⁶	0.998	±933 · 10 ⁻⁶	0.993	±2 · 10 ⁻³	0.993	±2 · 10 ⁻³	0.999 98	±9 · 10 ⁻⁶	0.999 77	±169 · 10 ⁻⁶
	Sample	876 · 10 ⁻⁶	±288 · 10 ⁻⁶	1 · 10 ⁻³	±620 · 10 ⁻⁶	0.999	±348 · 10 ⁻⁶	0.997	±1 · 10 ⁻³	0.987	±3 · 10 ⁻³	0.985	±6 · 10 ⁻³	0.999 96	±24 · 10 ⁻⁶	0.999 82	±126 · 10 ⁻⁶
	Vertex	269 · 10 ⁻⁶	±72 · 10 ⁻⁶	263 · 10 ⁻⁶	±78 · 10 ⁻⁶	0.999	±480 · 10 ⁻⁶	0.998	±2 · 10 ⁻³	0.990	±3 · 10 ⁻³	0.990	±4 · 10 ⁻³	0.999 96	±29 · 10 ⁻⁶	0.999 85	±217 · 10 ⁻⁶
k = 7	Sample	886 · 10 ⁻⁶	±513 · 10 ⁻⁶	1 · 10 ⁻³	±996 · 10 ⁻⁶	0.999	±746 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.987	±9 · 10 ⁻³	0.988	±8 · 10 ⁻³	0.999 96	±35 · 10 ⁻⁶	0.999 92	±69 · 10 ⁻⁶
	Vertex	220 · 10 ⁻⁶	±79 · 10 ⁻⁶	271 · 10 ⁻⁶	±160 · 10 ⁻⁶	0.999	±342 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.991	±5 · 10 ⁻³	0.992	±5 · 10 ⁻³	0.999 98	±5 · 10 ⁻⁶	0.999 91	±38 · 10 ⁻⁶
	Sample	876 · 10 ⁻⁶	±288 · 10 ⁻⁶	1 · 10 ⁻³	±620 · 10 ⁻⁶	0.999	±348 · 10 ⁻⁶	0.997	±1 · 10 ⁻³	0.987	±3 · 10 ⁻³	0.985	±6 · 10 ⁻³	0.999 96	±24 · 10 ⁻⁶	0.999 82	±126 · 10 ⁻⁶
k = 8	Vertex	269 · 10 ⁻⁶	±72 · 10 ⁻⁶	263 · 10 ⁻⁶	±78 · 10 ⁻⁶	0.999	±480 · 10 ⁻⁶	0.998	±2 · 10 ⁻³	0.990	±3 · 10 ⁻³	0.990	±4 · 10 ⁻³	0.999 96	±29 · 10 ⁻⁶	0.999 85	±217 · 10 ⁻⁶
	Sample	886 · 10 ⁻⁶	±513 · 10 ⁻⁶	1 · 10 ⁻³	±996 · 10 ⁻⁶	0.999	±746 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.987	±9 · 10 ⁻³	0.988	±8 · 10 ⁻³	0.999 96	±35 · 10 ⁻⁶	0.999 92	±69 · 10 ⁻⁶
	Vertex	220 · 10 ⁻⁶	±79 · 10 ⁻⁶	271 · 10 ⁻⁶	±160 · 10 ⁻⁶	0.999	±342 · 10 ⁻⁶	0.998	±1 · 10 ⁻³	0.991	±5 · 10 ⁻³	0.992	±5 · 10 ⁻³	0.999 98	±5 · 10 ⁻⁶	0.999 91	±38 · 10 ⁻⁶

Fig. 5.1: Test set performance metrics for Juliet and natural-negative projects. These plots correspond to the metrics reported in table 5.7 but use the complementing metric for the y-axis and log scaling. This is necessary for legibility as the original y-axis values are saturated near 1 for most models. Note the use of log-log axes for false discovery rate (FDR) vs. false positive rate (FPR).

Table 5.8: Juliet performance metrics using a $k = 10$ model, decomposed per (CWE, variant) pair.

Common Weakness Enumeration	Scope	Dataset Size				
		Basic	Control	Data Copy	Data IPA	All
HARD_CODE_KEY	Sample	—	13	1	12	26
	Vertex	—	398	18	345	761
HTTP_RESPONSE_SPLITTING	Sample	8	324	3	35	370
	Vertex	395	25 321	112	1184	27 012
LDAP_INJECTION	Sample	—	59	2	9	70
	Vertex	—	8248	276	897	9421
SQL_INJECTION_JDBC	Sample	7	625	2	81	715
	Vertex	875	101 448	399	8822	111 544
UNVALIDATED_REDIRECT	Sample	—	41	1	5	47
	Vertex	—	3132	18	219	3369
XPATH_INJECTION	Sample	2	141	3	16	162
	Vertex	191	15 833	280	1001	17 305
XSS	Sample	1	174	2	65	242
	Vertex	32	13 431	80	4124	17 667
Total	Sample	18	1377	14	223	1632
	Vertex	1493	167 811	1183	16 592	187 079

Common Weakness Enumeration	Scope	ROC AUC					Average Precision				
		Basic	Control	Data Copy	Data IPA	All	Basic	Control	Data Copy	Data IPA	All
HARD_CODE_KEY	Sample	—	1.0000	—	1.0000	1.0000	—	1.0000	1.0000	1.0000	1.0000
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000	1.0000	0.9993
HTTP_RESPONSE_SPLITTING	Sample	1.0000	1.0000	1.0000	1.0000	0.9970	1.0000	1.0000	1.0000	1.0000	0.9977
	Vertex	0.9926	0.9993	1.0000	0.9822	0.9980	0.9461	0.9961	1.0000	0.8890	0.9860
LDAP_INJECTION	Sample	—	1.0000	1.0000	—	1.0000	—	1.0000	1.0000	1.0000	1.0000
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000	1.0000	1.0000
SQL_INJECTION_JDBC	Sample	1.0000	1.0000	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000
	Vertex	1.0000	1.0000	—	1.0000	1.0000	1.0000	0.9999	—	1.0000	0.9999
UNVALIDATED_REDIRECT	Sample	—	1.0000	—	—	1.0000	—	1.0000	1.0000	1.0000	1.0000
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	0.9998	1.0000	1.0000	0.9992
XPATH_INJECTION	Sample	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000	1.0000	1.0000
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000	1.0000	1.0000
XSS	Sample	—	1.0000	—	0.9970	0.9993	—	1.0000	1.0000	0.9981	0.9997
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	1.0000	1.0000	0.9990	0.9999
Total	Sample	1.0000	0.9998	1.0000	0.9936	0.9987	1.0000	0.9998	1.0000	0.9960	0.9989
	Vertex	0.9982	0.9999	1.0000	0.9990	0.9998	0.9804	0.9994	0.9997	0.9930	0.9983

