CERT: Continual Pre-Training on Sketches for Library-Oriented Code Generation

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Abstract

Code generation is a longstanding challenge, aiming to generate a code snippet based on a natural language description. Usually, expensive text-code paired data is essential for training a code generation model. Recently, thanks to the success of pre-training techniques, large language models are trained on large-scale unlabelled code corpora and perform well in code generation. In this paper, we investigate how to leverage an unlabelled code corpus to train a model for library-oriented code generation. Since it is a common practice for programmers to reuse third-party libraries, in which case the text-code paired data are harder to obtain due to the huge number of libraries. We observe that library-oriented code snippets are more likely to share similar code sketches. Hence, we present CERT with two steps: a sketcher generates the sketch, then a generator fills the details in the sketch. Both the sketcher and the generator are continually pre-trained upon a base model using unlabelled data. Furthermore, we craft two benchmarks named PandasEval and NumpyEval to evaluate library-oriented code generation. Experimental results demonstrate the impressive performance of CERT. For example, it surpasses the base model by an absolute 15.67% improvement in terms of pass@1 on PandasEval. Our work is available at https://github.com/microsoft/PyCodeGPT.

1 Introduction

Code generation, aiming to generate a code snippet for a given natural language description, is a longstanding challenge in the artificial intelligence community. Usually, to train a code generation model with good performance, the massive amount of code snippets paired with natural language descriptions are indispensable [Sun et al., 2019; Lu et al., 2021]. However, it is costly and time-consuming to annotate such a dataset. To alleviate this problem, inspired by GPT-3’s powerful zero-shot natural language generation ability [Brown et al., 2021], recent years have witnessed a trend to train large language models using large-scale code corpora (e.g., GitHub), and expect these models to work well directly on code generation tasks, without fine-tuning on expensive text-code pairs. For example, Codex shows that a 12B parameters language model can solve 28.8% of standalone Python programming problems1.

In this paper, we focus on investigating whether and how

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1Work done during the internship at Microsoft Research Asia.

1It is measured on HumanEval [Chen et al., 2021a] with pass@1.
language models pre-trained on code corpora (without fine-tuned on pairwise labelled data) can generate library-oriented code snippets rather than standalone ones. During software development, it is a common practice for programmers to reuse third-party libraries (e.g., Pandas and NumPy) to implement needed functionalities. It is not easy for programmers to learn how to use these libraries properly. For example, according to our statistics, more than 40% of StackOverflow questions with “Python” tag also have at least one library tag. Moreover, for library-oriented code generation, the necessity of training the model without pairwise labelled data is raised, as programmers usually need to reuse different libraries in different scenarios, and it is extremely costly to label sufficient text-code pairs that cover most of these libraries.

Compared to standalone code snippets, library-oriented code snippets are more likely to share similar sketches. Sketch is the code structure after anonymizing the user-defined terms in the code, such as variable names, method names, constants, etc., which has also been identified as an API usage pattern in previous research litterateurs on software data mining [Zhong et al., 2009; Wang et al., 2013; Niu et al., 2017]. An example is shown in Figure 1. After anonymizing variables and constants, multiple code snippets using the Pandas APIs may have the same (or similar) sketch. Based on this observation, a natural idea to improve library-oriented code generation is to decompose this task into two subtasks: generating the sketch and then filling in the details. Many methods based on this idea have been proposed in different code generation tasks (e.g., Coarse-to-Fine [Dong and Lapata, 2018] and PlotCORDER [Chen et al., 2021b]) and have shown that this idea can effectively improve the quality of generated code snippets. However, these methods are proposed for the fine-tuning process, in which high-quality text-code pairs are required to derive supervision signals for the two-step generation. Therefore, in our scenario that no pairwise labelled data is provided, a research question arises: how to leverage the insight of sketching to enhance the language model pre-training on unlabelled code corpora, thus improving the quality of generated library-oriented code snippets?

To meet the challenge, we propose CERT (for sketCher and gEneRaToR), a continual pre-training approach on sketches for library-oriented code generation. In CERT, a sketcher firstly focuses on predicting a sketch, which omits user-defined details; then, a generator uses the sketch as a prompt to generate the complete code. Both the sketcher and the generator are continually pre-trained based on a base language model for code, using unlabelled code corpora rather than pairwise labelled data. In addition, we craft two evaluation benchmarks for Python libraries, called PandasEval and NumpyEval, each including 101 programming problems using Pandas and NumPy, respectively. We perform extensive experiments on CERT. Results indicate that CERT has superior performance on library-oriented code generation. We further draw several insights via thorough analysis.

