WheaCha: A Method for Explaining the Predictions of Code Summarization Models

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The last decade has witnessed a rapid advance in learning-based program analysis tools. While the black-box nature of these systems may produce powerful predictions, it cannot be directly explained, posing a threat to the continuing application of machine learning technology in programming language research. Recently, attribution methods have emerged as a popular approach to interpreting model predictions based on the relevance of input features. Although their feature importance ranking can provide insights of how models arrive at a prediction from a raw input, they do not give a clear-cut definition of the key features models use for the prediction. In this paper, we present a new method, called WheaCha, for explaining the predictions of code summarization models, a broad class of code models that predict the name of a method given its body. Although WheaCha employs the same mechanism of tracing model predictions back to the input features, it differs from all existing attribution methods in crucial ways. Specifically, WheaCha divides an input method into "*wheat*" (*i.e.*, the defining features that are the reason for which models predict the label that they predict) and the rest "*chaff*" (*i.e.*, the auxiliary features that may help models predict the label that they predict) for any prediction of a learned code summarization model.

We realize WheaCha in a tool, HuoYan, and use it to explain four prominent code summarization models: code2vec, code2seq, sequence GNN, and extreme summarizer. Results show (1) HuoYan is efficient — taking on average under fifteen seconds to compute the *wheat* for an input method in an end-to-end fashion (*i.e.*, including the model prediction time); (2) the *wheat* that all models use to predict input methods is made of simple syntactic or even lexical properties (*i.e.*, identifier names), nevertheless, they are often intuitive and well-aligned to the features humans would have used for inferring the name of the same methods; (3) some of the most noteworthy attribution methods do not precisely capture the *wheat* that models use for prediction. Finally, we show *wheat* naturally lends itself to a novel, powerful attack mechanism on code summarization models. An extensive evaluation shows our attack mechanism significantly outperforms the state-of-the-art in both non-targeted and targeted attacks, and more importantly, in many cases renders a popular defense technique — adversarial training — almost non-existent.

Our work opens up this exciting, new direction of studying what models have learned from source code.

Additional Key Words and Phrases: Code Summarization Models, Explainability, Attribution Methods

1 INTRODUCTION

Riding on the major breakthroughs in deep learning methods along with the ever-increasing public datasets and computation power, modern machine learning (ML) models, such as neural networks, have been increasingly applied to solve programming language tasks, and achieved remarkable success in a variety of problem domains: code summarization [Alon et al. 2019a,b; Fernandes et al. 2019], program repair [Chen et al. 2019; Sakkas et al. 2020; Wang et al. 2020], and program verification [Ryan et al. 2020; Si et al. 2018; Yao et al. 2020]. Despite those accomplishments, neural networks mostly operate in a black-box manner, making it difficult to get insight into their internal mechanism of work. This lack of transparency has become an impediment to the use of learning-based program analysis tools, especially in security-critical settings (*e.g.*, malware detection) as the degree to which their predictions can be trusted is rather unclear. From a scientific standpoint,

improving the transparency of neural models is also essential to the soundness of science. Because their inability to provide explanations for their decisions not only weakens the validity but also hinders the openness of scientific discovery.

```
void f(int position) {
  super.initQueue();
  if (position > mItems.size())
    return;

  mItems.add(position, dummyItem);
  notifyItemInserted(position);
  if (debug)
    log("Add item;");
}
```

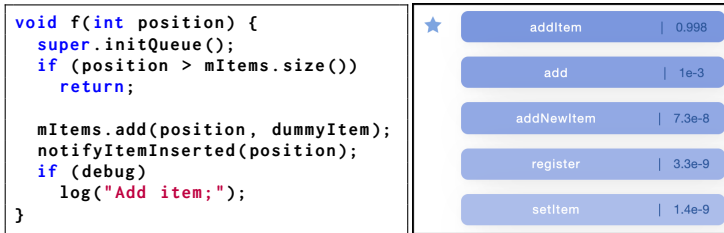| ★	addItem	0.998
	add	1e-3
	addNewItem	7.3e-8
	register	3.3e-9
	setItem	1.4e-9

Fig. 1. An example method whose name is correctly predicted by code2seq [Alon et al. 2019a]. The top-five predictions made by code2seq are shown on the right. Throughout the paper, we will use this program as our running example.

Review of Attribution Methods. In the past few years, significant progress has been made in explaining the predictions of ML models. A prominent class of explainability techniques, called attribution methods, has sparked a lot of interest in the ML community. The idea is to assign an attribution score to each input feature *w.r.t.* a particular output of a network. In general, attribution methods can be classified into two categories: perturbation-based and backpropagation-based. The former refers to those that make perturbation to input features and observe the impact on later neurons in the network. Zeiler et al. [2011] is a typical example in the image classification domain. In particular, it occludes different segments of an input image and visualizes the change in the activation of later layers. The strength of perturbation-based methods lies in their visibility, that is, one can directly visualize the marginal effect of any input feature via perturbation. Compared to the perturbation-based methods, backpropagation-based methods can hardly relate their outcome to a variation of the output. However, they can compute the attributions for all input features in a single forward and backward pass through the network, resulted in higher efficiency. As an early attempt, Simonyan et al. [2014] proposed using the gradient of the output *w.r.t.* pixels of an input image to compute a saliency map of the image. A key drawback of this approach is its inability to address the saturation problem, namely, gradients can be tiny at certain inputs that may yield significant activations within the network [Glorot and Bengio 2010; Shrikumar et al. 2017a]. Integrated Gradients [Sundararajan et al. 2017], a well-known explainability technique, offers a solution to the saturation problem. Instead of computing the gradients at only the current value of the input, they propose to integrate the gradients as the inputs are scaled up from a pre-set starting value to their current value. We defer a detailed survey on the attribution methods to Section 7.

Insights of WheaCha. While the attribution methods can be readily applied to explain the predictions of learning-based program analysis tools, such as producing a ranking on the importance of different parts of the input program *w.r.t.* a model prediction, they do not give a clear-cut definition of the critical features that models use for that prediction. Considering the simplest case in which there exists a "sweet-spot" in the ranking that separates the critical features from the rest, then how to determine the "sweet-spot" is rather unclear. To address this shortcoming, this paper presents a new explanation method, WheaCha (*i.e.*, *Wheat* and *Chaff*), for interpreting the predictions of code summarization models, ML systems that predict the name of a method given its body (Figure 1 depicts an example which we use as the running example). Unlike the existing attribution methods that assign a relevance score to each input feature, WheaCha classifies an entire input into two kinds of features: the defining features, namely *wheat*, that are the reason models predict the label that

```
void addItem(int position) {


  mItems.add(dummyItem);


}
```

```
void initQueue(int position) {
  super.initQueue();
  if (position > mItems.size()) return;
  mItems.add(position, dummyItem);
  notifyItemInserted(position);
  if (debug)  log("Add item;");
}
```

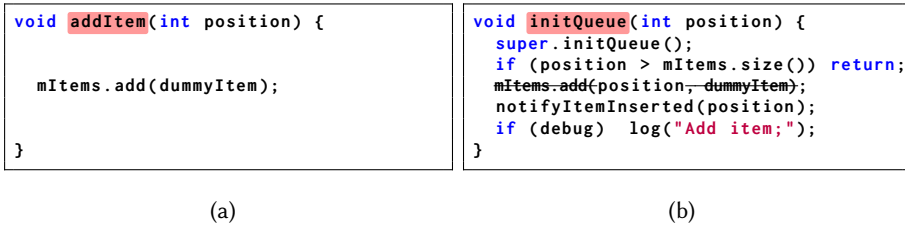(a)   (b)

Fig. 2. A statement in the example program that satisfies the two constraints.

they predict, and the remaining features, namely *chaff*, that may help models predict the label they predict. A natural question arises: how do we define *wheat* for an input program given a particular model prediction? Our insight is to observe how models react to a pair of complementary prediction samples derived from the original input. Technically, we formulate the following two constraints to quantify the influence of *wheat*. That is, the very same model must (1) preserve its prediction when the original input becomes the *wheat* alone; and (2) change its prediction when the original input becomes the *chaff*. Below we illustrate these two constraints with our running example. Figure 2a shows that the expression, `mItems.add(dummyItem);`, alone preserves the prediction, `addItem`, code2seq makes for the original input, thus the first constraint is satisfied; Figure 2b shows that removing `mItems.add(dummyItem);` from the input program changes code2seq's prediction to `initQueue`, therefore the second constraint is also met. However, using only those two constraints, every input program is the defining features for itself — an uninteresting explanation for any model prediction. To address this issue, we impose the third constraint: the defining features must be the minimum set of features from the input program that satisfies the two existing constraints.
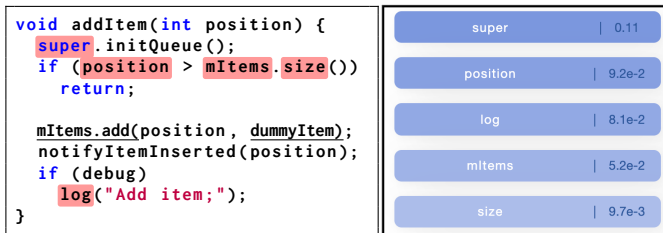
```
void addItem(int position) {
  super.initQueue();
  if (position > mItems.size())
    return;

  mItems.add(position, dummyItem);
  notifyItemInserted(position);
  if (debug)
    log("Add item;");
}
```

super	0.11
position	9.2e-2
log	8.1e-2
mItems	5.2e-2
size	9.7e-3

Fig. 3. For the prediction code2seq makes for the running example, the left shows the five most important features (highlighted within the shadow boxes) computed by Integrated Gradients and the *wheat* (underlined) found by WheaCha and verified by the exhaustive search. The ranking of the attribution scores of the five most important features is shown on the right.

Treating the three constraints as the *wheat* oracle, we find that the ranking produced by some of the most prominent attribution methods routinely underestimates the importance of *wheat*. Regarding code2seq's prediction for the running example, Figure 3 shows that none of the top-five important tokens computed by Integrated Gradients [Sundararajan et al. 2017] is part of the *wheat*, the underlined expression in the program. This finding is a strong rebuttal to the aforementioned "sweet-spot" hypothesis, and a firm confirmation that the existing attribution methods are unsuitable for *wheat* detection. In addition to the precise identification of the defining features, WheaCha offers another significant advantage. Compared to the backpropagation-based methods which currently dominate the literature of attribution methods, WheaCha easily backs up every explanation it

generates with simple, concrete evidence like the results shown in Figure 2a and 2b which end users can understand and appreciate without the expertise in machine learning models.

