Abstract

Over the past few years, deep learning (DL) has been continuously expanding its applications and becoming a driving force for large-scale source code analysis in the big code era. Distribution shift, where the test set follows a different distribution from the training set, has been a longstanding challenge for the reliable deployment of DL models due to the unexpected accuracy degradation. Although recent progress on distribution shift benchmarking has been made in domains such as computer vision and natural language process. Limited progress has been made on distribution shift analysis and benchmarking for source code tasks, on which there comes a strong demand due to both its volume and its important role in supporting the foundations of almost all industrial sectors. To fill this gap, this paper initiates to propose CodeS, a distribution shift benchmark dataset, for source code learning. Specifically, CodeS supports 2 programming languages (i.e., Java and Python) and 5 types of code distribution shifts (i.e., task, programmer, time-stamp, token, and concrete syntax tree (CST)). To the best of our knowledge, we are the first to define the code representation-based (token and CST) distribution shifts. In the experiments, we first evaluate the effectiveness of existing out-of-distribution (OOD) detectors and the reasonability of the distribution shift definitions, and then measure the model generalization of popular code learning models (e.g., the pre-trained language model, CodeBERT) on classification tasks using CodeS. The results demonstrate that 1) only softmax score-based OOD detectors perform well on CodeS, 2) distribution shift causes the accuracy degradation in all code classification models, 3) representation-based distribution shifts have a higher impact on the model than others, and 4) pre-trained models are more resistant to distribution shifts. We make CodeS publicly available, enabling follow-up research on the quality assessment of code learning models.

1 Introduction

Source code is the fundamental element of software, which has been the pillar to support almost all industrial sectors nowadays. The rapid advance of open source platforms (e.g., Github [1]), as well
as the large number of (both publically and industry internally) available software systems, bring challenges to traditional software analysis techniques, but offer new opportunities in understanding and reusing existing “big code” for software development by the data-driven approach. In particular, to enable the large volume of source code analysis, there comes a new trend in both software engineering and machine learning communities – machine learning for source code [2] in the last decade where deep neural networks (DNNs) have been widely employed for source code learning and achieved remarkable success in various tasks, e.g., code summarization [3], method naming [4], and source code classification [5].

In practice, the main activity of machine learning for source code remains at the stage of designing effective code representation techniques and model architectures, which are evaluated on the pure test data. Specifically, the most commonly used evaluation methodology of existing works is simply splitting a dataset into training, validation, and test sets and testing a model on the test set. In this way, the reported performance on the test set can only reflect the model performance on in-distribution data since the test set follows a similar distribution as the training set. However, with the rapid evolution of technology and software, new source code is programmed every day. Distribution shift often happens in the new data after the model has been deployed in the wild, which becomes a big challenge, and causes the model to produce unreliable predictions [6]. Here, distribution shift means that the test set follows a different data distribution from the training set. For example, in code learning models, compared to the training data, the new code data might be written by new developers (with different programming styles or habits) or collected from new projects using different techniques. Therefore, datasets with different types of distribution shifts are needed for the evaluation of code learning models.

Some recent progress has been made on building data distribution shift on domains like computer vision [7] and natural language processing [6] with data distribution shift has already gained considerable attention and multiple benchmarks have been constructed. For example, CIFAR-10-C [7] provides 15 types of algorithmically generated corruptions that generate data with different distributions from CIFAR-10. Wilds [6] collects natural datasets with distribution shifts including both image and text data in the wild. However, the study of data distribution shifts for the source code domain is still at a very early stage. Although some distribution shifts on source code [6, 8] are defined, they only considered rather simple scenarios, e.g., shifts from cross projects or time periods. The fine-grained and important features of source code data, for example, the frequency of represented token, are missed. Besides, existing datasets are not multi-language friendly because they only support one specific programming language such as only Java or Python. The above issues and challenges limit the use of these datasets and the generality of conclusions that were drawn.