Common Weakness Enumeration	Scope	Best ϕ Coefficient					Cross-Entropy				
		Basic	Control	Data Copy	Data IPA	All	Basic	Control	Data Copy	Data IPA	All
HARD_CODE_KEY	Sample	—	1.0000	0.0000	1.0000	1.0000	—	$137. \cdot 10^{-3}$	$9. \cdot 10^{-6}$	$205. \cdot 10^{-6}$	$69. \cdot 10^{-3}$
	Vertex	—	1.0000	1.0000	1.0000	0.9898	—	$5. \cdot 10^{-3}$	$545. \cdot 10^{-6}$	$216. \cdot 10^{-6}$	$3. \cdot 10^{-3}$
HTTP_RESPONSE_SPLITTING	Sample	1.0000	1.0000	1.0000	1.0000	0.9838	$860. \cdot 10^{-6}$	$2. \cdot 10^{-3}$	$6. \cdot 10^{-6}$	$601. \cdot 10^{-3}$	$58. \cdot 10^{-3}$
	Vertex	0.9509	0.9893	0.9999	0.8693	0.9780	$42. \cdot 10^{-3}$	$1. \cdot 10^{-3}$	$14. \cdot 10^{-6}$	$79. \cdot 10^{-3}$	$5. \cdot 10^{-3}$
LDAP_INJECTION	Sample	—	1.0000	1.0000	0.0000	1.0000	—	$2. \cdot 10^{-6}$	$60. \cdot 10^{-9}$	$20. \cdot 10^{-6}$	$4. \cdot 10^{-6}$
	Vertex	—	1.0000	1.0000	1.0000	1.0000	—	$115. \cdot 10^{-6}$	$213. \cdot 10^{-6}$	$258. \cdot 10^{-6}$	$131. \cdot 10^{-6}$
SQL_INJECTION_JDBC	Sample	1.0000	1.0000	0.0000	1.0000	1.0000	$2. \cdot 10^{-3}$	$5. \cdot 10^{-3}$	0.	$23. \cdot 10^{-3}$	$7. \cdot 10^{-3}$
	Vertex	1.0000	0.9981	0.0000	1.0000	0.9964	$356. \cdot 10^{-6}$	$109. \cdot 10^{-6}$	0.	$946. \cdot 10^{-6}$	$176. \cdot 10^{-6}$
UNVALIDATED_REDIRECT	Sample	—	1.0000	0.0000	0.0000	1.0000	—	$2. \cdot 10^{-3}$	$2. \cdot 10^{-6}$	$35. \cdot 10^{-3}$	$5. \cdot 10^{-3}$
	Vertex	—	0.9929	1.0000	0.9999	0.9871	—	$44. \cdot 10^{-6}$	$821. \cdot 10^{-6}$	$799. \cdot 10^{-6}$	$97. \cdot 10^{-6}$
XPATH_INJECTION	Sample	0.0000	1.0000	1.0000	1.0000	1.0000	0.	$983. \cdot 10^{-9}$	$914. \cdot 10^{-9}$	$13. \cdot 10^{-6}$	$2. \cdot 10^{-6}$
	Vertex	0.0000	1.0000	1.0000	1.0000	1.0000	0.	$25. \cdot 10^{-6}$	$20. \cdot 10^{-6}$	$258. \cdot 10^{-6}$	$38. \cdot 10^{-6}$
XSS	Sample	0.0000	1.0000	0.0000	0.9386	0.9809	0.	$487. \cdot 10^{-6}$	0.	$14. \cdot 10^{-3}$	$4. \cdot 10^{-3}$
	Vertex	0.0000	1.0000	1.0000	0.9850	0.9963	0.	$38. \cdot 10^{-6}$	$19. \cdot 10^{-6}$	$2. \cdot 10^{-3}$	$391. \cdot 10^{-6}$
Total	Sample	1.0000	0.9941	1.0000	0.9537	0.9865	$1. \cdot 10^{-3}$	$4. \cdot 10^{-3}$	$2. \cdot 10^{-6}$	$107. \cdot 10^{-3}$	$18. \cdot 10^{-3}$
	Vertex	0.9822	0.9958	0.9907	0.9835	0.9933	$11. \cdot 10^{-3}$	$313. \cdot 10^{-6}$	$78. \cdot 10^{-6}$	$7. \cdot 10^{-3}$	$954. \cdot 10^{-6}$

Fig. 5.2: **ROC** and **AP** for the Juliet subset of the primary dataset. Performance values for FindSecBugs [10] at different confidence thresholds are marked for comparison.

limited to using vertex features, the no-vertex-features **CBOW** baseline is able to exceed random-guessing using the sample’s vertex count via its bias’ coefficient. What was surprising was the unexpected informativeness of the edge features and the graph structure itself, as evidenced by the $k = 5$ model achieving a best ϕ Coefficient of 0.76 and 0.83 per sample and vertex, respectively.

5.4 Transferring to Unseen Projects

The fitted models were applied to the natural-defective dataset (see section 5.1.3) in order to evaluate their ability to transfer from synthetic defect examples to unseen natural defects. The sample-level ATP(0.2) and **ROC** was measured for all natural-defective projects, as well as the ϕ Coefficient for labelled projects. Positive samples for **CWEs** not present within the training set were excluded as these would affect the ϕ Coefficient. Labels were provided for unlabelled samples which received a prediction ≥ 0.2 by at least one model, encompassing roughly 10% of the unlabelled dataset.

The models used in this experiment were fitted against the entire primary dataset, except for the development subset ($\approx 10\%$), using the same protocol as the primary evaluation. The results are tabulated in table 5.10, and fig. 5.3. The **ROC** plot in fig. 5.3 includes reported performance values for three open source static analyzers for comparison [90], each of which make use of interprocedural analyses.