Identifying the defining features from an input program is a challenging task. With a token-based representation, a program composed of n tokens will yield a search space of 2^n candidates (*i.e.*, every token may or may not be part of the defining features). Even after taking into account the syntactic and semantic constraints, the search space will not shrink dramatically. As a result, a brute-force search would be computationally intractable for any non-trivial program.

Our solution is based on the finding from Wang and Christodorescu [2019] — few simple code edits, albeit preserving the property of interest for input programs, frequently cause models to alter their predictions — we hypothesize that models heavily utilize small, fragmented program features for predictions. To confirm our hypothesis, we conduct a preliminary study in which we test how models respond to new programs obtained via systematic reduction of the input programs. Quite surprisingly, we find that almost always an input program can be reduced to very few statements (*i.e.*, ≤ 3) for which models make the same prediction as they do for the original program. This observation indicates that a small code fragment may already contain the defining features that models need for making the correct prediction. Therefore, a more efficient approach is to first detect such code fragments, and then locate the defining features within them. At the technical level, we present "*Reduce* and *Mutate*", a coarse-to-fine method for identifying the defining features that code summarization models use to predict method names. Given a method P for which a model M predicts a label L. First, we find a global minimal program $\tilde{P}$ for P that satisfies the first two above-mentioned constraints (*coarse-grained* search). Second, we mutate the expressions in $\tilde{P}$'s statements to pinpoint the program properties that led to the satisfaction of the two constraints (*fine-grained* search). We declare such properties the defining features M uses to predict L for P.

We realize our approach in a tool, called HuoYan, and use it to evaluate four code summarization models: code2vec [Alon et al. 2019b], code2seq [Alon et al. 2019a], sequence GNN [Fernandes et al. 2019], and extreme summarizer [Allamanis et al. 2016]. We study code summarization models due to the tremendous impact they made to the programming language field. All research works above not only have gathered a large number of citations since their publication, but also display significant potential for practical applications in software engineering (*e.g.*, API discovery and automatic code review). Results show (1) first, HuoYan is efficient: taking on average less than fifteen seconds to compute the defining features; (2) the defining features that all evaluated models use for predicting all test methods in Java-small, Java-med, and Java-large [Alon et al. 2019a] are simple as they never exceed fifteen tokens, many times down to the name of a single variable, however, we observe that such features, despite their simplicity, often capture the key properties of input methods. (3) Integrated Gradients and SHAP [Lundberg and Lee 2017], two among the most prominent attribution methods, do not precisely identify the defining features as those they assign higher attribution scores frequently miss out on the defining features.

Apart from powering an explanation method, we show that the defining features can be used to create adversarial examples for attacking the code summarization models. Our intuition is straightforward: given the overwhelming influence of the defining features on model predictions, we can trick models to make wrong predictions by tampering with the defining features of an input program in a semantics-preserving manner (*i.e.*, non-targeted attack). If it is required that models must be fooled to predict a certain label L, then we inject into an input program the defining features of another program with the label L (*i.e.*, targeted attack). Differing from the state-of-the-art attack which adopts a gradient-based method [YEFET et al. 2020], ours is a black-box approach, therefore, it does not require the knowledge of models' internal information, thus having wider applicability. Furthermore, we have conducted a head-to-head comparison between YEFET et al.

[2020] and our method. Results show our defining features-based attack is significantly more effective than YEFET et al. [2020] in both non-targeted and targeted attacks with or without adversarial training [Goodfellow et al. 2015], a popular approach to improving model robustness.

This paper makes the following contributions:

- A method for explaining the predictions of code summarization models.
- A definition of the defining features, the reason for which code summarization models predict the label that they predict.
- A method for identifying the defining features that code summarization models use to predict method names.
- An implementation, HuoYan, which we use to evaluate four prominent code summarization models: code2vec, code2seq, sequence GNN, and extreme summarizer. Results show that (1) HuoYan is efficient: taking on average less than fifteen seconds to compute the defining features; (2) all evaluated models use simple syntactic or even lexical properties for prediction; (3) Integrated Gradients and SHAP, two existing attribution methods do not precisely identify the defining features;
- A mechanism for attacking code summarization models that significantly outperforms the state-of-the-art regardless of the employment of adversarial training.

The rest of the paper is structured as follows. Section 2 gives the formalization. Section 3 illustrates our method for finding the defining features. Section 4 details our methodology. Section 5 provides an example application of the defining features. Next, we present our evaluation of HuoYan (Section 6). Finally, we survey related work (Section 7) and conclude (Section 8).

2 FORMALIZATION

We consider a machine learning model M as a program (with semantics $\llbracket M \rrbracket$) which executes on an input (*e.g.*, an image, a document, a piece of code, *etc.*) and returns a prediction as output. Given a prediction L that M makes for an input program P (*i.e.*, $\llbracket M \rrbracket(P) = L$), the key challenge for WheaCha is to identify the defining features M uses for this prediction. Below, we give a formal definition of *wheat*, which is at the core of WheaCha. In principle, our definition applies to any machine learning model that takes programs as inputs and makes predictions about their properties.

Definition 2.1. (*The Defining Features*) The defining features M uses for predicting the label of P is a set of statements/expressions $\tilde{P}$ such that (1) $\tilde{P}$ is a *constituent* of P: $\tilde{P}$'s token sequence, denoted by $(t_n^{\tilde{P}})_{n \in \mathbb{N}}$, is a *subsequence* of P's denoted by $(t_m^P)_{m \in \mathbb{N}}$. Formally, $(t_n^{\tilde{P}})_{n \in \mathbb{N}} = (t_{m_k}^P)_{k \in \mathbb{N}}$ where $(m_k)_{k \in \mathbb{N}}$ is a strictly increasing sequence of positive integers. (2) $\tilde{P}$ is *sufficient*: M makes the same prediction for $\tilde{P}$ as it does for P (*i.e.*, $\llbracket M \rrbracket(P) = \llbracket M \rrbracket(\tilde{P}) = L$); specifically for code summarization models which only take single methods as inputs, we always replace the body of P with $\tilde{P}$ to construct valid inputs. (3) $\tilde{P}$ is *necessary*: M makes a different prediction for $P \setminus \tilde{P}$ than it does for P (*i.e.*, $\llbracket M \rrbracket(P \setminus \tilde{P}) \neq \llbracket M \rrbracket(P)$) where $P \setminus \tilde{P}$ denotes the operation that subtracts program $\tilde{P}$ from P (Definition 2.2). Finally (4) $\tilde{P}$ is *minimal*: there does not exist another set of statements/expressions $\tilde{P}'$ such that $\tilde{P}'$ satisfies the above three requirements, and $|\tilde{P}'| < |\tilde{P}|$ where $|\cdot|$ denotes the length of a sequence.

Here we discuss the intuition behind Definition 2.1. First, the *constituent* requirement captures an obvious intuition, that is, the defining features must be part of an input method. Second, the *sufficient* requirement is also quite intuitive — as the defining features, they must singlehandedly lead models to predict the same label as before without the rest of the input. However, the satisfaction of *sufficient* requirement alone does not suffice one to be the defining features. Consider the following example in Figure 4. Even though Figure 4a shows the statement, `log("Add item;");`, manages

```
void addItem(int position) {


  log("Add item;");


}
```

```
void addItem(int position) {
  super.initQueue();
  if (position > mItems.size()) return;
  mItems.add(position, dummyItem);
  notifyItemInserted(position);
  if (debug)  log("Add item;");
}
```

(a)   (b)

Fig. 4. A statement that satisfies the *sufficient* but not *necessary* requirement.

```
void item(int position) {


  mItems(dummyItem);


}
```

```
void addItem(int position) {
  super.initQueue();
  if (position > mItems.size()) return;
  mItems.add(position, dummyItem);
  notifyItemInserted(position);
  if (debug)  log("Add item;");
}
```

(a)   (b)

Fig. 5. The expression `.add`, albeit being part of the defining features, is in fact unnecessary.

to preserve the prediction, `addItem`, the model makes for the original input (*i.e.*, the *sufficient* requirement is satisfied), it can *not* be the reason for which code2seq makes this prediction because removing it from the input program does not have any impact on code2seq as illustrated in Figure 4b. In fact, the prediction result in Figure 4b suggests that code2seq does not even need `log("Add item;");` let alone use it as the defining features to predict the example program. To address this issue, we design the *necessary* requirement: the removal of the defining features from the input program, which we call the *subtraction* operation (Definition 2.2), must lead models to predict different labels than they did for the original input.

Definition 2.2. (*Subtraction*) Given a program P and a set of statements/expressions $\tilde{P}$, $P \setminus \tilde{P}$ means for each statement/expression S in $\tilde{P}$, first locate the subtree from the Abstract Syntax Tree (AST) of P, which is equivalent to the AST of S; then remove the located subtree from the AST of P. Finally, serialize the resultant AST of P's back to a program in source format.

Now a contradiction seems to arise as Figure 4a suggests `mItems.add(dummyItem);` is an unnecessary feature (*i.e.*, code2seq does not need it for making the correct prediction) while Figure 2b suggests the exact opposite. Technically, what Figure 4a implies is `log("Add item;");` alone generates sufficient signals to lead code2seq to predict `addItem`. This in fact is an easier requirement to satisfy as our large-scale evaluation shows that the vast majority of programs have multiple sufficient features, however, many of such features are overwhelmed by the competing signals sent by other features in the same input which would lead models to predict different labels. This is precisely what happened in Figure 2b. In the absence of the real defining features, `mItems.add(dummyItem);`, the statement, `log("Add item;");`, does not generate as strong a signal as `super.initQueue();` which is actually the defining features of the program in Figure 2b. To sum up, an input feature's satisfaction of the *sufficient* requirement does not give any indication on the necessity of the remaining features in the same input, thus the contradiction dissolves. Note that the sole satisfaction of the *necessary* requirement is also inadequate. Figure 5 presents an example in which the necessary feature, `mItems(dummyItem);`, can not be the defining features without the expression, `.add`, which in fact does not satisfy the *necessary* requirement. In particular,
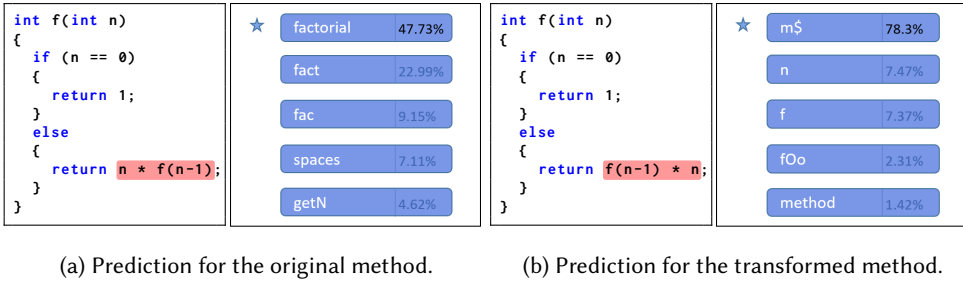
(a) Prediction for the original method.   (b) Prediction for the transformed method.