In this paper, we introduce CodeS, a distribution shift benchmark dataset for source code learning. Overall, CodeS covers five types of code-level distribution shifts from two perspectives, natural distribution shift and representation-based distribution shift. For natural distribution shift, we introduce cross task shift, cross programmer shift, and time period shift. For representation-based distribution shift, we define token frequency shift and concrete syntax tree (CST) similarity shift. Specifically, to build the datasets of CodeS, we first collect three in-distribution sets: two are collected from existing code classification datasets (Java250 and Python800), and one is crawled from the AtCoder site [9] by ourselves. Afterward, for each set, we generate five versions of data shift as described above. Finally, CodeS contains 16 groups of in/out-of-distribution (ID/OOD) data with two programming languages, i.e., Java and Python.

Based on the constructed datasets, we conduct experiments to investigate 1) the effectiveness of existing OOD detectors in distinguishing ID and OOD source code data, 2) the rationality of the definitions of source code distribution shift, and 3) the generalization ability of existing source code models on classification tasks. For the rationality exploration, we employ existing OOD detectors to quantify the shift degree. Generally, the more different the two sets are, the easier the OOD detector can distinguish them. The experimental results demonstrated that only the simple softmax score-based OOD detector performs well on our dataset. The representation-based distribution shifts have higher impact on the performance of the models, where the token distribution shift brings the biggest accuracy degradation.

To summarize, the main contributions of this paper are:
Table 1: Comparison between our developed CodeS dataset and existing datasets.

| Programming Language | Task | Programmer | Time-stamp | Token | CST |
|-----------------------|------|------------|------------|-------|-----|
| Wilds [6]            | Python |✓          | ✓          | ✓     | ✓   |
| Li et al. [8]        | Java  | ✓          | ✓          | ✓     | ✓   |
| Nie et al. [10]      | Java  | ✓          | ✓          | ✓     | ✓   |
| CodeS                | Python, Java | ✓        | ✓          | ✓     | ✓   |

- We propose CodeS\(^1\), a benchmark dataset that provides fine-grained distribution shift datasets for source code learning. To the best of our knowledge, this is the first benchmark that covers two programming languages (Java and Python) and five types of distribution shifts.
- We perform a comprehensive evaluation of the effectiveness of existing OOD detectors and the rationality of the defined distribution shift.
- We performed an in-depth investigation on popular source code classification models using CodeS and demonstrated that code representation-based (token and CST) distribution shifts cause significant degradation in model performance.

2 Related Work

**Source code learning.** Since source code can be represented as text data (e.g., sequence of tokens) and structural data (e.g., data flow), deep neural networks have been employed for learning such representations to solve different tasks in recent years [2]. In which, source code classification is one of the widely studied tasks for code understanding, and many source code classification applications have been proposed. Alon et al. [4] proposed the very early work, Code2Vec, which aims at predicting the function name of a code snippet by learning the distributed code representations. Lu et al. [11] proposed a large-scale dataset CodeXGLUE for code understanding. It supports 2 code binary classification tasks that are related to the privacy and vulnerability of code, clone detection and defect detection. More recently, researchers from IBM [12] proposed CodeNet which contains source code solution classification tasks with multiple programming languages, e.g., Java and Python. Different from existing works that only consider clean datasets without data shift, we construct the dataset including both clean data and distribution shift data, which can be better used to measure the performance of trained models from a more practical perspective.

**Distribution shift in source code.** Some works have studied the distribution shift in source code data. Table 1 lists the overview of the comparison between existing datasets and CodeS. More detailed, Wilds, proposed by Koh et al. [6], is the first work that mentioned the data distribution shift problem for code completion in source code learning. Wilds first defined the cross-project distribution shift that the shift might come from the data biases of different code repositories. Besides, Li et al. [8] conducted an empirical study to investigate the prediction uncertainty of models under three types of distribution shifts, code collected from different projects, code written by different programmers, and code collected across different time periods. The authors found that the uncertainty metrics proposed in the computer vision domain are not fully applicable for source code tasks, e.g., code summarization and code completion. Moreover, in the latest work, Nie et al. [10] discussed that the trained models should be evaluated in different methodologies according to the real use cases in the code summarization task. For example, in the evolution scenario, the developers should consider if the model trained at time \(t_0\) can still be used at time \(t_1\) in the future, which can be another data distribution shift. Compared to the above works, CodeS provides datasets with more comprehensive and fine-grained distribution shifts, i.e., more programming languages and more diverse data shift. Furthermore, based on the benchmarks, we evaluate the rationality of our distribution shift definitions using OOD detectors.

