CodeComplex: Dataset for Worst-Case Time Complexity Prediction

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Abstract

Reasoning ability of large language models (LLMs) is a crucial ability, especially in complex decision-making tasks. One significant task to show LLMs' reasoning capability is code time complexity prediction, which involves various intricate factors such as the input range of variables and conditional loops. Current benchmarks fall short of providing a rigorous assessment due to limited data, language constraints, and insufficient labeling. They do not consider time complexity based on input representation and merely evaluate whether predictions fall into the same class, lacking a measure of how close incorrect predictions are to the correct ones. To address these dependencies, we introduce CodeComplex, the first robust and extensive dataset designed to evaluate LLMs' reasoning abilities in predicting code time complexity. CodeComplex comprises 4,900 Java codes and an equivalent number of Python codes, overcoming language and labeling constraints, carefully annotated with complexity labels based on input characteristics by a panel of algorithmic experts. Additionally, we propose specialized evaluation metrics for the reasoning of complexity prediction tasks, offering a more precise and reliable assessment of LLMs' reasoning capabilities. We release our dataset and baseline models publicly to encourage the relevant (NLP, SE, and PL) communities to utilize and participate in this research. Our code and data are available at `https://github.com/sybaik1/CodeComplex`.

1 Introduction

Large language models (LLMs) demonstrate significant potential in complex decision-making tasks, with their inference capabilities being particularly valuable in software development (Austin et al., 2021; Jain et al., 2021). To further test LLM's inferencing abilities, we showcase this domain of predicting the code time complexity, which requires the consideration of numerous intricate factors. For example, factors such as algorithmic structure (Turing, 1936; Bentley et al., 1980), data input size, and resource constraints can all influence the time complexity of code (Nogueira, 2012; Hutter et al., 2014). Understanding and optimizing these factors is crucial for improving the performance of complex algorithms and generating efficient code (Peng et al., 2021; Lu et al., 2021).

Despite the existence of benchmarks for the time complexity analysis, such as CoRCoD (Sikka et al., 2020), and TASTY (Moudgalya et al., 2023), these benchmarks have limitations on their current state. Notably, CoRCoD is the only publicly available dataset that is small in size, and while TASTY considers both time and space complexity, its dataset remains undisclosed. Consequently, there is a clear need for a comprehensive and publicly accessible benchmark that addresses these shortcomings.

Our work aims to fill this gap by introducing CodeComplex, a dataset designed to be the definitive benchmark for evaluating LLMs' time complexity inference abilities. CodeComplex offers several distinct advantages over existing benchmarks. First, it provides a larger and more diverse dataset, encompassing a broad range of programming languages beyond the limited scope of CoRCoD, which focuses solely on Java. Second, our dataset encompasses a more comprehensive set of labeled complexity classes that cover general-use problem-solving algorithms, enabling a more detailed analysis. Thirdly, CodeComplex considers the representation of input data, distinguishing between numeric values and input size indicators, which is critical for accurate complexity analysis. Lastly, we suggest detailed metrics that allow for a more nuanced assessment of LLMs' performance, moving beyond simple class-based evaluations.

In summary, our contributions are as follows:

1. Comprehensive dataset: We present a novel

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dataset with a comprehensive range of algorithmic problems that includes bilingual programming languages, offering a significant expansion upon existing benchmarks.

2. Detailed complexity analysis: We annotate the code complexity through complexity analysis of the representation of input data, distinguishing between numeric interpretations and input size indicators.

3. Robustness of evaluation metrics: We implement precise evaluation metrics for a rigorous and nuanced assessment of LLMs' time complexity inference, facilitating accurate comparisons with state-of-the-art baselines.

Through these contributions, CodeComplex aims to advance the study of LLMs inference capabilities with the task of predicting code time complexity, ultimately fostering the development of optimized software. Our benchmark sets a new standard for the evaluation of LLMs, providing a robust and comprehensive tool for researchers and practitioners alike.

2 Related Work

The LLMs have led to numerous advances in the field of natural language processing (Brown et al., 2020; Chowdhery et al., 2023). Therefore, recent research is ongoing to improve the reasoning ability of LLMs. Numerous prompt engineering techniques emerged, such as zero-shot, few-shot, chain of thought, and prompt changing (Wei et al., 2022; Wang et al., 2023; Yao et al., 2023). Specifically, the chain of thought prompting was proposed to encourage them to engage in inferential thinking, with the subsequent application of arithmetic, commonsense, and sentiment reasoning. The methodologies demonstrated that when the LLMs' reasoning was improved, their capability to perform a range of tasks was enhanced.

Nevertheless, it is evident that LLMs are still constrained in their capacity to reason about complex tasks. The enhancement of LLM's capacity to reason effectively in complex domains is highly dependent upon the availability of a domain-specific and sophisticated dataset. In the field of code time complexity, some representative complex tasks have been proposed as a method for improving the reasoning ability of LLM models. Recently, Sikka et al. (2020) explored code complexity prediction using machine learning-based methods. They curated the CoRCoD dataset comprising 929 annotated Java codes. These codes were enriched with various hand-engineered features extracted from the code, encompassing counts of loops, methods, variables, jumps, breaks, switches, and the identification of specific data structures or algorithms like priority queues, hash maps, hash sets, and sorting functions. Employing machine learning classification algorithms such as K-means, random forest, decision tree, SVM, and more, they made predictions based on these diverse features. Additionally, they explored graph2vec (Narayanan et al., 2017), a neural graph embedding framework that operates on a program's AST and achieves comparable performance results.

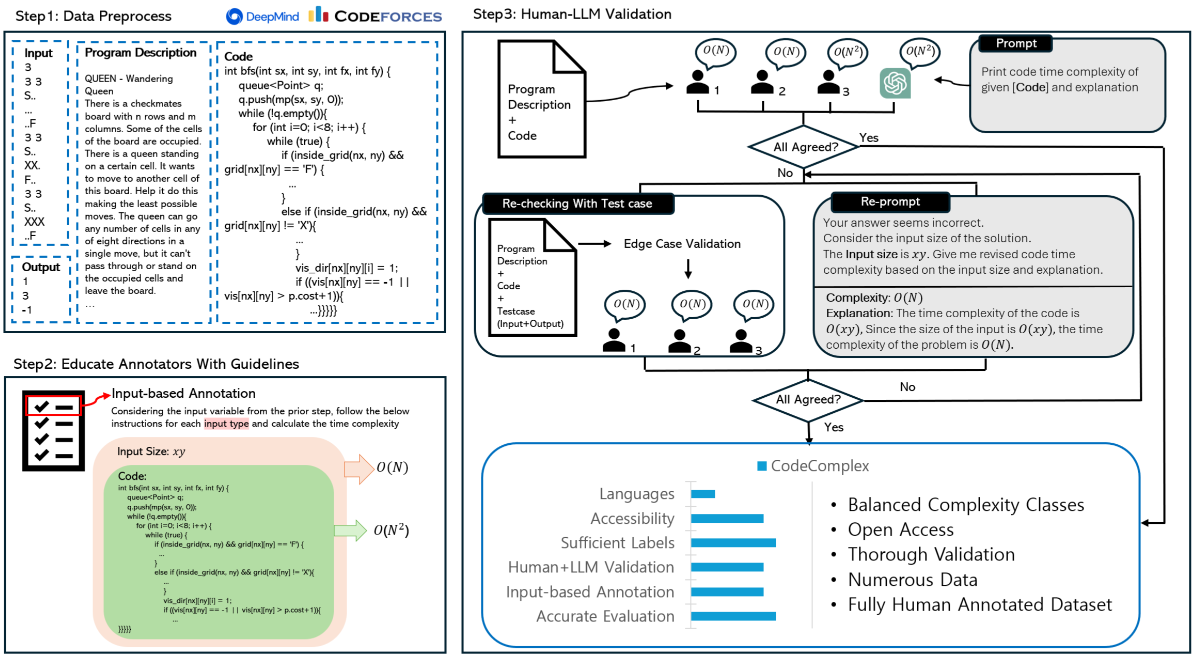
Another exploration by Prenner and Robbes (2021) scrutinized the potential of pre-trained programming language understanding models, particularly CodeBERT (Feng et al., 2020), for predicting code complexity. Their experiments showcased promising results, suggesting that pre-trained models could serve as a viable solution in this domain. In the most recent development, Moudgalya et al. (2023) tackled the analysis of time and space complexity using language models. They leveraged codes sourced from GeeksForGeeks[1] and CoRCoD, alongside a dataset comprising 3,803 Java codes. Their work showcased the viability of fine-tuning pre-trained language models such as GraphCodeBERT (Guo et al., 2021) for predicting both time and space complexity, thereby opening new avenues for exploration in this field.

3 The CodeComplex Dataset

The CodeComplex dataset contains a collection of codes written in two languages, Java and Python, from a competitive programming platform. Our dataset originates from Codeforces and collects data from CodeContests (Li et al., 2022), a competitive programming dataset tailored for machine learning applications created by DeepMind. It comprises 9,800 codes, evenly split between Java and Python, with 4,900 codes each. We have categorized these codes into seven distinct complexity classes: constant ($O(1)$), linear ($O(n)$), quadratic ($O(n^2)$), cubic ($O(n^3)$), logarithmic ($O(\ln n)$, $O(n \ln n)$), and exponential. Each class contains a minimum of 500 Java and Python codes.

