SimSCOOD: Systematic Analysis of Out-of-Distribution Behavior of Source Code Models

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Abstract

While large code datasets have become available in recent years, acquiring representative training data with full coverage of general code distribution remains challenging due to the compositional nature of code and the complexity of software. This leads to the out-of-distribution (OOD) issues with unexpected model inference behaviors that have not been systematically studied yet. We contribute the first systematic approach that simulates various OOD scenarios along different dimensions of data properties and investigates the model behaviors in such scenarios. Our extensive studies on six state-of-the-art models for three code generation tasks expose several failure modes caused by the out-of-distribution issues. It thereby provides insights and sheds light for future research in terms of generalization, robustness, and inductive biases of source code models.

1 Introduction

There has been increasing success in applying large language models to various source code understanding and generation tasks. Large language models for codes such as CodeBERT (Feng et al., 2020), GraphCodeBERT (Guo et al., 2021), PLBART (Ahmad et al., 2021), and CodeT5 (Wang et al., 2021) are pre-trained for auto-regression using large-scale source code datasets, and serve as universal initialization for a variety of downstream tasks. These tasks include code summarization (Alon et al., 2019; LeClair et al., 2020), text-to-code generation (Bunel et al., 2018; Iyer et al., 2018; Gupta et al., 2020), code translation (Nguyen et al., 2013; Rozière et al., 2020; Roziere et al., 2022), and program repair (Tufano et al., 2018; Chen et al., 2019; Hajipour et al., 2021).

Considering these source code models play crucial roles in automatic software development, it is equally crucial, if not more, to foresee and understand any unexpected models’ behaviors in different scenarios beyond in-distribution train/test splits.

Despite having access to the large code datasets to pre-train and fine-tune these models, it remains challenging in practice to have a full coverage of general code distribution. This mainly stems from the compositional structures of programs and the complexity of software. For instance, given a programming language, the number of valid programs scales exponentially w.r.t. the language elements.

Therefore, it is unclear how these models behave in out-of-distribution (OOD) (Shen et al., 2021). For example, there is a lack of existing studies revealing how these models generalize to programs with unseen language elements or unseen semantics. A common way to study model behaviors in various OOD scenarios is to collect testing datasets in the complementary domains of the training dataset domain (Shen et al., 2021). However, because the underlying true distribution of source code is intractable, it is barely feasible to justify if two raw datasets share a domain or not. Not to mention the substantial costs to enumerate and constitute a variety of OOD testing datasets.

Simulating various OOD scenarios by masking out sub-regions of training data distribution is an
alternative way to systematically study the model behaviors (Schott et al., 2022; Wiles et al., 2022). There are several distribution dimensions based on data properties. In the source code domain, we have access to the rich structural information to model the source code distribution based on the complexity, syntax, and semantics of programs. For example, in terms of the syntax dimension, we can mask out all the data with if statements to create a syntax-based OOD scenario.

In this work, we propose a systematic approach to analyzing the behaviors of large language models in various OOD scenarios. By leveraging the lexical, syntax information, and contextual embeddings of programs, we simulate the OOD scenarios by masking out the source code distribution in the complexity, syntax, and semantics dimensions (Figure 1).

To summarize, the contributions of this paper are in five thrusts. 1. Our work pioneers to investigate the behaviors of the source code pre-trained models in OOD scenarios. 2. We propose a systematic approach to simulate a variety of OOD scenarios by masking out sub-regions of source code distribution along the complexity, syntax, and semantics dimensions. 3. We conduct extensive experiments on six different pre-trained source code models with three code generation tasks, where we analyze several properties of the pre-trained models, including architecture, objective function, and pre-trained dataset size. 4. We provide insights in the generalization, robustness, and inductive biases of source code models, which expose catastrophic failure modes of unseen language elements. 5. Our analysis of data/model properties sheds light for the construction of future datasets/research on OOD of code models to provide better training distributions accounting for generalization and inductive biases.

2 Related Work

Large Language Models for Code Understanding and Generation. With the availability of large-scale code datasets (Husain et al., 2019; Ahmad et al., 2021), there are growing interests in employing large language models to develop a unified pre-training model for source code understanding and generation. CuBERT (Kanade et al., 2020) and CodeBERT (Feng et al., 2020) are the first two models that employ pre-training in the source code domain. CuBERT mainly focuses on program understanding tasks, and CodeBERT extends the RoBERTa-based model (Liu et al., 2019) to understand and generate source code in various programming languages. Guo et al. (2021) extend CodeBERT by using a semantic-aware objective function. Svyatkovskiy et al. (2020) employ GPT-based (Raffel et al., 2020a), which uses decoder-only architecture, for the code completion task. PLBART (Ahmad et al., 2021), designed on top of BART (Lewis et al., 2020), proposes a unified encoder-decoder model for various code generation and understanding tasks. Apart from these, CodeT5 (Wang et al., 2021) is another encoder-decoder approach based on T5 (Raffel et al., 2020b) architecture. In our work, we focus on generation tasks to spot weak and strong points of the models in generating rare and unseen language elements and functionalities.

Out-of-Distribution Analysis in Natural Languages and Programming Languages. Despite the importance of OOD analysis and detection in production (Shen et al., 2021), there are surprisingly much fewer efforts to investigate OOD behaviors of NLP and PL approaches (Arora et al., 2021). Recently, Hendrycks et al. (2020); Kong et al. (2020) study the behavior of pre-trained large language models in OOD scenarios. These works mainly focus on NLP-related classification tasks. Even though they show that the pre-trained models are better calibrated, there is still room for improvement. Arora et al. (2021) categorize OOD data into background shift and semantic shift, and find that model calibration and density estimation have different behaviors on each type of OOD data. Xiao et al. (2020) propose an OOD detection approach for neural machine translation models. They employ a Bayesian-based approach to detect OOD data in translation tasks. Bui and Yu (2021) propose an energy-bounded-based approach to detect OOD source codes in program-related tasks such as code classification. In our work, we systematically investigate the behaviors of the pre-trained models in various OOD scenarios. We aim to spot the strengths and weaknesses of different pre-trained models in OOD scenarios w.r.t unseen levels of program complexity, syntax, and semantics.