Fig. 6. A simple, natural, semantically-preserving transformation causes code2vec to change its prediction. Note that the probability of the top-one prediction is even higher on the transformed method.

Figure 5a shows `mItems(dummyItem);` violates the *sufficient* requirement, thus is not the defining features. Figure 5b demonstrates the missing piece, `.add`, is unnecessary.

It's possible that there are multiple $\tilde{P}$ that satisfy the *constituent*, *sufficient*, and *necessary* requirement considering the body of P is already the defining features for P itself. To this end, we argue that $\tilde{P}$ should be the globally minimum sequence of tokens since it's the most precise — neither itself nor any of its subsequences can be further reduced into a smaller sequence of tokens.

Given Definition 2.1, we prove that the defining features always exist for any input program for which models make a prediction.

Theorem 2.1 (Existence of The Defining Features). *Given a prediction L that M makes for an input program P, the defining features $\tilde{P}$ that models use to predict the label of P always exists.*

PROOF. Assume otherwise, so that the defining features $\tilde{P}$ does not exist for P.

Because the body of P, B_P, satisfies *constituent*, *sufficient*, and *necessary* requirement in Definition 2.1. It has to be the *minimal* requirement that B_P violates, meaning, there exists a set of statements/expressions P' that also satisfies all but the *minimal* requirement, and $|(t_n^{P'})_{n \in \mathbb{N}}| < |(t_n^{B_P})_{n \in \mathbb{N}}|$. Since P' is not the defining features either, we can infer that P' is also not *minimal*.

Because the domain that contains all sets of statements/expressions whose token sequence is a subsequence of P's is finite, and the size of the candidate programs will monotonically decreases (*i.e.*, $|(t_n^{P'})_{n \in \mathbb{N}}| < |(t_n^{B_P})_{n \in \mathbb{N}}|$, $|(t_n^{P''})_{n \in \mathbb{N}}| < |(t_n^{P'})_{n \in \mathbb{N}}|$, and so on), there will be a global minimal set of statements/expressions $\tilde{P}$ that satisfies all requirements in Definition 2.1, which implies that $\tilde{P}$ is the defining features for P. This contradicts the assumption that $\tilde{P}$ does not exist for P.   □

3 OVERVIEW

In principle, finding the defining features out of an input program requires an exponential time algorithm. However, by utilizing a key insight of ours, we show *Reduce* and *Mutate*, a coarse-to-fine technique that can compute the defining features[1] in a much more efficient fashion.

While deep neural networks have been gaining increasing levels of interest in programming languages research, Wang and Christodorescu [2019] cautioned that models of source code are notably unstable with their predictions. Simple, natural, and semantically-preserving transformations frequently cause models to alter their predictions. Here we use an example to demonstrate their finding. Figure 6a depicts the original method which is correctly predicted by code2vec to be *factorial*; Figure 6b depicts the transformed method, albeit semantically equivalent, is totally

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[1]The outcome of *Reduce* and *Mutate* may not satisfy the *minimal* requirement in Definition 2.1, a fact we explicitly acknowledge later in the paper, nonetheless, we use the term the *defining features* for consistency and brevity.
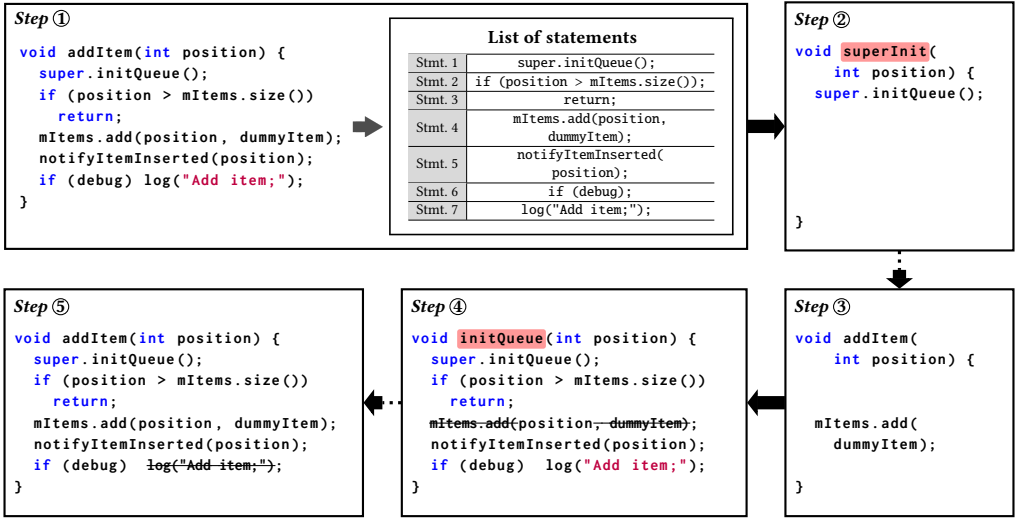
Fig. 7. High-level steps of *Reduce*

mishandled. None of the top-five predictions even remotely resemble the ground truth considering that all we changed is the order of the operands in a multiplication expression. Other models used in our evaluation — code2seq, sequence GNN, and extreme summarizer — do not even give the correct predictions for the method in Figure 6a. Besides, they also change their predictions on the transformed method.

Their finding suggests that models don't evenly distribute their attention across the entire structure of the method, instead, they focus on a small fragment of code. Using this key insight, we can aggressively prune the search space of the defining features by first identifying its surrounding code fragment (*i.e.*, the goal of *Reduce*), and then locate its constituent program properties (*i.e.*, the goal of *Mutate*).

3.1 Reduce

Because the fragment of code that contains the defining features for an input program is usually small, the search can be made very efficient by testing out the smaller code fragments first. Figure 7 illustrates the high-level steps of *Reduce* using our running example.

First, we flatten the input method into a list of statements (*Step* ①), which helps to form all the code fragments. We then traverse the fragments in the ascending order of their size, starting with those that contain only one statement. We pick *Stmt. 1* `super.initQueue()` as the first statement to check. Because it does not satisfy the *sufficient* requirement (*Step* ②), we move on to the next statement. We skip the verification of *Stmt. 2* and *Stmt. 3* which are both invalid. Later, we find that *Stmt. 4* `mItems.add(position, dummyItem);` satisfies both the *sufficient* (*Step* ③) and *necessary* requirement (*Step* ④). To avoid missing other candidates, we continue the traversal until reaching the last statement *Stmt. 7* `log("Add item;");` which is shown to violate the *necessary* requirement (*Step* ⑤). Because we already found a minimal code fragment that satisfies both requirements, the process completes, and *Stmt. 4* is the output of the *Reduce* step.
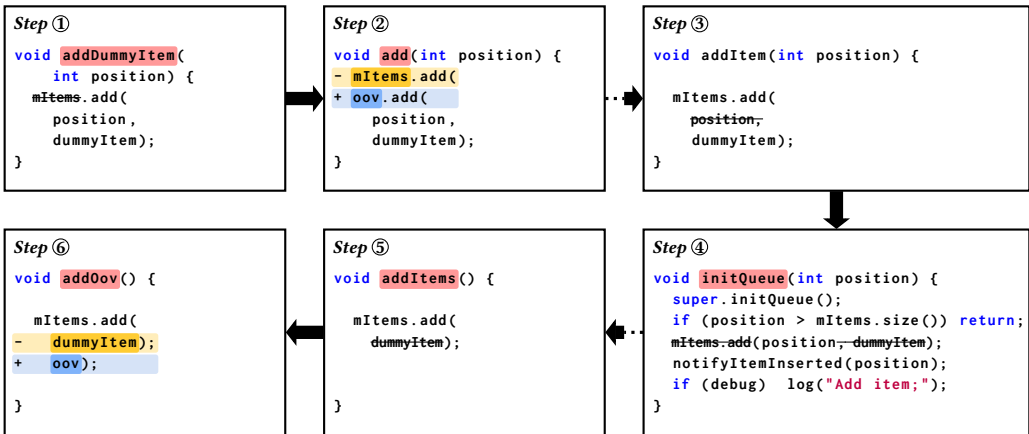
Fig. 8. High-level steps of *Mutate*. - expression (*resp.*, + expression) signals removed (*resp.*, added) lines.

3.2 Mutate

The features discovered in the *Reduce* step lie at the level of statements (*i.e.*, coarse-grained), thus they are likely to contain redundant elements. To pinpoint the fine-grained defining features, we mutate the program discovered in the *Reduce* step in an attempt to identify the minimal features that keep the *sufficient* and *necessary* requirement satisfied.

Since the number of tokens in the defining features is not guaranteed to be so small as that of the statements in the minimal code fragment, the style of search adopted by the *Reduce* step is likely to be inefficient for the *Mutate* step. For this reason, we only remove parts of the code fragment repeatedly until either the *sufficient* or *necessary* requirement is no longer satisfied. Worth mentioning that a significant difference between the two steps is *Mutate* does not adopt solely a program reduction approach to identifying the fine-grained defining features. As an example, suppose a code fragment is already successfully reduced to a field access expression, `foo.bar`. We then attempt to further reduce the expression into a single identifier `foo`. If `foo` turns out to be invalid, we will mutate `foo` back into a field access expression, this time with an out-of-vocabulary field name instead of `bar` — `foo.oov`[2]. Our rational is even if `foo.bar` satisfies both the *sufficient* and *necessary* requirement, it is still possible that models use the *type* of the syntactic structure — field access expression — associated with the object `foo` rather than the specific name of its field — `bar` — as the defining features. To deal with features of this kind that are not explicitly presented, we mix the deletion and modification operation in the *Mutate* step to pinpoint both the explicit and implicit fine-grained features.