2 Task Formulation

Before diving into the details of our proposed approach, we start with a formal description of the task. Code generation is to solve a programming problem: generate target code based on context. Context contains natural language problem description in the form of code comments, and a code snippet that includes statements such as import, function header and variable definition; target code is a code snippet that solves the programming problem described in the context. Formally, let $x = (x_1, x_2, \ldots, x_N)$ denote the context, where each $x_n$ can be either a code token or a natural language token. Given $x$, the code generation model can be formulated as $y = XM(x)$, where $y = (y_1, y_2, \ldots, y_M)$ denotes the target code and each $y_n$ is a code token.

For standalone code generation, the programming problem is expected to be solved by a code snippet without using third-party libraries; conversely, for library-oriented code generation, the target code $y$ contains library API calls. Two examples of library-oriented programming problems can be found in Figure 2. Note that carefully labelled context and target code pairs are indispensable for model fine-tuning, while our proposed approach only requires continual pre-training on unlabelled code corpora.

3 Methodology

In this section, we introduce our base models, followed by the details of our proposed approach CERT.

3.1 Base Models

Codex [Chen et al., 2021a] is a milestone pre-trained model that can generate decent code, but it is not publicly available. Several attempts have been made to reproduce Codex’s powerful code generation capability, e.g., CodeClippy and CodeParrot, but their performance in Python are not satisfactory. To this end, we present PYCODEGPT, a pre-trained language model, which has the ability to generate pretty good standalone Python code, for example, achieving 8.33% pass@1 on HumanEval [Chen et al., 2021a]. Especially, PYCODEGPT is a 110M parameters model based on GPT-Neo [Black et al., 2021]. We collected 60.6M raw python files with a total size of 330GB. After a series of data pre-processing strategies, such as de-duplicating python files, cleaning and formatting the contents, etc., the final pre-training corpus contains about 13.0M high-quality python

3https://github.com/CodedotAI/gpt-code-clippy
4https://huggingface.co/transformersbook/codeparrot
5More details about PYCODEGPT are in Appendix.
files with the size of 96GB. PyCodeGPT is pre-trained for 200K steps and 100B tokens on a cluster of 16 NVIDIA V100 GPUs with 32GB memory. The pre-training time is about 2 days. We summarize the three key points that make PyCodeGPT powerful: 1) a large amount of carefully cleaned data for pre-training; 2) a newly trained tokenizer, which is specialized in python; and 3) a resampling strategy that prioritizes high-quality data. Besides PyCodeGPT, we also regard CodexGen (MONO 350M) [Nijkamp et al., 2022] as one of our base models, which is by far the best performing publicly available model on HumanEval.

3.2 CERT

As mentioned in Section 2, code generation is to generate target code \( y \) based on context \( x \). Since we observe that library-oriented code snippets are more likely to share similar sketches, we present a novel approach CERT and decompose the code generation model \( \mathcal{M} \) into two modules: a sketcher \( \mathcal{M}_S \) and a generator \( \mathcal{M}_G \). Figure 3 shows the overview of CERT with a concrete example in Pandas. Given \( x \) as the input, the sketcher predicts \( s \), which is the sketch of the target code \( y \). The sketcher generates multiple candidate sketches (200 in our experiments) and we choose the one that appears the most. Then, the input of the generator is the concatenation of \( s \) and \( x \). Formally, the process of CERT can be written as \( s = \mathcal{M}_S(x) \) and \( y = \mathcal{M}_G(s; x) \). Note that if the sketch \( s \) is already a complete code snippet without anonymous symbols, we directly take it as the final prediction instead of using the generator; and if the sketch \( s \) is an empty sequence, we directly feed \( x \) into the generator.

We build the sketcher and generator on the top of the base model (PyCodeGPT or CodexGen) by continual pre-training. At first, we extract the python files that use a specific library (e.g., Pandas) from the whole pre-training corpus (13.0M files mentioned in Section 3.1), and obtain the sub-corpus denoted by \( D \). Then, we will detail the continual pre-training process of the sketcher and generator for this library.