\(^1\)The dataset is available at: https://github.com/testing-cs/CodeS.git
Data type: ID
Task: Contest-004-Task A: Tak and Hotels (ABC Edit)
Program:
```python
a, b, c = map(int, input().split())
if a % c == 0:
    print((b-a)//c+1)
else:
    print((b-(a//c+1)*c)//c+1)
```

Data type: OOD
Task: Contest-048-Task B: Between a and b
Program:
```python
N, K, X, Y = [int(input()) for i in range(4)]
fee = 0
for i in range(1, N+1):
    if (i <= K):
        fee += X
    else:
        fee += Y
print(fee)
```

Figure 1: An example of task distribution shift. Two programs target different tasks using Python.

Data type: ID
Programmer: penicillin0
Program:
```python
a, b, c = map(int, input().split())
print('YES') if b-a == c-b else print('NO')
```

Data type: OOD
Programmer: juppy
Program:
```python
a, b, c = map(int, input().split())
if b-a == c-b:
    print('YES')
else:
    print('NO')
```

Figure 2: An example of programmer distribution shift. Both users submit programs to AtCoder Beginner Contest: 058, Task A – A + l. Programming language: Python.

3 The CodeS Dataset

3.1 Examples of distribution shifts

We show two examples of code distribution shifts collected from the submissions on programming contest site, AtCoder [9]. Figure 1 shows the first distribution shift from the task difference. The two simple programs were submitted to two contests targeting different tasks. The ID program is to print Tak’s total accommodation fee, and the OOD one is to print the number of integers between a and b. Accordingly, if a model is trained on submissions of Contest 044 (Task A) and never sees the submissions of Contest 048, it is quite challenging in recognizing the unseen task. Such a task difference will produce the data distribution shift. Figure 2 presents an example where the distribution shift is from the programmer change. Concerning the programming habits, different programmers might solve the same task with different code styles. For instance, suppose the ID program has the if-else statement in one line, while the OOD uses the standard format where the conditions and actions are separated by new lines. Thus, the orders of tokens from these two programs are different which could introduce distribution shifts.

3.2 Dataset construction

CodeS contains three collections of data, Python75, Java250-S and Python800-S. Here, we introduce the distribution shift definitions and how we build each set accordingly.

**Distribution shift definition.** We design five types of distribution shifts for source code from two perspectives: natural distribution shift and representation-based distribution shift. Natural distribution shift comes from the common code style changes that the model could face every day, which includes the change of task, time period, and programmer. We utilize the submission tags (time, task, and user) as shown in Figure 3 (Appendix B) to divide data into ID and OOD sets. On the other hand, since source code is often transformed to different representations, such as the linear sequence of tokens and concrete syntax tree (CST) [13, 14], we also consider distribution shifts from the representation
aspect. Compared to the natural distribution shift, the representation-based shift is more fine-grained and can reflect the implicit difference in data features.

• Task distribution shift – ID data and OOD data target different tasks.
• Programmer distribution shift – ID data and OOD data target the same task but come from different programmers. As mentioned in Section 3.1, due to the programming habit, the distribution shift can happen across different programmers.
• Time distribution shift – ID code and OOD code target the same task but are written in different time periods. Assessing [15] and maintaining [16] the model performance over time is critical to ensure the reliability and security of models. This is because the code can be improved or new users appear over time.
• Token distribution shift – ID code and OOD code target the same task but the frequencies of tokens that appear to them are different. In source code learning, transforming code into numeral vectors is fundamental to make it executable for deep learning models [17]. A linear sequence of tokens is the typical and most important code representation, which is usually processed via tokenization, or lexical analysis. A token is the basic unit of the representation and can be a function name, an operator, or a punctuation sign. In practice, each token is represented by an integer to be compatible with models. Given token sequences of two source code files, the straightforward difference is the appearance of tokens.
• CST distribution shift – ID code and OOD code target the same task but have different CST representations. The concrete syntax tree (also known as the parse tree or derivation tree) is another popular code representation, which includes the syntactic structure of code files. The difference between code files can be represented by the distance between CSTs.