We annotated all 9,800 codes with experts,

[1]https://www.geeksforgeeks.org/



QUEEN - Wandering Queen
There is a checkmates board with n rows and m columns. Some of the cells of the board are occupied. There is a queen standing on a certain cell. It wants to move to another cell of this board. Help it do this making the least possible moves. The queen can go any number of cells in any of eight directions in a single move, but it can't pass through or stand on the occupied cells and leave the board.
...

```
int bfs(int sx, int sy, int fx, int fy) {
    queue<Point> q;
    q.push(mp(sx, sy, 0));
    while (!q.empty()){
        for (int i=0; i<8; i++) {
            while (true) {
                if (inside_grid(nx, ny) &&
grid[nx][ny] == 'F') {
                    ...
                }
                else if (inside_grid(nx, ny) &&
grid[nx][ny] != 'X'){
                    ...
                    }
                    vis_dir[nx][ny][i] = 1;
                    if ((vis[nx][ny] == -1 ||
vis[nx][ny] > p.cost+1)){
                        ...}}}}}
```

Considering the input variable from the prior step, follow the below instructions for each input type and calculate the time complexity

```
int bfs(int sx, int sy, int fx, int fy) {
    queue<Point> q;
    q.push(mp(sx, sy, 0));
    while (!q.empty()){
        for (int i=0; i<8; i++) {
            while (true) {
                if (inside_grid(nx, ny) && grid[nx][ny] == 'F') {
                  ...
                }
                else if (inside_grid(nx, ny) && grid[nx][ny] != 'X'){
                    ...
                    }
                    vis_dir[nx][ny][i] = 1;
                    if ((vis[nx][ny] == -1 || vis[nx][ny] > p.cost+1)){
                        ...
}}}}}
```

Print code time complexity of given [Code] and explanation

Your answer seems incorrect.
Consider the input size of the solution.
The **Input size** is xy. Give me revised code time complexity based on the input size and explanation.

Complexity: $O(N)$
Explanation: The time complexity of the code is $O(xy)$, Since the size of the input is $O(xy)$, the time complexity of the problem is $O(N)$.

Figure 1: Overview of the CodeComplex dataset creation process.

which include the 317 Java codes in the CoRCoD dataset from Codeforces. It is worth mentioning that the CoRCoD, a previous dataset used for code complexity prediction, categorizes Java codes into five complexity classes: $O(1)$, $O(n)$, $O(n^2)$, $O(\ln n)$, and $O(n \ln n)$. However, it suffers from imbalanced class distribution, evident in Table 1, with a relatively small size of 929 Java code samples in total. Our expansion significantly enhances the dataset's value for research, particularly concerning DL-based models outlined in Section 4.

Class	CoRCoD	CodeComplex	
	Java	Java	Python
$O(1)$	143	750 (+ 62)	791
$O(n)$	382	779 (+ 117)	853
$O(n^2)$	200	765 (+ 48)	657
$O(n^3)$	0	601	606
$O(\ln n)$	54	700 (+ 18)	669
$O(n \ln n)$	150	700 (+ 72)	796
exponential	0	605	528
Total	929	4,900 (+ 317)	4,900

Table 1: Statistical difference between CoRCoD and CodeComplex. Numbers in parentheses imply the number of codes from CoRCoD.

3.1 Data Collection

The original corpus of code is from CodeContests, which collected 128 million codes from Codeforces. The corpus only contained information about the contest ID, problem, username, language, acceptance, and statistics (runtime and memory). We extracted the selected problems from this corpus and identified each code's complexity.

Code samples were selected within the matching candidates with the following conditions. First, we checked the relevance of the problem. There are many problems within a coding competition, but not all of them fall into the scope of complexities we seek to compromise. Therefore, the problems were first analyzed to check whether or not they were in the complexity class of our dataset. If the problem was determined to be in one of the seven complexity classes, then we marked the problem as a candidate for the dataset. This helps to establish a clear base dataset for the complexity domain. Second, we checked the completeness and correctness of the code. We filtered codes that are available to pass the given problem in the contest, meaning that the code is functional, self-contained, and correct on the given task. One of the reasons for using code competition data is that we can check if the code is correct for the problem. Lastly, we wanted a large pool of code samples for a given problem. We took code samples from problems with abundant submissions. This helped to clarify the problem's robustness and variation.

Consider the following Python program that solves a problem with $O(1)$ time complexity:

```python
buf = input()
hand = buf.split()
t = []
for i in range(3):
    t.append([])
    for j in range(9):
        t[i].append(0)
for x in hand:
    idx = 0
    # Following lines are omitted.
```

Despite the short length of the code, it is not trivial to understand that the time complexity of the above code is actually constant, which implies that the number of instructions for executing the program does not depend on the input size. In fact, the problem description says that the input always consists of three strings separated by whitespace and, therefore, the size of the list hand is actually constant. Hence, it is impossible to correctly calculate the time complexity of a code only by analyzing the code, as the problem description sometimes has a big hint to determine the time complexity.

3.2 Data Preprocessing

Data preprocessing is an important step in preparing datasets for analysis or machine learning tasks. In this process, we utilize *dead code elimination* and *comment removal*. Dead code elimination involves removing any code that does not contribute to the functionality or output of the program, thereby reducing unnecessary clutter. From each code, we marked irrelevant codes and unreachable codes as dead codes. Irrelevant code involves variables, functions, and classes that were never used or never called, and unreachable code involves conditional statements that cannot be satisfied and statements that cannot be reached because of control statements such as continue and return.

On the other hand, comment removal entails stripping out any comments within the codebase, which are meant for human understanding. We removed the comments since the fragments could be exploited by the models to improve the accuracy of predicting the time complexity of models.

3.3 Annotation Process

Our primary objective is to create a solid foundation for accurately classifying time complexities. To achieve this, we have meticulously designed a procedure to generate a robust dataset with minimal noise and high quality. We specifically filter 'correct' Java and Python codes, ensuring they pass all test cases, including hidden ones. These codes form the basis of our statistical population. Categorizing problems based on problem-solving strategies involves leveraging annotations from CodeContests.Each problem in the dataset is associated with a plausible problem-solving strategy, such as brute force, dynamic programming, or backtracking, as outlined in CodeContests. Following this initial categorization, a detailed analysis of each problem is conducted. This analysis considers input and output variables, utilized data structures, and the overall workflow of the code. Subsequently, the code for each problem is annotated based on its specific input characteristics. More precisely, we take the largest input variable as the main factor in calculating the overall time complexity. By analyzing the code, we consider each control sequence on the code to determine if the input impacts a control segment or is constant. Note that we assume a *unit-cost RAM model* that requires the same cost for accessing all memory locations for calculating the time complexity. Our core annotation process adheres to four key rules:

1. Consider the input size and the output size as parameters to determine time complexity, with measurement based on the largest parameter among the input variables.

2. Account the impact of used packages and libraries, such as hashmap, sorting, and string-matching algorithms, on time complexity.

3. Treating each test case within a single input separately for complexity measurement.

4. Classifying cases with fixed constants as having a constant time complexity.

The annotation was held by three annotators who have expertise in the algorithm. In the initial annotation step, each annotator annotated each problem independently. Each reasoned on how we judged the input and annotated the time complexity.

During the agreement process, the annotators collaborated closely to reconcile any discrepancies in their annotations. We engaged in thorough discussions, sharing our reasoning and insights to reach a consensus on the appropriate time complexity classification for each problem. In cases where disagreements arose, the annotators carefully evaluated the evidence and considered alternative perspectives before arriving at a mutually acceptable classification. The involvement of ChatGPT

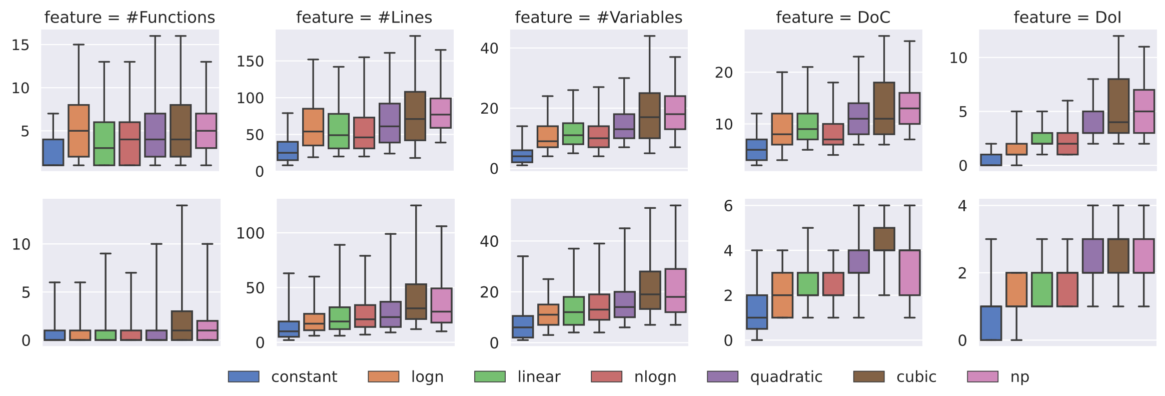


Figure 2: Statistics of CodeComplex dataset. The first and second lines are for Java and Python codes, respectively.

serves as a neutral advisor to validate the annotations and offer additional perspectives on complex cases. Through open communication and collaborative decision-making, the annotators ensure the accuracy and reliability of the final dataset. However, it is essential to note the significant impact of input formats and constraints on the actual time complexity of algorithmic problems. These constraints often lead to deviations from the ideal time complexity. Think of a scenario in which the input exploits the problem constraints in time complexity. Despite the problem of having a quadratic time complexity, the provided input constraints may result in linear running time. Moreover, determining the parameter for complexity measurement becomes crucial when faced with multiple input parameters. Additionally, certain code submissions optimize execution based on problem constraints, thus influencing code complexity assessment.