Inductive Bias in Large Language Models. Erhan et al. (2010) show that unsupervised pre-training provides inductive bias by playing a regularization role in downstream tasks. More recently, Rytting and Wingate (2021) reveal that prior knowl-
edge embedded in large language models provides useful inductive bias for textual reasoning tasks. In our work through extensive experiments, we demonstrate that the pre-trained models for source codes provide inductive bias to generate unseen language elements. We analyze the dark and bright sides of this inductive bias in our systematic setups. Wan et al. (2022) show that pre-trained large language models for source codes capture the syntax structure of source codes in the intermediate representations. Troshin and Chirkova (2022) introduce different probing tasks to investigate if these models capture syntax and semantic information of the source code. They show that the encoder part preserve most syntax and semantic information. Based on the findings of Troshin and Chirkova (2022), in our work, we employ the encoder part of CodeT5 (Wang et al., 2021) to model the semantics of the programs in continuous space.

3 SimSCOOD: Simulation of Source Code Out-of-Distribution Scenarios

In this work, we propose a systematic approach to investigate the program model behaviors on OOD data by simulating the OOD scenarios in multiple dimensions. Our simulation strategy allows us to construct measurable OOD scenarios of real-world data without additional costs of accessing another dataset. More importantly, by simulating the OOD scenarios, we have the control over different properties of OOD scenarios. We achieve this by masking out specific sub-regions of data distribution.

These OOD scenarios span over three data dimensions, including complexity, syntax, and semantics. These dimensions cover different aspects of the programs. In complexity-based OOD scenarios, where we model the programs based on their implementation difficulty, we study how the models behave if we mask out programs in different complexity levels and analyze their behaviors in interpolation and extrapolation scenarios. Here interpolation is OOD cases in the middle part of the distribution, and extrapolation refers to OOD cases on the tails. Syntax-based scenarios enable us to study the models by masking out specific language elements. More interestingly, using syntax-based scenarios, we can analyze to what extent each model can generate unseen language elements. Using semantic-based scenarios, we can investigate how the models behave if we mask out the data with specific functionalities (e.g., getter functions in Java). Benefited from these scenarios, we can also implicitly quantify how well the models compose different code language elements to achieve unseen or rare functionality.

Here, we experiment with different pre-trained models and probe their behaviors in each scenario. We achieve this using our new approach that systematically constructs various scenarios to challenge the OOD performance of each model. As a result, the distribution of source code can be characterized using the forementioned dimensions that we call properties in the following. We model the joint distribution of the source code as \( q(p_1, \ldots, p_n) \) where each \( p_i \) is a specific property of the source code in distribution \( q \). Given this distribution we can sample a dataset \( \mathcal{D} = \{x_1, \ldots, x_N|x_i \sim q(p_1, \ldots, p_n)\} \).

To create each OOD scenario we need to sample a new dataset \( \hat{\mathcal{D}} = \{x_1, \ldots, x_N|x_i \sim \hat{q}(p_1, \ldots, p_n)\} \) where \( \hat{q}(p_1, \ldots, p_k) = 0 \), meaning the samples with properties \( p_f, \ldots, p_k \) are masked out. Note that we just formulated OOD scenarios with categorical properties, whereas it also holds for continuous properties by \( p(a < p_i < b) \) with \( a < b \) and \( a, b \in \mathbb{R} \).

To sample dataset \( \hat{\mathcal{D}} \) we get inspiration from the rejection sampling technique (Casella et al., 2004). Here, \( \hat{q}(p_1, \ldots, p_n) \) is our target distribution and we consider \( q(p_1, \ldots, p_n) \) as our proposal distribution. We reject or accept the sample data \( x \sim q(p_1, \ldots, p_n) \) using the following step function,

\[
    f(x) = \begin{cases} 
        1 & \text{if } P(x) \notin \hat{\mathcal{P}} \\
        0 & \text{if } P(x) \in \hat{\mathcal{P}} 
    \end{cases}
\]

(1)

where \( P(x) \) returns the properties of data \( x \), and \( \mathcal{P} \) are the properties that we do not want the sampled data \( x \) to contain. Using the rejection sampling technique with a hard-decision function (Equation 1) we can construct dataset \( \hat{\mathcal{D}} = \{x_1, \ldots, x_N|x_i \sim \hat{q}(p_1, \ldots, p_n)\} \) with accepted samples, and also have access to dataset \( \tilde{\mathcal{D}} = \{x_1, \ldots, x_N|x_i \sim \tilde{q}(p_1, \ldots, p_n)\} \) which are all of the rejected samples. To examine model behaviors in each OOD scenario, we train models using \( \tilde{\mathcal{D}} \) data, and test them on test set of \( \hat{\mathcal{D}} \). Figure 2 depicts an overview of the complexity-, syntax-, and semantic-based scenarios. In the following, we provide the details of the each OOD scenario and how we simulate the training and test sets. (subsections 4.1).
3.1 Complexity-based Out-of-Distribution Scenarios

We first simulate OOD scenarios based on different program complexity levels. One simple yet effective feature of the complexity is the size of the programs (Fenton and Neil, 1999). We use the histogram of program token sizes to represent the distribution of a given dataset. See Figure 2 left as an example. To create each OOD scenario, according to the rejection sampling technique, we draw samples from the distribution and reject only the samples in the histogram’s specified sub-region.

As an example, in one of the OOD scenarios, we can consider token size between 120 and 135 as OOD testing data. Then \( \hat{D} = \{ x \sim \hat{q}(p_1, \ldots, p_n) \} \) where \( q(120 < p_i < 135) = 0 \) is the accepted data in the rejection sampling technique. Experimenting with the complexity-based OOD scenarios enables us to analyze how program models generalize to interpolate and extrapolate over distribution gaps.