**Sketcher.** Given the library-oriented sub-corpus \( D \), we perform the sketching operation on each file \( d \in D \). An example is shown in the upper part of Figure 5. The sketching operation is used to anonymize the user-defined terms in the code file with our pre-defined symbols. The file after sketching is denoted as \( \hat{d} \). We design three different types of sketching operations: 1) only anonymizing the user-defined constants (Default CERT); 2) only anonymizing the user-defined names, including function names, class names, and variable names (CERT-N); and 3) anonymizing both the user-defined constants and names (CERT-NC). For example, in Figure 5, the constant ‘user_1’ is anonymized with the pre-defined symbol ‘string’. The details of pre-defined symbols are shown in Figure 4. Then, we continually pre-train the base model on the library-oriented corpus after sketching, and we obtain the sketcher model. The pre-training objective is the same as that of the base model. We pre-train the model for 100K steps on a cluster of 8 NVIDIA V100 GPUs with 32GB memory.

**Generator.** In order to prepare the pre-trained corpus for the generator, we firstly split the original file \( d \) and the sketching file \( \hat{d} \) into \( K \) blocks\(^6\), and obtain \( d = (d_1, d_2, \ldots, d_K) \) and \( \hat{d} = (\hat{d}_1, \hat{d}_2, \ldots, \hat{d}_K) \). Each block is a relatively complete code snippet, such as a function or a class. Note that before splitting, we remove the natural language code comments from the sketching file \( \hat{d} \). Then, the two files are cross-merged to give a merged file \( \tilde{d} = (d_1, \hat{d}_1, d_2, \hat{d}_2, \ldots, \hat{d}_K, d_K) \). This is to mimic the process of having a sketch as a prompt for each block. An example is shown in the lower part of Figure 5. Then, the base model is continually pre-trained on all the merged files \( \tilde{d} \) and we obtain the generator model. As with the sketcher model, we continually pre-train for 100K steps.

4 Benchmark Construction

Third-party libraries are widely used in reality, while little work has been done to evaluate library-oriented code generation. To meet this challenge, we craft PandasEval and NumPyEval, two benchmarks for library-oriented code generation in Python. Each sample in the benchmarks is a programming problem consisting of context and target code. The programming problems are solved using libraries, where Pandas is for PandasEval, and NumPy is for NumPyEval. The benchmarks are expected to be diverse, authentic, high quality, moderately difficult, and unseen during pre-training.

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\(^5\)CodeGen was released during the review period of this paper.

\(^6\)We use pip-tools: autopep8, docformatter and redbaron.
In order to craft programming problems using libraries, we refer to StackOverflow, a Q&A website for programmers. There are plenty of real-world programming problems posted by real users, which helps us to improve the authenticity of our data. Specifically, we search for posts using the library tag on StackOverflow, and select those with high votes. To ensure quality, we only refer to posts with accepted answers. We go through a post’s question and its accepted answer, then manually organize them into the form needed for our benchmarks, containing both context and target code. We also polish all programming problems so that the problem descriptions are clear and the codes are correct. Note that we keepish all programming problems so that the problem descriptions, containing both context and target code. We also polish them manually into the form needed for our benchmarking.

As a result, we craft 101 programming problems for PandasEval and NumpyEval, respectively. Each programming problem is equipped with test cases for evaluation. For the programming problems in the form of a function, such as the bottom one in Figure 2, we create 20 test cases for each of them. For the others that contain no functions, such as the top one in the Figure 2, we provide 1 test case to check the correctness of predicted variable (e.g., out in Figure 2). In total, 64% programming problems in PandasEval and 30% in NumpyEval are equipped with 20 test cases. In addition, we craft programming problems that refer to StackOverflow rather than GitHub, and also carefully organize and polish the problems, so that we can ensure they are unseen by the pre-trained models.

## 5 Experiments

In this section, we evaluate CERT on PandasEval and NumpyEval to verify its effectiveness.