Table 5.9: Feature-set ablation evaluation for primary dataset, using baseline and $k = 5$ models. Of note is the surprising effectiveness of the no-vertex-features variant of the $k = 5$ model (highlighted in light blue).

Model	Scope	Features				Cross-Entropy		Avg. Precision		Best ϕ Coeff.		ROC AUC	
		Instr.	Type	Member	Const.	Train	Test	Train	Test	Train	Test	Train	Test
cbow	Sample					2	2	0.481	0.480	0.085	0.078	0.505	0.524
					✓	$428 \cdot 10^{-3}$	$402 \cdot 10^{-3}$	0.974	0.976	0.838	0.848	0.977	0.979
				✓		$149 \cdot 10^{-3}$	$92 \cdot 10^{-3}$	0.938	0.960	0.815	0.821	0.960	0.970
			✓			$476 \cdot 10^{-3}$	$475 \cdot 10^{-3}$	0.780	0.768	0.523	0.526	0.828	0.829
		✓				$618 \cdot 10^{-3}$	$630 \cdot 10^{-3}$	0.828	0.814	0.672	0.661	0.889	0.877
				✓	✓	$80 \cdot 10^{-3}$	$80 \cdot 10^{-3}$	1.000	1.000	0.983	0.982	1.000	1.000
			✓	✓		$88 \cdot 10^{-3}$	$80 \cdot 10^{-3}$	0.973	0.975	0.877	0.881	0.980	0.982
		✓		✓		$87 \cdot 10^{-3}$	$77 \cdot 10^{-3}$	0.980	0.961	0.867	0.852	0.984	0.976
			✓	✓	✓	$18 \cdot 10^{-3}$	$18 \cdot 10^{-3}$	1.000	1.000	0.991	0.995	1.000	1.000
		✓		✓		$39 \cdot 10^{-3}$	$32 \cdot 10^{-3}$	0.990	0.991	0.929	0.931	0.992	0.993
		✓	✓	✓	✓	$25 \cdot 10^{-3}$	$8 \cdot 10^{-3}$	0.999	1.000	0.976	0.989	0.999	1.000
		Vertex				$140 \cdot 10^{-3}$	$136 \cdot 10^{-3}$	0.030	0.029	0.035	0.031	0.468	0.479
					✓	$66 \cdot 10^{-3}$	$68 \cdot 10^{-3}$	0.418	0.407	0.420	0.421	0.909	0.903
				✓		$39 \cdot 10^{-3}$	$41 \cdot 10^{-3}$	0.655	0.664	0.618	0.623	0.957	0.955
			✓			$54 \cdot 10^{-3}$	$54 \cdot 10^{-3}$	0.409	0.425	0.417	0.433	0.931	0.936
		✓				$61 \cdot 10^{-3}$	$60 \cdot 10^{-3}$	0.328	0.339	0.351	0.361	0.938	0.940
				✓	✓	$20 \cdot 10^{-3}$	$20 \cdot 10^{-3}$	0.896	0.893	0.825	0.819	0.990	0.990
			✓	✓		$27 \cdot 10^{-3}$	$27 \cdot 10^{-3}$	0.797	0.801	0.691	0.690	0.989	0.989
		✓		✓		$22 \cdot 10^{-3}$	$22 \cdot 10^{-3}$	0.801	0.784	0.685	0.673	0.989	0.989
			✓	✓	✓	$8 \cdot 10^{-3}$	$8 \cdot 10^{-3}$	0.959	0.961	0.863	0.866	0.998	0.999
		✓		✓		$17 \cdot 10^{-3}$	$18 \cdot 10^{-3}$	0.840	0.839	0.726	0.727	0.992	0.991
		✓	✓	✓	✓	$8 \cdot 10^{-3}$	$7 \cdot 10^{-3}$	0.963	0.969	0.869	0.880	0.999	0.999
k=0	Sample					2	2	0.470	0.470	0.000	0.000	0.500	0.500
					✓	$486 \cdot 10^{-3}$	$467 \cdot 10^{-3}$	0.707	0.719	0.455	0.474	0.751	0.776
				✓		$365 \cdot 10^{-3}$	$392 \cdot 10^{-3}$	0.697	0.656	0.424	0.381	0.730	0.691
			✓			$934 \cdot 10^{-3}$	$943 \cdot 10^{-3}$	0.560	0.559	0.253	0.249	0.562	0.558
		✓				2	2	0.470	0.469	0.019	0.000	0.500	0.500
				✓	✓	$300 \cdot 10^{-3}$	$300 \cdot 10^{-3}$	0.708	0.705	0.451	0.454	0.759	0.761
			✓	✓		$331 \cdot 10^{-3}$	$345 \cdot 10^{-3}$	0.676	0.687	0.402	0.418	0.715	0.716
		✓		✓		$312 \cdot 10^{-3}$	$297 \cdot 10^{-3}$	0.673	0.699	0.398	0.429	0.706	0.739
			✓	✓	✓	$227 \cdot 10^{-3}$	$238 \cdot 10^{-3}$	0.722	0.728	0.484	0.507	0.782	0.776
		✓		✓		$381 \cdot 10^{-3}$	$373 \cdot 10^{-3}$	0.675	0.684	0.402	0.412	0.712	0.721
		✓	✓	✓	✓	$208 \cdot 10^{-3}$	$215 \cdot 10^{-3}$	0.724	0.727	0.453	0.463	0.774	0.771
		Vertex				$149 \cdot 10^{-3}$	$152 \cdot 10^{-3}$	0.031	0.032	0.000	0.000	0.500	0.500
					✓	$125 \cdot 10^{-3}$	$126 \cdot 10^{-3}$	0.168	0.169	0.307	0.308	0.646	0.644
				✓		$105 \cdot 10^{-3}$	$99 \cdot 10^{-3}$	0.290	0.268	0.419	0.398	0.842	0.839
			✓			$107 \cdot 10^{-3}$	$108 \cdot 10^{-3}$	0.169	0.165	0.287	0.281	0.857	0.854
		✓				$120 \cdot 10^{-3}$	$127 \cdot 10^{-3}$	0.064	0.067	0.191	0.195	0.769	0.768
				✓	✓	$77 \cdot 10^{-3}$	$77 \cdot 10^{-3}$	0.436	0.438	0.510	0.510	0.928	0.929
			✓	✓		$77 \cdot 10^{-3}$	$74 \cdot 10^{-3}$	0.337	0.331	0.438	0.437	0.940	0.940
		✓		✓		$78 \cdot 10^{-3}$	$77 \cdot 10^{-3}$	0.315	0.322	0.411	0.417	0.927	0.926
			✓	✓	✓	$57 \cdot 10^{-3}$	$56 \cdot 10^{-3}$	0.469	0.468	0.532	0.526	0.968	0.967
		✓		✓		$78 \cdot 10^{-3}$	$81 \cdot 10^{-3}$	0.335	0.345	0.437	0.446	0.938	0.939
		✓	✓	✓	✓	$52 \cdot 10^{-3}$	$51 \cdot 10^{-3}$	0.476	0.472	0.534	0.526	0.967	0.967
k=5	Sample					$156 \cdot 10^{-3}$	$133 \cdot 10^{-3}$	0.919	0.927	0.763	0.756	0.932	0.936
					✓	$14 \cdot 10^{-3}$	$15 \cdot 10^{-3}$	0.994	0.994	0.934	0.941	0.994	0.994
				✓		$28 \cdot 10^{-3}$	$48 \cdot 10^{-3}$	0.980	0.974	0.880	0.867	0.983	0.979
			✓			$63 \cdot 10^{-3}$	$51 \cdot 10^{-3}$	0.953	0.958	0.776	0.793	0.954	0.961
		✓				$50 \cdot 10^{-3}$	$46 \cdot 10^{-3}$	0.977	0.980	0.836	0.852	0.977	0.981
				✓	✓	$28 \cdot 10^{-3}$	$31 \cdot 10^{-3}$	0.998	0.997	0.970	0.970	0.998	0.997
			✓	✓		$32 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	0.983	0.983	0.891	0.884	0.986	0.986
		✓		✓		$23 \cdot 10^{-3}$	$16 \cdot 10^{-3}$	0.996	0.997	0.955	0.964	0.996	0.997
			✓	✓	✓	$10 \cdot 10^{-3}$	$13 \cdot 10^{-3}$	0.999	0.998	0.979	0.968	0.998	0.997
		✓		✓		$7 \cdot 10^{-3}$	$9 \cdot 10^{-3}$	0.999	0.999	0.967	0.971	0.999	0.999
		✓	✓	✓	✓	$39 \cdot 10^{-3}$	$31 \cdot 10^{-3}$	0.997	0.996	0.962	0.961	0.997	0.996
		Vertex				$20 \cdot 10^{-3}$	$20 \cdot 10^{-3}$	0.883	0.892	0.818	0.829	0.996	0.996
					✓	$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.986	0.987	0.922	0.927	0.999	1.000
				✓		$5 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	0.970	0.964	0.938	0.931	0.999	0.999
			✓			$10 \cdot 10^{-3}$	$11 \cdot 10^{-3}$	0.918	0.923	0.846	0.850	0.997	0.996
		✓				$15 \cdot 10^{-3}$	$15 \cdot 10^{-3}$	0.949	0.951	0.869	0.864	0.998	0.998
				✓	✓	$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.998	0.998	0.987	0.987	1.000	1.000
			✓	✓		$3 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	0.973	0.972	0.933	0.928	0.999	0.999
		✓		✓		$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.996	0.997	0.970	0.970	1.000	1.000
			✓	✓	✓	$1 \cdot 10^{-3}$	$883 \cdot 10^{-6}$	0.998	0.999	0.988	0.988	1.000	1.000
		✓		✓		$2 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.998	0.997	0.979	0.982	1.000	1.000
		✓	✓	✓	✓	$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.997	0.998	0.976	0.976	1.000	1.000