Figure 8 illustrates the procedure of the *Mutate* step. As depicted in *Step* ① and ②, it turns out that neither reducing `mItems` nor mutating `mItems` into `oov` satisfies the *sufficient* requirement. Next, we could not remove any part of the *Stmt. 4* `mItems.add(position, dummyItem);` until reaching *Step* ③ and ④, in which we manage to reduce `position` without violating either of the *sufficient* or *necessary* requirement, respectively. In this case, we will continue to reduce `mItems.add(dymmyItem);`. Since the expression can not be reduced any further (*Step* ⑤ and ⑥ show the result of dealing with the last feature `dymmyItem`), we conclude that `mItems.add(dummy-`

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[2]out-of-vocabulary words are those models have never encountered during training. Thus, replacing a token with an out-of-vocabulary word erases the influence of the replaced name on models. Throughout the paper, we use `oov` to represent out-of-vocabulary words for simplicity and clarity.

`Item`) is the defining features that code2seq uses for predicting the running example. Apparently, the features are quite intuitive which humans are also likely to use for this prediction.

4　THE REDUCE AND MUTATE METHOD

In this section, we give a detailed presentation of *Reduce* and *Mutate* for identifying the defining features that code summarization models use for prediction.

4.1　Reduce

Algorithm 1 gives the functionality of the *Reduce* step. The `for` loop at line 3 gradually increases the size of the subsets drawn from the list of flattened statements (line 2) while searching for the minimal code fragments. The function `SelectionUtil` first creates a subset with the parameter `k`, then invokes `Verify`, another function that checks the validity of the created subset against the *sufficient* and *necessary* requirement. Once the created subset is found out to be valid, we add it to the collection of all minimal subsets `fragments` (line 28). Below, we present the technical details about two functions: `Flatten` (line 2) and `Reconstruct` (line 26).

The goal of the `Flatten` function is to reduce an input method into a set of statements. Specifically, for a non-control statement such as declarations, assignments, or method calls, `Flatten` directly adds them to the set (line 17); for a control statement such as `if` statement or `while` loop, `Flatten` first adds the predicate of the control statement (*e.g.*, `if (condition)`) with an empty body as a separate statement to the set (line 14); and then in order to process statements in their body, we recursively call function `Flatten` with the body of the control statement as the function argument (line 15). The function terminates when we completely flatten the input program. Note that we bind certain code structures as a single statement to ensure the syntactic validity of the added statements. For example, `case` or `default` labels will be automatically added with the `switch` predicate whenever a `switch` statement is flattened.

`Reconstruct` function (line 26) returns two new programs: one for verifying against the *sufficient* requirement (*i.e.*, `suff_mth`) and the other for verifying against the *necessary* requirement (*i.e.*, `nec_mth`). Regarding the construction of `suff_mth`, when the selected combination, denoted by `set`, contains only one element, we place the single statement inside the body of *suff_mth* while copying the method header from `method`, otherwise, we rearrange the statements in `set` to reflect the syntactic structure of the input method. For example, an assignment statement will be placed back into the body of a `for` loop if that was the syntactic structure the input method possesses originally. To construct `nec_mth`, we simply subtract the statements in `set` from the original input `method` (Definition 2.2).

Minimality　Algorithm 1 traverses the subsets of P in the ascending order of the cardinality while checking the validity of each subset against the two requirements, therefore, the first subset it finds is the smallest among all. Furthermore, Algorithm 1 only collects the subsets that have the same size as the first subset it finds. Therefore, Algorithm 1 always returns the minimal sets of statements that satisfy the two requirements.

Time Complexity　We analyze the running time of Algorithm 1. In theory, the algorithm runs in exponential time. However, considering over eight hundred thousand test methods in Java-small, Java-med, and Java-large as the inputs, Algorithm 1 runs in cubic time in the worst case because the size of the minimal code fragment never exceeds three for each of the evaluated models. Furthermore, since the minimal region of three statements rarely occurs, we argue the average-case complexity, which we analyze below, is a more accurate measure of Algorithm 1's performance in practice.

Algorithm 1 Find the minimal fragment of code in a method.

1: **procedure** FindMinimalFragment(*method*, *model*)
2:      statements ← Flatten(method)
            ▷ traversing all subsets in the ascending of the cardinality; '-1' excludes the entire set.
3:      **for** k ← 1 **to** statements.size - 1 **do**
4:          fragments ← SelectionUtil(statements, k, method, model)
5:          **if** fragments ≠ ∅ **then**
6:              **return** fragments
7:          **end if**
8:      **end for**
9: **end procedure**

10: **function** Flatten(*method*)
11:     stmts ← ∅
12:     **foreach** stmt ∈ *method*.statements **do**
13:         **if** stmt **is** ControlStmt **then**   ▷ if stmt is a control statement
14:             stmts ← stmts ∪ stmt.predicate
15:             stmts ← stmts ∪ Flatten(stmt.body)
16:         **else**
17:             stmts ← stmts ∪ stmt
18:         **end if**
19:     **end foreach**
20:     **return** stmts
21: **end function**

22: **function** SelectionUtil(*statements*, *k*, *method*, *model*)
23:     sets ← *CombinationsOfKStatement*(statements, k)   ▷ getting combinations of size k
24:     fragments ← ∅
25:     **foreach** set ∈ sets **do**
26:         suff_mth, nec_mth ← *Reconstruct*(set, method)
27:         **if** *Verify*(suff_mth, nec_mth, model) **then**   ▷ check the validity of set
28:             fragments ← fragments ∪ set
29:         **end if**
30:     **end foreach**
31:     **return** fragments
32: **end function**

We focus on the process of traversing the subsets of `statements` in Algorithm 1 since the remaining steps take $O(1)$ time. On average, the traversal takes t_{ave} to execute:

$$t_{ave} = \sum_{k=0}^{\infty} p_k t(k)$$

$$= \sum_{k=0}^{\infty} p_k (k * t_{one}) = t_{one} \sum_{k=0}^{\infty} p_k k$$

where $t(k)$ denotes the average time taken to traverse k subsets; and p_k denotes the probability of an input causing k subsets to be traversed. Since the average time taken to traverse one subset
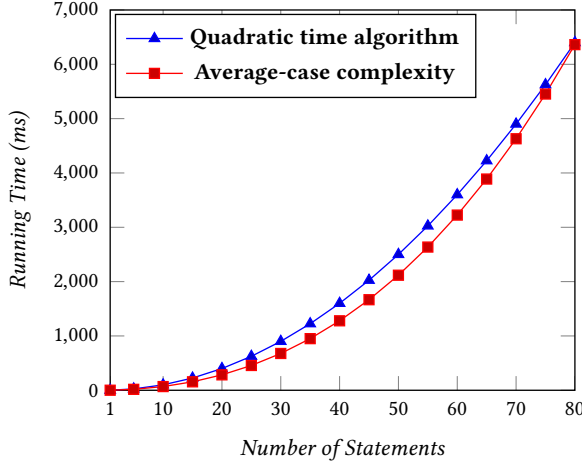
Fig. 9. Average-case complexity of Algorithm 1.

is independent of the total number of subsets Algorithm 1 requires, we replace $t(k)$ with $k * t_{one}$ where t_{one} is the average time taken to traverse one subset.

Now, incorporating the distribution of our inputs:

$$t_{ave} = t_{one} \sum_{k=1}^{|P|^3} p_k k \; (p_k = 0 \text{ when } k = 0 \text{ or } k > |P|^3)$$

$$< t_{one}(p_{|P|}|P| + p_{|P|^2}|P|^2 + p_{|P|^3}|P|^3)$$

where P denotes the set of statements in an input method. The last step is derived based on an overly conservative approximation that Algorithm 1 will always traverse the maximum number of subsets to find the minimal subset *e.g.*, $|P|$ for size of 1, $|P| * (|P| - 1)$ for size of 2 and $|P| * (|P| - 1) * (|P| - 2)$ for size of 3.

Assigning the probability according to the distribution of over eight hundred thousand test methods in the three datasets for code2seq (all other evaluated models have similar distributions).

$$t_{ave} < t_{one}(0.406|P| + 0.589|P|^2 + 0.005|P|^3) \tag{1}$$

Figure 9 plots the upper bound of t_{ave} (*i.e.*, the right side of Equation 1) *w.r.t.* the number of statements in a method assuming t_{one} takes one millisecond. We adopt the interquartile range to exclude outliers in the three datasets based on the number of statements in a method. This measure determines the cut-off value to be around 80, which covers more than 99% of the methods in the three datasets. Clearly, Algorithm 1 runs even faster than a quadratic algorithm with the same constant factor t_{one} most of the time. Given the scale and generality of the experimented inputs, we believe the average-case complexity would apply to any arbitrary set of methods for the four evaluated models.

4.2 Mutate

In the *Mutate* step, we aim to pinpoint the defining features within the minimal code fragment discovered by the *Reduce* step.

Algorithm 2 gives the details. At a high-level, we perform a postorder traversal on the AST of the minimal statements. For each node operation, we consider the following two cases. If a node

---

Algorithm 2 Find the defining features in the minimal code fragment.