	TASTY	CODAIT	CoRCoD	CodeComplex
Provided # of Languages	2	1	1	2
Label Categories	7	6	5	6
Accessibility	X	X	O	O
Input-based Annotation	X	X	X	O

Table 2: Comparison between CodeComplex and other time complexity prediction datasets.

The CodeComplex dataset offers a meticulously curated collection of algorithmic problems and corresponding Java and Python code submissions. It serves as a foundation for accurately classifying time complexities and problem-solving strategies. Figure 2 demonstrates basic statistics of the codes for the number of lines, functions, variables, depth of code (DoC), and depth of iterations (DoI). Moreover, both Java and Python solutions displayed comparable characteristics when considering the depth of iterations, reflecting nested loops. However, a distinctive trait of Python code was its abundance of variables, potentially attributed to Python's lack of explicit variable declaration requirements. This inherent difference in variable declaration mechanisms might contribute to the observed discrepancy in variable counts between the two languages within our dataset. Table 2 summarizes the strengths of our dataset.

3.4 Dataset Overview

Various data We have collected the dataset to include multiple problems upon various algorithm categories. Each complexity class includes problems from dynamic programming, brute force, dynamic programming, divide and conquer, and much more. The dataset provides the problem tags from Codeforces, which the user can use to verify the algorithm categories. Also, we can see in Figure 2, that our dataset is not biased in the number of functions or variables for a given complexity class. The traditional models in Table 3 fail to verify the complexity class from these features, which further shows that the solution codes have an even distribution among the complexity classes.

Balanced complexity classes One of the significant strengths of our dataset is the careful balancing of complexity classes. Balanced classes prevent bias in the reasoning process of LLMs and enable more accurate and generalized model performance by providing a comprehensive learning experience across all possible scenarios. However, in Tables 1, the CoRCoD dataset exhibits imbalances among the classes. In contrast, our dataset provides balanced class data, ensuring an accurate and reliable prediction result of LLM models.

Open access In previous research on benchmarking the time complexity of code, it was observed that open data sources for code complexity prediction are notably scarce, with CoRCoD being one of the few available datasets. In contrast, our dataset is an open-source resource, providing an accessible and practical solution for researchers and practitioners in the field.

Fully human generated and annotated dataset The Codecomplex dataset is labeled manually by three human annotators and all final decisions and verifications are made by humans. Also, the source codes are collected from the codes before LLMs became present, which makes them free of machine-generated codes.

Thorough validation During the process of code complexity annotation, a thorough validation was conducted. Three annotators annotated using structured guidelines and cross-validated each other's annotations and the reasoning process. Also, we used ChatGPT as a failsafe precaution to validate the labels. If the response from ChatGPT disagrees, the annotators re-evaluated the code through edge case validation.

4 Experiments

As a preliminary study on code complexity prediction using a large-scale dataset, we conduct experiments with well-known machine learning-based solutions and LLMs. First, we try to replicate the result by Sikka et al. (2020) by employing traditional models such as decision tree (DT), random forest (RF), and support vector machine (SVM). Second, we use pre-trained programming language models (PLMs) such as CodeBERT (Feng et al., 2020), GraphCodeBERT (Guo et al., 2021), UniXcoder (Guo et al., 2022), PLBART (Ahmad et al., 2021), CodeT5 (Wang et al., 2021), and CodeT5+ (Wang et al., 2021). Note that we can further categorize these models into two groups where the first group (CodeBERT, GraphCodeBERT, and UniXcoder) only uses encoder architecture, and the second group (PLBART, CodeT5, and CodeT5+) exploits encoder-decoder architecture. Finally, we test the dataset on closed-source LLMs, ChatGPT3.5, ChatGPT4.0 (OpenAI, 2024), Gemini Pro (Google, 2024), and test open source LLMs Llama (Touvron et al., 2023), CodeGemma, Gemma1 and Gemma2 (Team et al., 2024), Mistral-Nemo (Jiang et al., 2023), Qwen2 and Qwen2.5 (Yang et al., 2024) from an instruction-tuned and a fine-tuned version of our dataset.

4.1 Experimental Settings

We divide the CodeComplex into training and test datasets by a 9 to 1 ratio for both Java and Python. As a result, the training and test datasets comprise 8,820 and 980 codes, respectively. Hyperparameters and methods to fine-tune each model can be found in section B.

4.2 Evaluation Metric

Hierarchy Complexity Score(HC-Score) To effectively evaluate the reasoning capabilities of LLMs on our dataset, we propose a novel metric called the Hierarchy Complexity Score (HC). Traditional accuracy metrics treat all incorrect answers equally. In contrast, the HC-Score is designed for tasks with a clear hierarchy, such as code time-complexity. It penalizes predictions in proportion to their hierarchical distance from the correct answer. The HC-Score is calculated with the following formula:

$$\text{HC}(P, R) = \frac{1}{N}\sum_{i=1}^{N}\left(1 - \frac{|p_i - r_i|}{\text{Number of class}}\right),$$

where N is the total number of samples, $P = p_1, \ldots, p_N$ is the set of model predictions, $R = r_1, \ldots, r_N$ is the set of correct answers (references), and $|p_i - r_i|$ is the hierarchical distance between a prediction and the correct answer. For example, think of a case of predicting a $O(n \log n)$ class as an $O(n)$ class. We would give a score of $6/7$ for this case, penalizing the 1 class near miss.

For more flexible evaluation, we can adapt this metric by introducing a "scoring window," which limits the penalty range. This Windowed HC-Score (HC_w) assigns a score of zero to predictions that fall outside a specified distance. Also, we can expand this metric by reducing the scoring window of a single class. The formula is:

$$\text{HC}_w(P, R) = \frac{1}{N}\sum_{i=1}^{N} max\left(0, 1 - \frac{|p_i - r_i|}{w}\right),$$

where w is the size of the scoring window. If the distance $|p_i - r_i|$ is greater than or equal to w, the score for that instance becomes 0. Predictions that closely approximate the correct result incur minimal penalties, while those with substantial errors are penalized more heavily. This nuanced scoring system aims to provide a more precise assessment of an LLM's reasoning abilities by accounting for the complexity of the tasks at hand. Our contribution is the introduction of this refined evaluation metric, which offers a discriminative and comprehensive tool for assessing model performance. The HC-Scored metric facilitates a deeper understanding of LLM capabilities, guiding further advancements in the development of sophisticated language models.

5 Results & Analysis

We present some selected interesting experimental results and analysis for various scenarios in the following Section. Full experimental results can be found in the Appendix C due to the lack of space.

5.1 Comparison of Java and Python

Java and Python are both popular programming languages, each with its unique features and characteristics that influence code structures and development practices. One key difference between Java and Python is the syntax typing. Java has to declare variables with their data types beforehand, but Python variables can be assigned without explicit type declarations.

Model	**Java**			**Python**		
	F1	HC	HC_2	F1	HC	HC_2
Decision Tree	44.4	82.3	56.1	37.3	79.9	50.9
Random Forest	41.9	80.0	51.9	40.0	80.3	52.6
SVM	24.3	71.9	39.1	17.2	66.8	36.0
CodeBERT	77.3	90.9	80.2	73.3	88.7	76.5
GraphCodeBERT	85.5	94.1	87.4	80.8	92.2	83.5
UniXcoder	**86.5**	**94.6**	**88.2**	**85.4**	**94.0**	**87.4**
PLBART	85.3	94.3	87.1	77.2	91.0	80.7
CodeT5	82.4	93.1	84.8	75.5	89.9	79.1
CodeT5+	85.8	**94.6**	88.0	78.2	91.0	81.2
Gemini Pro	29.7	80.1	48.6	33.4	80.2	51.8
ChatGPT 3.5	52.9	87.0	66.2	44.2	83.4	59.9
ChatGPT 4.0	60.6	90.0	72.7	52.7	87.2	67.4

Table 3: Performance comparison between Java and Python. Macro F1 score and HC scores are displayed.

UniXcoder was the best of the listed modes, and even the wrong answers lie in a similar class which is hard to distinguish. The HC scoring metric always boosts the score since it grants some score to wrong predictions. However, we can see by the HC score that LLMs are more affected than the traditional and program language models. Since LLMs try to reason parts of the codes and combine those results into a whole answer, LLMs tend to land closer to the correct answer if the parts are analyzed correctly.

5.2 Effect of Code Length

Intuitively, it is natural to assume that the shorter the code is, the easier it is to predict the complexity. To confirm our assumption, we categorize codes into four groups according to the number of tokens of the codes. If a code has less than or equal to 128 tokens, then the code falls into the first group (G1). If a code has more than 128 tokens and less than or equal to 256 tokens, then it falls into the second group (G2). The third group (G3) has codes with more than 256 tokens and less than or equal to 512 tokens. Lastly, group G4 has the longest codes, where each code has more than 512 tokens.

Figure 3 shows the experimental results on the four groups. It is easy to see that the experimental results confirm our assumption as the performance gets worse as the code becomes longer. We can see that the performance is quite similar in tendency except group G4. PLMs tend to have limits to their token size limiting their performance, however, the traditional methods rely on robust features of longer codes leading to better performance.