### Evaluation Metrics

We use pass@k as the metrics. When k code samples are generated per problem, pass@k indicates the fraction of correct ones. But computing pass@k in this way may have high variance. Hence, we follow Chen et al. [2021a] to generate n ≥ k code samples per problem (n = 200 in our experiments) and count the number of correct samples c. If n − c < k, then pass@k = 1; otherwise, pass@k = 1 − \( \prod_{i=n-c+1}^{n} (1 - k/i) \). Note that a predicted code is correct if it can pass all the test cases.

**Implementation Details.** We implement our approach using PyTorch [Paszke et al., 2019], HuggingFace’s transformers library [Wolf et al., 2019], and DeepSpeed⁸. In the training phase of PYCODEGPT, we set the batch size to 10, the window size to 1024, the learning rate to 5e-4, the gradient accumulation steps to 4 and the weight decay to 0.1. The settings of sketcher and generator are the same as PYCODEGPT. We use the mixed-precision of FP16 to accelerate the pre-training. In inference phase, we set the temperature to one of \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}. The best performance is reported across the above hyper-parameters.

### 5.1 Main Results

Before evaluating CERT, we would like to evaluate our base model PYCODEGPT on HumanEval [Chen et al., 2021a] compared to several advanced pre-trained models. As shown in Table 1, PYCODEGPT (110M) achieves competitive 8.33% pass@1. It largely exceeds other models with comparable parameters, e.g., AlphaCode (89M) [Li et al., 2022], CodeClippy (125M), and CodeParrot (110M), and also is better than the larger model GPT-Neo (1.3B).

| Model               | pass@1 | Model               | pass@1 |
|---------------------|--------|---------------------|--------|
| GPT-Neo 120M        | 0.75   | GPT-Neo 1.2B        | 4.79   |
| AlphaCode 89M       | 4.30   | CodeParrot 110M     | 3.80   |
| Codex 12M           | 4.94   | Codex 12M           | 8.27   |
| Codex 2.5B          | 21.36  | Codex 12B           | 28.81  |
| PYCODEGPT 110M      | 8.33   | CODEGEN-MONO 350M   | 12.76  |

⁷https://stackoverflow.com

⁸https://github.com/microsoft/DeepSpeed
CERT. The file numbers are about 0.61M for Pandas and 2.62M for Numpy. Baselines include our base models Py-
CodeGPT and CodeGEN; PyCodeGPT-XL and Code-
GEN-XL, which are continual pre-trained PyCodeGPT and
CodeGEN on the extracted library-oriented files; and
advanced pre-trained models for code, like CodeTS [Wang et
al., 2021], CodeGPT [Lu et al., 2021], CodeClippy and
CodeParrot. Table 2 summarizes the performance.
CERT consistently outperforms all the baselines by a large
margin. The absolute improvements over PyCodeGPT and
CodeGEN are shown in red, which are significant, for
example, 12.60% pass@1 for CERT and 13.43% pass@1 for
PyCodeGPT-CERT on NumpyEval. The results demonstrate
the effectiveness of CERT with the idea of leveraging sketches for library-oriented code generation.

Additionally, we would like to investigate the performance
of CERT with respect to the number of API calls involved in
the target code. We divided the programming problems in
each benchmark into four parts based on the number of
APIs. As shown in Figure 6, compared to PyCodeGPT, Py-
CodeGPT-CERT has a steady improvement on each part. It
indicates that CERT can improve the performance of library-
oriented code generation of varying difficulties.

Table 2: The pass@k (%) results on PandasEval and NumpyEval. The absolute improvements of CERT over the base model are highlight-
ed in red. Also, we report the performance of different sketch-
ing operations (CERT-N and CERT-NC) and the performance of CERTg trained for general code generation.

Table 3: The pass@k (%) results of PyCodeGPT and PyCodeGPT-CERTg on HumanEval.

5.2 Closer Analysis
We conduct some closer analyses to provide more insights.

Different Types of Sketching. As mentioned in Sec-
tion 3.2, we propose three types of sketching operations. By
default, CERT only anonymizes user-defined constants. The
other two types include CERT-N, which anonymizes only
user-defined names, and CERT-NC, which anonymizes both
user-defined constants and names. As shown in Table 2,
CERT with default setting achieves the best performance.
This observation may be related to the inherent character-
istics of Pandas and NumPy. They are commonly used in
data statistics and analysis, often involving manipulation
of the data constants. Thus, it is necessary to anonymize user-
defined constants. Anonymizing both user-defined constants
and names would probably make the sketches too abstract.