All models struggled with this task, despite the abundance of defects within in dataset. Most models achieved an excellent **ROC** for the majority of projects, but did so by being exhibiting relatively high specificity and low sensitivity. The OWASP Benchmark project, however, was particularly difficult for all models. None achieved a notable **ROC** or **AP** for this project, and all exhibited an abysmal best ϕ coefficient. This was not unexpected, as this particular test suite focuses heavily on defect variants requiring interprocedural analysis.

Interestingly, the most successful models for the natural-defective dataset were those with smaller neighbourhood upper bounds, e.g. $k \in [1, 5]$. Models with larger effective neighbourhoods, including the **CBOW** baseline, struggle to maintain a reasonable **ROC**.

Fig. 5.3: Performance metric curves for Natural-Defective dataset. The OWASP Benchmark's ROC includes the ROCs for three different conventional static analyzers for comparison (as reported by [90]).

Table 5.10: Quantitative sample-level performance results for the natural-defective dataset using models fitted against the primary dataset. Results inferior to a random classifier’s output are marked in red.

Model													
	cbow	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$	$k = 9$	$k = 10$	
$\{ x x \in \mathcal{D}, 0.2 \leq p(x)\}$	Java Vuln. Lab	5	58	57	56	31	23	33	23	16	18	17	
	OWASP Benchmark	32	983	962	947	582	422	867	987	104	396	97	
	STONESOUP Inj.	17	239	314	221	98	57	69	45	17	42	13	
	WebApps Piggybank	0	0	1	1	0	0	0	0	0	0	0	
	WebGOAT	20	54	90	42	25	24	10	12	11	3	1	
	All	74	1334	1424	1267	736	534	969	1077	155	457	129	
ATP(0.2)	Java Vuln. Lab	0	0.169	0.192	0.418	0.350	0.504	0.526	0.448	0.423	0.619	0.494	
	OWASP Benchmark	0.505	0.383	0.547	0.502	0.577	0.479	0.431	0.486	0.502	0.400	0.642	
	STONESOUP Inj.	0	0.006	0.009	0.021	0.033	0.039	0.011	0.027	0.022	0.038	0.037	
	WebApps Piggybank	0	0	0	0	0	0	0	0	0	0	0	
	WebGOAT	0.105	0.096	0.175	0.279	0.328	0.533	0.418	0.449	0.103	0	0.535	
	All	0.294	0.362	0.345	0.477	0.510	0.466	0.429	0.423	0.480	0.362	0.384	
ROC AUC	Java Vuln. Lab	0.378	0.954	0.956	0.977	0.982	0.985	0.976	0.981	0.967	0.926	0.963	
	OWASP Benchmark	0.552	0.551	0.549	0.537	0.509	0.549	0.509	0.513	0.514	0.525	0.494	
	STONESOUP Inj.	0.625	0.930	0.952	0.962	0.971	0.919	0.967	0.902	0.912	0.920	0.867	
	WebApps Piggybank	—	—	—	—	—	—	—	—	—	—	—	
	WebGOAT	0.341	0.983	0.993	0.985	0.986	0.957	0.952	0.856	0.853	0.710	0.596	
	All	0.425	0.905	0.897	0.911	0.879	0.872	0.919	0.918	0.762	0.905	0.774	
AP	OWASP Benchmark	0.576	0.571	0.601	0.596	0.591	0.583	0.539	0.555	0.560	0.556	0.524	
	All	0.576	0.571	0.601	0.596	0.591	0.583	0.539	0.555	0.560	0.556	0.524	
Best ϕ	OWASP Benchmark	0.114	0.138	0.164	0.152	0.172	0.109	0.041	0.068	0.095	0.084	0.029	
	All	0.114	0.138	0.164	0.152	0.172	0.109	0.041	0.068	0.095	0.084	0.029	