5.3 Experiments with LLMs

To predict the code time complexity, we use OpenAI's ChatGPT (version 3.5 and 4.0) and Google's Gemini-Pro for closed-source LLMs[2] and use the instruction-tuned versions of Gemma (9b and 27b), Llama3.1 (8B and 70B), Mistral-Nemo-2407 (12B), and Qwen2 (7B) for open-source LLMs. The prompt used for the experiments is given in Figure 5. The prompt specifies the role, the question on time complexity, the output format, and the answer choices. In summary of experimental results with LLMs, the biggest model, ChatGPT4.0 and Llama3.1 70B excel for both the base and fine-tuned versions. Also, we can see that ChatGPT4.0 has a high score on HC_2, which indicates that ChatGPT4.0 was able to infer the time complexity to a point, but failed in gathering information to conclude the correct complexity. We can see in Fig 4, LLMs sometimes fail on the final step of inference, which our HC scoring metric can capture. This is especially the case between Qwen2 and Qwen2.5, where Qwen2.5 is better on the F1 score but Qwen2 is better on the HC score. Our experiments show that ChatGPT4.0 indeed has the best inference capabilities. One thing to note is that some models, such as Gemma2 27B, are poor at analyzing time complexity. This was due to the instruction-tuned

[2]Accessed on 2024/2/12 for all closed-source LLMs

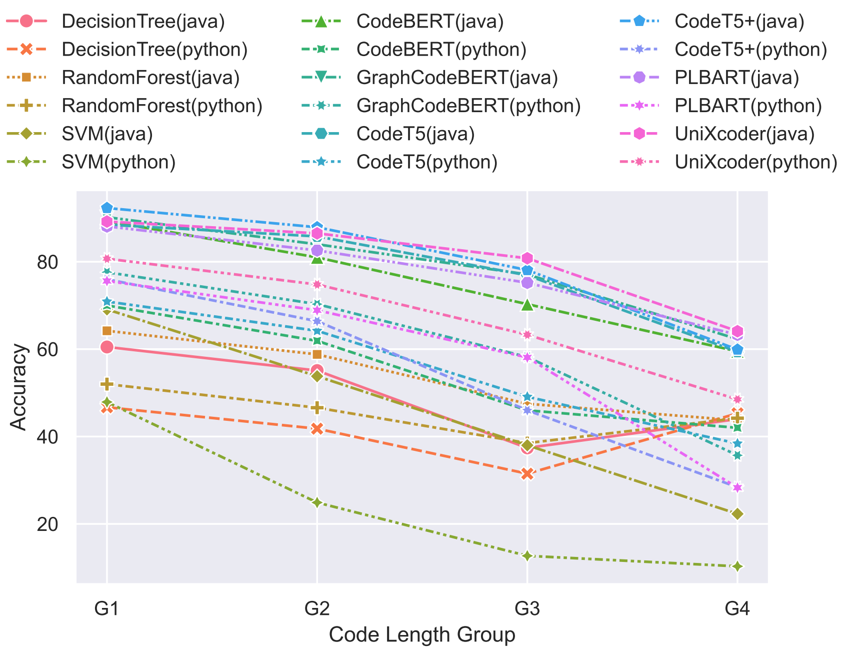


Figure 3: Classification performance of models for different length groups of codes.

LLM response example

"complexity": "linear", Here's why: the main logic of the code involves a binary search function, which has a time complexity of o(logn). However, the binary search is called only once, and the rest of the code runs in constant time. Therefore, the overall time complexity is dominated by the binary search, making it linear.

Figure 4: Wrong LLM response example.

	Method	Acc	F1	HC	HC_2	HC_3
	Gemini Pro	34.0	31.6	80.2	50.2	63.1
	ChatGPT 3.5	49.9	48.6	85.2	63.1	72.8
	ChatGPT 4.0	**56.9**	**56.7**	**88.6**	**70.1**	**78.4**
Inst	CodeGemma-7B	25.7	28.9	56.7	35.6	44.6
	Gemma2-9B	41.1	43.5	71.5	50.3	58.9
	Gemma2-27B	13.2	17.5	19.8	15.1	17.3
	Gemma1.1-7B	25.7	28.7	57.3	34.7	43.8
	Llama3.2-3B	22.9	22.8	60.6	33.1	43.4
	Llama3.1-8B	30.0	28.4	73.8	43.4	56.6
	Llama3.1-70B	**44.2**	43.8	**81.3**	**56.2**	**67.1**
	Mistral-12B	42.3	**44.3**	73.2	53.5	61.9
	Qwen2.5-7B	34.2	39.9	57.8	42.9	49.3
	Qwen2.5-14B	4.0	7.2	6.6	4.9	5.5
	Qwen2-7B	33.6	31.9	77.1	48.9	61.0
Fine-tuned	CodeGemma-7B	89.5	91.6	94.0	91.4	92.6
	Gemma2-9B	87.4	89.4	93.5	89.3	91.1
	Gemma2-27B	90.2	92.2	94.3	92.0	93.1
	Gemma1.1-7B	89.6	91.6	94.0	91.5	92.7
	Llama3.2-3B	88.2	89.4	94.9	91.1	92.8
	Llama3.1-8B	89.4	90.7	95.4	92.0	93.6
	Llama3.1-70B	**92.9**	**94.1**	**96.0**	**94.2**	**95.0**
	Mistral-12B	88.5	89.7	94.8	90.9	92.7
	Qwen2.5-7B	88.7	90.0	95.0	91.4	93.1
	Qwen2.5-14B	91.9	93.2	**96.0**	93.6	94.7
	Qwen2-7B	90.2	91.5	95.3	92.5	93.7

Table 4: Complexity prediction with accuracy, macro f1 score, and HC-Score for each LLM models

models failing to output a response when if it could not generate the desired output format. Gemma2 9B outputs the response ignoring the output format giving a better result than the 27B model. You can also see more results with smaller models in appendix C.

5.4 Qualitative Error Analysis

After investigating the common errors from extensive experiments with many baseline models, we find that the following problems are the root causes of most error cases.

Unused boilerplate codes Codes can include parts of codes that are irrelevant to the operation of the code. This can be because of coding habits or template codes for handy development. There are cases where the writer puts in ascii art in the comments. These methods add to the overall recognition load of understanding the codebase and can obscure the true flow of execution. Codes that include unused methods introduce noise, making it harder for models to recognize the overall structure.

Logarithmic loops The most common errors are from the logarithmic complexity class. Loops with logarithmic sizes, such as those found in binary search algorithms, can significantly affect the prediction of a code's time complexity. These loops have similar structures to normal linear loops, but inside the loop, they have additional variables or conditions that control the algorithm's flow. Unlike linear loops, this needs a thorough analysis of all contributing factors, ensuring a comprehensive understanding of the algorithm's performance characteristics. It seems like deep learning models lack the power to determine the contributing factors and figure out their meaning and impact.

Too much conciseness of Python Despite the famous zen of Python, it offers various ways to implement a loop such as classical for or while loop, list comprehension, and even lambda function. While the usage of list comprehension and lambda function makes Python codes much more concise and leads to statistics as in Figure 2, it also makes the complexity prediction task more challenging. The tendency is clearly seen especially when compared to Java in Table 3.

6 Conclusions

We have presented **CodeComplex**, the first large-scale, bilingual benchmark dataset designed to rigorously assess the reasoning abilities of LLMs in predicting the worst-case time complexity of programs. By providing a comprehensive and balanced collection of Java and Python codes, along with input-aware annotations and a novel Hierarchy Complexity Score (HC-Score), our work establishes a more nuanced foundation for evaluating model performance beyond simple accuracy. Our experiments with a wide range of models, from classical machine learning approaches to state-of-the-art LLMs, demonstrate that while current techniques show promise, a significant gap remains in achieving reliable performance for practical use cases, underscoring the need for continued research.

Looking ahead, we identify several key directions for future work to build upon this foundation. First, exploring more advanced prompting techniques is crucial. Leveraging methods like Chain-of-Thought prompting could elicit stronger zero-shot reasoning, moving models from pattern matching to more deliberate, step-by-step analysis. Second, to ensure models develop true algorithmic understanding, we propose conducting **code obfuscation tests**. Assessing performance on functionally identical but syntactically varied or intentionally complex code would test the robustness of models beyond familiar, memorized patterns. Third, the task itself can be evolved from classification to generation. Future work should investigate open-ended complexity generation, where models produce a symbolic expression (e.g., $O(n\sqrt{m})$) rather than selecting from a fixed set of classes. This would represent a far more sophisticated level of reasoning. Finally, the ability of models trained on CodeComplex to generalize is paramount. We suggest conducting transfer experiments by evaluating these models on other benchmarks, such as CoRCoD and problems from platforms like GeeksForGeeks, to measure out-of-domain performance gains and pave the way for more universally applicable code reasoners. Pursuing these directions will be essential in developing LLMs with the sophisticated and reliable inference capabilities required for the next generation of software development tools.

7 Limitations

Although this study offers insights into enhancing LLM reasoning abilities in complex tasks such as code time complexity prediction tasks, future research should address the following limitations. First, problem descriptions should be provided as part of the input for the completeness of the specification. As shown in examples in Section 3.1, it is necessary to consider problem specification to determine the intended time complexity of the problem, which will apply to most of the solution codes for the problem. Second, we need to deal with the unintended biases towards problem-specific information rather than implementation details learned due to the characteristics of our dataset. Finally, to fully address the inference capabilities of LLMs, we could use methods such as chain of thought prompting or tree of thought prompting to handle cases such as Fig 4 and give us more robust results.

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Note: the following appendices are in one-column format due to heavy code examples.

