Calibration and Correctness of Language Models for Code

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***Abstract*—Machine learning models are widely used, but can also often be wrong. Users would benefit from a reliable indication of whether a given output from a given model should be trusted, so a rational decision can be made whether to use the output or not. For example, outputs can be associated with a *confidence measure*; if this confidence measure is strongly associated with *likelihood of correctness*, then the model is said to be *well-calibrated*.**

A well-calibrated confidence measure can serve as a basis for rational, graduated decision-making on how much review and care is needed when using generated code. *Calibration* has so far been studied in mostly non-generative (*e.g.*, classification) settings, especially in software engineering. However, generated code can quite often be wrong: Given generated code, developers must decide whether to use directly, use after varying intensity of careful review, or discard model-generated code. Thus, calibration is vital in generative settings.

We make several contributions. We develop a framework for evaluating the calibration of code-generating models. We consider several tasks, correctness criteria, datasets, and approaches, and find that, by and large, generative code models we test are *not* well-calibrated out of the box. We then show how calibration can be improved using standard methods, such as Platt scaling. Since Platt scaling relies on the prior availability of correctness data, we evaluate the applicability and generalizability of Platt scaling in software engineering, discuss settings where it has good potential for practical use, and settings where it does not. Our contributions will lead to better-calibrated decision-making in the current use of code generated by language models, and offers a framework for future research to further improve calibration methods for generative models in software engineering.

***Index Terms*—LLM, Calibration, Confidence Measure**

I. Introduction

Generative large language models (LLMs) are now widely-used for code completion in IDEs. However, LLMs make mistakes: they can generate known buggy code [1], or code with risky vulnerabilities [2], [3]. Despite these risks, LLM "copilots" [4] are growing in popularity—thus there is a growing concern that bad LLM-generated code could be integrated into widely-used software. Given that LLMs might generate buggy code, how should a developer decide whether generated code is correct or not?

One possibility is to use the *confidence*, or probability assigned to the generated code by the LLM itself. Consider a developer who asks GPT-3.5 to complete some unfinished code. For example, given the prefix

```
def clear(self, tag: Optional[Hashable] = None) -> None:
```

the model generates the completion

```
self.jobs[:] = [job for job in self.jobs if job.tag != tag]
```

with an average per-token confidence of `91%`, suggesting high confidence (based on its training) that the code is a likely completion for the given prefix. However, this code is known to be buggy! In fact, when we test thousands of line completions, in cases where the average probability was greater than `90%`, only `52%` actually passed test cases. One can also find reverse examples, where the LLM has very little confidence, but the generated code is actually correct.

We make two observations. First, since LLMs can make mistakes, *users would benefit from a reliable indication of confidence that the generated code is actually correct*. Second, *such indications of confidence, when well-aligned with actual correctness, can support well-justified software quality control measures, and thus improve the reliability of the AI4SE ecosystem*. When an LLM-offered code suggestion is accompanied by a numerical "confidence" signal *e.g.*, a probability measure, then this signal *should be* well-aligned with the likelihood that the code is actually correct. Such a measure is said to be well-*calibrated*.

Calibration has been studied in other settings *e.g.*, classically in weather prediction and recently for software-related *classification* tasks [5]. In this paper, we study the calibration of *generative*[1] large language models, when used in practical software engineering settings, such as line-level code completion, function synthesis, and code-repair.

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[1]We note that the notion of *correctness* for generative tasks is quite different than for classification tasks, where the output is a label, rather than a sequence of tokens.

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A well-calibrated confidence measure would support rational risk-management in the development process, and help quality-improvement processes. For example, a development team might reasonably adopt a policy that: a) generated code associated with high confidence could be reviewed lightly and quickly accepted; b) suggestions with a medium confidence value should be reviewed more carefully before acceptance; and c) suggestions with a low confidence value should be simply rejected or the prompt should be adjusted.

Despite its importance and widespread use of LLMs in software engineering, the correctness and calibration of code-generating models currently is not well understood. In particular, it is currently unknown whether confidence measures provided by the LLMs themselves align well with actual code correctness.

This paper does an empirical study of the calibration of code-generating models using several prior techniques and explores approaches for improving calibration further. To this end, we describe an evaluation framework for the calibration of code-generating language models. We instantiate the framework for different tasks, *e.g.*, code synthesis, code completion, and program repair, using different correctness criteria (exact-match w.r.t. a reference solution and correctness-modulo-testing), and by applying the framework to different models. Based on this framework, we evaluate well-established techniques for estimating how a model's confidence align with actual correctness; then, based on our findings, we present improvements over existing techniques.

Our work yields several findings:

- The alignment of *confidence measures* provided by LLMs with standard notions of *code correctness* is poor, when evaluated on realistic datasets across different tasks, including completion, synthesis, and automated program repair. We observe generally high ECE (Expected Calibration Error, described in Section III-C) across all settings, ranging from 0.09 to 0.73, suggesting intrinsic LLM confidences are poor predictors of code correctness.
- We evaluate several *reflective* approaches to improve this alignment, and also *confidence rescaling* using known correctness labels. While rescaling generally improves calibration, reflective methods are rather inconsistent, working better in some settings than others.
- Finally, we focus on the most widely-used SE task for LLMs, *viz.* code completion, and use the instructable GPT-3.5 model, and few-shotting, in a reflective setting, and show that calibration improves substantially from the skill score[2] of 0 to a much higher level of 0.15.

Our work considers the important problem of providing developers with a reliable indication of whether generated code is correct, and (especially for the widely-used task of code completion) offers an approach, using BM25-aided [6] few-shotting, that has potential practical value.

[2]Brier Skill score, which we explain below in § III-C.

A. Research Agenda

Code LLMs are perhaps mostly widely-used for *code suggestion/completion*; other tasks include *code synthesis* and *program repair*.

RQ 1. How well is the confidence of language models in their output aligned with the empirical correctness of the output, specifically for common generative tasks, *viz.* function synthesis, line-level code completion, and program repair?

We evaluate the output for two different notions of correctness, *viz.*, exact-match with known correct code, and second, passing all given tests.

In general, the levels of alignment between the *intrinsic* confidence (*viz.,* directly provided by the LLM) and correctness is poor. This indicates need for better approaches to calibration. We then explore several engineering responses to the problem, listed in the following research questions. First, we consider the standard approach of confidence *rescaling*, using Platt scaling.

RQ 2. Can alignment between LLM confidence in generated code, and its correctness, be improved by confidence rescaling?

While confidence rescaling can help remedy over- and under-confidence, it does require some data to determine the parameters of the scaling function. We also analyze and discuss some considerations in obtaining this data, specifically for code-generation tasks.

Next, we investigate the possibility that the model is able to better calibrate upon *reflection*. We ask the model (using a separate reflective prompt) to consider its own generated code and judge its confidence in the quality.

RQ 3. Is confidence obtained by reflection better aligned with correctness?

Finally we investigate few-shotting, to see whether it helps calibration for the widely used task of code completion.

RQ 4. Can we use few-shot techniques to achieve better calibrated confidence for code completion, using an instruction-tuned model with in-context learning?

II. Background

A. Calibration

This concept originates in prediction problems like weather forecasting. Consider a weather model predicting a 70% confidence (probability) of rain the next day. If we ran this model for a while, and observed rain in 70% of the days where a forecast with 70% confidence was made, then we call it a well-calibrated model. A well-calibrated model's confidence in a given output, is quite close to the empirical relative frequency (likelihood) with which the output is actually correct.