3.2 Syntax-based Out-of-Distribution Scenarios

Each programming language has its own grammar which is a set of rules to define valid program statements. Using the grammar, we can parse each program into an abstract syntax tree (Guo et al., 2021) and have access to all of the language elements used in the program. For example, we can identify all the conditional (e.g., if) languages elements of each program. In this work, we leverage the grammatical information of the programming language to create syntax-based OOD scenarios. We use the histogram of language elements to model the syntax distribution of a given source code dataset. Figure 2 middle shows an example of how we construct a syntax-based OOD scenario by masking out specific language elements. To create an OOD scenario, using rejection sampling technique, we sample testing data \( \tilde{D} \) that does not contain certain language elements (e.g., while), namely, \( \mathcal{P} = \{ \text{while} \} \). We then train our model using \( \hat{D} \) which is the set of data that does not contain while, and test the model using \( \tilde{D} \). In order to set up systematic syntax-based OOD scenarios, we can replace while in \( \mathcal{P} \) with a traversal of other language elements. Using syntax-based OOD scenarios, in addition to analyzing model behaviors in such OOD, we can also explore the inductive biases from the pre-training procedure for various models. For example, we can count the frequencies of different pre-trained models that generate programs with unseen language element.

3.3 Semantic-based Out-of-Distribution Scenarios

The semantics of programs is our third way of modeling the distribution of a given source code dataset. However, it is not clear how we can model the semantics of the programs, especially in the cases where we do not have Input-Output examples or any meta-data. It has been shown that a large pre-trained model can be used to cluster the input data based on their semantics (Aharoni and Goldberg, 2020). Following the success of unsupervised domain clustering, in this work, we employ the pre-trained CodeT5 (Wang et al., 2021) encoder to map a dataset of programs to a set of continuous representation vectors. We then cluster the vectors to group programs with similar semantics. As a result, we are able to create semantic-based OOD scenarios, via the rejection sampling procedure, to reject all samples that belong to a specific cluster and accept the rest as \( \hat{D} \). Like other scenarios we can use \( \hat{D} \) as training data and \( \tilde{D} \) as test data. Semantic-based OOD scenarios allow us to analyze the model’s ability to deal with unseen or rare program semantics (functionality). We provide more implementation details in subsection 4.2.

4 Experiments

In this section, we first articulate the experiment setups, including the pre-trained program models, downstream tasks, and OOD data construction process. Then, we demonstrate the model’s performance in different OOD scenarios. We also analyze how well the model can generalize in various sce-
narios by revealing 50% of the masked data to the model. In the following, we call the 50% masked-out cases generalization scenarios. Furthermore, we investigate the inductive bias of the models in generating unseen language elements.

4.1 Setups

Pre-trained Models. We analyze the behavior of six widely-used pre-trained models for source code. These models are designed using a variety of architectures, pre-training objective functions, numbers of parameters, and pre-training dataset sizes. CodeBERT (Feng et al., 2020) is an encoder-only transformer-based model that is pre-trained using the CodeSerchNet dataset (Husain et al., 2019). This dataset consists of 2.1M pairs of individual functions and code documentation with 6.4M code-only data items across multiple programming languages. GraphCodeBERT (Guo et al., 2021) extends CodeBERT using a semantic-aware pre-training objective function. PLBART (Ahmad et al., 2021) is a BART-based (Lewis et al., 2020) encoder-decoder transformer that is pre-trained with a source code dataset of 470M Java functions and 210M Python functions, associated with 47M natural language descriptions. Additionally, we study PLBART CS which uses CodeSerchNet (Husain et al., 2019) as pre-training dataset. CodeT5 (Wang et al., 2021) employs T5 (Raffel et al., 2020) encoder-decoder architecture. In our implementations, we use CodeT5-base with 220M parameters and CodeT5-small with 60M parameters. We provide more models’ details in Appendix A.

Downstream Tasks. We study the behavior of the models on three different downstream tasks, including text-to-code generation, code refinement, and code translation. These tasks are part of the most challenging tasks in the CodeXGLUE benchmark (Lu et al., 2021). Text-to-code is the task of generating a program given a natural language description. In CodeXGLUE benchmark (Lu et al., 2021), CONCODE dataset (Iyer et al., 2018) is proposed for this task. Code refinement is the task of resolving the bugs in a given program by automatically generating a corrected program. We use the medium dataset of Tufano et al. (2019). Code translation is the task of translating the program from one programming language to another. We use the released dataset of Lu et al. (2021) to translate from CSharp functions to Java functions.

Evaluation Metrics. Exact match (Wang et al., 2021), and BLEU score (Papineni et al., 2002) have been commonly used to evaluate the model performance in the downstream tasks. The exact match metric evaluates if the generated code precisely matches the target code at token-level. BLEU score measures the n-gram overlap between the output and the target code. In this work, we mainly focus on the exact match metric to quantify the model’s behaviors. It has been shown that BLEU score is not necessarily correlated with the correctness of the programs (Hendrycks et al., 2021). We also report BLEU score results in Appendix D.

4.2 Data Construction and Fine-tuning

In the data construction process, for each scenario, we choose $\tilde{P}$ in a way that it counts for $\approx 3\%$ of the entire training data. In OOD scenarios, we mask out all of the data with properties $\tilde{P}$. For the generalization cases, we mask-out half (50%) of data with properties $\tilde{P}$ ($\approx 1.5\%$ of the entire training data). In all the scenarios, we infer the fine-tuned models on test data with $\tilde{P}$ properties. Note that, in the text-to-code task, we mask out the data based on the target data (code data rather than text data) properties. For the other tasks, we masked the data based on the input.