A Overview on CodeComplex Dataset

Our dataset construction process owes much to the recently released dataset called the CodeContests[3], a competitive programming dataset for machine learning by DeepMind. We constructed a dataset with the codes from the CodeContests dataset that are again sourced from the coding competition platform Codeforces. Our dataset contains 9,800 codes in seven complexity classes, where there are new 500 Java and Python source codes annotated with each complexity class. The seven complexity classes are constant ($O(1)$), linear ($O(n)$), quadratic ($O(n^2)$), cubic ($O(n^3)$), $O(\ln n)$, $O(n \ln n)$, and exponential. We also re-use 317 Java codes from CoRCoD as we confirmed that they also belong to the CodeContests dataset.

For constructing the dataset, we asked three human annotators who have more than five years of programming experience and algorithmic expertise to inspect the codes manually and classify them into one of the seven complexity classes. Once each human annotator reported the initial result, we collected the annotation results and inspected them once again by assigning the initial result to two different annotators other than the initial annotator. Finally, we have collected 9,800 complexity annotated codes of which there are 500 codes for each complexity class in both languages.

First, we selected several problems that are expected to belong to one of the considered complexity classes and submitted codes for the problems from Codeforces. The submitted codes contain both correct and incorrect solutions, and they are implemented in various programming languages such as C, C++, Java, and Python. We sorted out only the correct Java codes for our dataset construction.

In the second step, before delving into the time complexity of problems, we divide the problems by the problem-solving strategy such as sorting, DP (dynamic programming), divide-and-conquer, DFS (depth-first search), BFS (breadth-first search), A*, and so on. This is because it is helpful to know the type of problem-solving strategy used to solve the problem for human annotators to analyze the time complexity, and problems solved by the same strategy tend to have similar time complexity.

Third, we uniformly assign problems and correct codes for the problems to human annotators and let them carefully examine the problem-code pairs to label the time complexity of the codes.

Notice that there can be solutions with different time complexities for a problem depending on how to actually implement the solutions.

We, therefore, provide a specific guideline that contains instructions and precautions to annotators so that human annotators can assign correct and consistent labels to the assigned codes.

After the initial annotation process, we collect the results and assign them to different annotators to carefully cross-check the correctness of the initial annotation results. Primarily, we instruct the annotators again to carefully verify the results in accordance with the precautions provided in the annotation guideline.

A.1 Further Details on CodeComplex Dataset Construction

We gathered 128,000,000 submissions of Codeforces, where 4,086,507 codes are implemented in Java language. After discarding the incorrect codes (that do not pass all the test cases), there are 2,034,925 codes and 7,843 problems. Then the problems are split with their tags (e.g. sorting, dfs, greedy, etc) and given to the annotators with the guidelines in Section A.2. We were able to gather around 500 problems and 15,000 codes for the seven complexity classes.

As the complexity of codes for the same problem can vary depending on the implemented algorithms, it is obvious that the codes we inspect also have various complexity classes. However, we only target seven complexity classes that are the most frequently used complexity classes for algorithmic problems. Accordingly, there were some codes we inspected which belong to other complexity classes such as $O(n^5)$ or $O(\ln \ln n)$. We inspected around 800 problems and found out that the complexity classes of approximately 15 of the problems belong outside the chosen complexity classes. Although it is still possible that one might implement codes with complexity class that falls into the seven complexity classes, we simply rule out the problems from our dataset to ease the annotation process.

[3]https://github.com/deepmind/code_contests

During this process, we found out that many codes are not optimal for the given problem and some codes are too difficult to analyze due to their complex code structure. Moreover, there are many codes with a number of methods that are never used, mainly because the codes come from a coding competition platform and participants prefer just to include the methods that are frequently used in problem-solving regardless of the actual usage of the methods.

In the section below, we share the detailed guidelines provided to human annotators for a consistent and accurate annotation process.

A.2 Guideline of Production

Annotator Guideline

1. Check the variables that are described in the algorithm problems. Each algorithm implementation can have many variable instances and we only consider the variables that are given as inputs from the problems for calculating the time complexity.

* For convenience, we use n and m in the guideline to denote the input variable and $|n|$ and $|m|$ to denote the size of n and m.

2. Considering the input variable from the prior step, follow the below instructions for each input type and calculate the time complexity.

   (a) When only a number n is given as an input, calculate the time complexity proportional to n. Do the same thing when there are two or more variables. For instance, when only n is given as an input, the variable used to denote the time complexity of a code is n.

   (b) When a number n and m numeric instances are given as inputs, calculate the time complexity proportional to the one with higher complexity. For instance, when $m = n^2$, we compute the complexity of a code with m. If the implemented algorithm runs in $O(n^2) = O(m)$, it belongs to the linear complexity class.

   (c) If the input is given as constant values, the complexity of a given code also belongs to the constant class. For instance, if an algorithm problem states that exactly 3 numeric values are given as inputs, the solution code only uses the constant number of operations. Therefore, the code belongs to the constant class.

3. Consider the case where the code utilizes the input constraints of the problem. When the input is given by $n \leq a$, the code can use the fixed value a in the problem instead of using n. Mark these codes as unsuitable.

4. Consider the built-in library that the implemented algorithm is using (e.g. HashMap, sort, etc.) to calculate the time complexity of an entire code. For instance, given n numeric instances as inputs, when an implemented algorithm uses $O(n)$ iterations of built-in sort algorithm for n numeric instances, the time complexity for the algorithm is $O(n^2 \ln n)$.

5. When the code has unreachable codes, only consider the reachable code.

6. Mark the item that does not belong to any of the 7 complexity classes.

A.3 Statistics of CodeComplex

Table 5 shows basic statistics in numbers of our CodeComplex dataset. Each property is extracted using the abstract syntax tree of each language.

Property	$O(1)$		$O(n)$		$O(n^2)$		$O(n^3)$		$O(\ln n)$		$O(n \ln n)$		exponential		**Total**	
	Ja	Py	Ja	Py	Ja	Py	Ja	Py	Ja	Py	Ja	Py	Ja	Py	Ja	Py
#Problems	38	50	94	104	12	16	41	46	10	22	60	63	23	36	269	277
#Lines	31.7	19.7	60.9	29.3	72.7	36.6	82.3	48.3	66.0	22.2	59.4	30.7	85.6	43.6	64.5	31.9
#Functions	2.6	1.3	4.5	1.7	5.9	2.0	6.0	3.4	6.0	1.3	4.7	1.6	6.0	2.6	5.0	1.9
#Variables	5.3	9.7	12.2	15.5	15.2	18.6	19.4	24.3	11.2	12.3	11.6	16.0	19.4	24.5	13.2	16.7
DoC	5.7	1.5	10.2	2.5	12.2	3.4	13.6	4.2	9.4	2.3	8.5	2.6	14.2	3.5	10.4	2.8
DoI	0.6	0.5	2.7	1.0	4.0	1.0	5.5	1.0	1.8	0.8	2.4	0.9	5.6	0.9	3.1	0.9

Table 5: Statistics of codes from CodeComplex dataset. There are two values in each cell where the first value is about the Java codes and the second value is aboitemizeut the Python codes.

B Experiment Details for each Model

Hyperparameters For all pre-trained programming language models, we use the AdamW (Loshchilov and Hutter, 2019) optimizer with a warmup linear scheduler. The learning rate was set to 2e-6, epsilon to 1e-8, and the weight decay to 1e-2. We applied either the AutoTokenizer or the RobertaTokenizer. The models were fine-tuned for 15 epochs before using them for evaluation. For open-source LLMs, we used QLoRA and FSDP to train and test the models. We used a AdamW optimizer with a warmup linear scheduler. The learning rate was set to 2e-5, and used flash attention for training. The LoRA alpha and r values were both set to 16, with a dropout of 0.05. The quantization was set to 4 bits. We applied the basic AutoTokenizer and the basic chat template from the LLM model. Prompting was done in a similar manner to Fig 5, where it includes system messages to give a coding expert role if the LLM supports a system role. Otherwise, it is given as the header of the user message.

Prompt example

You are a world expert in investigating properties of a code that influences the time complexity.
The given code: "[code]"
Print "ONLY the time complexity in ONE WORD" of the given code in the answer from np, logn, quadratic, constant, cubic, linear and nlogn, do not print any other words in a json format.

Figure 5: LLM prompt examples used in our experiments.

C Full Experimental Results

C.1 Performance Per Complexity Class

We analyzed the results with responses that could be recognized as one of the seven classes. We can see in Table 6, Table 7 and Table 12, that the constant class and linear class are the most accurate among the classes. The direct correlation between the input size and the number of iterations makes these classes easy to analyze. However, models still face challenges in predicting the complexity of self-referential algorithms and control flows that are not in the main part of the algorithm, such as predicting between the $O(n \log n)$ class and $O(n^2)$ class. Failing to analyze loop controls leads to failing to differentiate the $O(n \log n)$ case from $O(n^2)$. This is well seen in the confusion matrix in Section E, where we can see many wrong predictions are between classes $O(n)$, $O(n \log n)$, and $O(n^2)$.

