Learning from Self-Sampled Correct and Partially-Correct Programs

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Abstract

Program synthesis aims to generate executable programs that are consistent with the user specification. While there are often multiple programs that satisfy the same user specification, existing neural program synthesis models are often only learned from one reference program by maximizing its log-likelihood. This causes the model to be overly confident in its predictions as it sees the single solution repeatedly during training. This leads to poor generalization on unseen examples, even when multiple attempts are allowed. To mitigate this issue, we propose to let the model perform sampling during training and learn from both self-sampled fully-correct programs, which yield the gold execution results, as well as partially-correct programs, whose intermediate execution state matches another correct program. We show that our use of self-sampled correct and partially-correct programs can benefit learning and help guide the sampling process, leading to more efficient exploration of the program space. Additionally, we explore various training objectives to support learning from multiple programs per example and find they greatly affects the performance. Experiments on the MathQA and GSM8K datasets show that our proposed method improves the PASS@k performance by 3.1% to 12.3% compared to learning from a single reference program with MLE.

1 Introduction

Developing models that can automatically generate programs from user specification (e.g., natural language, input/output pairs, etc) has been a longstanding challenge [14, 21]. Recent progress in neural program synthesis, especially using large language models pretrained on code [2, 6, 9], has shown promise in generating general-purpose programming languages. These models have been experimented on many different programming tasks, including math-word-problems [2, 10], jupyter notebook cell generation [5], common programming tasks [2, 25] or even competition level programming puzzles [17]. The performance of these models are often measured by the PASS@k

∗Majority of the work done during an internship at Microsoft Research.
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We perform experiments on two math programming tasks, namely MathQA-Python [2] and Grade-School-Math (GSM) [10], where the task is to generate python programs to solve math problems described in natural language descriptions. Results show that learning from self-sampled programs can improve the PASS@100 from 22.7% to 35.0% for GSM, and 25.1% to 28.2% for PASS@80 on a filtered version of MathQA-Python. Moreover, we find that adding partially-correct programs can outperform using only fully-correct programs by 2.7% on the GSM and it also shows improvement with MathQA-Python. Such performance boosts from our proposed methods are also consistent for whose intermediate execution states are consistent with known correct programs. This new technique allows the model to maximally utilize the self-sampled programs and more efficiently explore the program space. We also study various common loss functions for learning from multiple programs targets for a single specification, including augmented-MLE, Maximize Marginal Likelihood (MML) and $\beta$-smoothed MML [15].

We perform experiments on two math programming tasks, namely MathQA-Python [2] and Grade-School-Math (GSM) [10], where the task is to generate python programs to solve math problems described in natural language descriptions. Results show that learning from self-sampled programs can improve the PASS@100 from 22.7% to 35.0% for GSM, and 25.1% to 28.2% for PASS@80 on a filtered version of MathQA-Python. Moreover, we find that adding partially-correct programs can outperform using only fully-correct programs by 2.7% on the GSM and it also shows improvement with MathQA-Python. Such performance boosts from our proposed methods are also consistent for different model sizes for the pretrained code language models. Ablation on different loss functions show that MLE-Aug loss is the most effective in learning from multiple program targets and yields the most improvements over MLE loss.

2 Overview

Problem formulation. We consider the task of program synthesis from specifications written in natural language (NL). Given an NL description $x \in \mathcal{X}$ and a program executor $\mathcal{E} : \mathcal{Y} \rightarrow \mathcal{Z}$, the goal is to generate a program $y \in \mathcal{Y}$ that executes to the expected results $z^* \in \mathcal{Z}$, i.e., $\mathcal{E}(y) = z^*$.

Standard approach and its limitation. Given a program synthesis dataset, typically only one gold program $y^*$ is provided for each NL $x$, thus a parameterized model $P_\theta(y | x)$ is typically learned with the Maximum Likelihood Estimation (MLE) objective from the NL-Program pair $(x, y^*)$ as:

$$L_{\text{MLE}}(x, y^*, P_\theta) = - \log P_\theta(y^* | x)$$

The built-in assumption of using Eq. 1 for learning is that only the gold program $y^*$ is correct. However, this assumption is clearly untrue for the program synthesis problem as typically multiple programs can satisfy the same specification. With only one gold program, Eq. 1 would encourage the model to put all probability mass on $y^*$, which could easily lead to overfitting [2, 4, 10].

Overview of our approach. Because manually collecting multiple reference programs for each specification is a laborious process, in our work, we explore an alternate approach: where the model self-samples additional correct (or partially-correct) programs and learns from them during training. Fig. 1 shows an example: for the specification $x$, our model was able to self-sample a correct program $\hat{y}$ that is different from the gold program $y^*$ provided in the dataset. Looking at the program execution states shown on the right, we can see that both these programs execute to produce the sample desired output, $i.e.$, $\hat{z} = z^*$, as noted with dashed red boxes in Fig. 1. Taking one step further, our approach can also identify partially-correct programs from its self-sampled programs.

4For simplicity, we consider programs with no explicit inputs, i.e., inputs embedded as variable initialization.
A goods train runs at a speed of 72kmph and crosses a 250M long platform in 26 seconds. What is the length of the goods train?

We now formally present our approach. There are three main steps: 1) sampling the reference to prevent saving trivial variants. Concretely, we first perform filtering based on the linearized abstract syntax trees (ASTs) to eliminate the buffer to remove them. This process is essential to control the buffer quality for better learning.