Complexity-based Scenarios. To generate data for complexity-based scenarios, we characterize the dataset of programs based on the token size. For each scenario, $\tilde{P}$ specifies a continuous range of program token sizes. We consider five ranges in our experiments: $\tilde{P}_1 = \{[0\%, 3\%]\}$, $\tilde{P}_2 = \{[24\%, 27\%]\}$, $\tilde{P}_3 = \{[48\%, 51\%]\}$, $\tilde{P}_4 = \{[72\%, 75\%]\}$, and $\tilde{P}_5 = \{[97\%, 100\%]\}$. Note that $\tilde{P}_1 = \{[0\%, 3\%]\}$ represents the top 3% smallest programs, in terms of token size.

Syntax-based Scenarios. In syntax-based scenarios, we characterize programs datasets based on the histogram of language elements (e.g., syntex keyword if). For each task, we select five different language elements, corresponding to five syntax-based scenarios, each that covers $\approx 3\%$ of the entire data. For example, in text-to-code task $\tilde{P}_1 = \{\text{else}\}$. We provide details of the selected language elements in Appendix B.

Semantic-based Scenarios. In this work, we employ CodeT5 (Wang et al., 2021) encoder to characterize the semantics distribution of programs. We feed the tokenized programs to the CodeT5
encoder and obtain the corresponding feature vectors $V$ of size $768 \times t$, where $t$ is the size of the input program. We obtain the continuous representation of the programs by averaging the tokens’ embedding following (Koto et al., 2021). We then cluster the programs in continuous space using the K-means algorithm. We set the number of clusters $K = 35$ using the elbow method (Bholowalia and Kumar, 2014). To accelerate the clustering procedure, we perform dimensionality reduction PCA with the target dimension of 50. We determine the dimension in a way that all the components explain at least 80% of the data variance. To have different semantic-based scenarios, without losing generality, we randomly select five different clusters. Each cluster can represent a set of $\tilde{P}_i$ properties.

**Model Fine-tuning Details.** We fine-tune six pre-trained models for three different tasks in various scenarios. We stick to their defaults for fair comparisons. All our experiments are conducted using a single NVIDIA 40GB Ampere A100 GPU.

### 4.3 How Do Models Generalize in OOD Scenarios?

Figure 3 shows the overall results performance of different models in complexity-, syntax-, and semantic-based scenarios, respectively. Note that we separately provide results for the interpolation and extrapolation cases of the complexity-based scenarios. Figure 3a shows the model performance in the OOD scenarios where the models do not have access to the training data with $\tilde{P}$ properties. Result in Figure 3b show how well the models perform when they have access to the 50% of the training data with $\tilde{P}$ properties. Note that in Figure 3a and Figure 3b all of the results are the average of different scenarios. In complexity-based scenarios, we have five different scenarios, three for the interpolation cases and two for the extrapolation cases, so we report the average results for each case. In syntax-based and semantic-based scenarios, we report the average results of five different scenarios.

We conclude according to Figure 3a that: 1. Interpolation cases in the complexity-based OOD scenarios, as we expected, are the easiest OOD scenarios for the models in different tasks. 2. Syntax-based OOD scenarios are the most challenging scenarios for the models. 3. BERT-based models are the most susceptible models to the OOD data, especially in the syntax-based OOD scenarios. 4. Even though PLBART uses a 200x larger pre-training dataset compared to PLBART CS, we observe that in different OOD scenarios, especially in syntax-based and semantic-based scenarios, they have comparable performance.

**Model behaviors in complexity-based OOD scenarios.** In Figure 4, we provide the results of the models in five scenarios for three tasks. Scenarios span over the x-axis of the plots. For example, 0%-3% shows the results when we mask out the programs that are the top 0% to 3% program with the smallest token size. In these scenarios, 0%-3% and 97%-100% are the extrapolation cases because they are the ending bins, and the rest of the scenarios are thus interpolation cases. The y-axis of the plots in Figure 4 shows the exact match results of each model relative to when the model has access to 100.0% of the training data.

In Figure 4 we observe the most challenging parts are the extrapolation cases (0%-3% and 97%-100%). Especially, we observe that in the text-to-code task (Figure 4a), all models’ performance drastically drops. The interesting case is that the model performance drops significantly when we only mask out small-size tokens (0%-3%) from the programs. In the code translation task (Figure 4c), we observe that the models are more susceptible to removing programs with a larger size than smaller-size. We reason that code translation is an easier task than the two others as the models can easily learn to copy unseen or rare language elements. We provide more results in Appendix D.

**Model behaviors in syntax-based OOD scenarios.** In Figure 3a we show that syntax-based scenarios are the most challenging OOD scenarios for the models in different tasks. We reason that it challenges models more to generate unseen language elements than to compose a set of seen elements. We further observe more significant performance drops in text-to-code and code refinement tasks than in code translation tasks. This indicates that in translation tasks, the models learn to copy unseen or rare language elements.

Among the models, according to Figure 3a we observe that BERT-based models have the most significant performance drops. This shows that encoder-only models are more susceptible to the OOD scenarios than the encoder-decoder models. Another discovery is that PLBART performance drops more than PLBART CS, although PLBART uses 200x more pre-training data items.
Figure 3: Overall results of the model performance in different scenarios. (a) Relative exact match to the 100% baseline (without data mask-out) for different OOD scenarios. (b) Relative exact match to the 100% baseline for different generalization scenarios (access to 50% of the data of a certain property).

Model behaviors in semantic-based OOD scenarios. In Figure 3a we depict the performance of the models in different semantic-based OOD scenarios. We find smaller performance drops in semantic-based OOD scenarios compared to syntax-based ones. We reason that, in semantic-based ones, the models have the opportunity to learn to compose observed language elements to implement unseen or rare semantics. However, in syntax-based OOD scenarios, the models do not encounter particular language element(s) during the fine-tuning.

4.4 What Are the Inductive Biases of the Pre-trained Models?

In OOD scenarios, we explore the inductive biases of the models in different tasks. As an example, in Figure 3a, we ascribe the performance gain of the models in syntax-based scenarios to the inductive biases of the models. Furthermore, in syntax-based OOD scenarios, we systematically analyze to what extent each model’s inductive biases can provide enough information to generate unseen language elements. In the following, we examine the inductive biases of each model in generating unseen language elements.