Quality of Generated Sketches. Intuitively, it is easier to
generate a sketch than a complete code. Thus, we would like
to evaluate the quality of sketches generated by the sketcher
of CERT. We use exact match accuracy as the metric and in-
clude PyCodeGPT and PyCodeGPT-XL for comparison.
For PyCodeGPT and PyCodeGPT-XL, we anonymize the
user-defined constants in the predicted code to obtain the
sketch. As shown in Figure 7, our sketcher surpasses base-
lines by 15.20% and 14.21% on PandasEval and NumpyEval,
respectively. It indicates that the sketcher can generate high-
quality sketches, and such sketches further benefit the gener-
ator. Additionally, the generator does not necessarily require
an exactly correct sketch, as the sketch is just a prompt (A
case will be discussed in Section 5.3).

CERT for General Code Generation. Technically speaking,
CERT can also be used for general code generation tasks,
not just the library-oriented ones. Concretely, follow-

ing the procedure in Figure 5, we can continually pre-
train PyCodeGPT using the whole 13.0M python corpus
instead of the extracted library-oriented files, and obtain the
model we called CERTg. We evaluate CERTg for gen-
eral code generation on HumanEval compared to the base
Figure 8: Three library-oriented code generation cases.

| Benchmark | Model         | Size  | pass@1 | pass@10 | pass@100 |
|-----------|---------------|-------|--------|---------|----------|
| Pandas Eval | CODEGEN-CERT | 110M  | 68.04  | 62.08   | 56.64    |
| CODEGEN-CERT | 780M  | 52.40  | 46.90  | 41.04   | 35.04    |
| CODEGEN-CERT | 110M  | 31.47  | 46.42  | 41.42   | 36.42    |
| CODEGEN-CERT | 150M  | 32.00  | 49.45  | 44.45   | 39.45    |
| CODEGEN-CERT | 175M  | 16.25  | 22.15  | 17.15   | 12.15    |
| CODEGEN-CERT | 12B   | 34.42  | 55.75  | 45.75   | 35.75    |

Table 4: GPT-3 and Codex on PandasEval and NumpyEval.

Model PYCODEGPT. As shown in Table 3, they have similar pass@k results. This observation verifies our assumption that library-oriented code snippets are more likely to share similar sketches, so it is beneficial to use sketches as prompts in this situation. But in the general case, it is not useful. Meanwhile the results of CERTg on PandasEval and NumpyEval are in Table 2. CERTg is inferior to CERT, suggesting that extracting library-oriented files is essential for CERT to learn the knowledge of library-oriented sketches.

Evaluation of GPT-3 and Codex. We evaluate GPT-3 and Codex to see how these extremely large models perform on PandasEval and NumpyEval. As shown in Table 4, CERT is competitive with only 110M parameters. Such observation proves CERT’s powerful code generation capability in library-oriented programming problems.

5.3 Case Study

For a more comprehensive comparison, we show three cases in Figure 8. We show in turn the context, the golden target code, the predicted code of PyCodeGPT and PyCodeGPT-XL, the sketch generated by PyCodeGPT-CERT and the predicted code of PyCodeGPT-CERT. Case 1 is from PandasEval, both PyCodeGPT-CERT’s sketcher and generator reach the correct results, while the baselines do not. It reveals that sketcher and generator can work well together. Case 2 is from NumpyEval, the sketch predicts the correct sketch, which has no anonymous symbols, then this sketch is the final predicted code. It indicates that the sketch has the ability to predict code without user-defined constants. At last, in Case 3, the sketcher makes a wrong prediction pd.Series([[number*2]*3]], while the correct sketch is pd.Series([[number*2], number, ([number*2], number)*2]). But PyCodeGPT-CERT’s generator rectifies it and finally generates the correct code. Since the sketch acts only as a prompt, it is not necessarily to be perfectly correct, which endsow the generator with solid robustness.