CHAPTER 6

Conclusions

I demonstrated that a neural graph classifier fitted against a mixture of natural negative code and synthetic test suites can achieve excellent precision and **ROC**. When applied to unseen natural code, the models mostly retained their ROC, but exhibited poor precision and recall. None of the model variants were able to transfer to the OWASP Benchmark suite.

Summary of Contributions.

I implemented a new approach for detecting software defects caused by incorrect operation dependencies based upon learning to identify partial subgraphs within a program’s dependence graph. While whole graph classification is not a novel task in machine learning, to the best of my knowledge this combination of subgraph classification and application domain is novel.

I demonstrated that this approach can achieve excellent performance against an adapted subset of Juliet [60], and a very modest ability to transfer to unseen natural defective code. This approach even managed some minimal success against the OWASP Benchmark project, despite lacking any ability to perform interprocedural analyses due to simplifying assumptions.

6.1 Future Work

Interprocedural Analysis. In order to simplify the task, the scope of sample is limited to a single subroutine. This is a significant limitation as defects can easily span across several subroutines, if only via data-flow. One naive solution is to expand invocations up to some given depth by substituting invocations with their callee’s dependence graph. However, this

could dramatically increase the size of the graphs and would only be effective up to an expanded depth of k . A possible solution would be to infer which callees, including indirect callees, would be good candidates for inlining. Such an approach bears some similarities to MERLIN’s inference of source-sink-sanitizer triplets [12].

Symbol Vocabulary. As discussed in section 5.1.4.3, proper handling of the symbol vocabulary is important. Some adjustments were made, given the unusual nature of the symbol vocabulary, but these adaptations were kept to a minimum. It behooves us to consider this issue in more detail, particularly with regards the handling of rare symbols. Possibilities include adapting the techniques presented in Herbelot and Baroni [38] for initializing the embedding of a new symbol based on the symbol’s entity definition, e. g. using an embedding of a function as its initial representation, or its usage contexts.

Few Shot & Active Learning. Requiring hundreds of examples to learn a handful of variants for a single defect is not practical, nor necessarily possible for all defects. An application-specific defect specific might only have a small handful of instances; it would be perverse to require the user to deliberately create more. Ideally, the user should only have to annotate one or two instances of a defect before receiving feedback. Users should also be able to refine the inferred specification by correcting erroneous predictions with additional labelling, if so desired.

A practical tool must therefore support few-shot labelling, as well as active learning. This could include incremental vocabulary expansion by initializing new symbols using the embeddings of known symbols [38]. It may be difficult to generalize any kind of transfer learning to entirely novel defects, but it should be possible to apply to defect families, e. g. defects involving string concatenation, and defect variants, e. g. Juliet’s data and control flow variants.

APPENDIX A

Recurrence Connection Behaviour

Laurent and von Brecht [51] demonstrated the presence of strange attractors in the recurrent connections of some Long Short-Term Memorys (LSTMs) and Gated Recurrent Units (GRUs). These do not appear to be present within any of our fitted models, where all initial states seem to invariably collapse to $\mathbf{0}$. Empirically, this holds both for models using our modified update equation eq. (4.3b) as well as models using the classic GRU update equation.

However, one can illustrate the dynamical behaviour mentioned in section 4.2, as shown in fig. A.1, which plots the evolution of $\mathbf{h}^t$ given null inputs (i. e. $\mathbf{f}_x = \mathbf{0}$) for classic GRUs, the modified update rules, and Laurent and von Brecht [51]’s Chaos-Free Recurrent (CFR) cell. The first and second columns of figs. A.1a and A.1b plot $\mathbf{h}^t$ given a uniformly random h_0 drawn from $[-1, 1]$. The first column illustrates the standard behaviour of the cell, while in the second column the input bias, $\mathbf{b}_z$ in eq. (4.3b), is set to $\mathbf{0}$ to remove the saturation effect. The third column illustrates the behaviour of the cell when $h^0 = \mathbf{0}$, leaving only the interaction of $\mathbf{b}_z$ with the cell’s recurrent connections. For the modified cell variant, these consists of the recurrent gate terms in eqs. (4.3c) and (4.3e).

The modified cells exhibit far more consistent behaviour, i. e. monotonic progression given null inputs, over time (fig. A.1d) than classic GRUs, while still being exhibiting some dynamical behaviour (figs. A.1b and A.1d). Note that unlike CFR cells, the modified GRU cell is not guaranteed to be consistent due to interactions between $\mathbf{b}_z$ and the gates’ recurrence terms. This can be demonstrated by the following single unit cell whose steady state roughly alternates between $h = 1$ and $h = 2$:

$$\mathbf{W}_z = \begin{bmatrix} 0 & 0 \end{bmatrix} \qquad \mathbf{b}_z = \begin{bmatrix} 1 \end{bmatrix} \qquad (\text{A.1a})$$

$$\mathbf{W}_u = \begin{bmatrix} 0 & 0 \end{bmatrix} \qquad \mathbf{b}_u = \begin{bmatrix} 100 \end{bmatrix} \qquad (\text{A.1b})$$

$$\mathbf{W}_r = \begin{bmatrix} 0 & -75 \end{bmatrix} \qquad \mathbf{b}_r = \begin{bmatrix} 100 \end{bmatrix} \qquad (\text{A.1c})$$

(a) Classic update: $\mathbf{h}^{t+1} = (1 - \mathbf{u}^t) \odot \mathbf{h}^t + \mathbf{u}^t \odot \tau(\mathbf{W}_z[\mathbf{r}^t \odot \mathbf{h}^t] + b_z)$ (b) Modified update: $\mathbf{h}^{t+1} = (1 - \mathbf{u}^t) \odot \mathbf{h}^t + \mathbf{u}^t \odot (\tau(b_z) + \mathbf{r}^t \odot \mathbf{h}^t)$

Fig. A.1: Normalized activations over time for classic GRUs, the modified GRUs, and CFR cells. A cell's activations are *consistent* if they are element-wise monotonic given a sequence of null inputs. Figure A.1d empirically demonstrates that both the modified GRU and CFR cell exhibit more consistent activations than classic GRU cells. This is not guaranteed for the modified GRU.