With well-calibrated rain-forecasting, a user has options for a *rational response*: at 20% confidence of rain, one might take a hat; at higher confidences, one might take an umbrella; if even higher, one might take the bus rather than walk, *etc.* From an earlier work by Jiang *et al.* [7]: given a model M,

an input X and true, expected correct output Y, a model output $M(X) = \hat{Y}$, (note that we won't always have $Y = \hat{Y}$) and a output probability $P_M(\hat{Y} \mid X)$ provided by the model, a perfectly calibrated model satisfies the following condition

$$P(\hat{Y} = Y \mid P_M(\hat{Y} \mid X) = p) = \mathrm{p}, \quad \forall \mathrm{p} \in [0, 1]. \qquad (1)$$

In other words, if we have perfectly-calibrated confidence p (the model's calculated probability of its prediction that the output is $\hat{Y}$), then this value equals the *empirical fraction* p of the cases where the actual output Y correctly matches the prediction $\hat{Y}$. Usually these probabilities don't perfectly match; there are various measures of the deviation, including *Brier Score* [8] and ECE (Expected Calibration Error) [9]

B. Why Calibration Matters for Code

Even powerful LLMs can make mistakes [1], potentially leading users to accept incorrect code. A well-calibrated confidence signal could help developers manage [4], [10] this risk. Consider the confidence p associated with generated code. A well-calibrated high-value of p would indicate a high empirical probabilty p that the code is correct, and so it could be simply accepted; a low value would indicate higher risk that the code is incorrect, and so should be rejected. A poorly calibrated model may lead to either unnecessary rejection of likely correct code, or ill-advised acceptance of likely incorrect code. We note that good calibration allows more nuanced, effective quality-control (Q-C) decisions, beyond simple binary decisions *e.g.*, carefully review each token of generated code, perhaps by several people, *vs.* just use it. Such a well-calibrated quality-control process has been used in medicine *e.g.*, for elder-care [11], and for decision-making in cancer-care [12]. Given the cost & consequences of properly addressing software quality, and the potential benefits of LLM-generated code, a well-calibrated confidence signal is highly desirable.

III. Research Methodology

We consider three generative tasks *i.e.*, function synthesis, line-level code completion, and program repair, where generative LLMs are directly applicable and widely-used (*e.g.*, completion in Copilot). In this section, we will discuss the tasks, datasets, models, and methodology of our approach.

A. Code Correctness

When evaluating calibration, we need a notion of correctness. For (non-generative) models outputting labels, classes, True/False, *etc.* correctness is simply an exact-match with ground-truth correct label. Exact-match *could* also be viewed as a notion of correctness for code, *e.g.*, with defect repair, where there is a known, incorrect "buggy" version, and a known "fixed" version. Generated code is correct only if it matches exactly the fixed version, given an appropriate prompt. However, this approach is **overly strict**; the generated code might match exactly, but still pass all tests. Other notions of correctness exist: code-review, formal verification, *etc.* We use test cases provided with the code as our preferred indication of correctness, as tests are widely used, and are easily automated.

While test-passing correctness offers the advantage of admitting different semantically identical forms, test cases maybe insufficient or incorrect[3]; tests can also be "flaky" [14]: the same test, on the same code, might pass, or fail.

B. Confidence Measures

We usually calculate a confidence measure (or probability) p, associated with generated output code C. We consider two categories of measures: *intrinsic probability*, which is calculated by the generative LLM *per se*, and *reflective probability*, obtained by *re*-invoking the model, instructing it to estimate its confidence in the correctness of the code just generated Our measures include:

Average Token Probability *(Intrinsic, p_{avg})* For an output sequence T of tokens $\tau_i, i = 1 \ldots n$, we collect the associated model probabilities $p(\tau_i)$, and then compute the mean $p_{\text{avg}}(\mathrm{T}) = \frac{1}{n} \sum_{i=1}^{n} p(\tau_i)$.

Generated Sequence Probability *(Intrinsic, p_{tot})* The full generated sequence confidence is calculated as the product of probabilities, $p_{tot}(\mathrm{T}) = \prod_{i=1}^{n} p(\tau_i)$.

Verbalized Self-Ask [15]–[17] *(Reflective, p_v)* We instruct the model to reflect jointly on the prompt, *and* the model-generated code, and then output a numeric value of its confidence in the generated code.

Extra logic is implemented for when the model fails to output a probability

Question Answering Logit [18] *(Reflective, p_B and p_{NB})* In this case, rather than prompting for a numerical score (as above), we ask for a **TRUE** or **FALSE** answer. The probability associated with the **TRUE** token is taken to be the confidence measure. Additionally, we extend this approach using *normalization*: the model can assign probability mass to multiple possible expressions of **TRUE** or **FALSE** or even other variations (e.g, " True", " true", " ",). Thus when extending to the normalized form (Ask T/F N), we take the fraction of probability mass "True" assigned between only "True" and "False".

Our experiments consider the four above: *average token probability*, *generated sequence probability*, *verbalized self-evaluation*, and *question answering logit*. In addition, as a baseline, we also used the *length* of the generated sequence. The length baseline is calculated based on the number of characters in the generated sequence, scaled such that 0 is the shortest value in the dataset, and 1 is the longest.

For reflective measures, we expected that a code generation model should perform well (and provide well-calibrated confidence scores for correctness): first, *for synthesis*, given just

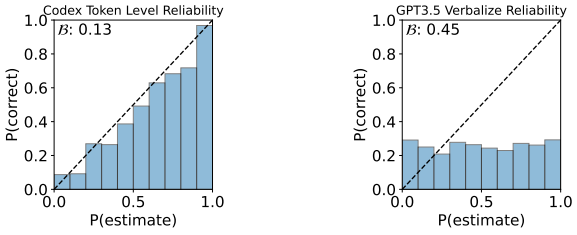
[3] *e.g.*, Liu *et al.* [13] report gaps in the test sets of HumanEval.

a good natural language description (without tests), of the desired function; second, *for completion & bug-fixing*, given the surrounding context. In both settings, we measure correctness using available hidden test cases. We also note that including hidden or failing tests in an LLM prompt is not common experimental practice for the tasks we analyze. [19]–[21].

C. Measures of Calibration

Using model's *confidence* in its generated output, and a way of determining *correctness*, one can compute measures of calibration. Calibration measures conceptually arise from the *Reliability Plot*, which plots correctness *vs.* confidence

Two reliability plots illustrating this method are shown in Figure 1. Figure 1a is for token-level code completions from CODEX; it shows the observed proportion of exact-match correct tokens (y-axis) *vs.* the predicted probability *i.e.*, confidence *as per* the language model, based on bucketing observations into subsets $S_1, S_2, \ldots S_n$. Here, there are $n = 10$ buckets, equally spaced by confidence measure. Each bucket has an associated bar whose height indicates the proportion (value $\in [0, 1]$) of correct samples in the bucket. The closer the bars in each S_i are to the diagonal line, the better the calibration.