6 Related Work

The most related work is the line of large pre-trained models for code. As for the encoder-style pre-trained models, they cannot be employed directly to generate code, such as CuBERT [Kanade et al., 2020], CodeBERT [Feng et al., 2020], and GraphCodeBERT [Guo et al., 2020]. As for the decoder-style or encoder-decoder-style ones, they are trained on large unlabelled code corpora and can work directly on code generation task, such as CodeTS [Wang et al., 2021], CodeGPT [Lu et al., 2021], PLBART [Ahmad et al., 2021], PolyCoder [Xu et al., 2022], CODEGEN [Nijkamp et al., 2022], AlphaCode [Li et al., 2022], and Codex [Chen et al., 2021a]. All of them focus on generating standalone code, while we investigate library-oriented code generation. Also, similar to our idea, there are several works leveraging code sketches, for example, Coarse-to-Fine [Dong and Lapata, 2018], BAYOU [Murali et al., 2018], SketchAdapt [Nye et al., 2019], and PLOTCODER [Chen et al., 2021b]. However, they require labelled text-code paired data for fine-tuning, while our models continually pre-train on unlabelled code corpora. For code generation benchmarks, there are few works, including APPS [Hendrycks et al., 2021], HumanEval [Chen et al., 2021a], and PlotCoder’s dataset [Chen et al., 2021b]. The former two ones focus on evaluating the capability of generating standalone code, and the last one is primarily devoted to generating plotting APIs and visualization code. PandasEval and NumpyEval are dedicated to evaluating the performance of library-oriented code generation.

7 Conclusion

In this paper, we propose a novel approach CERT for library-oriented code generation. It leverages the code sketches and consists of a sketcher and a generator. The sketcher and generator are continually pre-trained upon a base model using unlabelled code corpora. Also, we carefully craft two benchmarks to evaluate library-oriented code generation, namely PandasEval and NumpyEval. Experimental results and thorough analysis show the effectiveness of CERT. In future work, we are interested in code generation for private libraries with fewer data.
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A PYCODEGPT: A Democratizing Code Generation Model in Python

Large pre-trained language models, e.g., Codex [Chen et al., 2021a] and AlphaCode [Li et al., 2022], have recently achieved surprisingly promising results on modeling source code in several programming languages. However, most of the state-of-the-art models are not publicly available, hindering the progress of related research topics and applications. To this end, we propose a publicly available code pre-trained model for Python, named PYCODEGPT, to reproduce Codex with medium size.

A.1 Data Construction

It is well-known that large language models require extremely large amounts of data to exhibit its performance well. In this section, we present the process of data collection and the data pre-processing strategies to ensure data quality.

Data Collection We first crawl 7.6M repository pages hosted on GitHub. Then we consider the language distribution tags in each page to filter the repositories without Python files. As a result, we obtain 1.2M Python-related repository URLs. With the filtered repository URLs, we download all the contents of each repository from GitHub. Following Codex, we remove files over 1MB, as experienced developers usually avoid creating large source code files to maintain good readability. As a result, we get 60.6M raw Python files under 1MB, with a total size of 330GB. Among these files, we further filter out duplicated files, which has been recognized as an important step by CodeParrot. Finally, the number of unique files is reduced to 13.0M, with a total size of 96GB.

Data Pre-processing The data pre-processing strategies are summarized in three aspects.

• According to the strategies applied to Codex and CodeParrot, we consider each source code as text and focus on line length limit and alphanumeric rate. In detail, we filter the files which do not meet the four conditions: lines of code \( \geq 5 \), average line length \( \leq 100 \), maximum line length \( \leq 1000 \), and alphanumeric rate \( \geq 0.98 \). Note that, the fourth condition is applied after removing comments with alphanumeric rate \( < 0.5 \), which is one of the following strategies.

• We also remove the automatically generated or meaningless files, for example, files with the name \_init\_py, setup.py or \_pb2\_py, because these files can mislead the model during training. In addition, we remove some useless contexts from the Python files. Specifically, we remove the contexts with license description and comments with alphanumeric rate \( < 0.5 \), where license description appears as a comment in the head of the code.

• To ensure the training quality, we design two methods to perform Python syntax checking. The first method is to use Python’s built-in module ast to check the correctness of the syntax. This strategy filter out non-Python files largely, even if the file name ends with .py. The second method applies pattern matching to leave files containing more than two typical Python keywords (e.g., def, if, return, and for).

A.2 Model Training

We use GPT-Neo [Black et al., 2021] as our base model, which is comparable to GPT-3 [Brown et al., 2021] and has already been pre-trained on the Pile dataset [Gao et al., 2020]. In this section, we present the details of model training, including tokenization, resampling, and hyper-parameters.