APPENDIX B

Project	Samples		Vertices	
	Count	% Tot.	Count	% Tot.
Apache Commons Codec	677	0.43	22773	0.79
Apache Commons IO	1378	0.88	23022	0.79
Apache Commons Logging	283	0.18	4879	0.16
Apache HTTP	4213	2.70	62579	2.17
Apache XML	4414	2.83	69501	2.41
BouncyCastle	24114	15.47	760247	26.38
Capnproto Runtime	535	0.34	7244	0.25
dbus-java	467	0.29	15542	0.53
DexLib	4416	2.83	67883	2.35
ExtendJ	16613	10.66	238920	8.29
FasterXML	8382	5.37	139659	4.84
FuseSource hawtjni	78	0.05	1644	0.05
FuseSource Jansi	274	0.17	4333	0.15
Guava	11944	7.66	121553	4.21
Jasmin	135	0.08	14441	0.50
Java Unix Sockets	105	0.06	1234	0.04
JBoss	10519	6.75	167200	5.80
JCommander	365	0.23	5829	0.20
Keycloak	28430	18.24	403690	14.01
libpam4j	76	0.04	766	0.02
Misc. Example Code	104	0.06	1923	0.06
ObjectWeb ASM	1796	1.15	46740	1.62
Polyglot	3551	2.27	98378	3.41
Proprietary Tool 1	4428	2.84	43456	1.50
Scopt	461	0.29	5377	0.18
SLF4J	436	0.27	5023	0.17
Soot	25752	16.52	504885	17.52
Twitter4J	1778	1.14	35355	1.22
XMLPull	85	0.05	6813	0.23
Total	155809	100.0	2880889	100.0

Table B.1: Population statistics for natural-negative code dataset.

APPENDIX C

Metric Definitions

Aside from cross-entropy, there are three metrics particularly suited for our evaluations: The receiver operating characteristics (ROC), average precision (AP), and the ϕ coefficient.

The most important of these for our task is the ROC, which is defined as:

$$\text{ROC} = \frac{\textcolor{red}{TPR}}{\textcolor{red}{FPR}} = \frac{\text{TP} \text{ TN} + \text{FP}}{\text{FP} \text{ TP} + \text{FN}} \quad (\text{C.1})$$

A model with good **ROC** is *robust* in the sense that it is capable of ranking instances regardless of the classification threshold, which, in turn, can be adjusted for an unseen dataset.

The **AP** is defined as:

$$\text{AP} = \int_0^1 P_R(r) \, dr \quad (\text{C.2})$$

Where $P_R(r)$ is the precision at recall r . Equation (C.2) offers a more precise summary of the average precision than taking the area under the precision-recall curve. For situations where the recall is unavailable, i. e. partially labelled datasets (section 5.1.3 and section 5.4), the average precision weighed by threshold is used instead:

$$\text{APT}(i) = \int_i P_T(t) \, dt \quad (\text{C.3})$$

Where $P_T(t)$ is the precision at for the classifier score threshold t and $0 \leq i$ is a lower bound on the threshold selecting the subset of labelled samples considered.

The ϕ Coefficient is a correlation coefficient for two binary variables. Its domain is $[-1, 1]$, where 1, -1 , and 0 indicate complete agreement, complete disagreement, and no correlation, respectively. It is also insensitive to the class sizes, providing an effective summary of a binary confusion matrix [64]. The ϕ Coefficient can be computed from a confusion matrix

using:

$$\phi \text{ Coefficient} = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TN + FN)(TP + FN)(TN + FP)}} \quad (C.4)$$

APPENDIX D

Table D.1: Feature-set ablation evaluation for primary dataset, using baseline and $k = 5$ models. This table is equivalent to table 5.9, but includes samples from natural-negative projects (section 5.1.2) in the reported metrics.