For example, on the bottom left, we show a sampled program \( \hat{y} \) that is incorrect only because of an error in its last two lines. But we identify a subprogram \( \hat{y'}_{\leq 5} \) of it as partially-correct because the execution state \( s^5 \) for this subprogram matches the intermediate state \( s_5^\ast \) of a known correct program \( y^\ast \), which is noted as the solid red boxes in Fig. 1. Based on these observations and intuitions, we introduce our approach in the following sections.

3 Learning from Self-Sampled Programs

We now formally present our approach. There are three main steps: 1) sampling; 2) filtering; and 3) learning as shown in Alg. 1. Here we mainly introduce the self-sampling framework using only fully-correct programs and the extensions with partially-correct programs will be introduced in §4.

3.1 Online Sampling and Filtering

For each specification \( x \), we maintain a buffer \( B \) to save the different programs that are correct, i.e., execute to the expected results. Note that the buffers are persistent and cumulative across training epochs. To add more programs in \( B \), we perform online sampling and filtering as follows.

**Online sampling (line 2 in Alg. 1):** For each example \((x, y^\ast)\), the model samples a set candidate programs, i.e., \( \hat{y} = \{\hat{y}_i\}_{i=1}^T \sim P(y|x) \);

**Filtering incorrect programs (line 5 in Alg. 1):** As not all sampled programs in \( \hat{y} \) are correct (thus not suitable for learning), we filter out all incorrect programs in \( \hat{y} \), i.e., \( \hat{y}^* = \{\hat{y} \in \hat{y} : \epsilon(\hat{y}) = z^*\} \);

**Filtering duplicate programs (line 6 in Alg. 1):** Because the model can sample programs that are correct but are "trivial variants" of other correct programs (e.g., the program differs from another program only in whitespaces, comments or trivial statements like "x = x * 1.0"), we further filter the buffer to remove them. This process is essential to control the buffer quality for better learning. Concretely, we first perform filtering based on the linearized abstract syntax trees (ASTs) to eliminate the differences in whitespaces, etc.; then we set a constraint on maximum number of lines using \( y^\ast \) as the reference to prevent saving trivial variants.
We use $y$ we say two (sub)programs with Augmented MLE (MLE-Aug): This objective augments MLE with multiple targets by summing

$$- \log P_\theta(y^* | x)$$

$$- \sum_{y \in B} \log P_\theta(y | x)$$

$$- \sum_{y \in B} \nabla_\theta \log P_\theta(y | x)$$

$$- \sum_{y \in B} \frac{P_\theta(y | x)}{P_\theta(y^* | x)} - \nabla_\theta \log P_\theta(y | x)$$

$$- \beta \log \sum_{y \in B} P_\theta(y | x)^\beta$$

$$- \beta \sum_{y \in B} \frac{P_\theta(y | x)^\beta}{\sum_{y \in B} P_\theta(y | x)^\beta} - \nabla_\theta \log P_\theta(y | x)$$

Table 1: Comparison of loss functions and their gradients over multiple reference $B$. Note that they all degenerates to MLE when only the gold program is used as reference, i.e., $B = \{y^*\}$.

### 3.2 Learning from Multiple Targets

In this section, we discuss some common loss functions to learn from multiple targets for each specification. Empirically, we find that the distinction between those loss functions greatly affects the model performance (§ 5.3). The loss functions and their gradients are shown in Tab. 1.

**Augmented MLE (MLE-Aug):** This objective augments MLE with multiple targets by summing the loss from multiple programs in $B$, as if $(x, y) \forall y \in B$ is a set of different examples in the dataset.

**Maximum Marginal Likelihood (MML):** MML attempts to approximate $P_\theta(z^* | x)$ by marginalizing over the correct programs in $B$. However, for each program $\tilde{y} \in B$, the gradient of it is in proportion to the likelihood $P_\theta(\tilde{y} | x)$ given by the model. This typically results in the model still putting a majority of the weight on one of the programs in $B$ as noted in [15].

**$\beta$-smoothed MML ($\beta$-MML):** Proposed in [15], the $\beta$-MML objective is an extension of MML with $\beta \in [0, 1]$, where it recovers MML when $\beta = 1$ and is equivalent to MLE-Aug when $\beta = 0$.

### 4 Partially-Correct Programs

In § 3 we only show how to train the model with self-sampled fully-correct programs (FCPs). However, during the sampling process, the model can often encounter programs that are very close to being correct as they only have mistakes in the last few lines, as the examples shown in Fig. 1. Learning from FCPs only makes the model miss the opportunity to learn useful information from these programs. Moreover, while sampling a fully-correct program from scratch may not be hard for simpler domain-specific languages, it can be challenging for larger sparse program space. And if no FCP can be sampled, the method described in § 3 degenerates to MLE. Here we show how to mitigate this issue and more efficiently explore the program space by identifying and learning from partially-correct programs (PCPs).

### 4.1 Partial Correctness Definition

In the previous section, we define correctness of a program based on its final execution result $z = \mathcal{E}(y)$. Here we define partial correctness based on intermediate execution states of programs. The distinction is also shown in Fig. 1 (solid red boxes vs. dashed red boxes).

**Program state.** Given a program $y = (u_1, ..., u_t)$ where $u_i$ is the $i$-th statement, we define the execution state $s_i$ of a subprogram $y_{\leq i} = (u_1, ..., u_i)$ as the set of values of all variables in the current scope of subprogram $y_{\leq i}$. For example, given a subprogram "$a=b; c=a+b$", its program state is $\{1, 3, 4\}$. Note that the state representation is name-agnostic as variable names are not used, because there could be programs that are equivalent but use different intermediate variable names. We use $T(y_{\leq i}) = s_i$ to denote the evaluation of $y_{\leq i}$ to obtain its state $s_i$, where $T : \mathcal{Y} \rightarrow \mathcal{S}$ is called a tracing function. For simplicity, we only consider multi-line sequential programs (i.e., no if-conditions or loops), and we leave the study of more complex programs to future work.