Figure 5 shows the frequencies of unseen or rare language elements relative to the frequencies in ground truth programs. We consider a language element as unseen if it does not appear in training data, and we consider it rare if it just counts for $\approx 1.5\%$ of the training data items. We report the average results of five different unseen language elements during fine-tuning. Note that the solid bars show the results when models do not see the language elements, and the hatched bars show the results when models have access to 50% of the data with those language elements.

Figure 4: Model performance in different complexity-based OOD scenarios in terms of relative exact match compared to the 100% baselines (without data mask-out). We provide results for (a) text-to-code, (b) code refinement and (c) code translation tasks.

Figure 5 shows that the models are able to generate unseen language elements in different tasks. More interestingly, we observe that models can gain a large margin in generating those elements with just 50% of the masked-out language elements ($\approx 1.5\%$ of the training data). We can also see that in the translation task, the models can generate almost as much as ground truth cases, which again shows that the models learn to copy unseen and rare language elements. Here, text-to-code is the most challenging task in generating language elements. The main reason is that the models need to learn the mapping from natural language to the programs. We further observe that BERT-based models provide less informative inductive biases to generate unseen elements than the other models.
Figure 5: Frequencies of generating unseen and rare language elements relative to the frequencies of the language elements in ground truth data. Solid and hatched bars show the results when models do not see the language elements and when the models have access to 50% of data with those elements, respectively.

Figure 6: Histograms of negative log-likelihood density for different models in syntax-based OOD scenarios (0.00%) and in full distribution scenarios (100.00%). We provide results for Code refinement task. Lower negative log-likelihood means higher confidence.

4.5 Models Confidence Is not a Reliable Alternative Metric

Figure 6 provides the confidence distributions of different code refinement models in syntax-based OOD scenarios and in in-distribution scenario (when the model has access to all the data). The x-axes of these plots show the negative log-likelihood of the generated code, similar in spirit to Xiao et al. (2020). Results of the other tasks and models are provided in Appendix D. We find that we can not distinguish the in-distribution from OOD data cleanly by relying on the model confidence. We conclude that it is not possible to easily detect OOD data solely based on the model confidence.

5 Discussion

Our systematic experimental approach exposes the fragility of the pre-trained models for source code, in several OOD scenarios. Our results validate that there is no best model in dealing with OOD scenarios. However, we show that BERT-based models are the most susceptible to OOD data. We advocate that future models need to be examined in OOD scenarios. Furthermore, they need to be either well-calibrated or guarded using OOD detector.

In our experiments, we show that syntax-based OOD scenarios are the most challenging OOD cases for all of the models. More interestingly, we also show that the models can gain high improvement by just adding a few relevant data to the training set ($\approx 1.5\%$ of the training set). This evidences how catastrophic a model might fail if it is not updated with the data of newly introduced language elements or APIs. This aspect needs to be taken into account in dataset construction, as current models have a hard time dealing with missing data at training time.

Furthermore, our results show that pre-trained models can be fine-tuned to generate unseen language elements in various downstream tasks. This could lead to the failure of the models and, in some extreme points, causes security and privacy issues. As an example, the model could generate a deprecated API or element, or there can even be cases when the pre-trained dataset might be poisoned in the first place (Schuster et al., 2021).

6 Conclusion

In this work, we propose a systematic approach to investigate the behaviors of pre-trained models in OOD scenarios. Given the data, we simulate OOD scenarios based on the program’s complexity, syntax, and semantics. Using the simulated scenarios, we shed light on the model fragility in the OOD scenarios, potential misbehavior or dangers of these models, and the necessity to improve dataset construction in the future. We also reveal the model impotence to handle each considered OOD dimension and to what extent we can improve the generalization of the models by exposing the relevant data. Furthermore, we investigate how well the models can generate unseen language elements, and we discuss the potential threats of these inductive biases. We will release the implementation of our work to
support future systematic analysis of source code model behavior in OOD scenarios.

Limitations

One of the limitations of our approach is about the computational cost. To investigate the model behavior in each dimension, we need to fine-tune individual models. This makes our investigation computationally expensive. Furthermore, in this work, we focus on the code generation tasks as they provide more fine-grained results to investigate the model behavior. It would also be interesting to investigate how the models perform in OOD scenarios in understanding tasks, such as clone detection or defect detection.

In our work, we leverage the contextual embedding of source code to model the semantics of the source codes. We use K-means clustering to group programs based on their semantics. Even though we check if these clusters represent specific meaning (we provide examples of cluster semantics in Appendix C), we do not measure how well these programs are clustered in terms of their semantics. The performance of the clustering algorithm can be measured using datasets with meta-data about the semantics of each data item, which we do not have access to in this study.
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A Pre-trained Models

Here, we provide more detail about the pre-trained models we used in our experiments.

A.1 BERT-based Models

CodeBERT (Feng et al., 2020) is an encoder-only transformer-based model that is pre-trained using CodeSearchNet dataset (Husain et al., 2019). This dataset consists of 2.1M pairs of individual functions and code documentations with 6.4M code-only data items across multiple programming languages. This model uses a 12-layer RoBERTa-based (Liu et al., 2019) architecture with 125M parameters. It is trained using masked language modeling (MLM) and replaced token detection objective.

Guo et al. (2021) proposed GraphCodeBERT by extending CodeBERT (Feng et al., 2020) using a semantic-aware pre-training objective function. They incorporate data-flow information in the pre-training stage to encode the semantic information of the program.

A.2 PLBART

PLBART (Ahmad et al., 2021) is a BART-based (Lewis et al., 2020) encoder-decoder transformer that consist of six encoder and decoder layers. (Ahmad et al., 2021) use a pre-training dataset of source code for 470M Java and 210M Python functions, and their corresponding 47M code-related natural language descriptions. There are three different variants of this model: (i) PLBART consist of 140M parameter, (ii) PLBART Large, which is a 12-layers encoder-decoder with 400M parameters, and (iii) PLBART CS, which uses CodeSearchNet (Husain et al., 2019) as a pre-training dataset. PLBART (Ahmad et al., 2021) uses denoising function similar to BART-base (Lewis et al., 2020) model.