(a) Well Calibrated (b) Poorly Calibrated

Fig. 1: *Sample calibration plots demonstrating well-* vs. *poorly- calibrated.*

We note here that CODEX is a large model, well-trained on the task of token-level completion; thus, it is both well-calibrated and generally correct on the simple token-level completion task. However, for notions of correctness farther from the training objective, such as line-level code completion and test-passing, CODEX's *intrinsic* probability may not be as well-calibrated. An example (Figure 1b) where the confidence is not well-calibrated is GPT-3.5 for line completion using verbalized confidence (*i.e.*, asking it to write its confidence; see Section III-B).

We study two measures of calibration: Brier Score [8] and ECE [9]. Both measure the deviation from perfect calibration. As before (following [22]), we assume a model M, input X, actual desired output Y, and model prediction $M(X) = \hat{Y}$. In our case, both Y and $\hat{Y}$ are code, rather than a single label. Calibration measures indicate the extent to which the deviations of $\hat{Y}$ from the desired Y are actually aligned with the model's confidence in its output, $\hat{Y}$.

From the calibration plot, with the evaluation set T bucketed into subsets $S_i, i = 1 \ldots m$ s.t. $\bigcup_i S_i = T$, $\forall i \in 1 \ldots m$. We estimate correctness in each bucket as the fraction of predictions in that bucket which are "correct" (as discussed in § III-A); confidence is the average estimated probability from the model in that bucket:

$$\text{corr}(S_i) = \frac{1}{\mid S_i \mid} \sum_{x_i \in S_i} \mathbb{1}(\checkmark M(x_i)) \tag{2}$$

$$\text{conf}(S_i) = \frac{1}{\mid S_i \mid} \sum_{x_i \in S_i} \hat{p}_i \tag{3}$$

where the model generates the code $M(x_i)$ with confidence (probability) $\hat{p}_i$, and $\checkmark M(x_i)$ indicates that the generated code is correct, as per the operative experimental definition. For a perfectly calibrated M, we would have $\text{corr}(S_i) = \text{conf}(S_i) \quad \forall i \in 1 \ldots m$. In practice, we observe deviations from this ideal. Expected Calibration Error (ECE) [9] is a typical measure of calibration, calculated as the weighted average of these deviations.

$$ECE = \sum_{i=1}^{m} \frac{\mid S_i \mid}{\mid T \mid} |\text{corr}(S_i) - \text{conf}(S_i)| \tag{4}$$

ECE is intuitive, but can mislead; as seen below, a naïve predictor whose confidence is always the base rate would yield a deceptively low ECE value. An alternative measure, the Brier score, $\mathcal{B}$ [8] avoids this issue; it is calculated as follows:

$$\mathcal{B} = \frac{1}{\mid T \mid} \sum_{i=1}^{|T|} (\hat{p}_i - \mathbb{1}(\checkmark M(x_i)))^2 \tag{5}$$

One can achieve an optimal Brier of $\mathcal{B} \approx 0$ when confidently estimating $\hat{p}_i \approx 1$ when the code is correct, and estimating $\hat{p}_i \approx 0$ when the code is incorrect for each sample.

For comparison, consider using the *Unskilled Reference Brier Score,* $\mathcal{B}_{ref}$, attainable by a naïve, "unskilled" model, which simply assigns the base-rate p_r as its confidence for every prediction. Here, all prediction confidence values are in one bin, the value p_r; and the empirical correctness in this single bin *is* the base rate p_r; so $ECE \approx 0$ which is misleading (thus exemplifying one of the weaknesses of ECE). The closed-form Brier Score for this unskilled predictor is:

$$\mathcal{B}_{ref} = p_r(1 - p_r) \tag{6}$$

In a 50-50 coinflip scenario (assuming *heads* is *correct*), a naïve predictor that randomly guesses *correct* with 50% confidence receives $\mathcal{B}_{ref} = 0.5 * (1 - 0.5) \approx 0.25$. Higher base rates yield lower $\mathcal{B}_{ref}$; *e.g.*, for the MBPP dataset [20], GPT-3.5 generates test-passing solutions for about 72% of the programming problems; here always guessing *correct* with 72% confidence results in $\mathcal{B}_{ref} = 0.72 * 0.28 \approx 0.20$. With well-calibrated confidence scores, a "skilled" model can achieve Brier Scores lower than this unskilled $\mathcal{B}_{ref}$ value; if a model does worse, it is indicative of poor calibration. Thus, one commonly reports a *Skill Score* (SS), calculated thus:

$$SS = \frac{\mathcal{B}_{ref} - \mathcal{B}_{actual}}{\mathcal{B}_{ref}} \tag{7}$$

Positive SS (perfect score = 1.0) indicates improvement over baseline $\mathcal{B}_{ref}$; negative indicates worse calibration than the baseline. Small positive values of SS can sometimes indicate good skill. For example, the *Deutsche Wetterdienst*

(German weather forecasting service) considers 0.05 Skill Score to be a minimum threshold for a good forecast quality[4]. As another data point, the American data journalism site *538* reports a skill of around 0.13 in forecasting World Cup games[5], which is in the range of what we observe in our experiments for best case code generation by LLMs; but these LLM performance numbers are just a starting point, and can be expected to improve in the future. ECE (Equation 4) and Brier Score (Equation 5) serve slightly different purposes: the Brier Score is calculated for each sample, and measures *both* the ability to correctly discriminate output categories, *and* calibration of the output probability. The ECE measures just calibration; but it can be misleadingly low, as noted above for the unskilled predictor. Additionally binning must be done carefully, since it can affect ECE scores [23].

D. Rescaling Approaches

Machine learning models are not always calibrated. Guo *et al.* [22] discuss ways of rescaling probability estimates to better match observations. A common approach is Platt scaling [24], where a logistic regression is fit to the logit values of the prediction *i.e.*, the $\ln$ of the measured confidence probability. This optimizes two parameters, a linear scaling multiplier and a bias *i.e.*, intercept, that shifts the value.

To reduce the likelihood that the scaling overfits & skews our results, we rescale over five folds; *i.e.*, we fit a logistic regression on a random 4/5 of data and apply it to 1/5 of data, before sliding over and doing each combination of 4/5.

Besides Platt scaling, temperature rescaling has also been used [18], [22], [25]: this approach applies a scalar multiplier on the logits representing each class *e.g.*, a multiclass image classifier. In our binary confidence case, this has similar expressivity to Platt scaling without an intercept. Other approaches include histogram binning [26], isotonic regression [27], *inter alia* [22], [28]. These approaches are more parameterized; given the data limitations in our experimental setup *e.g.*, a few hundred examples in function synthesis, they pose higher risk of overfitting.

As we discuss in Section IV, Platt scaling does improve calibration, with some caveats.

E. Tasks & Dataset

Task	Dataset	Dataset Size	Correctness Measure	Confidence Measure	Calibration Metric
Function synthesis	HumanEval	164	Test-passing Correctness	Average Token Probability, Generated Sequence Probability, Verbalized Self-Evaluation, Question Answering Logit	Brier Score, ECE
	MBBP Func	880			
Line-level Completion	DyPyBench	1,988	Test-passing Correctness, EM		
Program Repair	Defects4J 1-line	120			
	ManySStubs4j	3,000	Exact-Match (EM)		

TABLE I: List of tasks with associated datasets and measures.

1) Function Synthesis: This task aims to generate Python functions from "Docstrings".[6] Correctness is determined by functional testing.