Tokenization The tokenizer of GPT-Neo models is based on GPT-2 [Radford et al., 2019] tokenizer, which applies the byte-level version of Byte Pair Encoding (BPE) [Sennrich et al., 2016]. The tokenizer is trained on the Pile dataset with a vocabulary of 50K. Since the distribution of source code words differ from that of natural text, the original GPT-Neo tokenizer is not very effective for encoding Python source code. Thus, we follow CodeParrot to train a new byte-level BPE tokenizer from scratch on our collected code data. Finally, we set the vocabulary size to 32K, which allows us to encode code using approximately 40% fewer tokens.

| Hyper-parameter     | Value       |
|---------------------|-------------|
| Learning Rate       | \( 5 \times 10^{-4} \) |
| Optimizer           | AdamW       |
| Adam \( \beta \)    | 0.9, 0.95   |
| Adam \( \epsilon \) | 10^{-8}     |
| Weight Decay        | 0.1         |
| Warmup Steps        | 100K        |
| Learning Rate Decay | Cosine      |
| Batch Size (tokens) | 480K        |
| Training Steps      | 200K steps, 100B tokens |
| Context Window      | 1024        |

Table 5: Hyper-parameters in pre-training.

\( ^9 \) It makes our model only target the English version.
Resampling  Since different files have different importance for training, we design a data resampling strategy to make high-quality files appear more often, while keeping a balance to make each file appear at least once throughout the training process. In detail, we evaluate the quality of a Python file in two aspects: repository star count and unit test function rate. The repository star count is determined by GitHub users and is the main factor in measuring repository quality. We do not use the star count directly for filtering data because most files have very few stars. The unit test function rate is the number of unit test functions divided by the number of functions. We introduce it to reduce the weight of files used for testing, because test files often contain a lot of user-defined numeric constants or string constants.

Hyper-parameters  PyCODEGPT shares the same configurations with original GPT-Neo 125M model except for the vocabulary size. It is trained on 16 V100 (32GB) GPUs for about 2 days. Table 5 lists the hyper-parameters.

A.3 Experiments  We conduct experiments on HumanEval and CodeXGLUE to show the effectiveness of PyCODEGPT.

| Model          | Params | pass@k  |
|---------------|--------|---------|
|               |        | k=1     | k=10    | k=100   |
| Parameter Scale: ~100M |        |         |         |         |
| TabNine       | 2.58%  | 4.35%   | 7.59%   |         |
| GPT-Neo       | 0.75%  | 1.88%   | 2.97%   |         |
| CodeParrot    | 3.80%  | 6.57%   | 12.78%  |         |
| PolyCoder     | 2.13%  | 3.35%   | 4.88%   |         |
| Codex         | 8.22%  | 12.81%  | 22.40%  |         |
| AlphaCode     | 4.3%   | 12.2%   | 20.0%   |         |
| PyCODEGPT (Ours) | 110M  | 8.33%   | 13.36%  | 19.13%  |
| Parameter Scale: ~500M |        |         |         |         |
| PolyCoder     | 400M   | 2.96%   | 5.29%   | 11.59%  |
| Codex         | 300M   | 13.17%  | 20.37%  | 36.27%  |
| CodeParrot    | 679M   | 16.22%  | 25.7%   | 40.95%  |
| AlphaCode     | 302M   | 11.6%   | 18.8%   | 31.8%   |
| AlphaCode     | 685M   | 14.2%   | 24.4%   | 38.8%   |
| CODEGEN-MONO  | 350M   | 12.76%  | 23.11%  | 35.19%  |
| Parameter Scale: ~1B |      |         |         |         |
| GPT-Neo       | 1.3B   | 4.97%   | 7.47%   | 16.30%  |
| CodeParrot    | 1.5B   | 3.85%   | 8.03%   | 14.96%  |
| AlphaCode     | 1.1B   | 17.1%   | 28.2%   | 45.3%   |
| Parameter Scale: ~2B |      |         |         |         |
| GPT-Neo       | 2.7B   | 6.41%   | 11.27%  | 21.37%  |
| PolyCoder     | 2.7B   | 5.59%   | 9.84%   | 17.68%  |
| CodeParrot    | 2.5B   | 21.36%  | 35.42%  | 59.50%  |
| CODEGEN-MONO  | 2.7B   | 23.70%  | 36.64%  | 57.01%  |
| Parameter Scale: ~6B |      |         |         |         |
| GPT-J         | 6B     | 11.62%  | 15.74%  | 27.74%  |
| CODEGEN-MONO  | 6.1B   | 26.13%  | 42.29%  | 65.52%  |
| Parameter Scale: >10B |     |         |         |         |
| Codex         | 12B    | 28.81%  | 46.81%  | 72.31%  |
| CODEGEN-MONO  | 16.1B  | 29.28%  | 49.86%  | 75.00%  |