**State-based equivalence and partial correctness.** Given this representation of the program state, we say two (sub)programs $y_1$ and $y_2$ are equivalent if and only if $T(y_1) = T(y_2)$, i.e., those two programs produces the exact same set of variable values. Even though this is a conservative way for defining program equivalence, it is sufficient for the programs we study in this work. Based on program equivalence, we recursively define partial correctness as follows: (1) A fully-correct program
Here we introduce how the saved partially correct programs can be used to guide and accelerate the learning of programs. In §3.1, we described the simple correctness-based method to identify which programs to save in $B$. However, as mentioned in §4, if a program $\hat{y}$ does not produce the expected output $z^*$ but its subprogram $y_{\leq i}$ is partially-correct, the model can still learn from $y_{\leq i}$. Since any subprogram of a partially correct program is itself partially correct, the task here is to find the longest subprogram that is partially correct. We can achieve this simply by traversing the subprograms in decreasing order of the length to find the longest subprogram $\hat{y}_{\leq i}$ with state $s_i$ that is identical to any of the states from a saved program.

Guided-Sampling (line 2 in Alg. 1): In §3.1, we mentioned that full programs are sampled for each specification $x$ as $\hat{y} \sim P_\theta(y|x)$. Instead of sampling from scratch, we sample from partially-correct programs to improve efficiency. This partial-correctness-based sampling process is described in more detail in Alg. 2. Because the sampling process is guided by the partially correct programs and the generation length is reduced, the model can explore the program space more efficiently. Note that since the empty program $y^0$ is in the buffer $B$ since initialization, the model can still generate and explore the space from scratch.

Identify partially correct programs (line 5 in Alg. 1): In §3.1, we described the simple correctness-based method to identify which programs to save in $B$. However, as mentioned in §4, if a program $\hat{y}$ does not produce the expected output $z^*$ but its subprogram $y_{\leq i}$ is partially-correct, the model can still learn from $y_{\leq i}$. Since any subprogram of a partially correct program is itself partially correct, the task here is to find the longest subprogram that is partially correct. We can achieve this simply by traversing the subprograms in decreasing order of the length to find the longest subprogram $\hat{y}_{\leq i}$ with state $s_i$ that is identical to any of the states from a saved program.

Filtering subprograms (line 6 in Alg. 1): With the inclusion of partially correct programs, we need to slightly change the two filtering criteria in §3.1. For deduplication, while we still use AST to rule out changes to the programming style, we also check if the partially correct program $\hat{y}_{\leq i}$ is a subprogram of another known partially correct program in $B$. For the same reason, when saving a new partially correct program $\hat{y}$, we need to prune out any existing programs in $B$ that is a subprogram of $\hat{y}$. As for the length constraint, the same principle still applies, but now it is compared against other partially correct programs that executes to the same state.

Learning from partially correct programs: As partially-correct programs are subprograms $y_{\leq i}$ missing the later part $y_{>i}$, with an auto-regressive left-to-right generation model, the learning of $P_\theta(y_{>i}|y_{\leq i})$ is independent of $y_{>i}$. Thus the learning objectives in §3.2 do not need to change with the inclusion of partially correct programs for learning. The only difference is that the end-of-sequence "<eos>" token is not appended to the PCPs as those programs are not yet finished.

In practice, we use a state $\rightarrow$ subprogram dictionary and the lookup takes a negligible amount of time.

### Algorithm 2 SamplePrograms ($x$, $P_\theta$, $B$) with partial correctness

**Input**: Model $P_\theta(y|x)$; the specification $x$ and a set of partially correct programs $B$

**Output**: Program samples $\hat{Y}$

1: Select $y_{\leq i} \in B \setminus \{y\in E(\hat{y}) = z^*\}$ uniformly at random
2: Sample a set of completions $\hat{y}_{\leq i} \sim P_\theta(y_{>i}|y_{\leq i}, x)$
3: $\hat{Y} \leftarrow \{\hat{y}_{\leq i}||\hat{y}_{>i}\}_{\hat{y}_{>i} \in Y_P} \leftarrow \text{concatenation} \leftarrow y_{>i}$
4: return $\hat{Y}$

is also partially correct; (2) Given a set of known partially-correct programs $B$, a (sub)program $y$ is partially-correct if and only if there exists a subprogram $y^*_{\leq i}$ from a program $y^*$ in $B$ that is semantically equivalent to $y$:

$$\exists y^* \in B. \exists j \leq |y^*| \text{ s.t. } T(y^*_{\leq j}) = T(y)$$

From the definitions, it is easy to see that all subprograms of a partially-correct program are themselves partially correct, including the empty program. An intuition for this definition is that for any partially correct program $y_{\leq i}$, there must be some completion of it $y_{>i}$ such that $y = [y_{\leq i}]y_{>i}$ is fully correct. Note that we initialize $B$ with the empty program $y^0$ and the gold program $y^*$, and with self-sampling, more PCPs and FCPs will be added in $B$.

**4.2 Learning with Partially Correct Programs**

Here we introduce how the saved partially correct programs can be used to guide and accelerate the sampling process, as well as the changes in the two filtering process. Due to space limit, we show the full training update algorithm with partial correctness in Appendix C.
5 Experiments

5.1 Experimental Setup

Datasets. We evaluate on two math programming datasets, in which Python code is generated to solve math problems described in natural language. We chose this domain as our main evaluation benchmarks as it involves moderately difficult numerical reasoning tasks that requires program execution, which is ideal to studying our technique. We leave the extension to general programs to future work and more discussion is in § 6.