We use HUMANEVAL [19] and MBPP [20] datasets. One caveat: the samples in these datasets largely constitute artificial problems, specifically assembled to test the code-synthesis capacity of LLMs; measurements (both accuracy and calibration) over these datasets may not generalize to real-world software development. Even so, these datasets provide a valuable datapoint for assessing model calibration.

We restructure all MBPP problems into a function synthesis task by placing the prompt inside the tested method as a Docstring, making it comparable to HUMANEVAL. Additionally we exclude approximately 75 problems where the reference solution fails to pass the provided test cases[7].

2) Line-level Code Completion: Code completion is currently the most important and widely-deployed generative task, with tools like GitHub Copilot [19]. Completion performance has been studied at both the token and line levels [29]–[32]. However, *calibration* for this vital, widely-deployed task has so far not been evaluated in detail

The current decoder-only GPT models [19], [33] are *already trained* to generate the next token at low average cross-entropy given all the prior tokens, following the condition $p(token \mid prior\ tokens)$. Unsurprisingly, we found such autoregressively-trained models are *per se* well-calibrated at the token level. In this work, we will primarily focus on line-level completion. While several datasets exist for this problem [34], [35], we use DYPYBENCH [36], a new dataset consisting of 50 popular open-source Python projects, including test suites for these projects. The test suites allow a test-correctness measure, in addition to the highly restrictive exact-match (*viz.*, the original line).

DYPYBENCH consists of complex real-world projects, each with hundreds of thousands of lines of Python code, and totaling over 2.2 million lines of Python code. We ran all test suites for each project with coverage reporting enabled, extracted all functions from the projects, following [37], and selected 1,988 functions with at least 3 lines in the body, 100% test coverage, and at least one line in the "Docstring".

3) Program Repair: Program repair is a well-studied problem in software engineering [38]. Several studies report that LLMs are effective at this task [21], [39], [40]. However, LLM *calibration* for program repair is not well-understood. This paper focuses on small, pre-localized single-line bugs. We leverage the widely-used Defects4J dataset [41], which includes real-world examples of buggy programs, with fixes and test-sets. We extract 120 single-line bugs from DEFECTS4J dataset. However, with only 120 samples, we may not obtain a comprehensive view of calibration. Therefore, we included another dataset, ManySStubs4J [42] (abbr. SSTUBS), which consists of single-line repairs. Following the setup of the SSTUBS dataset, the bug might be localized to a sub-

[4]www.dwd.de/EN/ourservices/seasonals_forecasts/forecast_reliability.htm

[5]projects.fivethirtyeight.com/checking-our-work/

[6]Docstrings are code comments that explain the code's purpose and usage. Further discussed in § III-E2.

[7]Due to either buggy reference code/tests, or possibly missing environment/networking/compute-time requirements.

expression of the line[8]. We sample (uniformly at random) 3,000 examples from this dataset. SSTUBS does not provide test-sets; so the only evaluation metric available is the exact-matching of the generated text to the ground truth bug-free text.

F. The Models

We explore confidence calibration for three code generation models. These include OpenAI GPT-3.5[9], OpenAI CODEX [19], and CODEGEN2-16B [43]. We sample from the models with temperature of 0, consistent with the reality that busy developers typically look at just the first suggestion in the completion [44]. For function synthesis task, temperature zero is most accurate and is fairly standard practice when doing pass@1 with only one solution to generate and present [13], [19].

IV. RESULTS

We begin with a brief overview of the findings on the correctness- & confidence- measures of LLMs on the various tasks, and then provide detailed results on the calibration-related research questions.

	All Pass@1			Exact-Match		
	CodeGen2	Codex	GPT-3.5	CodeGen2	Codex	GPT-3.5
SStubs	-	-	-	0.73%	**27.77%**	20.27%
DyPyBench	28.84%	32.96%	**33.22%**	19.68%	23.60%	**23.96%**
Defects4J	0.00%	**23.33%**	19.17%	0.00%	**19.17%**	15.00%
HumanEval	23.17%	47.24%	**64.60%**	-	-	-
MBPP	29.08%	61.79%	**72.04%**	-	-	-

TABLE II: Performance comparison of models on tasks. Metrics are All Pass at Rank 1 (**All Pass@1**), meaning all project test cases passed with the line completion on first and only sample (at $t = 0$), and Exact-Match, meaning the line completion was an exact string match with the original project line. Exact-Match is not commonly used for function synthesis tasks, since the generated output is longer and less likely to match. SStubs dataset does not have test cases. Boldface signifies high performing model for task and metric.

A. RQ 1: How well are language models' confidence in their output aligned with the empirical correctness of their output, specifically for common generative tasks, viz. function synthesis, line-level code completion, and program repair?

1) Overall Correctness: Correctness performance rate of the various models on the various tasks and datasets, are presented in Table II. Specifically, we report the fraction of samples passing all test cases for a given model and dataset, and the percentage of exact-matches. We found that GPT-3.5 worked well for both function synthesis (HUMANEVAL and MBPP), and line-level code completion, whilst CODEX generally performed well on program repair. The DYPYBENCH benchmark reflects the most popular use of LLMs, *viz.*, for code completion.

[8]Note, due to data processing errors, 3 Defects4J examples have slightly mis-localized bugs. We leave these as-is, reasoning that model confidence should be robustly well-calibrated even with slight localization noise, ideally giving a lower confidence of a fix if the location is noisy.

[9]The gpt-3.5-turbo-instruct model, https://platform.openai.com/docs/models/gpt-3-5-turbo

2) Correctness: Test-passing vs. *Exact-match:* As per § III-A, we evaluate correctness both on test-passing and exact-match. Our experiment included two datasets (DEFECTS4J and DYPYBENCH), where both methods of measuring correctness were available. Since DEFECTS4J consists of only 120 samples, we present the results for DYPYBENCH; in this case, as per Table II, GPT-3.5 performed best, with approximately 33% of generated code passing all available tests, and approximately 24% matching exactly.

In this setting (DYPYBENCH/GPT-3.5), we cross-tabulate performance across the two correctness-measuring methods. We note that approximately **half** the test-passing generations did *not* match the original code exactly; furthermore 6.89% of the cases where the code matched exactly, did not pass all the test cases. Upon careful study we found that these tests were "flaky", depending on network conditions, execution order, and other variable execution environment conditions. This aligns with [36], the author of this dataset, who observed an overall 7% failure rate, but noted that 31 out of 50 projects had zero failed tests. *This illustrates the relative merits/demerits of each correctness-evaluating approach, in practical SE settings.* Since the correctness performance is different with these two notions of correctness, the *calibration* is also different, as we see below.

3) Confidence Measures: As might be expected, the two intrinsic measures p_{avg} & p_{tot} are usually somewhat, and sometimes strongly, positively correlated with each other within the same model, dataset, and task.

4) Calibration without Rescaling: Table III presents the results for Line Completion, Function Synthesis, and Program Repair for each model and the raw confidence measure, without any rescaling method. We find raw confidence measures are poorly calibrated, with inconsistent exceptions. In fact, the raw baseline rate (using the average fraction correct without considering the individual generation) is hard to beat; the best skill-score is around 0.05.

For line completion, the p_{tot} confidence measure is slightly worse than the baseline rate; calibration error is modest ($ECE \sim 0.15$). The total probability improves on the average probability, which is overconfident: the average token probability exceeds the $\sim 30\%$ overall success rate.