Model	Scope	Features				Cross-Entropy		Avg. Precision		Best ϕ Coeff.		ROC AUC	
		Instr.	Type	Member	Const.	Train	Test	Train	Test	Train	Test	Train	Test
cbow	Sample				✓	$207 \cdot 10^{-3}$	$208 \cdot 10^{-3}$	0.234	0.222	0.341	0.337	0.861	0.870
				✓		$35 \cdot 10^{-3}$	$39 \cdot 10^{-3}$	0.954	0.937	0.859	0.848	0.997	0.997
				✓		$19 \cdot 10^{-3}$	$16 \cdot 10^{-3}$	0.929	0.943	0.876	0.902	0.997	0.998
			✓			$64 \cdot 10^{-3}$	$55 \cdot 10^{-3}$	0.723	0.749	0.714	0.743	0.987	0.989
		✓				$58 \cdot 10^{-3}$	$56 \cdot 10^{-3}$	0.818	0.788	0.818	0.810	0.992	0.992
			✓	✓	✓	$7 \cdot 10^{-3}$	$6 \cdot 10^{-3}$	0.998	0.998	0.973	0.977	1.000	1.000
			✓	✓		$11 \cdot 10^{-3}$	$10 \cdot 10^{-3}$	0.956	0.962	0.905	0.927	0.998	0.998
		✓		✓		$13 \cdot 10^{-3}$	$13 \cdot 10^{-3}$	0.960	0.969	0.899	0.911	0.998	0.998
			✓	✓	✓	$4 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.999	0.993	0.985	0.989	1.000	1.000
		✓		✓		$9 \cdot 10^{-3}$	$6 \cdot 10^{-3}$	0.983	0.983	0.939	0.957	0.999	0.999
		✓	✓	✓	✓	$3 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	0.999	1.000	0.987	0.991	1.000	1.000
		Vertex				$35 \cdot 10^{-3}$	$36 \cdot 10^{-3}$	0.016	0.015	0.062	0.059	0.729	0.719
				✓	✓	$16 \cdot 10^{-3}$	$17 \cdot 10^{-3}$	0.408	0.411	0.426	0.422	0.976	0.977
				✓		$12 \cdot 10^{-3}$	$11 \cdot 10^{-3}$	0.627	0.657	0.604	0.621	0.988	0.989
			✓			$16 \cdot 10^{-3}$	$16 \cdot 10^{-3}$	0.359	0.408	0.396	0.432	0.980	0.983
		✓				$15 \cdot 10^{-3}$	$15 \cdot 10^{-3}$	0.335	0.310	0.376	0.387	0.984	0.984
				✓	✓	$6 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	0.875	0.894	0.809	0.825	0.997	0.997
			✓	✓		$7 \cdot 10^{-3}$	$7 \cdot 10^{-3}$	0.760	0.788	0.674	0.693	0.996	0.997
		✓		✓		$7 \cdot 10^{-3}$	$7 \cdot 10^{-3}$	0.757	0.784	0.659	0.679	0.996	0.997
			✓	✓	✓	$3 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.946	0.955	0.849	0.859	0.999	1.000
		✓		✓		$6 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	0.821	0.852	0.715	0.742	0.998	0.998
		✓	✓	✓	✓	$2 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.960	0.966	0.865	0.876	1.000	1.000
		k=0 Sample				$222 \cdot 10^{-3}$	$222 \cdot 10^{-3}$	0.045	0.046	0.007	0.000	0.488	0.500
				✓	✓	$52 \cdot 10^{-3}$	$51 \cdot 10^{-3}$	0.668	0.670	0.642	0.653	0.974	0.976
				✓		$37 \cdot 10^{-3}$	$34 \cdot 10^{-3}$	0.661	0.662	0.639	0.648	0.975	0.980
			✓			$93 \cdot 10^{-3}$	$94 \cdot 10^{-3}$	0.394	0.383	0.413	0.450	0.926	0.934
		✓				$162 \cdot 10^{-3}$	$159 \cdot 10^{-3}$	0.111	0.119	0.261	0.277	0.812	0.821
				✓	✓	$25 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	0.715	0.701	0.665	0.690	0.985	0.986
			✓	✓		$37 \cdot 10^{-3}$	$33 \cdot 10^{-3}$	0.650	0.650	0.636	0.648	0.976	0.979
		✓		✓		$37 \cdot 10^{-3}$	$36 \cdot 10^{-3}$	0.648	0.666	0.639	0.653	0.978	0.981
			✓	✓	✓	$24 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	0.700	0.681	0.677	0.693	0.985	0.986
		✓		✓		$36 \cdot 10^{-3}$	$36 \cdot 10^{-3}$	0.651	0.661	0.641	0.651	0.978	0.981
		✓	✓	✓	✓	$25 \cdot 10^{-3}$	$24 \cdot 10^{-3}$	0.711	0.695	0.674	0.676	0.985	0.986
		Vertex				$38 \cdot 10^{-3}$	$38 \cdot 10^{-3}$	0.007	0.008	0.000	0.000	0.472	0.500
				✓	✓	$32 \cdot 10^{-3}$	$33 \cdot 10^{-3}$	0.151	0.146	0.299	0.302	0.659	0.672
				✓		$26 \cdot 10^{-3}$	$25 \cdot 10^{-3}$	0.209	0.203	0.281	0.299	0.799	0.815
			✓			$27 \cdot 10^{-3}$	$28 \cdot 10^{-3}$	0.085	0.083	0.186	0.199	0.893	0.907
		✓				$30 \cdot 10^{-3}$	$32 \cdot 10^{-3}$	0.026	0.027	0.117	0.121	0.842	0.843
				✓	✓	$18 \cdot 10^{-3}$	$19 \cdot 10^{-3}$	0.357	0.350	0.408	0.423	0.913	0.924
			✓	✓		$21 \cdot 10^{-3}$	$20 \cdot 10^{-3}$	0.234	0.226	0.286	0.304	0.943	0.956
		✓		✓		$22 \cdot 10^{-3}$	$22 \cdot 10^{-3}$	0.227	0.223	0.285	0.297	0.943	0.947
			✓	✓	✓	$16 \cdot 10^{-3}$	$15 \cdot 10^{-3}$	0.376	0.366	0.411	0.422	0.973	0.977
		✓		✓		$20 \cdot 10^{-3}$	$21 \cdot 10^{-3}$	0.240	0.231	0.297	0.307	0.958	0.960
		✓	✓	✓	✓	$16 \cdot 10^{-3}$	$14 \cdot 10^{-3}$	0.378	0.379	0.413	0.438	0.976	0.980
		k=5 Sample				$10 \cdot 10^{-3}$	$14 \cdot 10^{-3}$	0.925	0.874	0.833	0.826	0.994	0.989
				✓	✓	$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.996	0.989	0.964	0.951	1.000	0.999
				✓		$4 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	0.975	0.961	0.910	0.922	0.998	0.997
			✓			$8 \cdot 10^{-3}$	$10 \cdot 10^{-3}$	0.935	0.939	0.861	0.862	0.997	0.996
		✓				$5 \cdot 10^{-3}$	$6 \cdot 10^{-3}$	0.972	0.961	0.888	0.882	0.998	0.998
				✓	✓	$3 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.995	0.994	0.966	0.989	1.000	0.999
			✓	✓		$4 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	0.979	0.971	0.919	0.919	0.998	0.998
		✓		✓		$2 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.994	0.987	0.954	0.948	1.000	0.999
			✓	✓	✓	$1 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.998	0.994	0.975	0.981	1.000	0.998
		✓		✓		$1 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.997	0.994	0.968	0.968	1.000	1.000
		✓	✓	✓	✓	$2 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	0.995	0.993	0.953	0.969	1.000	0.999
		Vertex				$4 \cdot 10^{-3}$	$5 \cdot 10^{-3}$	0.882	0.840	0.807	0.802	0.999	0.997
				✓	✓	$1 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.986	0.979	0.926	0.916	1.000	1.000
				✓		$2 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	0.959	0.953	0.915	0.926	1.000	0.999
			✓			$4 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	0.889	0.896	0.827	0.825	0.999	0.998
		✓				$2 \cdot 10^{-3}$	$3 \cdot 10^{-3}$	0.951	0.938	0.867	0.851	1.000	0.999
				✓	✓	$624 \cdot 10^{-6}$	$456 \cdot 10^{-6}$	0.996	0.996	0.977	0.985	1.000	1.000
			✓	✓		$2 \cdot 10^{-3}$	$1 \cdot 10^{-3}$	0.968	0.958	0.920	0.930	1.000	0.999
		✓		✓		$894 \cdot 10^{-6}$	$683 \cdot 10^{-6}$	0.994	0.990	0.957	0.964	1.000	1.000
			✓	✓	✓	$402 \cdot 10^{-6}$	$619 \cdot 10^{-6}$	0.998	0.996	0.981	0.984	1.000	0.999
		✓		✓		$793 \cdot 10^{-6}$	$534 \cdot 10^{-6}$	0.995	0.996	0.969	0.978	1.000	1.000
		✓	✓	✓	✓	$597 \cdot 10^{-6}$	$555 \cdot 10^{-6}$	0.996	0.997	0.969	0.973	1.000	1.000