- MathQA-Python: MathQA-Python consists of 19.2K training examples of NL and Python program pairs [2]. However, we find the raw dataset to contain many programs that share the same NL/program templates and only differ in concrete number across the train/dev/test sets;

- MathQA-Python-Filtered: To better understand the generalization of the trained models, we derive a deduplicated version of the dataset by first merging the train and dev data and then perform the template-based deduplication. Partly inspired by [12], we re-split the train and dev set based on the question templates, and 6.8K training data is left after such filtering process. We will release the processing scripts for replication and comparison.

- GSM5.5K-Python: The grade-school-math (GSM8K) dataset [10] contains 7.5K training data. Since it only provides natural language solutions with math formulas and does not have a dev set, we first reserved 20% of the training data as dev set, then automatically converted the formulas to Python code in the same style as MathQA-Python. As the result, we run our experiments with the 5.5K successfully converted training data with Python solutions. Note that the natural language solutions are not used as input to the models in our experiments.

Evaluation metrics: Following recent work in neural program synthesis [2, 6, 10], we use PASS@k as our main evaluation metric. It allows the model to sample k programs for each specification and the task is considered solved if any one of the k programs is correct, then the average PASS@k is calculated on the test/dev set. More details (e.g., temperature) can be found in Appendix A.

Model training: We use GPT-Neo [3] as our program synthesis model and mainly study two model sizes, 125M and 2.7B. Following previous work [2], we evaluate on the same model checkpoint with the best PASS@1 score, but note that it might not be the best checkpoint for other k values (more discussion in Appendix E). Detailed hyperparameter settings can also be found in Appendix A.

5.2 Main Results

Learning from self-sampled programs improves PASS@k. Fig. 2 shows the performance on two datasets by learning from self-sampled FCPs and PCPs using MLE-Aug, compared with MLE on single gold program. We can see that our proposed method can greatly improve PASS@k, especially for higher k values. By inspecting the k generated programs for each task, we find that there is more diversity in the programs that the model generates using our method. More specifically, we calculate the ratio of unique programs from the 100 samples for the comparison in Fig. 2a and find that while 30.5% of them are unique for our approach but only 20.8% for the model trained with MLE. By comparing different base model sizes, we can see that learning from self-sampled programs can help with both small and large program synthesis models, with a 12.3% and 9.0% PASS@100 improvement on GSM5.5K-Python for GPT-Neo-125M and GPT-Neo-2.7B, respectively. We also compare our method with previous work on the original test sets of Grade-school-math and MathQA-Python. The results are shown in Tab. 2 and Tab. 3. We can see that our method improves over all previous methods on MathQA-Python. On Grade-school-math, some of the prior works are evaluated on a different format of NL inputs than ours, so they are not directly comparable. We test Codex using the same input in a few-shot setting, and we find that our method achieves better PASS@1 while being significantly worse in PASS@100 compared with Codex.\footnote{Due to the little information we have about Codex (e.g., model size, training data), it is hard to derive any conclusion. However, we found that the programs Codex generates are much more diverse.}

Partially correct programs improve model performance. We next show our results on whether partially-correct programs help with learning in Tab. 4. First, we observe that using using partial correctness not only results in PCPs being saved and learned from, it also boosts the number of FCPs being found with the guided-sampling process. As a result, most PASS@k performances drop if we do not include partially correct programs in the buffer, as the model learns from a smaller number of
Figure 2: Main results on the dev set of GSM5.5K-Python and MathQA-Python-Filtered datasets comparing our proposed learning approach and the common MLE objective. All our methods include partially-correct programs and use the MLE-Aug loss for learning.

| Models | PASS@80 |
|--------|---------|
| Previous work: |
| Codex Davinci$^\dagger$ [6] | 42.0 |
| LaMDA 8B$^\ast$ [2] | 74.7 |
| LaMDA 68B$^\ast$ [2] | 79.5 |
| LaMDA 137B$^\ast$ [2] | 81.2 |
| GPT-Neo 125M |
| w/ MLE | 83.2 |
| w/ self-sampling FCP only | 84.4 |
| w/ self-sampling FCP + PCP | 84.7 |
| GPT-Neo 2.7B |
| w/ MLE | 18.8 |
| w/ self-sampling FCP only | 16.7 |
| w/ self-sampling FCP + PCP | 19.5 |

Table 2: Compare with previous methods on the original test set of MathQA-Python dataset. $^\ast$: model not pretrained on code. $^\dagger$: few-shot learning results

| Models | PASS@1 | PASS@100 |
|--------|--------|----------|
| Previous work: |
| OpenAI 6B$^\ast$ [10] | 21.8 | 70.9 |
| PaLM-Coder 540B$^\dagger$ [9] | 50.9 | - |
| LaMDA 137B$^\ast$ [2, 9] | 7.6 | - |
| Codex Cushman$^\dagger$ [6] | 5.0 | 58.0 |
| Codex Davinci$^\dagger$ [6] | 17.0 | 71.0 |
| GPT-Neo 2.7B |
| w/ MLE | 18.8 | 34.0 |
| w/ self-sampling FCP only | 16.7 | 39.2 |
| w/ self-sampling FCP + PCP | 19.5 | 41.4 |

Table 3: Compare with previous methods on the original test set of GSM8K dataset. $^\ast$: model not pretrained on code. $^\dagger$: few-shot learning results. $^\clubsuit$: different setting from ours

FCPs and PCPs. Interestingly, when comparing different base model sizes, we can find that while the sum of FCP and PCP programs sampled and saved in the buffer are about the same (i.e., 2.36 and 2.31), around 42% of them are FCP for the small model while it is 65% for the larger model. This is because those PCPs are slowly converted to FCPs with the guided-sampling process. The difference percentage of PCPs left in the buffer also reflects the model’s ability in program completion. We perform the same experiments on MathQA-Python-Filtered and observe similar performance improvement with GPT-Neo-2.7B but no clear advantage of adding PCPs for the 125M model. The corresponding results are shown in Appendix B due to space limit.