For function synthesis with raw measures, p_{tot} exhibits very poor calibration for GPT-3.5 and CODEX, but not for CODEGEN2 on HUMANEVAL, while the best intrinsic measure for MBPP is p_{avg} for GPT-3.5 and CODEX. The intrinsic measures are inconsistent; with average probability showing indicators of better calibration for GPT-3.5 and CODEX, but not for CODEGEN2.

For program repair, intrinsic measures are consistently below the base rate for both models and are as such, poorly calibrated. There are several caveats here. First, DEFECTS4J is a small dataset, so findings may not generalize. Second, CODEGEN2 performs poorly on DEFECTS4J. Since CODEGEN2 is a smaller model without instruction tuning and relatively more limited reasoning

		Line Completion			Function Synthesis						Program Repair					
		DyPyBench			HumanEval			MBPP			Defects4J			SStubs		
Model	Metric	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE
GPT-3.5	Total Prob	**0.23**	**-0.03**	0.15	0.62	-1.70	0.63	0.71	-2.50	0.71	0.25	-0.63	0.28	0.24	-0.50	0.25
	Avg Prob	0.41	-0.87	0.46	0.27	-0.18	0.23	**0.22**	**-0.09**	**0.14**	0.68	-3.39	0.73	0.64	-2.94	0.69
	Ask T/F	0.25	-0.13	0.16	0.34	-0.47	0.37	0.33	-0.64	0.38	**0.15**	**+0.05**	**0.04**	**0.16**	**-0.01**	**0.04**
	Ask T/F N	0.25	-0.15	**0.15**	**0.23**	**+0.01**	0.19	0.22	-0.11	0.16	0.20	-0.30	0.24	0.22	-0.34	0.23
	Verbalize	0.43	-0.92	0.42	0.28	-0.24	0.22	0.24	-0.17	0.17	0.58	-2.72	0.60	0.50	-2.09	0.53
	Length	0.44	-0.99	0.46	0.23	-0.03	**0.15**	0.22	-0.10	0.16	0.53	-2.43	0.60	0.53	-2.26	0.60
	Unskilled	0.22	0.00	0.00	0.23	0.00	0.00	0.20	0.00	0.00	0.15	0.00	0.00	0.16	0.00	0.00
Codex	Total Prob	**0.23**	**-0.02**	0.16	0.44	-0.77	0.45	0.60	-1.52	0.60	0.25	-0.39	0.24	0.20	0.00	0.09
	Avg Prob	0.46	-1.07	0.50	0.34	-0.38	0.35	**0.24**	**-0.03**	**0.19**	0.66	-2.68	0.69	0.58	-1.90	0.62
	Ask T/F	0.24	-0.09	0.12	0.37	-0.47	0.36	0.49	-1.06	0.50	**0.18**	**+0.01**	**0.07**	**0.19**	**+0.03**	**0.02**
	Ask T/F N	0.23	-0.06	**0.07**	**0.32**	**-0.29**	**0.30**	0.42	-0.79	0.43	0.25	-0.41	0.27	0.23	-0.14	0.18
	Verbalize	0.38	-0.74	0.35	0.42	-0.67	0.40	0.38	-0.61	0.33	0.47	-1.65	0.50	0.43	-1.14	0.42
	Length	0.43	-0.95	0.45	0.44	-0.77	0.44	0.56	-1.35	0.56	0.50	-1.79	0.55	0.56	-1.78	0.59
	Unskilled	0.22	0.00	0.00	0.25	0.00	0.00	0.24	0.00	0.00	0.18	0.00	0.00	0.20	0.00	0.00
CodeGen2	Total Prob	**0.21**	**-0.02**	0.15	**0.23**	**-0.30**	**0.23**	0.29	-0.41	0.29	-	-	-	-	-	-
	Avg Prob	0.44	-1.16	0.50	0.60	-2.39	0.66	0.58	-1.80	0.61	-	-	-	-	-	-
	Ask T/F	0.23	-0.10	**0.14**	0.25	-0.38	0.24	**0.25**	**-0.19**	**0.21**	-	-	-	-	-	-
	Ask T/F N	0.33	-0.59	0.35	0.39	-1.19	0.45	0.39	-0.88	0.43	-	-	-	-	-	-
	Verbalize	0.42	-1.04	0.41	0.43	-1.39	0.42	0.40	-0.94	0.38	-	-	-	-	-	-
	Length	0.47	-1.28	0.51	0.38	-1.14	0.42	0.33	-0.58	0.28	-	-	-	-	-	-
	Unskilled	0.21	0.00	0.00	0.18	0.00	0.00	0.21	0.00	0.00	-	-	-	-	-	-

TABLE III: Calibration measured as raw, non-scaled Brier Score ($\mathcal{B}$, ↓ lower better), Skill Score (SS, ↑ higher better), and Expected Calibration Error (ECE, ↓ lower better), with respect to "all passed" notion of correctness, except SStubs which is "exact-match". CodeGen2 repair values are omitted as it does not perform the task with greater than 1% accuracy. The "Unskilled" row corresponds to a naive approach where the confidence is always returned as the base correctness rate, with Skill Score (SS) always zero by definition.

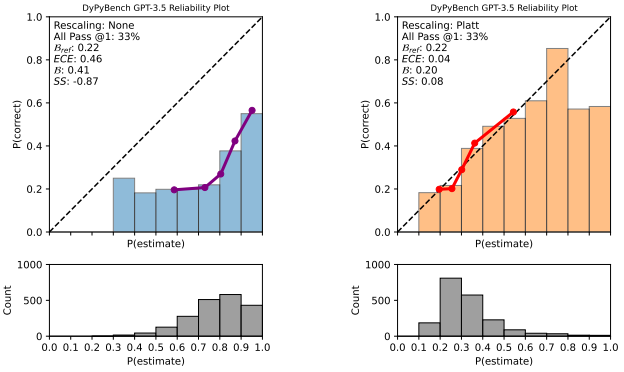
capabilities it gets "distracted" by the buggy version shown in the prompt: it often just repeats the buggy lines. With very few correct outputs, the estimation of the confidence measure becomes unreliable. Therefore, we have removed the CODEGEN2 results from Table III. A final caveat is that SSTUBS uses only exact-match as a correctness measure, which is quite different from a test passing measure.

In general, non-scaled confidence measures are only well calibrated for exact match on code completion; for test-passing correctness, they are poorly calibrated.

B. RQ 2: Can alignment between LLM confidence in generated code, and its correctness, be improved by confidence rescaling?

Table IV shows the results after applying Platt scaling to all measures (See § III-D). Figure 2a shows a reliability plot before rescaling, and its equivalent after rescaling in Figure 2b. Rescaling can improve calibration. Considering all values, ECE improves from an average of 0.32 to 0.03. For just those measures with a post-scaling SS of at least 0.05, ECE improves from 0.38 to 0.05.

a) Understanding "Bucket Collapse": Platt scaling can lead to deceptively low ECE. If a confidence measure is poorly aligned with correctness, Platt-scaling can rescale (squash) all the confidence values to the baseline rate; this places all samples in a single confidence value bucket where probability exactly matches the baseline rate of correctness, resulting in an ECE near 0. This indicates the problem of only considering ECE. SS and Brier, on the other hand, would reveal the poor utility of the confidence measure. Thus when applying rescaling, it is important to consider Skill Score, rather than only Brier and ECE.