Method	$O(1)$	$O(\ln n)$	$O(n)$	$O(n \ln n)$	$O(n^2)$	$O(n^3)$	exponential	Micro	Macro
Decision Tree	64.4	55.9	15.2	65.2	68.8	32.9	34.4	48.6	48.1
Random Forest	66.2	57.7	28.2	68.6	60.2	36.0	62.6	43.9	54.2
SVM	49.7	40.0	65.1	42.7	74.6	23.5	18.0	28.1	44.8
CodeBERT	86.1	60.9	68.1	18.8	33.6	73.1	84.8	60.5	59.4
GraphCodeBERT	88.7	53.5	51.9	28.9	38.8	78.1	85.5	60.4	60.0
UniXCoder	83.1	54.8	54.1	15.9	33.9	76.9	88.1	57.7	56.6
PLBART	86.6	52.7	61.9	34.8	36.4	76.2	88.1	52.1	61.9
CodeT5	81.8	43.7	69.4	40.7	33.9	72.0	85.6	**60.7**	**60.3**
CodeT5+	90.7	50.8	64.2	14.1	27.0	74.9	86.8	58.0	56.1
ChatGPT 3.5	54.0	55.8	74.1	28.0	67.7	79.8	85.73	43.6	35.6
ChatGPT 4.0	64.2	43.4	70.9	72.8	56.2	67.2	42.2	54.8	45.7
Gemini Pro	33.2	15.4	59.4	7.1	72.4	8.1	19.4	30.1	21.4

Table 6: Complexity prediction accuracy of classification methods for each complexity class on Java.

Method	$O(1)$	$O(\ln n)$	$O(n)$	$O(n \ln n)$	$O(n^2)$	$O(n^3)$	exponential	Micro	Macro
Decision Tree	45.0	39.8	37.0	62.4	42.1	65.8	6.6	38.8	42.7
Random Forest	52.9	53.4	44.8	63.4	42.0	69.4	18.5	40.8	49.2
SVM	43.1	25.3	78.6	52.1	14.0	20.7	13.7	23.6	35.4
CodeBERT	68.0	66.1	31.7	46.9	40.6	63.8	25.6	51.2	49.2
GraphCodeBERT	68.5	56.9	61.9	51.4	56.8	68.1	34.8	**58.1**	**57.3**
UniXCoder	63.0	59.8	51.7	50.4	51.0	63.8	36.9	55.0	54.4
PLBART	72.1	62.3	51.9	46.3	48.5	59.3	24.2	54.0	52.4
CodeT5	68.9	47.1	44.5	41.4	43.6	51.8	38.3	48.9	48.4
CodeT5+	65.9	54.9	58.9	23.4	40.3	66.3	24.6	49.8	47.7
ChatGPT 3.5	44.4	46.4	83.0	12.3	60.6	29.8	19.6	41.8	35.6
ChatGPT 4.0	54.7	33.0	80.0	39.6	61.4	78.3	34.2	51.7	41.9
Gemini Pro	35.9	19.5	72.0	8.4	61.3	23.2	16.6	35.1	28.5

Table 7: Complexity prediction accuracy of classification methods for each complexity class on Python.

	Method	$O(1)$	$O(\ln n)$	$O(n)$	$O(n \ln n)$	$O(n^2)$	$O(n^3)$	exponential	Micro	Macro
Inst	CodeGemma-7B	85.9	85.5	76.5	72.6	83.5	86.8	90.2	25.7	24.4
	Gemma2-9B	86.7	91.5	78.5	84.8	81.9	87.0	82.6	41.1	36.1
	Gemma2-27B	81.0	90.7	84.8	84.2	85.8	86.9	90.3	13.2	13.6
	Gemma1.1-2B	79.9	89.2	74.3	84.1	60.1	86.9	61.8	12.8	9.1
	Gemma1.1-7B	83.7	90.6	76.9	76.1	82.1	85.6	80.7	25.7	23.3
	Llama3.1-8B	83.7	90.3	58.5	78.4	79.1	87.9	89.7	30.0	23.4
	Llama3.1-70B	87.3	90.4	69.7	75.5	86.1	90.0	92.2	**44.2**	**36.6**
	Llama3.2-1B	79.2	89.4	78.8	82.4	83.6	86.7	75.1	8.2	9.2
	Llama3.2-3B	84.4	89.5	78.4	82.9	56.7	87.0	82.2	22.9	17.8
	Mistral-12B	88.6	91.1	76.1	88.5	78.3	88.6	83.0	42.3	**36.6**
	Qwen2.5-1.5B	80.0	90.0	82.4	84.1	86.3	86.8	85.3	1.4	2.2
	Qwen2.5-7B	85.3	91.9	79.3	84.6	80.9	87.1	91.5	34.2	34.1
	Qwen2.5-14B	80.2	90.6	82.7	84.4	85.7	86.7	89.2	4.0	6.5
	Qwen2-7B	89.1	91.3	76.0	84.1	51.9	88.2	90.9	33.6	25.7
Fine-tuned	CodeGemma-7B	97.9	97.7	96.2	96.8	97.8	98.4	98.8	89.5	80.1
	Gemma2-9B	97.0	97.7	95.0	96.8	96.5	98.1	98.2	87.4	78.2
	Gemma2-27B	97.8	98.2	96.3	97.1	98.1	98.3	99.1	90.2	80.8
	Gemma1.1-2B	96.9	97.3	94.6	94.5	94.6	97.2	98.4	84.6	75.7
	Gemma1.1-7B	98.3	98.1	96.1	96.9	97.3	98.2	98.8	89.6	80.1
	Llama3.1-8B	98.1	98.4	95.1	96.1	96.8	98.5	98.6	89.4	79.4
	Llama3.1-70B	98.4	99.0	97.6	97.9	97.8	99.0	99.0	**92.9**	**82.4**
	Llama3.2-1B	96.4	97.6	91.4	94.5	95.1	97.9	97.9	83.9	74.8
	Llama3.2-3B	97.4	97.9	93.7	95.8	97.3	98.5	98.5	88.2	78.5
	Mistral-12B	97.6	98.3	93.7	96.1	96.9	98.6	98.7	88.5	78.8
	Qwen2.5-1.5B	98.2	97.9	94.8	95.3	96.5	98.6	98.7	88.6	78.7
	Qwen2.5-7B	98.3	98.2	94.8	95.3	96.3	98.9	98.7	88.7	78.9
	Qwen2.5-14B	98.5	98.2	96.6	97.8	97.9	99.1	98.7	91.9	81.5
	Qwen2-7B	98.1	98.0	95.4	96.3	98.1	98.7	98.7	90.2	80.1

Table 8: Complexity prediction accuracy of classification methods for each complexity class on open source LLMs.

Method	**G1**	**G2**	**G3**	**G4**	**G1**	**G2**	**G3**	**G4**
	Java				Python			
Decision Tree	57.2	45.6	40.0	38.2	57.2	45.6	40.0	38.2
Random Forest	62.3	46.8	40.6	26.4	62.3	46.8	40.6	26.4
SVM	48.9	18.1	18.1	16.6	48.9	18.1	18.1	16.6
CodeBERT	72.4	62.8	60.7	48.0	56.9	46.9	37.5	22.8
GraphCodeBERT	74.6	61.7	49.8	39.4	60.3	57.8	44.1	30.8
UniXCoder	58.6	54.4	43.2	31.2	58.6	54.4	43.2	31.2
PLBART	74.3	65.1	62.5	52.8	60.6	49.4	39.9	23.2
CodeT5	69.5	56.5	52.4	42.4	53.6	48.1	36.5	19.5
CodeT5+	72.8	63.5	53.0	44.4	56.4	42.4	30.7	29.8

Table 9: Prediction performance on different code length groups.

Model	**w/o Desc.**		**with Desc.**	
	Ja	Py	Ja	Py
ChatGPT 3.5	**43.38**	**43.14**	42.51	36.55
ChatGPT 4.0	55.42	51.57	**57.61**	**54.28**

Table 10: Complexity prediction performances of LLMs with and without a problem description in the prompt by the help of information retrieval.

C.2 Does Problem Description Help?

A critical aspect in accurately determining the worst-case time complexity of a given code is the comprehensive understanding of the problem specifications. In certain instances, these specifications may indicate that some inputs are constant, significantly influencing the complexity analysis. The absence of a full and detailed specification can lead to an incomplete or incorrect assessment of the worst-case time complexity.

Table 10 shows that problem descriptions actually help LLMs perform better as ChatGPT 4.0 is known to have real-time access to the information on the web. Note that the performance becomes worse for ChatGPT 3.5 when problem IDs are provided, as ChatGPT 3.5 does not utilize the problem descriptions, only from problem IDs.

C.3 Effect of Dead Code Elimination

Table 11 shows the effect of dead code elimination on prediction performance. Given the nature of codes submitted to competitive programming platforms, there are a lot of redundant variables, methods and even classes in the codes. Due to Java's complicated IO functions and limited built-in data structures, there are many codes related to the implementation of IO and data structures. Removing such fragments helps the models concentrate on the program structure and results in enhanced prediction accuracy. On the other hand, it appears that the dead code elimination does not help improve the performance on Python as the Python codes are already more concise than the Java codes due to its own language design principle.

Model	After		Before	
	Ja	Py	Ja	Py
Decision Tree	**48.6**	**38.8**	47.6	21.1
Random Forest	**43.9**	**40.8**	43.2	23.0
SVM	**28.1**	**23.6**	27.1	21.5
CodeBERT	**60.5**	51.2	59.7	**52.0**
GraphCodeBERT	**60.4**	58.1	57.8	**60.2**
UniXcoder	**57.7**	55.0	57.2	**55.3**
PLBART	**62.1**	54.0	61.2	**55.4**
CodeT5	**60.7**	48.9	60.2	**49.8**
CodeT5+	**58.0**	49.8	57.4	**50.0**
ChatGPT 3.5	**54.1**	45.4	53.8	**46.16**
ChatGPT 4.0	59.9	**53.7**	**59.7**	53.8
Gemini Pro	32.4	**35.1**	**34.0**	33.5

Table 11: Performance comparison before and after dead code processing.