A.3 CodeT5

CodeT5 (Wang et al., 2021) employ T5 (Raffel et al., 2020b) encoder-decoder architecture. The authors use CodeSearchNet (Husain et al., 2019) with 1.2M pairs of functions’ code with corresponding documentation, and 0.8M code-only data items. In our experiments, we use CodeT5-base with 220M parameters and CodeT5-small with 60M parameters. This model uses MLM objective and identifier-aware objective function in the pre-training procedure.

B List of Language Elements

In syntax-based scenarios, we consider one element in each scenario and mask-out the source code with that particular element. Here, we provide the details of five language elements used in our experiments. Note that, in each study, we pick an element that covers ≈ 3% of the training data. We conduct our syntax-based experiments based on the following language elements of each tasks,

1. **Text-to-Code**: \{ `else`, `floating_point_type`, `unary_expression`, `array_access`, `true` \}

2. **Code Refinement**: \{ `while_statement`, `long`, `array_creation_expression`, `break`, `>=` \}

3. **Code Translation**: \{ `for`, `true`, `array_creation_expression`, `||` (or), `conditional_expression` \}

C Do the clusters represent programs with specific semantics?

Table 1 provides semantics of five random clusters (out of 35) in text-to-code tasks. We randomly check 20 source codes in each cluster to check their semantics.

Table 1: Semantics of five clusters in text-to-code task.

| Cluster ID | Semantic                |
|------------|-------------------------|
| 0          | Property setter functions |
| 1          | Property string getter functions |
| 6          | Initialize object        |
| 11         | Using getter function    |
| 17         | String concatenation     |

D More experimental results

D.1 BLEU-score Results

Table 2 and Table 3 provide BLEU score results for syntax-based and semantic-based OOD scenarios, respectively. As we mention in subsection 4.1, the BLEU score is not necessarily correlated with the correctness of the programs. (Hendrycks et al., 2021). For example, Wang et al. (2021) show that in the code refinement task, the BLEU score of a naive copy of the input code can be as good as the state-of-the-art methods. In Table 2 we can observe the performance drop of the models in all three tasks in OOD scenarios compared to the 100% baseline. In Table 3 we can also see the
performance drops in OOD scenarios of text-to-code compared to 100% baseline. However, in code refinement and translation, we can see a few performance drops in OOD scenarios compared to the other scenarios.

Table 4, Table 5, and Table 6 provide BLEU score results for complexity-based scenarios in text-to-code, code refinement, and code translation tasks. We provide results for five different scenarios. The first (0% − 3%) and last scenarios (97%−100%) show the results for the extrapolation cases, and the rest of the scenarios are the interpolation cases. In the three tasks, we can observe again that extrapolation cases are more challenging than interpolation cases. We can see that by comparing the OOD scenarios with the 100% baseline.

D.2 Qualitative examples

In Figure 7, Figure 8, Figure 9, and Figure 10 we provide qualitative results where the CodeT5 model was able to generate unseen language element. Figure 7 shows an example where the model generates unseen true element for text-to-code task. However, in the generated code, we can see the model does not use the keyword true correctly. Figure 8 provides another example of text-to-code task in generating unseen unary_expression. In the generated example of the code at line 2 we can see that the models does not use unary expression “!” (not) correctly to implement the desired functionality of the target code. This indicates that the inductive biases in generating unseen elements in these models can cause security and vulnerability issue. Figure 9 shows an example of code refinement task. In line 6 of the generated code, the model can generate a break statement, which was unseen to the model. However, by comparing the generated code with the target code, we can see that the model could not generate break element in line 9 of the target code. Figure 10 shows an example of the translation task. In line 4 of the generated code, we can observe that the model generates the for statement exactly like the target code while it does not observe any example with for statement during fine-tuning. This is a qualitative example that indicates that in the translation task, the models learn to copy the unseen and rare elements.

D.3 More Results of Complexity-based Scenarios

Figure 11 provides the results for the models in five complexity-based scenarios. We provide the results for the generalization scenarios, where we reveal 50% of the masked data with certain properties to the model. Here, we can also see that the extrapolations part are the most challenging scenario for the models. Furthermore, we can see that the left extrapolation part (0 − 3%) is less challenging for the models in different tasks compared to the right part (97 − 100%). We can see large gaps between the models in code translation tasks (Figure 11c), especially for the PLBART CS. This is because in this task, we have low test data, and just a few changes can drop or raise the exact match results of the models sharply.

D.4 More Results of Models’ Confidence

Figure 12 provides models’ confidence results of text-to-code, code refinement, and code translation in syntax-based scenarios. In this figure (Figure 12), we can see that the confidence distributions of in- and out-of-distribution data for the text-to-code task are less distinguishable than the other tasks. In general, we can see that we can not cleanly distinguish in- and out-of-distribution data for all tasks and models.