(a) DyPyBench, nonscaled reliability plot

(b) DyPyBench, Platt scaled reliability plot

Fig. 2: Reliability plots for DYPYBENCH line-level code completion tasks, with respect to All Pass @1 correctness measure and Average Token Probability confidence measure. GPT-3.5 was used for both experiments. Bottom histogram represents number of samples in each bin. $\mathcal{B}_{ref}$ refers to the unskilled predictor Brier, ECE to Expected Calibration Error, $\mathcal{B}$ to Brier Score, and SS to Skill Score. Red & purple lines represent scaled & non-scaled quantile bins rather than evenly spaced bins with 1/5 of the data at each point. The left nonscaled plot shows over-confidence, as the confidence estimate is high, but the actual correctness is low. The scaled plot (right) improves calibration.

b) Results: After rescaling, only the intrinsic measures show skill improvement over the baseline rate for line completion. p_{avg} and p_{tot} are similarly calibrated. The calibration and skill appears roughly consistent between all three models in this case. Rescaling improves calibration results for function synthesis. The p_{tot} measure reaches a SS of 0.15 for HUMANEVAL. Rescaling useful improvement for reflective prompts as well bringing SS and ECE to similar values (discussed further in Section IV-C). For program repair, rescaling doesn't improve skill score, for any measure.

		Line Completion			**Function Synthesis**						**Program Repair**					
		DyPyBench			HumanEval			MBPP			Defects4J			SStubs		
Model	Metric	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE	$\mathcal{B}$	SS	ECE
GPT-3.5	Total Prob	0.21	+0.07	0.03	**0.20**	**+0.15**	0.09	0.19	+0.07	0.05	0.16	-0.05		**0.16**	**+0.03**	
	Avg Prob	**0.20**	**+0.08**	0.04	0.23	-0.02		0.20	0.00		0.16	-0.03		0.16	+0.02	
	Ask T/F	0.22	0.00		0.20	+0.12	0.11	0.18	+0.09	0.06	**0.15**	**+0.05**		0.16	0.00	
	Ask T/F N	0.22	0.00		0.20	+0.14	0.07	**0.18**	**+0.11**	0.04	0.15	+0.04		0.16	+0.01	
	Verbalize	0.22	0.00		0.24	-0.05		0.20	+0.02		0.17	-0.09		0.16	0.00	
	Length	0.22	0.00		0.24	-0.03		0.20	+0.01		0.16	-0.06		0.16	0.00	
	Unskilled	0.22	0.00		0.23	0.00		0.20	0.00		0.16	0.00		0.16	0.00	
Codex	Total Prob	**0.20**	**+0.09**	0.03	0.22	+0.11	0.08	0.22	+0.06	0.04	0.18	-0.01		**0.19**	**+0.05**	0.02
	Avg Prob	0.20	+0.09	0.04	**0.22**	**+0.14**	0.07	**0.21**	**+0.12**	0.06	0.18	-0.02		0.19	+0.05	0.02
	Ask T/F	0.22	0.00		0.24	+0.03		0.24	0.00		0.18	0.00		0.19	+0.04	
	Ask T/F N	0.22	0.00		0.24	+0.03		0.24	0.00		0.18	-0.01		0.20	+0.02	
	Verbalize	0.22	0.00		0.26	-0.02		0.24	-0.01		**0.18**	**0.00**		0.20	0.00	
	Length	0.22	+0.01		0.26	-0.03		0.24	-0.01		0.20	-0.10		0.20	0.00	
	Unskilled	0.22	0.00		0.25	0.00		0.24	0.00		0.18	0.00		0.20	0.00	
CodeGen2	Total Prob	**0.19**	**+0.08**	0.04	0.18	0.00		0.21	0.00		-	-		-	-	
	Avg Prob	0.19	+0.07	0.02	0.17	+0.03		0.21	0.00		-	-		-	-	
	Ask T/F	0.21	0.00		0.18	-0.01		**0.20**	**+0.01**		-	-		-	-	
	Ask T/F N	0.21	0.00		**0.17**	**+0.04**		0.21	0.00		-	-		-	-	
	Verbalize	0.21	0.00		0.18	-0.01		0.21	0.00		-	-		-	-	
	Length	0.21	0.00		0.18	-0.02		0.21	0.00		-	-		-	-	
	Unskilled	0.21	0.00		0.18	0.00		0.21	0.00		-	-		-	-	

TABLE IV: Calibration measured as Platt-scaled Brier Score ($\mathcal{B}$, ↓ lower better), Skill Score (SS, ↑ higher better), and Expected Calibration Error (ECE, ↓ lower better), with respect to "all passed" notion of correctness, except SStubs which is "exact-match". In cases where the SS is less than 0.05, the ECE is omitted. This is because an estimate without any signal will become Platt-scaled to approximately the base rate. This will *appear* as one well calibrated bin, resulting in an ECE near zero, but does not provide information. CodeGen2 repair values are omitted as it does not perform the task with greater than 1% accuracy.

c) Is Rescaling a Panacea for Calibration?: Rescaling typically improves calibration; it has been used in settings other than generative models of code, with other notions of correctness [22], [25], [45]–[49]. However, there are disadvantages. First, "bucket collapse" (see § IV-B0a) can mislead with deceptively low ECE. Second, some correctness data is needed to fit rescaling parameters. When sweeping through various sized bootstrapped subsets of the data, we find that it can take over 64 data points for the rescaling to result in positive skill and lower ECE, with improvements continuing into 100s of data points. When using the full data, the rescaling between tasks can vary dramatically. Ideally, we want confidence measures which are reliable and allow trustworthy auditing even when applying language models to new software engineering tasks. To study how close we are to this, we fit rescaling parameters to one task, and then apply it to the other tasks[10]. We find it is viable to use rescaling between tasks of the same domain with similar base rates, such as within the program synthesis tasks. For example, for GPT-3.5 when fitting p_{NB} (results in next section) rescaling to each of two function synthesis tasks, and then applying it to the other, we observe an average drop of SS from 0.14 → 0.12, and average drop of ECE from 0.07 → 0.05. However, applying the p_{total} rescaling fit on DyPyBench to the function synthesis tasks, results in an average SS change of 0.12 → -1.28 and ECE change of 0.08 → 0.54, indicating a lack of robustness. These reasons suggest one must be careful when analyzing and reporting calibration results based on rescaling, and highlights the need for further work on confidence measures that might be more directly calibrated.

[10]See supplementary appendix on arxiv:2402.02047 for figures showing variation given amount of data points and transfer between tasks.

Without rescaling, total probability p_{total} shows hints of calibration. With rescaling, there is a possible 10-20% improvement over baseline rates and good calibration, but it is inconsistent as skill is poor for CodeGen2 on Function Synthesis.

> Rescaling is an effective technique for improving calibration, but metric improvements ($\mathcal{B}$ and ECE) may be misleading by matching the base rate in a "bucket collapse" scenario or can lack generalization.

C. RQ 3: Is confidence obtained by reflection better aligned with correctness?

The two logit-based reflective measures p_B & p_{NB} are usually strongly positively correlated with one another, since they are calculated from similar numbers. The reflective verbalized self-ask confidence measure p_v, and the two logit-based reflective confidence measures have no consistent relationships.