Raw data preparation. The raw data of Python75 is collected from the AtCoder site [9], where contests are continuously announced. Hence, there are many new submissions and new programmers in the contests. We selected the submissions from 75 tasks in 25 contests based on the following conditions: 1) the language should be Python3, and 2) the tasks have at least 1,000 submissions and 3) the status of the submission is accepted (AC). In total, we collected 200,462 programs for Python75. The detailed information of Python75 can be found in Appendix B. The raw data of Java250-S and Python800-S are from Java250 and Python800 provided by the Project CodeNet [13]. In total, Java250-S and Python800-S contain 75000 and 240000 programs.

Shift dataset creation. For each type of distribution shift, we create a dataset consisting of the training set, ID test set, and OOD test set extracted from the raw data. The training and ID test sets share the same data distribution and both contribute to training a model. The OOD test set is used to evaluate the generalization ability of the trained model. Table 2 shows the details of each dataset.

Table 2: Data information (number of classes, data size in each class) of each distribution shift dataset.

| Data collection | Programmer, Time, Token, CST | Task |
|-----------------|-------------------------------|------|
|                 | #Classes | #Training | #ID test | #OOD test | #ID Classes | #OOD classes | #Training | #ID test | #OOD test |
| Python75        | 75       | 732       | 134      | 134       | 65          | 10          | 846       | 154      | 1000      |
| Java250-S       | 250      | 180       | 60       | 60        | 200         | 50          | 225       | 75       | 300       |
| Python800-S     | 800      | 180       | 60       | 60        | 640         | 160         | 225       | 75       | 300       |

• Task distribution shift – We firstly randomly divide all tasks into the given number (#ID Classes and #OOD Classes in Table 2) of ID and OOD tasks. Next, in each ID task, we randomly select the number of #Training and #ID test code files as the training and ID test data, respectively. Finally, in each OOD task, a number of #OOD test code files are randomly selected as the OOD test data.
• Programmer distribution shift - We follow the strategy used by Li et al. [8] to prepare this type of data. Specifically, for each task, we first randomly select specific programmers and consider their submissions as the OOD test data, the submissions from other users (at least two submissions) are added into training and ID test sets.
• Time distribution shift - For each task, we sort the source code files according to the submission time and take the newest files as OOD test data2. The earlier code files are randomly split into the training and ID test sets, respectively.

2The time tag of Java250 and Python800 is unavailable, hence we do not create datasets with the time shift.
• Token distribution shift - For each task, we first build a density distribution of each token sequence based on the histogram (the bin number is equal to the total number of token types) [18]. Then we discriminate the tokens that are only used by some sequences but never used by the others, based on which the code files are divided into ID and OOD sets. The ID set is further randomly split into the training and ID test sets. In this paper, we use the publicly available tokenizer tool provided by Puri et al. [13] to generate the token representations. Examples can be found in Appendix C.

• CST distribution shift - For each task, we calculate the average distance between each file and the others by the Robinson-Foulds distance between two CSTs. The ones with greater distances are grouped into the OOD set, and the ones with smaller distances are grouped into the training and ID test sets. We use the parse tree generator provided by Puri et al. [13] to obtain the CST presentations. Examples can be found in Appendix C.

4 Experimental setup

We first investigate the performance of different OOD detectors. Then we explore the shift degree by different shift types based on OOD detectors and the model performance. Finally, we analyze the generalization ability of modes with different code representations on classification tasks when dealing with distribution shifts.

4.1 DNNs

We consider 5 DNNs with different code representations. CNN (Sequence) is a model with both max and average global pooling operations (doublePoolClassDNN). MLP (Bag) is a DNN with dense layers (denseDNN). Both CNN (Sequence) and MLP (Bag) are provided by the Project CodeNet [13]. Besides, we apply 3 Pre-trained models (RoBERTa, CodeBERT, and GraphCodeBERT) provided by the CodeXGLUE project [19] in our experiments. Each pre-trained model is fine-tuned using the training set. More detailed model information can be found in Appendix A.