1: **procedure** FINDFEATURES(*mini_met*, *method*, *model*)
2:     root ← *Parse*(mini_met).root
3:     MUTATE(root, root, method, model)   ▷ mini_met is the minimal fragment of method
4:     **return** root
5: **end procedure**

6: **function** MUTATE(*node*, *root*, *met*, *model*)
7:     **foreach** child ∈ node.children **do**
8:         MUTATE(child, root, met, model)
9:     **end foreach**
10:     count ← node.children.size
11:     node_bck ← node   ▷ backing up node
12:     **if** count == 0 **then**
13:         **if not** DELETENODE(node, node_bck, root, met, model) **then**   ▷ removing node
14:             MUTATENODE(node, node_bck, root, met, model)   ▷ if fails, mutating node
15:         **end if**
16:     **end if**
17: **end function**

18: **function** DELETENODE(*node*, *node_bck*, *root*, *met*, *model*)
19:     node ← *Delete*(node)
20:     **return** ISVALID(node, node_bck, root, met, model)
21: **end function**

22: **function** MUTATENODE(*node*, *node_bck*, *root*, *met*, *model*)
23:     node ← *Replace*(node, oov)   ▷ mutating node into **oov** node
24:     **return** ISVALID(node, node_bck, root, met, model)
25: **end function**

26: **function** ISVALID(*node*, *node_bck*, *root*, *met*, *model*)
27:     suff_mth, nec_mth ← *ReconstructByNode*(root, node, met)
28:     **if** *Verify*(suff_mth, nec_mth, model) **then**
29:         **return** True
30:     **end if**
31:     node ← *RestoreNode*(node_bck)   ▷ reverting to the backup node
32:     **return** False
33: **end function**

---

does not have any child node, then we first try deleting the node (line 13). If the resultant program no longer satisfies both the *sufficient* and *necessary* requirement, we will mutate the node into one with an out-of-vocabulary value (line 14). As explained in Section 3, the reason we attempt the deletion operation prior to the mutation operation is that even when an expression can not be further reduced, we may only need to retain its syntactic structure without the specific identifier names. If a node has children nodes, the parent node will be kept intact to preserve the status of its

```
void addItem(int position) {          void set(int position) {
  super.initQueue();                    super.initQueue();
  if (position > mItems.size())         if (position > mItems.size())
    return;                               return;
                                  +       clean = dummyItem;
                                  -       mItems.add(position, dummyItem);
  mItems.add(position, dummyItem);  +     mItems.add(position, clean);
  notifyItemInserted(position);         notifyItemInserted(position);
  if (debug)  log("Add item;");         if (debug)  log("Add item;");
}                                     }
```

(a) (b)

Fig. 10. An example of non-targeted attack.

children. Note that whenever we attempt to delete a node, we may delete addition nodes (*i.e.*, the minimal set of nodes required) just to ensure the syntactic validity of the resultant programs. If the node happens to be irremovable, we simply skip the deletion operation. The same strategy also applies to mutation operations.

For other functions not explicitly defined in Algorithm 2, `Parse` extracts the AST out of a method, `Delete` removes a node, `Replace` replaces a node with a new node, `ReconstructByNode` constructs method `suff_mth` for verifying against the *sufficient* requirement and method `nec_mth` for verifying against the *necessary* requirement, and finally *RestoreNode* reverts a node back to the saved node.

Minimality Obviously, the result of Algorithm 2 may not satisfy the *minimality* requirement in Definition 2.1. In principle, it satisfies the *1-tree-minimality* [Misherghi and Su 2006] property because no node can be further removed from the AST of the defining features. On the other hand, the style of search adopted in *Reduce* also can not guarantee the global minimality of its outcome because the defining features may exist in a non-minimal code fragment that *Reduce* can not find. This is the reason that we only consider *1-tree-minimality* in the *Mutate* step, especially given that (1) the size of the defining features is already small, thus the explanations to be generated will be informative to end users; (2) the current algorithm is highly efficient.

Time Complexity Since Algorithm 2 performs a linear traversal on the AST of the input program, it has a complexity $O(n)$ where n is the number of the nodes in the tree. Given the dominance of *Reduce* in terms of the time complexity, our method — *Reduce* and *Mutate* — runs in exponential time in theory and quadratic time in practice.

5 AN APPLICATION OF DEFINING FEATURES

This section presents an application of the defining features: creating adversarial examples for attacking the code summarization models. As a brief background, an adversarial examples is a special type of data created by systematically perturbing the model inputs. Szegedy et al. [2013] are the first to discover the existence of adversarial examples in the image classification domain: visually indistinguishable perturbations cause models to alter their predictions made for the original image. In this work, we create adversarial examples by manipulating the defining features in two different manners. For non-targeted attack, we simply alter the defining features of original inputs while making certain that their semantics is still preserved. Figure 10 shows a successful attack on code2seq with our running example. In particular, we create an adversarial example by changing the identifier from `dummyItem` to `clean` (Figure 10b). While YEFET et al. [2020] also utilize variable renaming as an attack method, our approach is significantly more effective since it pinpoints the right identifier in the program to change. In addition to variable renaming, our generation of adversarial examples features three other semantics-preserving program transformations (Figure 11).

```
int contains(String target,          int addChildRequest(long          void addItem(List<T> items) {
  List<String> Items) {                   duration) {...                    ...
    ...                                 childDurationsSum =                 items.add(generateItem());
    if (Items.indexOf(target)!=-1)       childHits + duration;             log("Item added.");
    ...                                   ...                               ...
}                                     }                                  }
```

```
 int contains(String target,          int addChildRequest(long          void addItem(List<T> items) {
   List<String> Items) {                  duration) { ...                   ...
  ...                                  childDurationsSum =                 log("Item added.");
  if (Items.contains(target))           duration + childHits;             items.add(generateItem());
  ...                                    ...                               ...
}                                     }                                  }
```

(a) API substitution   (b) Operands swapping   (c) Statements reordering

Fig. 11. Three semantically-preserving program transformations. The top row describes the original methods, and the bottom row describes the transformed methods.

```
public void setClassLoader(Object obj) {      public void addItem(Object obj) {
                                              + if (secure_hash("a") == 0)
                                              +   mItems.add(dummyItem);
  if (obj == null)                              if (obj == null)
    return;                                       return;
  else if (!(obj instanceof ClassLoader))      else if (!(obj instanceof ClassLoader))
    return;                                       return;
  else {                                        else {
    digester.set(classLoader);                    digester.set(classLoader);
    return;                                        return;
  }                                             }
}                                             }
```

(a)   (b)

Fig. 12. An example of targeted attack.

For targeted attack, we first obtain the defining features of a program which has the label which we attempt to fool models to predict, and then inject it into the original input. Similarly, for the purpose of preserving the input's semantics, we make the injected defining features deadcode by placing them under a `if` predicate that is always evaluated to false. The example in Figure 12 tells the whole story — Figure 12b shows that with the defining features of our running example, we manage to fool code2seq to predict `addItem` for the original input which was correctly predicted to be `setClassLoader` (Figure 12a). Note that we synthesis the `if` condition based on secure hash functions to prevent the compiler, which can de deemed as the first line of defense, from recognizing them as deadcode and removing them from the input method.

6 EVALUATION

We realize our method *Reduce* and *Mutate* in a tool, called HuoYan, which extracts the defining features that code summarization models use for prediction. In this evaluation, we first deploy HuoYan to explain several prominent code summarization models. Then we evaluate if other explanation methods can find the defining features that HuoYan finds. Next, we evaluate the effectiveness of our attacks to code summarization models based on the defining features. Finally, we demonstrate WheaCha's potential to be a universal explanation method for all code models.

6.1 Evaluation Subjects

Models. code2vec [Alon et al. 2019b], code2seq [Alon et al. 2019a], sequence GNN [Fernandes et al. 2019], extreme summarizer [Allamanis et al. 2016], and LiGER [Wang et al. 2020] are among the most notable code summarization model in the literature. We include every model except LiGER in our experiments. The reason is LiGER incorporates program executions as a feature dimension for

Table 1. Compare reimplementations (**bolded**) to originals for all evaluated models.

Models	Java-small			Java-med			Java-large		
	Precision	Recall	F1	Precision	Recall	F1	Precision	Recall	F1
code2vec	18.51	18.74	18.62	38.12	28.31	32.49	48.15	38.40	42.73
code2vec	**19.23**	**17.72**	**18.44**	**40.32**	**28.89**	**33.66**	**48.90**	**37.26**	**42.29**
code2seq	50.64	37.40	43.02	61.24	47.07	53.23	64.03	55.02	59.19
code2seq	**48.72**	**35.46**	**41.05**	**61.91**	**46.38**	**53.03**	**63.78**	**54.41**	**58.72**
sequence GNN	—	—	51.4	—	—	—	—	—	—
sequence GNN	**49.94**	**47.35**	**48.61**	**58.46**	**45.73**	**51.32**	**61.82**	**50.32**	**55.48**
extreme summarizer	50.25	24.62	33.05	60.82	26.75	37.16	60.71	27.60	37.95
extreme summarizer	**51.27**	**22.28**	**31.06**	**61.28**	**27.38**	**37.85**	**58.37**	**29.72**	**39.39**

predicting method names, thus, they have rather limited applicability and generality. As a concrete piece of evidence, LiGER is evaluated on less than 10% of the methods in Java-med and Java-large since the vast majority do not trigger interesting executions for LiGER to learn (*i.e.*, either do not compile or are not covered sufficiently by dynamic executions).

Datasets. We use Java-small, Java-med, and Java-large, three public datasets Alon et al. [2019a] propose for the code summarization task. All of them are large collections of Java methods they extracted from projects on GitHub. We have re-trained code2vec, code2seq, sequence GNN and extreme summarizer using their implementations open-sourced on GitHub. Table 1 shows the performance of all re-trained models is either comparable or superior to the originals. Note that we only use the methods in the test sets for models to predict in case they over-fit to the training sets.

Baseline. We design a simple baseline method that replaces *Reduce* with a new functional module that repeatedly removes statements until the remaining code no longer satisfies both the *sufficient* and *necessary* requirement. Then, we invoke *Mutate* to identify the defining features. We compare HuoYan with this baseline for every test method in Java-small, Java-med, and Java-large using every evaluated model.

Hardware. All experiments are conducted on five Red Hat Linux servers each of which has 64 Intel(R) Xeon(R) 2.10GHz CPU, 755GB RAM and four NVIDIA Tesla V100 GPU with 32GB of GPU memory each.

6.2 Performance of HuoYan

We evaluate the performance HuoYan for the *Reduce* and *Mutate* step separately. As depicted in Table 2, HuoYan is fast, taking on average around half of a second in both steps. Note this does not take into account the time models spend on predicting, which is mostly independent of our method. For this reason, we measure the number of forward passes through the network that is invoked by HuoYan while searching for the defining features. Table 3 shows that in almost all cases HuoYan requires on average less than ten forward passes in total to find the defining features. Our results show that HuoYan is efficient in finding the defining features.

Regarding the utility of WheaCha, we measure the time HuoYan spends generating explanations end-to-end. Table 4 shows HuoYan takes significantly longer thanks to the contribution of model prediction time. However, by simply paralleling the *Reduce* step (*i.e.*, checking the validity of each code fragment that contains no more than three statements in parallel), HuoYan displays a much more reasonable performance. Finally, Table 2-5 show the baseline is comparable to HuoYan in every aspect mentioned above.

6.3 Makeup of the Defining Features

Now, we give the details regarding the defining features HuoYan found that each evaluated model uses to predict the methods in the three test sets.