Table 6: Experimental results of models under different parameter scales on the HumanEval Dataset. For AlphaCode, we report the pre-trained decoder-only results from their paper. For TabNine, we do know the parameter scale, so we put it to the first scale group.

Results on HumanEval  HumanEval [Chen et al., 2021a] contains 164 hand-written code generation problems. As mentioned in Section 5, the evaluation metric is pass@k. We use the same parameters as those used by Codex, except for the stop sequences. The stop sequences include `\n:class`, `\n#`, `\n`, `\nprint`, and `\nif`. We generate 200 programs and apply nucleus sampling using p = 0.95. As in previous work, we try various temperatures (from 0.1 to 1.0 with the interval of 0.1) and report the best result for each k.

Table 7 shows the experimental results. Even though the original GPT-Neo models (125M, 1.3B and 2.7B) and GPT-J 6B [Wang and Komatsuzaki, 2021] are trained on the dataset containing GitHub files, they do not achieve satisfactory performance on HumanEval compared to Codex. For the open-source CodeParrot models (110M and 1.5B), as we mentioned before, they outperform the corresponding ones of GPT-Neo but still not enough to compare with Codex. AlphaCode [Li et al., 2022] also evaluates their decoder-only model on HumanEval, and the performance is slightly worse than Codex. PolyCoder [Xu et al., 2022] is pre-trained on several programming languages, and it shows even worse performance than CodeParrot. However, our pre-trained 110M model can obtain comparable performance to Codex 85M and outperform CodeParrot 110M by 4.53% on pass@1, 6.79% on pass@10 and 6.35% on pass@100. During our paper review, CODEGEN [Nijkamp et al., 2022] also provided code generation models of various sizes from 350M to 16.1B and obtained good performance. We omit CodeT5, CodeGPT, and CodeClippy, since they all get 0% on pass@1, pass@10, and pass@100.

Results on CodeXGLUE  CodeXGLUE [Lu et al., 2021a] is a benchmark for programming language understanding and generation tasks. In total, CodeXGLUE provides datasets for 14 tasks, in which the dataset PY150 is for code completion task. Table 7 shows the experimental results. Note that we fine-tuned PyCODEGPT and CodeParrot on PY150 training dataset. The results show that CodeGPT is worse than the fine-tuned CodeParrot. However PyCODEGPT wins the CodeParrot with 3.02% higher score on token level completion accuracy. On line level completion, PyCODEGPT also achieves 2.67% and 2.02% higher accuracy on exact match and edit similarity, respectively.

| Model          | Params | Token Level | Line Level |
|---------------|--------|-------------|------------|
|               |        | Accuracy    | EM         | ES         |
| LSTM          | –      | 58.00%      | 17.93%     | 50.05%     |
| Transformer   | –      | 73.20%      | 36.65%     | 67.51%     |
| GPT-2         | 117M   | 74.22%      | 38.55%     | 68.94%     |
| CodeGPT       | 124M   | 74.93%      | 39.11%     | 69.69%     |
| CodeGPT-Adapted | 124M   | 75.11%      | 39.65%     | 69.84%     |
| CodeParrot    | 110M   | 77.22%      | 42.10%     | 71.07%     |
| PyCODEGPT (Ours) | 110M  | 80.24%      | 44.77%     | 73.09%     |

Table 7: Experimental results on CodeXGLUE Code Completion task dataset PY150. Results of LSTM, Transformer, GPT-2, CodeGPT and CodeGPT-Adapted are from Lu et al. [2021]. Exact match and edit similarity are abbreviated as EM and ES.