---

**Input text:** returns true if the predicate evaluates to true with respect to the specified scan.

(a) Target Code

```
1 boolean function (Scan arg0) {
2    for (Term loc0: terms)
3        if (!loc0.isSatisfied(arg0)) {
4            return false;
5        }
6    return true;
7 }
```

(b) Generated Code

```
1 boolean function (Scan arg0) {
2    return true(terms.containsAll());
3 }
```

Figure 7: An example of generated code by CodeT5 in syntax-based OOD scenario for the text-to-code task. Here true is unseen language element.
Table 2: BLEU score results of models for text-to-code, code refinement and code translation in syntax-based scenarios. OOD refers to the OOD scenarios, Gen denotes to generalization scenarios (access to 50% of the data with certain properties), and Full refers to 100% baseline (when model has access to 100% of training set).

| Models     | Text-to-Code | Code Refinement | Code Translation |
|------------|--------------|-----------------|------------------|
|            | OOD          | Gen            | Full            | OOD            | Gen            | Full            | OOD          | Gen            | Full            |
| CodeT5     | 24.08        | 25.20          | 27.01           | 83.05          | 89.19          | 89.88           | 65.39        | 72.06          | 73.31           |
| CodeT5 Small | 20.38      | 21.64          | 24.05           | 85.41          | 90.78          | 90.06           | 64.38        | 71.10          | 73.38           |
| PLBART     | 17.16        | 18.91          | 20.98           | 82.32          | 90.00          | 89.09           | 66.38        | 72.06          | 73.31           |
| PLBART CS  | 20.99        | 21.75          | 25.67           | 83.04          | 89.33          | 89.50           | 69.49        | 71.17          | 71.43           |
| GCBERT     | -            | -              | -               | 79.44          | 90.36          | 91.10           | 52.54        | 62.70          | 65.38           |
| CBERT      | -            | -              | -               | 80.26          | 91.11          | 91.14           | 47.09        | 59.27          | 61.98           |

Table 3: BLEU score results of models for text-to-code, code refinement and code translation in semantic-based scenarios. OOD refers to the OOD scenarios, Gen denotes to generalization scenarios (access to 50% of the data with certain properties), and Full refers to 100% baseline (when model has access to 100% of training set).

| Models     | Text-to-Code | Code Refinement | Code Translation |
|------------|--------------|-----------------|------------------|
|            | OOD          | Gen            | Full            | OOD            | Gen            | Full            | OOD          | Gen            | Full            |
| CodeT5     | 44.58        | 45.43          | 48.48           | 85.68          | 86.54          | 86.54           | 82.83        | 83.64          | 83.64           |
| CodeT5 Small | 37.01      | 40.13          | 46.67           | 86.78          | 88.91          | 88.85           | 79.81        | 79.98          | 81.59           |
| PLBART     | 36.52        | 40.00          | 44.70           | 86.58          | 87.23          | 86.86           | 79.18        | 83.40          | 80.63           |
| PLBART CS  | 36.46        | 39.21          | 42.69           | 86.77          | 86.88          | 87.2           | 81.71        | 83.48          | 79.78           |
| GCBERT     | -            | -              | -               | 88.36          | 88.95          | 89.73           | 74.43        | 77.44          | 77.04           |
| CBERT      | -            | -              | -               | 88.71          | 89.35          | 89.24           | 70.67        | 79.14          | 76.25           |

Input text: set a default spacing value. This is used as a fallback when no spacing has been set for a particular direction.

(a) Target Code

```java
1 boolean function (int arg0, float arg1) {
2     if (mDefaultSpacing == null) {
3         mDefaultSpacing = newSpacingResultArray ();
4     }
5     if (!FloatUtil.floatsEqual(
6         mDefaultSpacing[arg0], arg1)) {
7         mDefaultSpacing[arg0] = arg1;
8         return true;
9     }
10    return false;
11 }
```

(b) Generated Code

```java
1 void function (int arg0, float arg1) {
2     if (mValueFlags != 0) {
3         throw new Error("srini_string");
4     }
5     mDefaultSpacing[arg0] = arg1;
6     mValueFlags = mValueFlags;
7 }
```

Figure 8: An example of generated code by CodeT5 in syntax-based OOD scenario for text-to-code task. Here unary_expression is unseen language element.
Table 4: BLEU score results of models for text-to-code in complexity-based scenarios. OOD refers to the OOD scenarios, Gen denotes to generalization scenarios (access to 50% of the data with certain properties), and Full refers to 100% baseline (when model has access to 100% of training set).

| Models       | 0%-3% OOD | 0%-3% Gen | 0%-3% Full | 24%-27% OOD | 24%-27% Gen | 24%-27% Full | 48%-51% OOD | 48%-51% Gen | 48%-51% Full | 72%-75% OOD | 72%-75% Gen | 72%-75% Full | 97%-100% OOD | 97%-100% Gen | 97%-100% Full |
|--------------|-----------|-----------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| CodeT5       | 15.69     | 16.86     | 25.95      | 38.61       | 50.48       | 51.46       | 39.57       | 49.95       | 43.09       | 42.40       | 46.30       | 48.84       | 14.50       | 23.51       | 22.22       |
| CodeT5 Small | 32.86     | 38.27     | 42.88      | 64.67       | 74.25       | 74.95       | 61.52       | 66.57       | 74.95       | 44.76       | 66.43       | 50.39       | 19.33       | 23.51       | 27.79       |
| PLBART       | 58.77     | 60.82     | 68.01      | 70.67       | 77.43       | 80.68       | 60.37       | 57.88       | 58.14       | 35.82       | 39.29       | 42.81       | 17.27       | 18.78       | 19.11       |
| PLBART CS    | 12.74     | 26.13     | 24.64      | 39.89       | 49.35       | 49.59       | 38.89       | 42.53       | 44.6        | 36.33       | 46.35       | 43.85       | 9.23        | 15.33       | 15.30       |

Table 5: BLEU score results of models for code refinement in complexity-based scenarios. OOD refers to the OOD scenarios, Gen denotes to generalization scenarios (access to 50% of the data of a certain property), and Full refer to 100% baseline (when model has access to 100% of training set).