Finding the Minimal Code Fragments. We follow Algorithm 1 to identify the minimal code fragment of a given method. Table 6 depicts the size of the fragment in terms of the number of statements it consists of (*e.g.*, mean and median). For all models, the minimal region is very small, containing around two on average with a median of one or two.

Finding the Defining Features. Next, we follow Algorithm 2 to pinpoint the fine-grained features within the minimal code fragments presented above. Table 7 gives the number of tokens the defining features are composed of (*e.g.*, mean and median). Surprisingly, the defining features that sequence GNN uses are the smallest while it is supposedly the most expressive model that also utilizes semantic properties of input programs for prediction. We conjecture the reason being its expressiveness helps itself to pick up the small features to distinguish the labels in the test set whereas the other models suffer from the disadvantage of exclusively learning from syntactic properties. Overall, we find that none of the defining features that any evaluated model uses to predict any method in the three test sets exceed fifteen tokens. This result indicates that existing code summarization models use simple program properties for prediction. and the explanations to be generated based on such properties, albeit not guaranteed to be the global minimum, still help end users to understand how input features influence the model predictions.

```
void init(                    void sort(int[] array) {
    CipherParameters            boolean swapped = true;
    params) {                   for (int i = 0; i < array.length
                                    && swapped; i++) {
                                  swapped = false;
    reset();                      for (int j = 0; j < array.length
                                      - 1 - i; j++) {
    cipher.init(true,               if (array[j] > array[j+1]) {
    params);                          int temp = array[j];
                                      array[j] = array[j+1];
                                      array[j+1]= temp;
                                      swapped = true;
}                             }}}}
```

```
void init() {                 void sort(int[] array) {
  init;                         swapped;
}                             }
```

Fig. 13. Lexical defining features. First (*resp.*, second) row is the original methods (*resp.*, defining features).

Comparing HuoYan against the Baseline. We perform a comprehensive, head-to-head comparison between HuoYan and the baseline method. In particular, for each method in the three test sets

Table 2. Time taken by HuoYan (in seconds). Hereinafter, bolded (*resp.*, normal) numbers denotes HuoYan's (*resp.*, baseline's) results.

Models	Java-small		Java-med		Java-large	
	Reduce	Mutate	Reduce	Mutate	Reduce	Mutate
code2vec	0.56	0.54	0.72	0.83	0.63	0.89
	0.48	**0.45**	**0.58**	**0.69**	**0.57**	**0.75**
code2seq	0.64	0.65	0.71	0.78	0.65	0.68
	0.52	**0.53**	**0.56**	**0.53**	**0.54**	**0.56**
seq-GNN	0.64	0.77	0.66	0.59	0.71	0.78
	0.57	**0.61**	**0.55**	**0.47**	**0.58**	**0.58**
extreme	0.65	0.78	0.90	0.83	0.84	0.89
	0.58	**0.67**	**0.73**	**0.66**	**0.67**	**0.72**

Table 3. The Avg # of forward passes through the network invoked by HuoYan when identifying the defining features that each model uses for prediction.

Models	Java-small		Java-med		Java-large	
	Reduce	Mutate	Reduce	Mutate	Reduce	Mutate
code2vec	3.63	2.65	4.21	4.23	2.66	2.54
	2.62	**1.94**	**3.31**	**3.06**	**2.10**	**1.55**
code2seq	5.21	3.56	8.45	4.69	8.98	4.56
	3.99	**2.20**	**6.91**	**2.93**	**6.73**	**3.04**
seq-GNN	5.68	4.98	5.21	6.52	4.23	4.52
	4.33	**3.08**	**3.77**	**4.35**	**3.31**	**3.79**
extreme	7.34	7.88	7.15	9.21	6.52	6.31
	6.37	**6.60**	**5.44**	**6.93**	**3.12**	**4.22**

Table 4. Avg. end-to-end time.

Models	Java-small	Java-med	Java-large
code2vec	16.36	21.55	14.33
	13.76	**14.37**	**10.71**
code2seq	10.66	15.93	16.77
	9.95	**11.91**	**11.53**
seq-GNN	23.74	26.34	21.69
	18.57	**22.07**	**19.79**
extreme	22.20	30.02	18.29
	19.31	**21.86**	**16.55**

Table 5. Avg. end-to-end time in parallel mode.

Models	Java-small	Java-med	Java-large
code2vec	11.42	12.80	9.59
	9.44	**10.91**	**8.77**
code2seq	7.36	9.05	11.59
	6.32	**6.76**	**7.07**
seq-GNN	15.34	20.88	16.11
	12.90	**14.20**	**13.72**
extreme	15.15	17.89	13.93
	13.44	**14.79**	**11.53**

```java
void checkDone() {

  boolean done = false;

  while (!done) {
    if (remaining() <= 0) {
      done = true;

    }
  }

}
```

```java
int nextInt() {
  while (st == null ||
    !st.hasMoreElements()) {
    try {
      st = new StringTokenizer(
        br.readLine());
    } catch (Exception e) {
      e.printStackTrace();
    }}
  return Integer.parseInt(
    st.nextToken());
}
```

```java
void checkDone() {
  while (!done) {
  }
}
```

```java
int nextInt() {
  return parseInt(
    nextToken());
}
```

Fig. 14. Syntactic defining features.

predicted by each evaluated model, we compare the defining features found by HuoYan and the baseline. We find that for less than 9% of all the test methods, the baseline manages to find the same defining features as HuoYan while HuoYan finds smaller defining features for the remaining over 91%. In other words, the baseline method never finds smaller defining features than HuoYan. Furthermore, when a method is flattened into no less than four statements, HuoYan always beats out the baseline method. The reason is simple: the baseline frequently removes the key statement, which can be a smaller piece of the defining features, and later overcompensate with more than necessary code fragments. Table 6 and 7 give the details of this comparison. In both cases, the defining features found by HuoYan are smaller.

Investigating the Substance of the Defining Features. We classify the defining features into three categories according to their constituent program properties: lexical, syntactic, and semantic.

- **Lexical:** If each of the statements in the defining features consists of a single identifier. Figure 13 depicts two examples, in both cases, the defining features consist of only one identifier.

Table 6. The # of statements in minimal fragments.

Models	Java-small		Java-med		Java-large	
	Mean	Median	Mean	Median	Mean	Median
code2vec	2.12	2.00	2.43	2.00	2.56	2.00
	1.66	**2.00**	**1.88**	**2.00**	**1.82**	**2.00**
code2seq	1.94	2.00	2.22	2.00	2.15	2.00
	1.39	**1.00**	**1.65**	**2.00**	**1.57**	**2.00**
seq-GNN	2.32	2.00	3.54	3.00	2.30	2.00
	1.60	**1.00**	**1.74**	**1.00**	**1.85**	**1.00**
extreme	3.18	3.00	2.64	2.00	2.28	2.00
	1.78	**2.00**	**1.61**	**2.00**	**1.89**	**1.00**

Table 7. The # of tokens in the defining features.

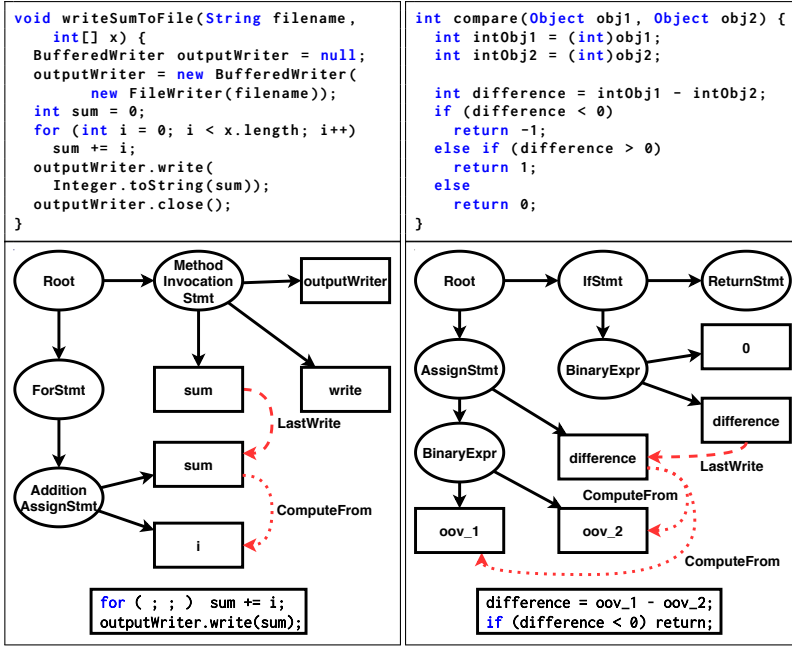| Models	Java-small		Java-med		Java-large	
	Mean	Median	Mean	Median	Mean	Median
code2vec	14.2	9.00	15.2	11.0	16.2	10.0
	8.53	**6.00**	**9.91**	**9.00**	**9.58**	**7.00**
code2seq	15.2	10.0	14.2	11.0	17.2	12.0
	8.04	**7.00**	**9.35**	**7.00**	**10.2**	**8.00**
seq-GNN	5.30	4.00	12.84	11.00	6.04	6.00
	7.74	**5.00**	**6.39**	**6.00**	**6.66**	**6.00**
extreme	10.6	9.00	9.20	8.00	11.41	9.00
	8.14	**6.00**	**8.83**	**6.00**	**9.72**	**7.00**

Fig. 15. Semantic defining features. Second row shows the AST of both the defining features, in which dash arrows denote the semantic edges. For clarity, the ASTs are simplified.

- **Syntactic:** If there is at least one of the statements in the defining features composed of a syntactic expression (Figure 14).
- **Semantic:** Sequence GNN is the only model which also takes in semantic properties as model inputs. In particular, Fernandes et al. [2019] use nine kinds of manually designed edges (described in the supplemental material), out of which seven can be deemed as semantic in nature, to enrich the original AST of input methods. Therefore, we define the defining features to be semantic if there is at least one of its statements whose AST is augmented with at least one semantic edge. Take the method compare in Figure 15 as an example, the three semantic edges — one LastWrite edge and two ComputeFrom edges — must be present in the AST of the defining features, otherwise the *sufficient* and *necessary* requirement are no longer satisfied at the same time. Thus, we classify this example as semantic. To determine whether sequence GNN used semantic properties in its defining features, we first run *Reduce* and *Mutate* as usual, then we remove all the semantic edges from the augmented AST of the obtained defining features. If the resulted tree no longer satisfies both the *sufficient* and *necessary* requirement, we categorize the defining features to be semantic, and add back the minimum set of the semantic edges necessary to make the defining features valid again.