4.2 Baseline

To investigate the effectiveness of different distribution shifts, we introduce the random manner to split data as a baseline. Namely, we randomly select a given number of samples for the training, ID test, and OOD test sets, respectively. The data size is the same as the programmer distribution shift as shown in Table 2. By default, this type of dataset has no distribution shift.

4.3 OOD detector

Four widely used OOD detectors are included, Maximum Softmax Probability (MSP) [20], Out-of-Distribution detector for neural networks (ODIN) [21], Mahalanobis [22], and Outlier Exposure (OE) [23]. The first three are simply softmax score-based given a pre-trained model, and the last one requires training a new neural network. A more detailed introduction can be found in Appendix D.

4.4 Evaluation measures

Accuracy is a basic performance measure of a given model, which measures the percentage of data being correctly classified. Given a pre-trained model, we measure its accuracy on the ID and OOD test sets, respectively. In general, a model will have greater accuracy on ID test data than on the OOD since its training data has the same distribution as the ID test set [6].

AUROC is short for the area under the receiver operating characteristics. This metric gives insights into how different the ID and OOD test sets are as well as the model’s ability to distinguish between ID and OOD data. An ideal OOD detector has the highest AUROC score of 100%.
5 Results Analysis

5.1 OOD detector analysis

Since the data with task distribution shift is real OOD data (these data are not in the classification target of the model), we can use ID/OOD data split based on task distribution shift and random split to evaluate the performance of OOD detectors. A high AUROC score obtained by the detector indicates that its discrimination ability is strong.

Table 3 shows the results. Concerning the random case, MSP, Mahalanobis, and OE detectors all have a score of around 50 regardless of the dataset. However, the ODIN detector achieves a much smaller (compared to 50) score (37.32) on Python800-S. Concerning the task distribution shift, MSP, Mahalanobis, and OE detectors perform better than the ODIN detector by giving higher scores. Particularly, ODIN outputs the lowest scores (less than 14) for Python800-S. The first conclusion we draw is that the ODIN detector performs the worst of all, which can not be used for our source code data. Furthermore, we found that the simplest MSP detector produces the best result where the difference between random and task distribution shift is larger than by the well-designed Mahalanobis and OE. For example, in Python800-S, MSP achieves 78.88 for the task distribution shift, while Mahalanobis and OE cannot well distinguish between ID and OOD sets by obtaining the AUROC score close to 50. These results show that it’s still challenging for source code OOD detection. Thus, the first application of CodeS is: researchers can use our dataset to design better OOD detectors for source code learning.

Table 3: AUROC scores by different OOD detectors. The ODIN and Mahalanobis detectors have a parameter of perturbation magnitude ($\epsilon$). Average means the average score of all parameter settings.