For function synthesis with raw measures, p_{NB} shows best calibration for GPT-3.5, slightly better than Unskilled, for HumanEval. For program repair, we observe the strongest best-case performance with regards to the metrics. Both GPT-3.5 and Codex show positive SS and low ECE for p_B, but they are inconsistent after normalization (p_{NB}). These metrics suggest with reflection, these models' confidence is calibrated regarding repair correctness; however, further analysis does not indicate good calibration on this task, from any confidence measure. We find that in general, the intrinsic *vs.* reflective measure values have no consistent relationship, even for a given model, dataset and task.

This lack of relationship may not necessarily be negative: *e.g.*, perhaps the model's reflective, prompted confidence may be better calibrated, as suggested by prior work [20], [50]. Without rescaling or few-shot prompting, reflective results are inconsistent. In some cases, such as GPT-3.5 HumanEval

and DEFECTS4J, there are signs of calibration with slightly positive SS values and ECE values less than 0.2. Normalizing the T/F values induces some difference; but there are inconsistencies *vis-à-vis* tasks and models. For nonscaled GPT-3.5 results, p_{NB} improves calibration in line completion and function synthesis by an average of -0.34 SS and 0.19 ECE, but not for program repair or for CODEGEN2. Rescaling generally removes any sign of a normalization trend. For the alternative reflective approach of verbalization, the probability is not well calibrated for these models on the studied SE tasks.

In some cases, the reflective approaches are best calibrated without rescaling (see Table III), and show signs of being more robust when reusing learned rescaling parameters on unseen tasks.

> Reflective approaches may be best calibrated "out-of-the-box" and in some settings when rescaled. However, in the tested settings, they do not improve significantly over intrinsic measures.

D. RQ 4: Can we use few-shot techniques to achieve better calibrated confidence for code completion, using an instruction-tuned model with in-context learning?

We investigated the impact of few-shotting *viz.* providing a model completion and correctness as part of the p_{NB} prompt, on calibration [18]. To effectively perform few-shotting, we need a model that is instruction tuned and sufficiently large, which is best matched by GPT-3.5. We explore few-shotting for the widely-used line completion task.

We perform the experiment with 5-shots consisting of prior completions from the same experiments presented in Table IV, the reflective question, and the ground truth True/False. We try two variants of this experiment, one where the examples are randomly selected, and one where they are chosen based on the similarity to the unanswered prompt. In both cases, we exclude the ground truth result for the unanswered prompt. We focus on Line Completion for this experiment as it represents widespread use and has a large number of examples available.

Confidence Measure	$\mathcal{B}\downarrow$	$SS\uparrow$	$ECE\downarrow$
0-Shot Reflect	0.25	-0.15	0.15
0-Shot Reflect (Rescaled)	0.22	0.00	
FS Random	0.29	-0.29	0.21
FS Random (Rescaled)	0.22	0.0	
FS BM25	0.20	0.08	0.10
FS BM25 (Rescaled)	0.19	0.15	0.02

TABLE V: Few-shot reflective prompting using GPT-3.5 for line completion. 'FS Random' refers to selecting random few-shot examples. 'FS BM25' retrieves more relevant known completions. ECE values when rescaled values SS are close to zero are omitted (to avoid confusion with "bucket collapse", Section IV-B0a)

For line completion, the non-scaled results using random examples did not result in improved calibration over the baseline p_{NB}, however using BM25 [6] to select similar examples yielded a positive SS of 0.08, which could be improved further by rescaling, up to 0.15. This result notably exceeds any other measure for DYPYBENCH, and significantly improves over the baseline p_{NB} SS of 0.

While random few-shotting requires limited extra data, BM25 is more similar to rescaling, in that it is dependent on a larger set of ground truths. This could be actualized by logging user completions, and building up ground truths (on if the completion was correct) based off the test case runs or acceptance of completions.

> Providing a few examples selected via BM25 when asking GPT-3.5 to reflect on its own completion output significantly improves reflective calibration.

Alternative and improved ways of prompting (*e.g.*, different verbalization formats [15], [17], fine-tuning [15], [18], chain-of-thought [17], [51], *etc.*) may alter these findings and are areas for future work.

V. DISCUSSION

Language models are now widely-integrated into Software Engineering practice, via tools like Copilot [32] and Didact[11]. We raise here the importance of calibration when integrating *generative* LLMs in coding practice. We evaluate the calibration of generative LLM use (especially code completion) with large samples of *realistic* data (DYPYBENCH, SSTUBS), using widely adopted models, as well as some more academic datasets (HUMANEVAL, MBPP).

a) Using a well-calibrated model–beyond simple defect prediction: To clarify how a well-calibrated model enables more well-grounded decision-making concerning generated outputs, as compared to as compared to a traditional process choosing a binary decision point—we consider GPT-3.5 working on code completion, where correctness is determined by test-passing, and confidence is assigned by few-shotting, average token probability. The base correctness (test-passing) rate of completions is about 33%. With few-shotting, we get a very high skill score of 0.15 (Section IV-D, Table V).

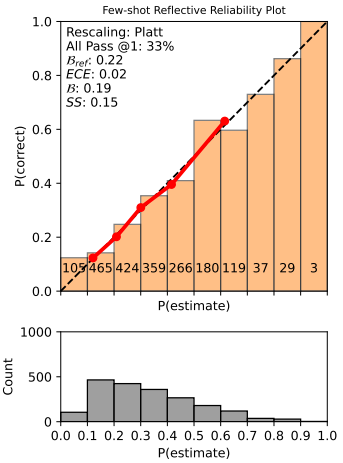


Fig. 3: *Few-shot reflective reliability plot, based on "FS BM25" row of Table V*

If we didn't have a well-calibrated model, we might very cautiously accept only those completions that are generated

[11] blog.research.google/2023/05/large-sequence-models-for-software.html

at a very high-confidence threshold; here, the FP rate could be low (of course TP rate would be low as well). While this may lower the risk of bad code, it also regrettably reduces the available help from the LLM. However, a well-calibrated confidence measure allows a more rational, graduated set of decisions. Such a well-calibrated measure is visualized in Figure 3. In this setting, for much of the confidence scale, a user could look at the confidence level, and get a very good idea of how likely the code is to be correct, and make a well-reasoned, situation-specific set of decisions to manage risk, and allocate reviewing resources, based on the model's confidence. This provides an illustration of the greater benefit provided a well-calibrated measure (high Skill level, low ECE) over one that is just providing good precision-recall trade-off (or, ROC curve); the latter does not allow such graduated deployment of quality-control effort. However, developers would need to learn to use calibrated probabilities in decision-making.

b) Beyond simple "correctness": In addition to the above uses, which considered a single notion of "correctness", one could consider a multi-class correctness prediction task, where the model could indicate the confidence in correctness (the absence of defects) from multiple perspectives: severity of possible defect, the kind of defect (relating to security, integrity, privacy, fairness, *etc.*) and defect complexity (indicating the cost or schedule impact of repairs). Drawing an analogy to classical forecasting, this is analogous to not just the probability it will rain, but probability it will be a drizzle or be a drenching thunderstorm.

c) Why calibration now?: We've always had bugs; poor-quality code isn't new. Our push for calibration, however, arises from the increasing amount of code generated by LLM. GitHub claims that up to 61% of code[12] in some systems is generated by LLMs. It is also known that LLMs make a lot of mistakes. A recent paper has reported [1] that LLMs, even when trained on *properly fixed* code, tends to recapitulate the *the old unfixed, buggy code* when prompted in context. However, LLMs do have very high capacity, and a demonstrated ability to usefully reflect [50], [52] on their generated text. Thus, we have both a high risk (of buggy code), and a chance to improve productivity. We believe that improved calibration could lead to better management of the risk-benefit of LLM-generated code. The studied correctness calibration is a stepping stone for more complex notions of confidence (like severity and localized confidence). Additionally, by studying code LLMs, we might make progress on the general safe deployment of capable generative models [10].

d) Summarizing per-token probabilities: To produce a summary confidence for generated token sequences in Tables III and IV, in Tables III & IV, we used (arithmetic mean) average & product to summarize the per-token probabilities. In this setting, it might be more reasonable to use geometric mean (as in [53]) to get a product value normalized for length; indeed, when we tried that, we found that Brier and skill scores improved marginally, but consistently so; future research could indicate whether these findings generalize.