Table 8 gives the detailed statistics on the classification for each model. Clearly, for all evaluated models, the defining features primarily consist of lexical properties.

6.4 Confirming the Minimality of the Defining Features

In this experiment, we set out to confirm the minimality of the defining features found by HuoYan. As explained earlier, finding the global minimum defining features requires exhausting all subsequences of the token sequence of the input method. Therefore, to lessen the computational burden, we limit

Table 8. Classification of the defining features that each model uses for prediction.

Models	Java-small			Java-med			Java-large		
	Lexical	Syntactic	Semantic	Lexical	Syntactic	Semantic	Lexical	Syntactic	Semantic
code2vec	59.27%	40.73%	–	51.34%	48.66%	–	50.22%	49.78%	–
code2seq	52.88%	47.12%	–	55.98%	44.02%	–	53.32%	46.68%	–
seq-GNN	77.60%	21.73%	0.67%	64.39%	32.96%	2.65%	71.25%	26.24%	2.51%
extreme	62.24%	37.76%	–	66.38%	33.62%	–	61.41%	38.59%	–

Table 9. Statistics on the selected methods for the minimality experiment.

Models	# of statements in methods				# of tokens in defining features				# of methods in total
	Min	Max	Mean	Median	Min	Max	Mean	Median	
code2vec	1.0	12.0	7.4	5.0	2.0	17.0	9.4	8.0	21,324
code2seq	1.0	15.0	7.2	6.0	2.0	16.0	10.1	9.0	18,105
seq-GNN	1.0	12.0	5.8	5.0	2.0	16.0	8.2	7.0	19,751
extreme	1.0	14.0	8.1	6.0	2.0	15.0	7.5	7.0	20,028

the evaluation data for this experiment to those methods that have either a small set of tokens or small defining features found by HuoYan (Table 9). We also diversify the data *w.r.t.* the size of the method and the defining features to make our results unbiased. To confirm the global minimality of the defining features for the selected methods, we exhaust all subsequences of the token sequence of the input method up to the size of the defining features, specifically, we start from the subsequences of size one, and gradually increases to the size of the defining features. To cope with such a heavy computational burden, we exhaustively generate the test candidates for each method beforehand in a parallel fashion; then we place them into separate batches to fully exploit the potential of our GPUs (*i.e.*, ≈10K test candidates per second per GPU). The whole experiment takes almost three months to complete.

We find that for 79,208 defining features that HuoYan identified, the brute-force search never finds a single instance where the defining features are smaller. Our results speak volume to the precision of our *Reduce* and *Mutate* method in finding the critical features that models use for prediction even if they are not guaranteed to be the global minimum.

6.5 Can Other Explainability Methods Find the Defining Features

In this experiment, we evaluate whether or not some of the most prominent attribution methods can also find the defining features that HuoYan finds. We choose Integrated Gradients [Sundararajan et al. 2017], a backpropagation-based method that computes the gradient of the predictions to the features to generate explanations, and SHAP [Lundberg and Lee 2017], arguably the state-of-the-art attribution method that has been widely used for explaining the predictions of image and natural language models. In particular, SHAP's explanation is based on the contribution of individual feature values to the model predictions. We also choose the attention mechanism [Bahdanau et al. 2015], which makes models pay greater attention to certain factors (*e.g.*, elements in an input) when processing the input data. Therefore, the features that are heavily attended to can be deemed as an explanation naturally. In theory, the three explainability methods may find the defining features that HuoYan does not, therefore, we only use the 79,208 methods whose defining features are verified to be ground-truth for this experiment.

First, we pick input features with top-*N*% highest attribution scores computed by the method. Then, we show the percentage of the programs that are fully covered by those input features (Table 10, 12 and 14). In addition, we also present on average the percentage of the defining features (measured by the number of tokens) that are covered by the selected input features (Table 11, 13

Table 10. Percentage of programs whose defining features are fully covered by Integrated Gradients.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	8.23	11.42	13.85	21.69	27.93
code2seq	2.08	4.16	4.98	10.36	22.97
seq-GNN	1.74	6.32	10.17	17.90	25.54
extreme	12.13	16.72	21.48	28.90	33.84

Table 11. Percentage of tokens in the defining features that are covered by Integrated Gradients.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	27.64	32.24	34.54	40.90	50.09
code2seq	13.74	16.48	17.68	33.51	46.78
seq-GNN	11.99	21.04	35.79	41.99	48.12
extreme	39.04	42.51	44.64	59.25	61.38

Table 12. Percentage of programs whose defining features are fully covered by attention-based explanation.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	52.50	60.00	62.50	64.91	69.22
code2seq	35.00	40.00	43.52	49.92	56.43
seq-GNN	41.36	45.81	51.27	56.92	60.14
extreme	35.71	40.48	44.72	47.83	50.18

Table 13. Percentage of tokens in the defining features that are covered by attention-based explanation.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	70.61	79.09	81.52	83.81	84.68
code2seq	59.04	68.00	69.71	71.35	72.10
seq-GNN	61.73	67.94	73.78	76.15	79.73
extreme	51.81	57.05	62.88	70.60	73.52

Table 14. Percentage of programs whose defining features are fully covered by SHAP.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	4.38	5.02	6.37	15.24	55.19
code2seq	3.42	5.71	8.06	12.55	48.57
seq-GNN	6.12	9.33	12.02	38.24	100.0
extreme	10.38	24.76	32.14	34.98	73.81

Table 15. Percentage of tokens in the defining features that are covered by SHAP.

Models	Top-N%				
	10%	30%	50%	70%	90%
code2vec	11.15	23.70	25.94	41.15	82.18
code2seq	14.18	20.05	24.05	37.76	76.93
seq-GNN	16.34	36.34	40.11	65.47	100.0
extreme	24.98	49.53	60.27	66.08	97.36

and 15). Quite unexpectedly, the attention mechanism turns out to be the top performer in this experiment. Up to the features that receive the top-70% attribution scores, attention beats the other two methods by a significant margin across all evaluated models. Another interesting observation we made about the attention is it can already cover a good amount of programs when only using the top-10% of the input features as the increases of the coverage slows down when more features are selected. This indicates the important role the attention plays in helping to model to learn the right features for prediction. As for the other two methods, SHAP's advantage over Integrated Gradients only stands out after the 50% mark, otherwise, their numbers are in the same ballpark. Overall, it's evident that none of those explanation methods are good at finding the defining features. As shown in Table 10, 12 and 14, even using half of the input tokens, there are still a significant amount of programs that are left uncovered even in the case of the attention mechanism.

6.6 Effectiveness of the Adversarial Attack

In this section, we evaluate our defining features-based adversarial attack on code summarization models. We choose DAMP [YEFET et al. 2020], the state-of-the-art attack, as the baseline in this experiment. Since code2vec is the only model that both YEFET et al. [2020] and our work use for evaluation, we compare our methods against DAMP in attacking code2vec. In addition, we also evaluate our attacks to code2seq, sequence GNN and extreme summarizer.

In the same setup as YEFET et al. [2020], we use code2vec trained on Java-large in both targeted and non-targeted attacks, in addition, only the correctly predicted methods in the test set are selected for this evaluation. The other three models used in these experiments are also trained on

Table 16. The robustness score of the four models (the lower robustness, the more effective the attack. A robustness score of zero indicates 100% success rate of the attack). Hereinafter, the first row denotes the best results that DAMP achieves from their two attack methods to code2vec. We list the results of our attacks to code2vec right below DAMP's for the ease of comparison. The last three rows show the results of our attacks to the other three models.

Methods	non-targeted	init	merge-From	size	isEmpty	clear	remove	value	load	add	run
DAMP	6.00	48.44	10.39	78.27	79.04	82.80	63.15	76.75	55.65	68.60	51.52
Our attack	**0.00**	**0.00**	**0.00**	**8.70**	**43.38**	**0.00**	**8.70**	**26.0**	**0.00**	**0.00**	**0.00**
code2seq	0.00	0.00	2.28	16.24	23.15	1.26	15.21	12.54	4.25	0.00	1.67
seq-GNN	0.00	0.00	5.21	19.28	32.15	0.00	8.34	32.17	0.00	8.68	0.00
extreme	0.00	0.00	6.73	8.49	24.97	10.21	0.00	22.45	9.68	0.00	6.53

Table 17. The robustness score of the four models after they are defended by adversarial training. The lower robustness, the more effective the attack. A robustness score of zero indicates 100% success rate of the attack.

Methods	non-targeted	init	merge-From	size	isEmpty	clear	remove	value	load	add	run
DAMP	68.80	78.17	98.91	99.39	98.91	85.09	89.29	99.47	88.29	95.90	94.48
Our attack	**0.00**	**5.39**	**65.22**	**91.30**	**86.96**	**4.35**	**65.22**	**73.91**	**0.00**	**17.93**	**0.00**
code2seq	34.21	20.38	76.21	93.21	95.21	10.28	72.32	58.32	62.85	20.30	10.74
seq-GNN	28.17	39.23	48.28	85.28	47.28	20.38	58.28	73.37	43.82	0.00	19.72
extreme	39.28	21.39	34.81	89.28	49.01	48.02	38.21	89.28	85.44	0.00	38.29

Java-large for their highest accuracy. For consistency, we only pick the methods that are correctly predicted by the respective model. We reuse all the desired adversarial labels in the targeted attack introduced by YEFET et al. [2020]. We also adopt the robustness metrics proposed in YEFET et al. [2020]. Specifically, in non-targeted attacks, robustness is defined as the percentage of examples in which the correctly predicted label was not changed to any other label. In targeted attacks, the robustness is the percentage of examples in which the correctly predicted label was not changed to the adversary's desired label. If the predicted label was changed to a label that is not the adversarial label, we consider the model as robust to the targeted attack. In both non-targeted and targeted attacks, their metrics imply that the lower model robustness, the higher effectiveness of the attack.

Table 16 shows the results of both non-targeted and targeted attacks for our methods and DAMP. In non-targeted attacks, our method, which achieves a 0.00% robustness score indicating the 100% success rate of the attack, is more effective than DAMP, which achieves a 6% robustness score. In targeted attacks, our method also performs significantly better than DAMP at all of the adversarial labels, especially, the label `init, mergeFrom, clear, load, add, run` for which our method achieves a 0.00% robustness score.