D Failure Cases

```
public class mad {
    public static void main(String[] args) {
        Scanner sc = new Scanner(System.in);
        int cura = 0, curb = 0;
        int ver;
        System.out.println("? 0 0");
        System.out.flush();
        ver = sc.nextInt();
        for (int i = 29; i >= 0; i--) {
            System.out.println("? " + (cura + (1 << i)) + " " + curb);
            System.out.flush();
            int temp1 = sc.nextInt();
            System.out.println("? " + cura + " " + (curb + (1 << i)));
            System.out.flush();
            int temp2 = sc.nextInt();
            if (temp1 != temp2) {
                if (temp2 == 1) {
                    cura += (1 << i);
                    curb += (1 << i);
                }
            } else {
                if (ver == 1) cura += (1 << i);
                if (ver == -1) curb += (1 << i);
                ver = temp1;
            }
        }
        System.out.println("! " + cura + " " + curb);
    }
}
```

The following example exhibits a failure example where our model predicts $O(2^n)$ for a code with $O(\ln n)$ complexity. We suspect that the primary reason is the usage of bitwise operators. When we filter the codes that use any bitwise operator at least once from our CodeComplex dataset, about 56 of the codes belong to the class $O(2^n)$. We find that many implementations for exponential problems rely on bitwise operators as they can efficiently manage the backtracking process by manipulating bit-level flags.

The following example demonstrates the case when our model predicts constant time complexity $O(1)$ for a code that runs in $O(n)$ time. We suspect that our model may have ignored the existence of the check method which actually determines the $O(n)$ time complexity or considered the argument of check as constant.

Method		Acc	F1	HC	HC_2	HC_3
	Gemini Pro	34.0	31.6	80.2	50.2	63.1
	ChatGPT 3.5	49.9	48.6	85.2	63.1	72.8
	ChatGPT 4.0	**56.9**	**56.7**	**88.6**	**70.1**	**78.4**
Inst	CodeGemma-7B	25.7	28.9	56.7	35.6	44.6
Inst	Gemma2-9B	41.1	43.5	71.5	50.3	58.9
Inst	Gemma2-27B	13.2	17.5	19.8	15.1	17.3
Inst	Gemma1.1-2B	12.8	10.5	53.5	22.6	32.7
Inst	Gemma1.1-7B	25.7	28.7	57.3	34.7	43.8
Inst	Llama3.2-1B	8.2	11.1	24.4	12.0	15.9
Inst	Llama3.2-3B	22.9	22.8	60.6	33.1	43.4
Inst	Llama3.1-8B	30.0	28.4	73.8	43.4	56.6
Inst	Llama3.1-70B	**44.2**	43.8	**81.3**	**56.2**	**67.1**
Inst	Mistral-12B	42.3	**44.3**	73.2	53.5	61.9
Inst	Qwen2.5-1.5B	1.4	2.0	4.6	2.2	2.9
Inst	Qwen2.5-7B	34.2	39.9	57.8	42.9	49.3
Inst	Qwen2.5-14B	4.0	7.2	6.6	4.9	5.5
Inst	Qwen2-7B	33.6	31.9	77.1	48.9	61.0
Fine-tuned	CodeGemma-7B	89.5	91.6	94.0	91.4	92.6
Fine-tuned	Gemma2-9B	87.4	89.4	93.5	89.3	91.1
Fine-tuned	Gemma2-27B	90.2	92.2	94.3	92.0	93.1
Fine-tuned	Gemma1.1-2B	84.6	86.5	92.7	88.0	90.0
Fine-tuned	Gemma1.1-7B	89.6	91.6	94.0	91.5	92.7
Fine-tuned	Llama3.2-1B	83.9	85.2	93.2	87.1	89.8
Fine-tuned	Llama3.2-3B	88.2	89.4	94.9	91.1	92.8
Fine-tuned	Llama3.1-8B	89.4	90.7	95.4	92.0	93.6
Fine-tuned	Llama3.1-70B	**92.9**	**94.1**	**96.0**	**94.2**	**95.0**
Fine-tuned	Mistral-12B	88.5	89.7	94.8	90.9	92.7
Fine-tuned	Qwen2.5-1.5B	88.6	89.8	95.2	91.6	93.3
Fine-tuned	Qwen2.5-7B	88.7	90.0	95.0	91.4	93.1
Fine-tuned	Qwen2.5-14B	91.9	93.2	**96.0**	93.6	94.7
Fine-tuned	Qwen2-7B	90.2	91.5	95.3	92.5	93.7

Table 12: Complexity prediction with accuracy, macro f1 score, and HC-Score for each LLM models

```java
public class abc {
    public static int check(StringBuilder s) {
        int countRemove = 0;
        if (!s.toString().contains("xxx")) return countRemove;
        else {
            for (int i = 1; i < s.length() - 1; i++) {
                if (s.charAt(i - 1) == 'x' && s.charAt(i) == 'x' && s.charAt(i + 1) == 'x') {
                    countRemove++;
                }
            }
            return countRemove;
        }
    }

    public static void main(String[] args) {
        Scanner sc = new Scanner(System.in);
        int n = sc.nextInt();
        String s = sc.next();
        StringBuilder sb = new StringBuilder("");
        sb.append(s);
        System.out.println(check(sb));
    }
}
```

The following is the case where our model predicts the quadratic time complexity $O(n^2)$ when the ground-truth label is $O(n \ln n)$. We guess that our model simply translates the nested `for` loops into the quadratic time complexity. However, the outer loop is to repeat each test case and therefore should be ignored. Then, the $O(n \ln n)$ complexity can be determined by the `sort` function used right before the nested loops.

```
public class round111A {
    public static void main(String[] args) {
        Scanner sc = new Scanner(System.in);
        int n = sc.nextInt();
        int[] coins = new int[n];
        for (int i = 0; i < n; ++i) coins[i] = sc.nextInt();
        Arrays.sort(coins);
        int ans = (int) 1e9;
        for (int i = 1; i <= n; ++i) {
            int sum1 = 0;
            int c = 0;
            int j = n - 1;
            for (j = n - 1; j >= 0 && c < i; --j, ++c) {
                sum1 += coins[j];
            }
            int sum2 = 0;
            for (int k = 0; k <= j; ++k) sum2 += coins[k];
            if (sum1 > sum2) {
                System.out.println(i);
                return;
            }
        }
    }
}
```

The following is the case when our model is confused with exponential complexity $O(2^n)$ with quadratic complexity $O(n^2)$. The code actually runs in exponential time in the worst-case but our model simply returns quadratic time complexity as it does not take into account the recursive nature of the method `solve`.

```
public class D {
    static int n, KA, A;
    static int[] b;
    static int[] l;
    static double ans = 0;

    public static void main(String[] args) throws IOException {
        Scanner in = new Scanner(System.in);
        n = in.nextInt();
        KA = in.nextInt();
        A = in.nextInt();
        b = new int[n];
        l = new int[n];
        for (int i = 0; i < l.length; i++) {
            b[i] = in.nextInt();
            l[i] = in.nextInt();
        }
        dp = new double[n + 2][n + 2][n * 9999 + 2];
        go(0, KA);
        System.out.printf("%.6f\n", ans);
    }
    public static void go(int at, int k) {
        if (at == n) {
            ans = Math.max(ans, solve(0, 0, 0));
            return;
        }
        for (int i = 0; i <= k; i++) {
            if (l[at] + i * 10 <= 100) {
                l[at] += i * 10;
                go(at + 1, k - i);
                l[at] -= i * 10;
            }
        }
    }

    static double dp[][][];

    public static double solve(int at, int ok, int B) {
        if (at == n) {
            if (ok > n / 2) {
                return 1;
            } else {
                return (A * 1.0) / (A * 1.0 + B);
            }
        }
        double ret = ((l[at]) / 100.0) * solve(at + 1, ok + 1, B) + (1.0 - ((l[at]) / 100.0)) *
        ↪  solve(at + 1, ok, B + b[at]);
        return ret;
    }
}
```

The following is the case when our model predicts $O(\ln n)$ for a code with $O(n^2)$ complexity. It is easily seen that the `inversions` function determines the quadratic time complexity by the nested `for` loops. We suspect that somehow our model does not take into account the `inversions` function in the complexity prediction and instead focuses on the modulo () operator to draw the wrong conclusion that the complexity is in $O(\ln n)$.

```
public class maestro {
    public static long inversions(long[] arr) {
        long x = 0;
        int n = arr.length;
        for (int i = n - 2; i >= 0; i--) {
            for (int j = i + 1; j < n; j++) {
                if (arr[i] > arr[j]) {
                    x++;
                }
            }
        }
        return x;
    }

    public static void main(String[] args) {
        Scanner sc = new Scanner(System.in);
        int n = sc.nextInt();
        long[] arr = new long[n];
        for (int i = 0; i < n; i++) arr[i] = sc.nextLong();
        long m = sc.nextLong();
        long x = inversions(arr) % 2;
        for (int i = 0; i < m; i++) {
            int l = sc.nextInt() - 1;
            int r = sc.nextInt() - 1;
            if ((r - l + 1) % 4 > 1) x = (x + 1) % 2;
            if (x == 1) System.out.println("odd");
            else System.out.println("even");
        }
    }
}
```

E Confusion Matrices for Models

This appendix provides a detailed visualization of model performance through a series of confusion matrices, offering a granular view of classification accuracy and error patterns for each of the seven complexity classes. Each figure presents a side-by-side comparison of a model's prediction results on the Java (left) and Python (right) datasets. The figures illustrate the performance of various models, with Figure 6 showing results for CodeBERT, Figure 7 for GraphCodeBERT, Figure 8 for PLBART, Figure 9 for UniXcoder, and Figure 10 for CodeT5+. These matrices map the true complexity labels against the labels predicted by the models. A common pattern revealed across these figures is the models' tendency to confuse hierarchically adjacent classes, such as mistaking $O(n \log n)$ for $O(n)$ or $O(n^2)$. This is visually evident in the heatmaps where significant numbers of misclassifications cluster around the main diagonal, underscoring the subtleties of the prediction task.