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Glossary

abstract syntax tree (AST) A syntax tree which only tracks variable lexemes, such as names or value literals. Non-variable lexical tokens, such as keywords or parentheses, are encoded by the tree’s construction.

average precision (AP) The mean precision of a classifier over all classification thresholds. 63

basic block A sequence of instructions. Execution of the block must begin at the head and may only transfer control at the tail. 5

Common Weakness Enumeration (CWE) A set of categories for classifying common defects. See MITRE [57]. 38

control-flow graph (CFG) A directed graph representing the possible paths of execution through a program. Vertices usually represent basic blocks rather than single instructions.

data-flow graph (DFG) A directed graph representing the producers and consumers of values within a program.

dead code Code unreachable from the program’s entry point.

domain specific language (DSL) A programming language specialized for a specific domain or task.

fully-connected layer (FC layer) A ubiquitous neural network layer consisting of a learned projection and bias. i. e. $FC(\mathbf{x}) = \mathbf{W}\mathbf{x} + \mathbf{b}$. Typically used in conjunction with a non-linearity.

Gated Recurrent Unit (GRU) A neural model designed for processing sequences. See section 2.3, and Cho et al. [19].

Gram matrix A Gram matrix is a positive semidefinite matrix $M \in \mathbb{R}^{|X| \times |X|}$ where $M_{ij} = \langle X_i \cdot X_j \rangle$, for the set of vectors X . A kernel matrix is a gram matrix where the inner products are computed by a kernel function $k : X \times X \rightarrow \mathbb{R}$. In practice, kernel matrices are not expected to be perfectly positive semidefinite [18, 86]. 15

induced subgraph Given $A = (V_A, E_A)$, $B = (V_B, E_B)$, $A \subset B$:

$$A \text{ is an induced subgraph} \iff \forall x \in V_A, y \in V_A. (x, y) \in E_B \rightarrow (x, y) \in E_A$$

intermediate representation (IR) A data structure modelling some aspect(s) of a program.

interprocedural analysis (IPA) An interprocedural analysis considers the program being analysed as a whole, rather than multiple disjoint subsets. Non-IPA analyses limit their scope to a single function at most.

Java virtual machine (JVM) A virtual machine created as a compiler target for Java, though other languages now target it as well. (e.g. Clojure, Kotlin, and Scala.)

lexeme A sequence of characters satisfying the pattern definition for a token. Often conflated with the token. 17

Long Short-Term Memory (LSTM) A neural model designed for processing sequences. See section 2.3, and Hochreiter and Schmidhuber [41].

minified source code Source code where all unnecessary whitespace (including comments) has been removed, and identifiers replaced with the shortest possible distinct names. This is often done for compression or cursory obfuscation. 19

multigraph A graph where multiple edges between two vertices is permitted. 14, 23, 24

multi-layer perceptron (MLP) A feed-forward network with at least one hidden layer. See section 2.3.

neighbourhood (graph) The (open) neighbourhood of a vertex v , $N(v)$, is the set of all incident edges and adjacent vertices; the *closed* neighbourhood also includes v itself. The k -neighbourhood of a vertex v , $N^k(v)$, is the subgraph defined by all vertices and edges within radius k from v . i.e. the 1-neighbourhood is equivalent to the closed neighbourhood. Note that directed edges are handled as if they were undirected. 22

out-of-vocabulary (OOV) Not present within a model's vocabulary. May also refer to a special symbol used as a substitute for OOV symbols.

partial subgraph A non-induced subgraph.

pure function A side-effect-free subroutine which always produces the same output given the same arguments. 24

receiver operating characteristics (ROC) A 2d plot comparing a classifier's true positive rate against its false positive rate. 56

right-hand-side expression (RHS) The value expression for an assignment operation. In many languages the assignment operator is an infix operator with the value expression appearing on the right and the destination on the left.

single static assignment (SSA) An IR where all variables have exactly one assignment. It is constructed by introducing fresh variables for every assignment and adding ϕ -nodes to select the correct SSA-variable depending on the executed control flow.

Structured Query Language (SQL) A domain specific language designed for querying databases.

subgraph Given graphs $A = (V_A, E_A)$, $B = (V_B, E_B)$:

$$A \subset B \iff V_A \subset V_B \wedge E_A \subset E_B$$

token A symbolic value representing a basic lexical unit. A token matches a specific pattern of characters (its lexeme), which is tracked for later processing.

e.g. A `NUMERIC_LITERAL` token could match multiple notations, such as 5, -0.22, or 5e-2. [17](#)

type A set of term-level values. e.g. In Java, the type `int` consists of the integers in the interval $[-2^{31}, 2^{31} - 1]$. [6](#), [28](#), [29](#)

Unicode Text Format 8-bits (UTF-8) A multi-byte encoding scheme for Unicode codepoints. It is backwards compatible with 7-bit ASCII.

uninhabited type A type consisting of an empty set of values. e.g. `void` in C-like languages.

void (type) An uninhabited type denoting the return type for subroutines which return no results. Functional languages often use the zero-tuple instead of `Void`. [29](#)