| OOD detector | $\epsilon$ | Python75 Random | Task | Java250-S Random | Task | Python800-S Random | Task |
|--------------|------------|------------------|------|------------------|------|--------------------|------|
| MSP          | 0          | 62.82            | 49.69 | 44.86            | 37.64 | 78.88              |      |
|              | 0.0005     | 62.83            | 49.69 | 44.85            | 37.63 | 78.88              |      |
|              | 0.001      | 62.83            | 49.69 | 44.85            | 37.63 | 78.88              |      |
|              | 0.0014     | 62.83            | 49.69 | 44.85            | 37.63 | 78.88              |      |
|              | 0.002      | 62.84            | 49.69 | 44.84            | 37.62 | 78.88              |      |
|              | 0.0024     | 62.84            | 49.69 | 44.84            | 37.62 | 78.88              |      |
|              | 0.005      | 62.86            | 49.70 | 44.81            | 37.59 | 78.88              |      |
|              | 0.01       | 62.90            | 49.71 | 44.76            | 37.55 | 78.88              |      |
|              | 0.05       | 63.50            | 49.85 | 44.30            | 37.20 | 78.88              |      |
|              | 0.1        | 64.55            | 50.00 | 43.61            | 36.73 | 78.88              |      |
|              | 0.2        | 67.20            | 50.27 | 41.87            | 35.73 | 78.88              |      |
|              | Average    | 63.46            | 49.79 | 44.40            | 37.32 | 78.88              |      |
| ODIN         | 0          | 51.78            | 49.58 | 49.55            | 51.21 |                    |      |
|              | 0.01       | 47.83            | 51.88 | 51.03            | 51.85 | 49.26              |      |
|              | 0.005      | 49.77            | 50.77 | 51.15            | 53.23 | 54.79              |      |
|              | 0.002      | 50.04            | 48.27 | 71.45            | 47.22 | 51.82              |      |
|              | 0.0014     | 49.07            | 52.25 | 70.78            | 48.55 | 53.14              |      |
|              | 0.001      | 47.32            | 49.95 | 71.80            | 47.41 | 51.82              |      |
|              | 0.0005     | 48.12            | 49.27 | 71.37            | 52.63 | 48.23              |      |
|              | Average    | 49.13            | 50.28 | 71.71            | 50.06 | 51.47              |      |
| Mahalanobis  | 0          | 51.83            | 49.58 | 49.55            | 51.21 |                    |      |
|              | 0.01       | 47.83            | 51.88 | 51.03            | 51.85 | 49.26              |      |
|              | 0.005      | 49.77            | 50.77 | 51.15            | 53.23 | 54.79              |      |
|              | 0.002      | 50.04            | 48.27 | 71.45            | 47.22 | 51.82              |      |
|              | 0.0014     | 49.07            | 52.25 | 70.78            | 48.55 | 53.14              |      |
|              | 0.001      | 47.32            | 49.95 | 71.80            | 47.41 | 51.82              |      |
|              | 0.0005     | 48.12            | 49.27 | 71.37            | 52.63 | 48.23              |      |
|              | Average    | 49.13            | 50.28 | 71.71            | 50.06 | 51.47              |      |
| OE           | 49.64      | 61.11            | 48.12 | 52.67            | 50.00 | 50.45              |      |

5.2 Shift degree

To explore the reasonability of our distribution shift definitions, we check the shift degree caused by each definition. Generally, task distribution shift should be the upper bound since it produces real OOD data with new classes. Table 4 shows the AUROC score and model accuracy on different distribution shifts. Concerning the model accuracy, regardless of the dataset, all types of distribution shifts (except for random splitting) cause performance degradation. This is consistent with the general finding that the distribution shift causes a performance drop [6].

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[6] Reference to a cited source about distribution shift's impact on performance.
Table 4: AUROC score and accuracy on different distribution shift. DNN: CNN (sequence). The accuracy improvement ↑ and degradation ↓ on the OOD test set are also listed. Average: average score of 4 OOD detectors. ODIN: $\epsilon = 0.0014$, $T = 1000$. Mahalanobis: $\epsilon = 0.0014$.

| Shift type | MSP  | ODIN | Mahalanobis | OE | Average | ID test | OOD test |
|------------|------|------|-------------|----|---------|---------|----------|
| Python75   |      |      |             |    |         |         |          |
| Random     | 50.16| 62.83| 49.07       | 49.64| 52.93   | 96.91   | 97.01 ($0.10 \uparrow$) |
| Task       | 91.33| 61.42| 70.54       | 61.11| 71.10   | 96.95   | -        |
| Programmer | 48.20| 83.23| 50.21       | 48.33| 57.49   | 96.53   | 96.47 ($0.06 \uparrow$) |
| Time       | 57.90| 76.80| 50.00       | 50.22| 58.73   | 97.51   | 92.64 ($4.87 \downarrow$) |
| Token      | 82.82| 71.16| 56.70       | 52.61| 65.82   | 97.50   | 61.04 ($36.46 \downarrow$) |
| CST        | 77.89| 70.43| 57.84       | 57.84| 66.00   | 96.98   | 71.17 ($25.81 \downarrow$) |

| Java250-S  |      |      |             |    |         |         |          |
| Random     | 50.06| 49.69| 52.25       | 48.12| 50.03   | 84.23   | 84.43 ($0.20 \uparrow$) |
| Task       | 80.99| 44.85| 70.78       | 52.67| 62.32   | 87.89   | -        |
| Programmer | 53.72| 49.36| 46.33       | 49.22| 49.66   | 85.86   | 82.84 ($3.02 \downarrow$) |
| Token      | 68.65| 52.28| 49.47       | 52.63| 55.76   | 89.01   | 65.85 ($23.16 \downarrow$) |
| CST        | 60.32| 41.85| 50.98       | 51.53| 51.17   | 86.69   | 75.91 ($10.78 \downarrow$) |