$^\dagger$Natural language explanations of the programs are used as input and the few-shot programs are not in the same format as ours.
Table 4: Comparing using self-sampled partially-correct programs (PCPs) and only using fully-correct programs (FCPs). Results are on the dev set of GSM5.5K-Python and MLE-Aug loss is used to learn from self-sampled programs. The number of FCPs does not include the original reference program.

| Models                  | # Progs. in $\mathcal{B}$ | PASS@k       |
|-------------------------|----------------------------|--------------|
|                         | FCP | PCP | $k=1$ | $k=5$ | $k=10$ | $k=20$ | $k=50$ | $k=100$ |
| GPT-Neo 125M            |     |     |       |       |        |         |            |          |
| w/ MLE                  | -    | -   | 7.4   | 10.6  | 12.7   | 15.3    | 19.2     | 22.7     |
| w/ self-sampling FCP + PCP | **1.00** | **1.36** |       |       |        |         |            |          |
| w/ self-sampling FCP only | 0.76 | -   | 7.6   | 13.1  | 16.5   | 20.5    | 26.8     | 32.3     |
| GPT-Neo 2.7B            |     |     |       |       |        |         |            |          |
| w/ MLE                  | -    | -   | 20.6  | 25.1  | 27.2   | 29.5    | 32.9     | 35.5     |
| w/ self-sampling FCP + PCP | **1.50** | **0.81** |       |       |        |         |            |          |
| w/ self-sampling FCP only | 1.26 | -   | **20.7** | 28.0  | 31.2   | 34.4    | 38.6     | 41.5     |

Table 5: Comparison of various loss functions (§ 3.2) with different self-sampling strategies. Results are on the dev set of GSM5.5K-Python with GPT-Neo 125M as the base model. Best performance within the same category is in **bold** and ones worse than MLE is underlined. $\beta = 0.25$ for $\beta$-MML.

| Self-Sampling | Loss Func. | # Progs. in $\mathcal{B}$ | PASS@k       |
|---------------|------------|----------------------------|--------------|
|               | FCP | PCP | $k=1$ | $k=5$ | $k=10$ | $k=20$ | $k=50$ | $k=100$ |
| -             | -    | -   | 7.4   | 10.6  | 12.7   | 15.3    | 19.2     | 22.7     |
| FCP only      | MML     | -   | 6.9   | 11.0  | 13.3   | 16.0    | 20.1     | 23.7     |
|              | MLE-Aug  | -   | **7.6** | **13.1** | **16.5** | **20.5** | **26.8** | **32.3** |
|              | $\beta$-MML | - | 7.5   | 11.7  | 14.5   | 17.9    | 23.1     | 27.3     |
| FCP + PCP     | MML     | 0.40 | 1.10  | 5.5   | 9.0    | 11.0    | 13.1     | 16.2     |
|              | MLE-Aug  | **1.00** | **1.36** | **7.5** | **13.6** | **17.5** | **22.1** | **29.2** | **35.0** |
|              | $\beta$-MML | 0.62 | 1.14  | 7.2   | 12.0   | 14.9    | 18.4     | 23.6     |

5.3 Ablation on Learning Objectives

We next study the effects of different objective functions described in § 3.2 for learning from multiple targets, including partially correct programs. Our experiment results on GSM5.5K-Python and GPT-Neo-125M with different learning objectives are shown in Tab. 5.

The choice of learning objectives matters for PASS@k. First, we observed that all three loss functions improves the model performance over MLE objective when learning from fully-correct self-sampled programs, which shows the benefits of learning from multiple targets. Second, we observed that the three learning objectives (MML, MLE-Aug, $\beta$-MML) results in very different model performance, especially in the PCP+FCP setup: the gap between MML and MLE-Aug is 16.3%. More specifically, we find the MML objective only marginally improves over MLE with only FCP and performs worse than MLE when also learning from PCPs. As discussed in § 3.2 and Tab. 1, MML would cause the model to put all weight on one program in the buffer, as the gradient is in proportional to the likelihood given by the model. As MLE already learns from the gold reference program, it is hard for MML to make improvements with self-sampled programs, and the performance may even decrease when MML puts all weight on a partially-correct program.

MLE-Aug loss can most effectively learn from multiple targets. We also note that MLE-Aug loss results in best performances in all setups. From Tab. 1 we can see that the gradients of MLE-Aug objective are equally distributed among the programs in the buffer, which leads to more diversity in its generation due to a more balanced source of learning signals. We can also observe a positive correlation between the size of the buffer and the PASS@k performance, note that this is a result of a virtuous circle during training: when a model has better performance, it can sample more FCP or PCP programs and more programs saved in the buffer leads to better model performance. Thus MLE-Aug objective leads to the most FCP and PCP being saved, as well as the best PASS@k performance. $\beta$-MML loss is proposed to alleviate the aforementioned issue for MML loss, but we do not observe an advantage of using it instead of the MLE-Aug loss in our experiments.
6 Limitations and Future Work

More general definition of partial correctness. In this work, we define partial correctness based on state-based program equivalence. As mentioned in §4.2, this is a conservative way for defining program equivalence as it requires exact match of the sets of variable values. We can relax this by, for example, only match the variables that will be referenced later and ignore the others. Besides, our correctness definition requires the existence of at least one fully-correct program and we use the gold program from the dataset. When only the gold execution results are provided for learning (i.e., no reference programs), we would need to sample an FCP that matches the gold execution result to begin with. We may also encounter spurious programs (i.e., incorrect programs yielding correct result by coincidence) but they can be addressed by adding more test cases.