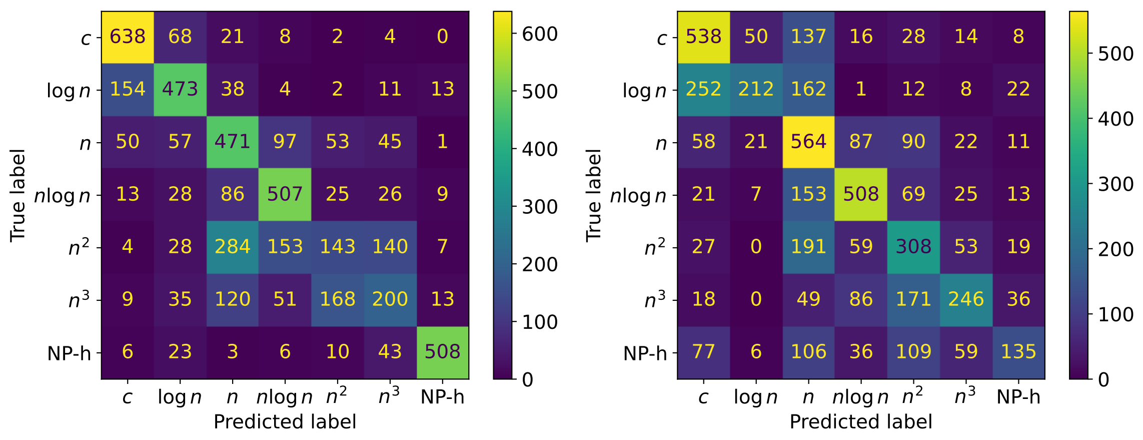

Figure 6: Confusion matrices of prediction results by CodeBERT on Java (left) and Python (right) datasets.

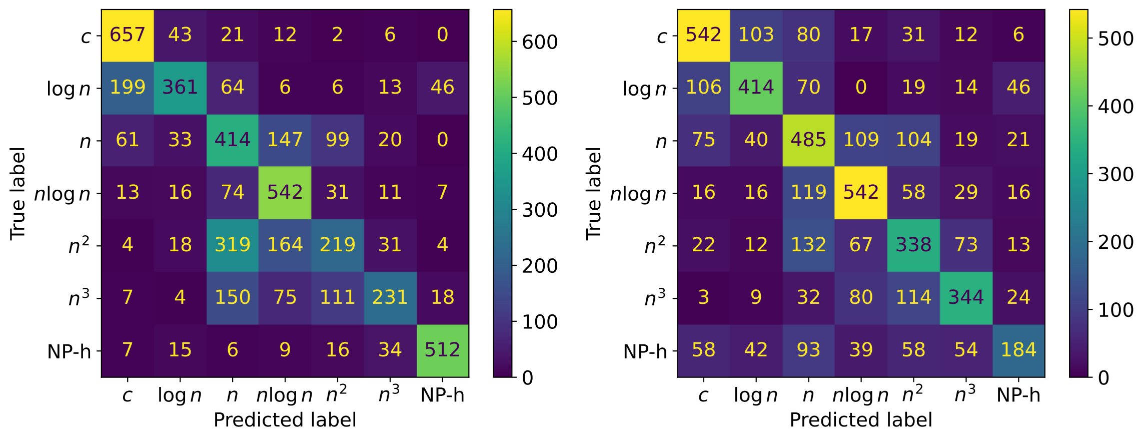

Figure 7: Confusion matrices of prediction results by GraphCodeBERT on Java (left) and Python (right) datasets.

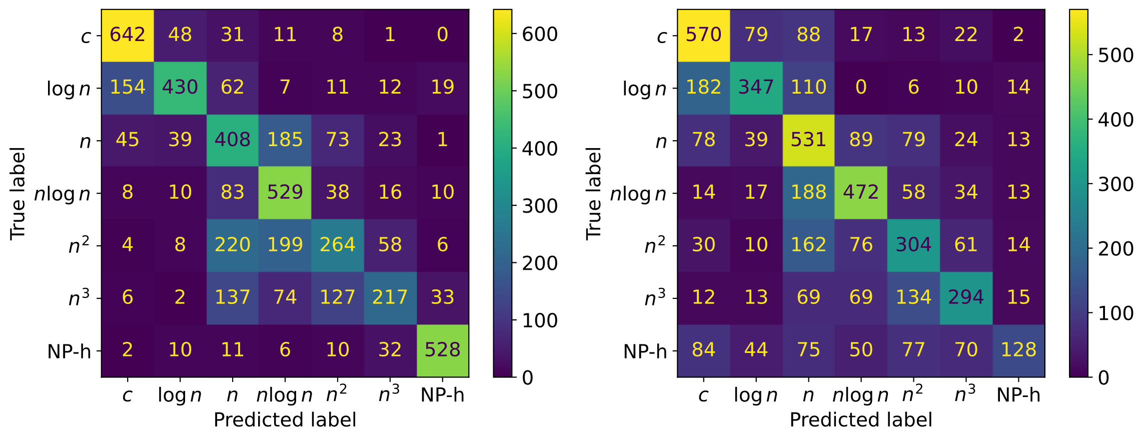

Figure 8: Confusion matrices of prediction results by PLBART on Java (left) and Python (right) datasets.

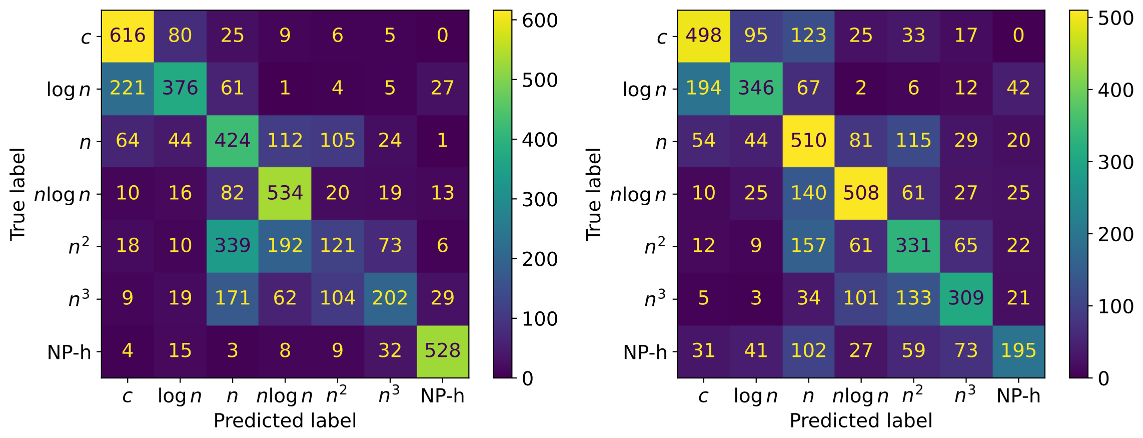

Figure 9: Confusion matrices of prediction results by UniXcoder on Java (left) and Python (right) datasets.

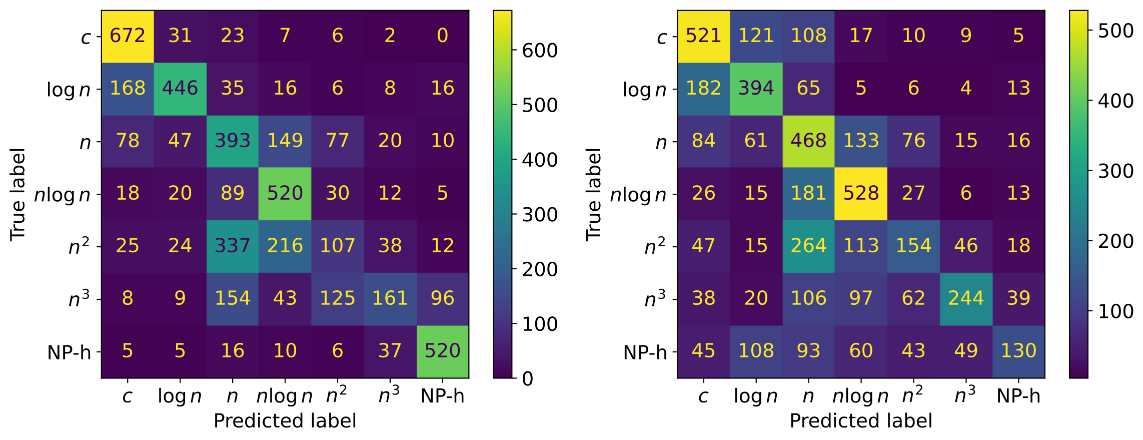

Figure 10: Confusion matrices of prediction results by CodeT5+ on Java (left) and Python (right) datasets.