| Python800-S |      |      |             |    |         |         |          |
| Random      | 49.67| 37.63| 48.55       | 50.00| 46.46   | 77.91   | 78.40 ($0.49 \uparrow$) |
| Task        | 78.88| 13.13| 53.14       | 50.45| 48.90   | 82.50   | -        |
| Programmer  | 58.10| 46.34| 54.30       | 62.45| 55.30   | 72.22   | 66.94 ($10.28 \downarrow$) |
| Token       | 64.47| 39.24| 50.52       | 50.00| 51.06   | 79.27   | 53.83 ($25.44 \downarrow$) |
| CST         | 49.74| 48.02| 48.26       | 50.00| 49.01   | 77.94   | 77.82 ($0.12 \downarrow$) |

Table 5: Average AUROC score and accuracy change over Python75, Java250-S, and Python800-S of different shift types. ↑ and ↓ indicate an accuracy improvement and degradation on the OOD test set, respectively.

| Shift type | MSP  | ODIN | Mahalanobis | OE | Average | Accuracy change (%) |
|------------|------|------|-------------|----|---------|---------------------|
| Python75   |      |      |             |    |         |         |
| Random     | 49.96| 50.05| 49.96       | 49.25| 49.81   | 0.26 ($\uparrow$) |
| Task       | 83.73| 39.80| 64.82       | 54.74| 60.77   | 6.07 ($\downarrow$) |
| Programmer | 53.34| 59.64| 50.28       | 53.33| 54.15   | -4.45 ($\downarrow$) |
| Time       | 57.90| 76.80| 50.00       | 50.22| 58.73   | -4.87 ($\downarrow$) |
| Token      | 71.98| 54.23| 52.23       | 51.75| 57.55   | -28.35 ($\downarrow$) |
| CST        | 62.65| 53.43| 52.36       | 53.12| 55.39   | -12.24 ($\downarrow$) |

On the other hand, concerning the AUROC scores, first, we can see that only MSP can produce scores with the same trend as the accuracy degradation. That means the greater the MSP score, the more drastic the accuracy decline. This finding future demonstrates that MSP is the best OOD detector among our considered ones. Then, we check the score of each definition. The results show that compared with the real OOD task distribution shift, all the other definitions have smaller scores, except the score produced by ODIN. This is reasonable since the model has some learned information on these data. Additionally, Table 5 shows the average AUROC score and accuracy change over Python75, Java250-S, and Python800-S. On average, the code representation-based (Token and CST) distribution shifts cause greater performance degradation than the natural distribution shifts (Programmer and Time) except for the task-based. More specifically, the token distribution shift affects the model accuracy the most. The average AUROC score also indicates the representation-based shifts are stronger than the natural ones. In conclusion, these results demonstrate that, in CodeS, the natural distribution shifts only introduce negligible data bias, while the new proposed representation-based distribution shifts are more challenging.

5.3 Model generalization analysis

Finally, we utilize CodeS to test the generalization ability of different models. Table 6 shows the accuracy of five models on the ID and OOD test sets. Regardless of the dataset and model, the accuracy of the randomly split ID and OOD test sets are similar (the greatest difference is 1.03% in Java250, MLP (Bag)). By comparing each model, we observe that the three pre-trained language models (RoBERTa, CodeBERT, and GraphCodeBERT) are more robust against the distribution shift.
than CNN (Sequence) and MLP (Bag). For example, in Python800-S with token distribution shift, all the pre-trained models can achieve more than 88% accuracy on the OOD test set while CNN (Sequence) and MLP (Bag) only achieve by up to 53.43% accuracy. This indicates that pretraining with diverse programming languages is helpful for producing models with better generalization ability on distribution shifted datasets. For instance, CodeBERT is pre-trained on natural language-programming language pairs in 6 programming languages (Python, Java, JavaScript, PHP, Ruby, and Go). In addition, by the accuracy drop on the OOD test sets, we can draw the same conclusion as the shift degree study – representation-based distribution shifts are more challenging. The second usage of CodeS is: CodeS opens the challenge for future improving the generalization of source code learning models.