More complex programs. The programs that we work with are straight-line programs, which do not contain conditions (e.g., if-else) or loops (e.g., while-do). Since most neural program synthesis models perform left-to-right auto-regressive generation, the changes to the control flow break the alignment between program generation and program execution [7, 8, 23]. There are two potential ways to extend our technique to address the problem. First, we can treat a branch or a loop as an atomic unit (i.e., a block whose state is the state after executing all statements within it), then we can apply state-based equivalence in the same way. Second, because our technique only requires execution after the full programs are generate, we can still evaluate and compare program states based on intermediate states.

7 Related Work

Code language models. Recently, there are several large language models that pre-trained on code. Most of these models such as CodeGPT [20], Codex [6], GPT-Neo [3], PolyCoder [28] and CodeGen [22] use a GPT-style decoder-only architecture and are trained using the causal language modelling objective. Other models such as CodeT5 [27] use encoder-decoder architecture and models such as [13] perform infilling of code rather than left-to-right completion. In our work, we use GPT-Neo as our base model, but our proposed method can be applied any of the above models.

Improving program synthesis with execution. There has been works on using execution to improve neural program synthesis by either using an executor to prune the search space [17–19] or conditioning the generation on a representation of the program states [7, 8, 11, 23, 24]. However, these methods require doing decoding and execution in tandem, which greatly slows down inference. In contrast, our work only uses execution during training.

Reinforcement learning for generating programs. As pointed out by [15], there are parallels between our work and the reinforcement learning setting with sparse rewards for generating programs [1, 4, 18, 26]. Similarly, our approach of identifying partial correctness of programs is similar to partial rewards. But instead of discounting an entire trajectory with a low reward as in RL, with programs, we are able to truncate the program to a partially-correct program and assign it the “full reward”, which is a main contribution of this work. Moreover, the application domain is different as we apply our approach to general-purpose languages such as Python with large code-LMs, while most other works test on domain-specific languages (DSLs).

8 Conclusion

We propose to let a program synthesis model sample additional program solutions for each specification and learn from the self-sampled programs that are correct or partially-correct. We define partial correctness by tracing and matching intermediate execution states. We experiment on different math programming tasks and show that such partially-correct programs can help more efficient exploration of the program space and provide useful learning signal, which improves the PASS@k performance. Overall, our proposed method can improve PASS@k from 3.1% to 12.3% compared to learning from a single program with MLE, and such improvement also generalizes to different model sizes.
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Appendix

A Experiment Setting Details

| Name                  | MathQA | Grade-school-math |
|-----------------------|--------|-------------------|
| # Training Steps      | 50K    | 25K               |
| Learning Rate (LR)    | 1.0e-4 |                   |
| Optimizer             | AdamW  |                   |
| Adam Betas            | (0.9, 0.999) |             |
| Adam Eps              | 1.0e-8 |                   |
| Weight Decay          | 0.1    |                   |
| LR Scheduler          | Linear w/ Warmup |         |
| # LR Warm-up Steps    | 100    |                   |
| Effective Batch Size  | 32     |                   |
| FP Precision          | FP 32 for 125M, FP16 for 2.7B | |
| Gradient Clipping     | 1.0    |                   |

Table 6: The hyperparameters used for model training on two different types of datasets.
### Table 7: Comparing using self-sampled partially-correct programs (PCPs) and only using fully-correct programs (FCPs). Results are on the dev set of MathQA-Python-Filtered and MLE-Aug loss is used. The number of FCPs does not include the original reference program.

| Models          | # Progs. in $B$ | PASS@$k$ |
|-----------------|-----------------|----------|
|                 | FCP             | PCP      | $k=1$ | $k=5$ | $k=10$ | $k=20$ | $k=50$ | $k=80$ |
| GPT-Neo 125M    |                 |          |       |       |        |        |        |        |
| w/ MLE          | -               | -        | 12.0  | 15.4  | 17.5   | 19.6   | 21.3   | 25.2   |
| w/ self-sampling FCP + PCP | 0.71  | 0.16  |       |        |        |        |        |        |
| w/ self-sampling FCP only | 0.43  |          | 13.5  | 17.4  | 19.5   | 21.9   | 25.8   | 28.0   |
| GPT-Neo 2.7B    |                 |          |       |       |        |        |        |        |
| w/ MLE          | -               | -        | 16.4  | 20.6  | 21.7   | 23.5   | 26.1   | 27.6   |
| w/ self-sampling FCP + PCP | 1.03  | 0.15  | 20.7  | 26.0  | 28.4   | 30.8   | 34.2   | 36.2   |
| w/ self-sampling FCP only | 1.00  | -      | 20.3  | 25.2  | 27.1   | 29.0   | 31.9   | 33.6   |

Hyperparameters. All hyperparameters for training is shown in Tab. 6. We use $\beta = 0.25$ in the experiments with $\beta$-MML, as a result of enumeration search among the values of $\{0.1, 0.25, 0.5, 0.9\}$. We use the default AdamW optimizer settings and slightly tuned the learning rate by trying out several values between 1.0e-3 and 1.0e-5. The difference in floating point precision is to fit the GPT-Neo 2.7B model into the memory of the GPUs. All experiments are conducted on V100-32GB GPUs.