| Models       | 0%-3% OOD | 0%-3% Gen | 0%-3% Full | 24%-27% OOD | 24%-27% Gen | 24%-27% Full | 48%-51% OOD | 48%-51% Gen | 48%-51% Full | 72%-75% OOD | 72%-75% Gen | 72%-75% Full | 97%-100% OOD | 97%-100% Gen | 97%-100% Full |
|--------------|-----------|-----------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| CodeT5       | 76.72     | 77.78     | 80.71      | 84.73       | 84.13       | 84.56       | 89.15       | 87.28       | 89.44       | 88.24       | 88.60       | 88.20       | 83.99       | 85.47       | 85.74       |
| CodeT5 Small | 78.37     | 81.77     | 80.95      | 85.73       | 87.74       | 87.57       | 87.93       | 89.19       | 88.72       | 87.78       | 87.78       | 87.91       | 84.70       | 87.99       | 86.13       |
| PLBART       | 79.80     | 82.53     | 83.49      | 86.09       | 87.82       | 88.16       | 87.72       | 86.88       | 87.52       | 86.4       | 86.6        | 84.45       | 81.31       | 81.31       | 84.80       |
| PLBART CS    | 80.40     | 82.62     | 84.16      | 85.63       | 88.35       | 87.70       | 87.43       | 88.23       | 88.52       | 86.81       | 87.56       | 87.245      | 82.36       | 82.36       | 84.19       |
| GCBERT       | 80.44     | 82.97     | 81.18      | 87.05       | 87.32       | 87.42       | 88.74       | 89.13       | 89.13       | 88.88       | 89.35       | 88.93       | 85.59       | 87.32       | 88.05       |
| CBERT        | 80.71     | 80.86     | 91.04      | 86.22       | 86.95       | 89.53       | 89.48       | 89.15       | 86.40       | 90.21       | 88.45       | 90.97       | 86.46       | 86.75       | 92.4        |

Figure 9: An example of generated code by CodeT5 in syntax-based OOD scenario for code refinement task. Here break is unseen language element.

(a) Target Code

```
1 public void METHOD_1(android.view.View view) {
2     switch(view.getId()) {
3         case VAR_1:  
4             int index = (VAR_2.METHOD_2()) - 1;
5             VAR_2.METHOD_3((index >= 0 ? index : (VAR_3.METHOD_4()) - 1));
6             break;
7         case VAR_4:
8             VAR_2.METHOD_3(((VAR_2.METHOD_2()) + 1) % (VAR_3.METHOD_4()));
9             break;
10     }
11 }
```

(b) Generated Code

```
1 public void METHOD_1(android.view.View view) {
2     switch(view.getId()) {
3         case VAR_1:  
4             int index = (VAR_2.METHOD_2()) - 1;
5             VAR_2.METHOD_3((index >= 0 ? index : (VAR_3.METHOD_4()) - 1));
6             break;
7         case VAR_4:
8             VAR_2.METHOD_3(((VAR_2.METHOD_2()) + 1) % (VAR_3.METHOD_4()));
9         }
10 }
```

Figure 10: An example of generated code by CodeT5 in syntax-based OOD scenario for code translation task. Here for is unseen language element.

(a) Target Code

```
1 public void addAll(BlockList < T > src) {
2     if (src.size == 0) return;
3     int srcDirIdx = 0;
4     for (; srcDirIdx < src.tailDirIdx; srcDirIdx++) addAll(src.directory[srcDirIdx], 0, BLOCK_SIZE);
5     if (src.tailBlkIdx != 0) addAll(src.tailBlock, 0, src.tailBlkIdx);
6 }
```

(b) Generated Code

```
1 public void addAll(BlockList < T > src) {
2     if (src.size == 0) return;
3     int srcDirIdx = 0;
4     for (; srcDirIdx < src.tailDirIdx; srcDirIdx++) {
5         addAll(src.directory[srcDirIdx], 0, BLOCK_SIZE);
6     }
7     if (src.tailBlkIdx != 0) {
8         addAll(src.tailBlock, 0, src.tailBlkIdx);
9     }
10 }
```
Table 6: BLEU score results of models for code translation in complexity-based scenarios. OOD refers to the OOD scenarios, Gen denotes to generalization scenarios (access to 50% of the data of a certain property), and Full refer to 100% baseline (when model has access to 100% of training set).

| Models    | 0%-3% OOD | 0%-3% Gen | 0%-3% Full | 24%-27% OOD | 24%-27% Gen | 24%-27% Full | 48%-51% OOD | 48%-51% Gen | 48%-51% Full | 72%-75% OOD | 72%-75% Gen | 72%-75% Full | 97%-100% OOD | 97%-100% Gen | 97%-100% Full |
|-----------|-----------|-----------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| CodeT5    | 46.77     | 53.29     | 59.94      | 71.76       | 73.34       | 76.33       | 70.31       | 74.15       | 77.49       | 65.44       | 67.48       | 68.15       | 54.11       | 71.65       | 71.43       |
| CodeT5 Small | 45.1      | 57.74     | 55.91      | 71.51       | 70.89       | 76.69       | 72.44       | 73.13       | 73.64       | 64.32       | 63.94       | 65.25       | 60.55       | 66.4        | 65.25       |
| PLBART    | 45.13     | 48.75     | 50.03      | 73.21       | 74.92       | 78.03       | 73.49       | 66.10       | 74.42       | 63.93       | 64.07       | 65.44       | 66.04       | 69.69       | 69.41       |
| PLBART CS | 49.92     | 51.21     | 56.15      | 71.28       | 73.21       | 77.6        | 72.5        | 72.11       | 72.08       | 64.74       | 63.95       | 60.76       | 62.54       | 68.2        | 67.26       |
| GCBERT    | 44.42     | 54.04     | 53.35      | 66.23       | 69.1        | 76.78       | 64.32       | 67.18       | 69.4        | 46.01       | 51.66       | 53.8        | 41.07       | 49.25       | 59.87       |
| CBERT     | 44.09     | 47.14     | 53.35      | 66.69       | 72.09       | 77.52       | 62.47       | 68.27       | 68.43       | 42.91       | 50.49       | 56.1        | 37.93       | 47.29       | 57.18       |

Figure 11: Results of models’ performance in different complexity-based scenarios. It shows the results when the models have access to 50% of the data with certain properties in each scenario. We provide results for (a) text-to-code, (b) code refinement and (c) code translation tasks.

Figure 12: Histogram of the negative log-likelihood density for different models in syntax-based OOD scenario (0.00%) and the full distribution scenario (100.00%). We provide results for text-to-code, code refinement, and code translation tasks.