[12] github.blog/2023-02-14-github-copilot-now-has-a-better-ai-model-and-new-capabilities

VI. Threats to Validity

a) Sample Size & Generalizability: While three of our datasets contain more than 800+ samples each, HumanEval and Defects4J datasets consist of only 164 and 120 samples, respectively. Results on these datasets may not generalize. However, we note that our study has a large and natural dataset for the *line-level code completion* task, which has current practical importance. Given the noise and variance we observe, we recommend future work push towards larger and more natural datasets, in particular for Function Synthesis & Repair.

While some of our treatments (*e.g.*, few-shotting) suggest substantial improvements in skill score (Table V), in other cases such as the different approaches to summarize per-token confidence differences, the differences are less clear. In future work, these differences could be judged more robustly using bootstrapped p-values and effect sizes.

b) Artificial vs. *real world data:* For function synthesis, we used the popular HumanEval and MBPP function synthesis datasets. These datasets contain small-ish Python programs that may not represent real-world software development functions. However, our other datasets, such as DyPyBench and SStubs are more representative of real-world, open-source GitHub projects.

c) Model Selection: Results might not generalize to all models, especially those with greatly differing training/fine-tuning or different architectures.

d) Experimental Design: Our exploration is not exhaustive; other SE tasks and datasets also could benefit from calibration studies. Additionally, the specific prompts we used for this paper surely played a role in our findings. Other prompts or problem phrasings (such as different forms of context for line-level code completion) may yield different results. Regarding test flakiness: the test "flake" rate of DyPyBench is not zero, but is quite low and not unrealistic [14].

Despite these caveats, our study, which includes three tasks and five datasets, provides a good starting point for further studies.

VII. Related Work

LLMs for code are extensively studied [54], [55]. While calibration has a long history in modeling [8], [56], it is not a frequently studied topic in the SE community. Early work moving into modern machine learning studied the calibration of smaller neural models performing classification tasks on text and images; while these early models were poorly calibrated *per se*, their performance could be improved by simple scaling [22] of their output probabilities. As models became larger, calibration was found to improve [57]. Pre-training was also found to improve calibration [25], [58]; however, these findings have been disputed [47].

More recent works evaluated LLM calibration on a wide variety of settings [7], [18], [25], [59]. Desai *et al.* [25]

studied non-code (natural language) tasks such as inference or paraphrasing, with only intrinsic measures using older-generation models (BERT and RoBERTA). Jiang *et al.* [7] studied calibration for natural language question-answering using just intrinsic measures. In contrast, we study calibration for three coding-related tasks, using both artificial and natural code datasets, and both intrinsic and reflective confidence measures, to evaluate calibration in the SE domain.

Other prior work has investigated tokens that might be edited. Vasconcelos *et al.* [60] discusses code model uncertainty for function-synthesis-style problems, and ran human evaluation of the usefullness of colored highlighting of uncertain tokens. They found highlighting a human-derived ground-truth of which tokens might be edited was helpful, and more useful than raw token probabilities from the model. Johnson *et al.* [61] developed method of highlighting likely edit tokens via a utility optimization algorithm comparing different file completions. We find exploring more on calibrated uncertainty for local areas be a interesting area for additional work.

Li *et al.* [49] investigate the calibration of Computer vision (CV) models from an operational perspective *i.e.*, the shift between training input and production inputs, presenting it as a software quality problem that can be addressed using Bayesian approaches. Minderer *et al.* [45] evaluate the calibration of at the time, state of the art CV models and find improved calibration with more recent models, notably those not using convolutions. Park *et al.* [46] study the effect of the mixup technique [62] on calibration in a natural language understanding (NLU) setting using older generation models (BERT and RoBERTa). Chen *et al.* [47] investigate the calibration of pretrained language models on various NLP tasks, also using older generation models (RoBERTa and T5). Bommasani *et al.* [48] introduce the HELM benchmark, which includes calibration as one of its seven metrics to evaluate language models in a natural language context. Huang *et al.* [63] explored LM uncertainty with a range of techniques and tasks, including both NLP and function synthesis tasks. They evaluated using correlation measures, rather than focusing on calibration. They explore interesting sample-based and perturbation techniques which could be explored more for calibration on diverse SE tasks. Other work [64] has explored training an ML model that sees code and execution results to estimate correctness probabilities for solution reranking. For natural language question answering tasks, work has explored improving calibration by training a model to adjust token logits [53], and training a model from LLM hidden states specifically around the ECE metric[65].

When suitably prompted, Kadavath *et al.* [18] found that LLMs can output well-calibrated scores on whether their own answers are correct or not, *viz.*, larger models "know what they know". While this work did investigate some function synthesis tasks (HUMANEVAL & an unpublished Python function dataset), they did so using only their private models, and ultimately focused on natural language tasks. Key *et al.* [59] developed an approach that given a natural language problem description, produces a confidence score for a sampled candidate solution based on generated specifications, allowing them to judge whether the LLM can solve the problem at all. Their metrics include calibration. Recent work has also explored calibration of software topics such as root cause analysis [66].

VIII. CONCLUSION

In this paper, we begin with the observation that while LLMs are often helpful (for example producing code-completions for developers) they often produce buggy code. We argue that a *well-calibrated* confidence score, could provide a reliable indication of whether the generated code was correct, and help more rational, graduated quality-control of of LLM-generated code We studied the calibration of intrinsic and reflective confidence measures in several practical settings (completion and repair) and a widely-used competitive setting (synthesis), across several LLMs. We find that LLMs are generally poorly calibrated out of the box, across a variety of confidence measures (both intrinsic and reflective) We then found that Platt scaling generally results in somewhat better calibrated confidence measures.

Finally, we focused in on a) coding task where LLMs are most widely-deployed, *viz.* code completion, and b) a very widely used instruction-tuned model, *viz.* GPT-3.5, and investigated whether a reflective, in-context learning approach (few-shotting) could provide better calibrated confidence measures. In this setting, we found that calibration improves substantially, reaching a skill score of 0.15, particularly with retrieval augmented few-shotting.

To our knowledge, our paper is the first to consider the problem of calibration in a real-world code generation setting. We do find that most models, both out-of-the-box and with simple reflection, don't provide reliable confidence measures. However, our results with retrieval-augmented few-shotting are very encouraging, and point towards a future where Language Models could provide developers with guidance on how to quality-control the code they generate.

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