PASS@$k$ evaluation. We use temperature sampling and sample $n$ programs with $T = 0.8$, where $n = 80$ for MathQA and $n = 100$ for GSM to evaluate PASS@$n$. We also report PASS@$\{5, 10, 20, 50\}$ using the $n$ samples and the unbiased estimator proposed in [6]. We use $T = 0.2$ to sample 1 program per specification and evaluate PASS@1.

Codex few-shot settings. We estimate the Codex [6] performance under the few-shot settings. More specifically, the prompt consists of a natural language task description "# Generate Python code to solve the following math word problems:" and four examples, following previous work [9]. Each example consists of the NL specification as a one-line comment and the gold program solutions. We evaluate PASS@$k$ for Codex using the same sampling methods as above.

Details for self-sampling. For self-sampling at training time, we sample one program per task in each mini-batch, i.e., $|\hat{Y}| = 1$ in Alg. 1 and Alg. 2. However, this is also scaled by the number of epochs, which makes the total number of programs we sample for each task throughout training to be around 235 for MathQA-Python-Filtered, 83 for MathQA-Python and 145 for GSM5.5K-Python. For sampling temperature, we use the same setting as inference time, with $T = 0.8$.

### B Partial Correctness Results on MathQA

Here we perform the same ablation study as § 5.2 to study the effect of using partially-correct programs on the MathQA-Python-Filtered dataset. The results are shown in Tab. 7. From these results, we can see a similar trend with Tab. 4 as adding PCPs typically leads to more FCPs being found. However, we do not observe any advantage of using PCPs for the GPT-Neo 125M model on this dataset. We think this is because with a small model, the number of PCPs can be found on MathQA (i.e., 0.16) is much smaller than that of GSM (i.e., 1.36).

### C Full Learning Algorithm with Partial Correctness

Our general learning framework is shown in Alg. 1 and it is further extended in § 4. Here we show a complete version of the algorithm with using partially-correct programs in Alg. 3. Additionally, here are the detailed explanation of the data structure and functions used in it:

- **Mapping $\mathcal{M}$**: This is a data structure that maps program state to a set of (sub)programs that execute to that state, i.e., $\mathcal{M} : S \rightarrow \mathcal{Y}^n$. In this mapping, we save all PCPs and their execution states, including all subprograms of any PCP. We use this to significantly speed up the lookup process as mentioned in § 4.2.

- **Function PartialCorrectnessCriteria**: Since all states for all known PCPs are saved in $\mathcal{M}$,
to know whether a subprogram $\hat{y}_{\leq i}$ is partially-correct, we only need to check if its state matches any of the known states for a PCP, i.e., if $s_i \in \mathcal{M}$;

- **Function isDuplicate($\hat{y}_{\leq i}$, $Y_S$):** As mentioned in § 4.2, we use AST and length constraint to rule out "trivial variants" and identify new PCPs to save in the buffer $\mathcal{B}$. Here the programs to compare are the set of programs $Y_S$ that reaches the same state, i.e., being state-based equivalent;

- **Function updateBuffer($\hat{y}_{\leq i}$, $\mathcal{B}$):** Here we not only need to add the new PCP into the buffer $\mathcal{B}$, but also need to prune out the saved programs that are subprograms of $\hat{y}_{\leq i}$;

- **Function updateMapping($\hat{y}_{\leq i}$, $\mathcal{M}$):** Here we need to save the states of all subprograms of an identified partially-correct program, thus we will loop through all subprograms of $\hat{y}_{\leq i}$ and obtain its execution state (similar to line 4 and 5 of Alg. 3), then update $\mathcal{M}$ accordingly. As mentioned above, existing PCPs may be a subprogram of the new PCP, so we also need to prune out such existing PCPs from the mapping $\mathcal{M}$.

### D Qualitative Analysis

In [Tab. 8] we show more examples of the fully-correct and partially-correct programs that the models found during self-sampling, from both the MathQA and GSM datasets. First, we can see that for some NL specification, it is possible that no FCP or PCP can be found with self-sampling, as in MathQA-Example-1 and MathQA-Example-2. Take MathQA-Example-2 as an example, the question is quite straightforward thus it leaves very little room for the existence of other correct programs, as the gold program is already very short. Moreover, we can also observe that the ways self-sampled FCP and PCP differ from the gold program vary a lot. In MathQA-Example-2, GSM-Example-1 and GSM-Example-2 the sampled FCPs complete the task with very different paths compared with the gold programs, and actually result in using fewer lines of code. Another way of getting FCP or PCP is to perform small and local perturbations, e.g., switch the two sides of an addition or reorder the two non-dependent statements, as shown in other examples. We find that these local perturbations are more common in general in both datasets, as such patterns are easier for the model to learn.

### E Tracking Training Progress

Here we shown the PASS@$k$ performance curve with respect to the training process in [Fig. 3].

**Learning from self-sampled programs mitigates overfitting.** From the curves, we can observe that for MLE, while PASS@1 and PASS@5 generally improves during training, other PASS@$k$ for higher $k$ actually decreases after reaching the peak performance in early epochs, which is consistent with previous findings [10]. This is due to overfitting: in the early stage of training,
Table 8: More examples of self-sampled fully-correct (FCP) and partially-correct programs (PCPs). "MathQA" denotes the MathQA-Python-Filtered dataset and "GSM" denotes the GSM5.5K-Python dataset. All programs are from the final buffer after training a GPT-Neo 2.7B model with learning from self-sampled FCP+PCP using the MLE-Aug loss.