To show the effectiveness of our attacks against defense techniques, we consider the adversarial training [Goodfellow et al. 2015], the same approach adopted by YEFET et al. [2020], which trains a model on the original training set, while learning to perform the original predictions and training on adversarial examples at the same time. After the adversarial training, the degradation of the precision, recall and F1 score for the re-trained code2vec model compared to the original is 7.30%, 1.65% and 4.42%, respectively, which is comparable to the one re-trained in DMAP's experiment, whose degradation of the precision, recall and F1 score is 1.91%, 7.04% and 5.02%. We leave the degradation scores of the other three models to the supplemental material for reviewers' perusal.

Table 17 shows the results of both non-targeted and targeted attacks for our method and DAMP after models are defended by adversarial training. After the re-training, our attack to code2vec still

Table 18. Performance of HuoYan in finding the defining features for CodeBert.

Evaluation items		Java-small	Java-med	Java-large
Avg. time taken by HuoYan (in seconds)	Reduce	0.73	0.75	0.78
	Mutate	0.52	0.67	0.65
Avg. # of forward passes through the network	Reduce	9.21	9.52	9.75
	Mutate	6.06	6.01	6.12
Avg. end-to-end time (in seconds)	Sequential	25.58	26.23	28.21
	Parallel	19.14	17.07	21.11
# of statements in minimal fragments	Mean	2.04	2.10	2.02
	Median	2.00	2.00	2.00
# of tokens in the defining features	Mean	6.64	7.82	9.01
	Median	5.00	7.00	8.00

achieves a 0.00% robustness score, a result that is substantially better than DAMP's 68.8%. Same for the targeted attacks, once again, our method outperforms DAMP at all adversarial labels by a wide margin, especially for the label `init, clear, load, add, run`. Overall, in six out of eleven attack scenes, our method makes adversarial training produce little to none effect. At this point, we conclude that our attack methods based on the defining features significantly outperform the state-of-the-art DAMP in all cases. The last three rows in Table 16 and 17 depict the results of our attacks to the other three models. Based on this evaluation, we conclude that our attack is highly effective in both non-targeted and targeted attacks with or without adversarial training on all the four models. This is yet another testament to the precision of *Reduce* and *Mutate* in finding the key features models use, which directly contributed to the power of our adversarial attacks.

6.7 Generalizing WheaCha to Explain Other Code Models

In this section, we demonstrate WheaCha can be generalized to explain other models of code, and potentially used as a universal explanation method for all models in the programming domain. We choose CodeBERT [Feng et al. 2020] as the evaluation target due to the two significant challenges it presents: (1) CodeBERT is built upon Bert [Devlin et al. 2019], which is powered by Transformer [Vaswani et al. 2017], a completely different network from all code summarization models we previously evaluated. (2) CodeBERT achieves the state-of-the-art results in two programming tasks: natural language code search and code documentation generation in six programming languages. If WheaCha was feasible to explain CodeBERT, it should be feasible to explain any code model. For this experiment, we explain CodeBert's prediction for every method in Java-small, Java-med, and Java-large in a code document generation task. Note that CodeBert's accuracy in this experiment is not relevant because our goal is to identify the defining features CodeBert uses for its predictions no matter they are right or wrong. The model we use is provided by Feng et al. [2020], which is pre-trained on 8.5M methods across six programming languages (including 2.1M Java methods) from CodeSearchNet [Husain et al. 2019]. Therefore, the model should be suitable for predicting the methods in our datasets.

Performance of HuoYan. As depicted in Table 18, HuoYan is efficient in dealing with CodeBert's predictions, taking on average less than 0.8 seconds for each input method and requiring on average less than ten forward passes through the network in both *Reduce* and *Mutate* steps. As for the time HuoYan spends on generating explanations end-to-end, HuoYan is slower when running in sequential mode, nevertheless, it becomes significantly faster once we parallel the *Reduce* step.

Makeup of the Defining Features The last two rows in Table 18 show that on average the number of statements in minimal fragments and the number of tokens in the defining features. Similar to

Table 19. Performance of Integrated Gradients, attention, SHAP in finding the defining features for CodeBert.

Models	Tasks	Top-N%				
		10%	30%	50%	70%	90%
Integrated Gradients	% of fully covered programs	6.23	10.33	13.12	20.90	29.50
	% of covered defining features	23.80	31.32	34.49	46.55	55.20
Attention-based	% of fully covered programs	41.97	48.44	52.02	58.19	63.12
	% of covered defining features	62.01	70.74	74.13	80.01	82.93
SHAP	% of fully covered programs	6.20	11.54	15.67	27.30	73.56
	% of covered defining features	17.00	31.38	40.22	56.88	94.46

the four code summarization models, CodeBert always uses less than three statements, and on average less than ten tokens in its defining features. The results are consistent with that of the four code summarization models, which demonstrate that HuoYan can be readily applied to explain CodeBert's predictions.

Evaluation of the Other Explainability Methods. We conduct the same experiment on the three other explanation methods for CodeBert. With the same metrics, the results in Table 19 gives very similar indications: first, the attention mechanism is the top performer in this experiment; second, SHAP outperforms Integrated Gradients after picking input features with top-50% highest attribution scores; and third, the three methods are not good at finding the defining features. With the same 50% mark for input features, they still miss a lot of programs in the three datasets.

7   RELATED WORK

In this section, we survey three strands of related work: attribution methods, explainability techniques for models of code, and code summarization models.

7.1   Attribution Methods

In machine learning field, attribution methods are usually classified into two categories: Perturbation-based and backpropagation-based. The former generates explanations by iteratively probing a trained machine learning model with different variations of the inputs. As a few representatives, Zeiler et al. [2011] visualized the neural activations of individual layers of a deep convolutional network by occluding different segments of the input image and generating visualizations using a deconvolution network (DeConvNet). Zintgraf et al. [2017] use a conditional sampling based multi-variate approach to generate more targeted explanations on image classification CNNs. The Interpretability Randomization Test (IRT) and the One-Shot Feature Test (OSFT) introduced by Burns et al. [2020] focuses on discovering important features by replacing the features with uninformative counter-factuals. To derive a representation that is understandable by humans, LIME [Ribeiro et al. 2016] tries to find importance contiguous superpixels (a patch of pixels) in a source image towards the output class. Lundberg and Lee [2017] present a unified framework, SHAP, which computes individual feature contributions towards that output prediction.

As for the backpropagation-based methods, Saliency maps [Simonyan et al. 2014] constructs attributions by taking the absolute value of the partial derivative of the target output with respect to the input features. Gradient*Input [Shrikumar et al. 2016] was then proposed to improve the sharpness of the attribution maps. The attribution is computed by taking the (signed) partial derivatives of the output with respect to the input and multiplying them with the input itself. Integrated Gradients [Sundararajan et al. 2017], similarly to Gradient*Input, computes the partial derivatives of the output with respect to each input feature. However, while Gradient*Input computes a single derivative, evaluated at the provided input x, Integrated Gradients computes the average gradient

while the input varies along a linear path from a baseline $\hat{x}$ to x. Layer-wise Relevance Propagation (LRP) introduced by Bach et al. [2015] is used to find relevance scores for individual features in the input data by decomposing the output predictions of the DNN. DeepLIFT [Shrikumar et al. 2017b], similar to LRP, assigns each unit i an attribution that represents the relative effect of the unit activated at the original network input x compared to some other reference input $\hat{x}$.

Compared to all the existing attribution methods which produce the ranking of feature importance, WheaCha gives a precise definition of the critical features models use for prediction. Another key drawback for many attribution methods is the lack of systematic procedure for justifying their explanations to end users who often do not have expert knowledge in machine learning. WheaCha, on the other hand, can easily back up its explanations with the prediction results that satisfy the *sufficient* and *necessary* requirement.

7.2   Explainability Techniques for Models of Code

Explainability techniques for models of code have also been attracting growing attention from the software engineering field. Bui et al. [2019] evaluate the impact of a specific code fragment by deleting it from the original program. Zheng et al. [2020] present an approach to capture real vulnerability signals from a model's prediction. They apply prediction-preserving input minimization using delta debugging. Tantithamthavorn et al. [2020] summarize three successful case studies on how explainable AI techniques can be used to make software defect prediction models more practical, explainable, and actionable. From the perspective of model robustness, prior works [Bielik and Vechev 2020; Ramakrishnan et al. 2020; YEFET et al. 2020] also show models of code primarily attend to simple syntactic features which have caused them to be vulnerable to adversarial attacks.

Unlike all the above-mentioned works, WheaCha is an explanation method for code summarization models, at its core, it's a formal definition of the defining features models use for prediction.

7.3   Code Summarization Models

Allamanis et al. [2016] tackle the problem of code summarization with a neural convolutional attentional model. Their model has a rather limited capacity as it only looks at tokens in a program. code2vec [Alon et al. 2019b] is the first to predict method names based on a large, cross-project corpus. The main idea is to decompose an AST into a collection of AST paths for models to learn. code2seq [Alon et al. 2019a] further extends code2vec by adding a decoder to predict method names as sequences of words. Fernandes et al. [2019] combine sequence models like recurrent neural networks with graph models like graph neural networks to summarize programs or documents. LiGER [Wang and Su 2020] is the first that combines both static and dynamic program features in the code summarization setting. CuBERT [Kanade et al. 2020] and CodeBERT [Feng et al. 2020], two models built upon Bert [Devlin et al. 2019], which tackle the problem of code search, code documentation, exception classification, variable-misuse localization, *etc.* Also related, Func2vec [DeFreez et al. 2018a,b] presents an embedding approach to finding function synonyms that help identifying relationships among program elements and aiding program understanding, debugging, and analysis.

8 CONCLUSION

In this paper, we present WheaCha, an explanation method for code summarization models. At the core of WheaCha, is the formal definition of *wheat*, the defining features models use for predicting input programs. Technically, we develop a method *Reduce* and *Mutate*, and a working implementation HuoYan which we use to explain code2vec, code2seq, sequence GNN, and extreme summarizer. We found that some of the most popular attribution methods routinely miss out on the defining features which are composed of simple syntactic or lexical properties. With a successful case study of CodeBert with HuoYan, we also show that WheaCha has the potential to be generalized into a universal explanation method for all models of code. Last, we present an example application of the defining features: creating adversarial examples to attack the code summarization models. Through an extensive evaluation, we find that our attack is significantly more effective than the state-of-the-art in both non-targeted and targeted attacks with or without the defense technique of adversarial training.

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