| NL Specs. | Gold Program | Self-Sampled FCP | Self-Sampled PCP |
|-----------|--------------|------------------|------------------|
| (MathQA-Example-1): The charge for a single room at hotel P is 70 percent less than the charge for a single room at hotel R and 10 percent less than the charge for a single room at hotel G. The charge for a single room at hotel R is what percent greater than the charge for a single room at hotel G? | n0=70.0 | n0=70.0 | - |
| | n1=10.0 | n1=10.0 | - |
| | t0=100.0-n0 | t0=100.0-n0 | - |
| | t1=100.0-n1 | t1=100.0-n0 | - |
| | t2=t0/t1 | t2=t0/t1 | - |
| | t3=t2*100.0 | t3=t2*100.0 | - |
| | t4=100.0-t3 | answer=t3-100.0 | - |
| | t5=t4/t3 | answer=t5*100.0 | - |
| (MathQA-Example-2): If John runs in the speed of 9 km/hr from his house, in what time will he reach the park which is 300m long from his house? | n0=9.0 | - | - |
| | n1=300.0 | - | - |
| | t0=n0*1000.0 | - | - |
| | t1=n1/t0 | answer=t1*60.0 | - |
| (MathQA-Example-3): A class consists of 15 biology students and 10 chemistry students. If you pick two students at the same time, what’s the probability that one is maths and one is chemistry? | n0=15.0 | n0=15.0 | n0=15.0 |
| | n1=10.0 | n1=10.0 | n1=10.0 |
| | t0=n0+n1 | t0=n0+n1 | t0=n0+n1 |
| | t1=n0/t0 | t1=n0/t0 | t1=n0/t0 |
| | t2=n1/t0 | t2=n1/t0 | t2=n1/t0 |
| | t3=t0-1.0 | t3=t0-1.0 | t3=t0-1.0 |
| | t4=n1/t3 | t4=n1/t3 | t4=n1/t3 |
| | t5=n0/t3 | t5=n0/t3 | t5=n0/t3 |
| | t6=t1*t4 | t6=t1*t4 | t6=t1*t4 |
| | t7=t5*t2 | t7=t5*t2 | t7=t5*t2 |
| | answer=t6+t7 | answer=t7+t6 | - |
| (GSM-Example-1): Ellie has found an old bicycle in a field and thinks it just needs some oil to work well again. She needs 10ml of oil to fix each wheel and will need another 5ml of oil to fix the rest of the bike. How much oil does she need in total to fix the bike? | n0=2 | - | - |
| | n1=10 | - | - |
| | n2=5 | - | - |
| | t0=n0+n1 | answer=n0+t0 | - |
| | t1=n1 | - | - |
| | t2=n0+n1 | - | - |
| (GSM-Example-2): There is very little car traffic on Happy Street. During the week, most cars pass it on Tuesday - 25. On Monday, 20% less than on Tuesday, and on Wednesday, 2 more cars than on Monday. On Thursday and Friday, it is about 10 cars each day. On the weekend, traffic drops to 5 cars per day. How many cars travel down Happy Street from Monday through Sunday? | n0=20 | n0=25 | n0=2 |
| | n1=100 | n1=2 | n1=25 |
| | n2=25 | n2=20 | n2=20 |
| | n3=2 | n3=100 | n3=100 |
| | n4=10 | n4=10 | n4=10 |
| | t0=n0/n1*n2 | t0=n0-n1 | t0=n0-n1 |
| | t1=n2-t0 | t1=n2/n3*n0 | t1=n2/t1 |
| | t2=t1+n3 | t2=t0-t1 | t2=t0-t1 |
| | t3=n4*n3 | t3=t2+n4 | t3=t2+n4 |
| | t4=t0+n3 | t4=n0-t3 | t4=n0-t3 |
| | t5=t4+n3 | answer=t4+n3 | answer=t4+n3 |
| | +t2+t3*t4 | - | - |

The model is less confident about its predictions thus the sampled k programs are very diverse, and while training continues, it overfits to the one gold program provided for learning thus leads to poor generalization when evaluated by PASS@k with high k values. [Fig. 3] also shows how our proposed self-sampling method can mitigate the overfitting problem, as it keeps improving or maintaining PASS@{5, 10, 20} while such performances start decreasing for MLE. Though it also shows improvements for PASS@{50, 100}, but the performance still decreases in later training stages.
Figure 3: How \( \text{PASS}@k \) on the dev set evolve during training. Results shown on GSM5.5K-Python dataset with GPT-Neo 125M model. Exponential moving average smoothing is applied for more clarity, but original curve is shown in shade.

Here we can also see the importance of suitable learning objective, as MML has almost no effect in mitigating such overfitting issue.

**Early stopping is needed when prioritizing high \( k \) value for \( \text{PASS}@k \).** In our experiments, we select the model checkpoint with the best \( \text{PASS}@1 \) performance to evaluate all \( \text{PASS}@k \). This setup aims to choose the best model that can solve the task with a small number of attempts (which corresponds to smaller \( k \) value), as studied in [2]. We can also observe that with our methods, the best \( \text{PASS}@1 \) checkpoint also yields the best or close to the best \( \text{PASS}@\{5, 10, 20\} \) performances. However, in certain applications where large number of attempts are allowed, \( \text{PASS}@k \) with high \( k \) values should be prioritized. An example is to generate candidate programs before reranking [10]. In this case, an earlier checkpoint (e.g., one with best \( \text{PASS}@100 \)) should be used instead, which is not the best checkpoint for \( \text{PASS}@k \) where \( k \) is small. Also note that our proposed method are not suitable for these applications, as we observe no improvement on the peak \( \text{PASS}@\{50, 100\} \) performances. We think this because when such peak performance is reached, it is still in the early stage of training thus not many FCPs or PCPs have been saved in the buffer yet.