Table 6: Model accuracy (%) on ID and OOD test sets given different DNNs and distribution shifts. The accuracy improvement ↑ and degradation ↓ on the OOD test set are also listed.

| Model          | Random Programming Time Token CST | Python75 | Java250-S | Python800-S |
|----------------|----------------------------------|----------|-----------|-------------|
|                | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test |
| CNN (Sequence) | 96.91   | 97.01 (0.11) | 98.35   | 96.47 (0.08) | 97.31   | 92.64 (14.81) | 97.50   | 61.04 (38.46) | 98.08   | 71.17 (23.81) |
| MLP (Bag)      | 92.22   | 92.07 (0.15) | 92.93   | 91.80 (1.13) | 92.35   | 88.13 (4.22) | 94.13   | 45.28 (48.85) | 93.53   | 63.45 (30.08) |
| RoBERTa        | 98.31   | 98.13 (0.18) | 98.35   | 98.46 (0.01) | 97.92   | 99.29 (1.36) | 98.28   | 95.02 (3.26) | 99.47   | 86.65 (12.82) |
| CodeBERT       | 98.37   | 98.29 (0.08) | 98.30   | 98.53 (0.23) | 98.06   | 99.44 (1.38) | 98.51   | 96.92 (1.59) | 99.52   | 87.04 (12.48) |
| GraphCodeBERT  | 98.49   | 98.34 (0.15) | 98.40   | 98.63 (0.23) | 98.11   | 99.52 (1.41) | 98.50   | 96.37 (2.13) | 99.52   | 87.17 (12.35) |

| Model          | Random Programming Time Token CST | Python75 | Java250-S | Python800-S |
|----------------|----------------------------------|----------|-----------|-------------|
|                | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test |
| CNN (Sequence) | 84.25   | 84.43 (0.2) | 85.86   | 82.84 (1.04) | -       | -       | 87.01   | 65.85 (23.16) | 86.69   | 75.91 (10.78) |
| MLP (Bag)      | 70.58   | 71.61 (0.03) | 72.40   | 71.59 (0.81) | -       | -       | 76.31   | 35.32 (40.99) | 76.03   | 50.86 (25.17) |
| RoBERTa        | 94.87   | 95.26 (0.39) | 95.53   | 95.04 (0.49) | -       | -       | 96.55   | 87.43 (9.12) | 96.79   | 87.47 (9.32) |
| CodeBERT       | 95.67   | 96.10 (0.43) | 96.29   | 96.25 (0.04) | -       | -       | 96.92   | 89.27 (7.65) | 97.41   | 88.63 (7.8)  |
| GraphCodeBERT  | 96.02   | 96.34 (0.32) | 96.56   | 96.51 (0.05) | -       | -       | 97.29   | 89.89 (7.4)  | 97.82   | 89.31 (8.51) |

| Model          | Random Programming Time Token CST | Python75 | Java250-S | Python800-S |
|----------------|----------------------------------|----------|-----------|-------------|
|                | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test | ID test | OOD test |
| CNN (Sequence) | 77.91   | 78.40 (0.49) | 77.25   | 66.94 (10.29) | -       | -       | 79.27   | 53.83 (25.44) | 77.94   | 77.82 (0.12) |
| MLP (Bag)      | 66.90   | 67.00 (0.10) | 67.29   | 63.39 (3.90) | -       | -       | 71.37   | 34.47 (36.90) | 66.39   | 67.77 (13.87) |
| RoBERTa        | 96.09   | 96.38 (0.29) | 95.73   | 96.15 (0.42) | -       | -       | 97.04   | 88.51 (8.53) | 95.72   | 97.31 (1.59) |
| CodeBERT       | 96.48   | 96.74 (0.26) | 96.19   | 96.99 (0.80) | -       | -       | 97.44   | 89.91 (7.53) | 96.19   | 97.77 (1.58) |
| GraphCodeBERT  | 96.69   | 96.89 (0.20) | 96.26   | 97.24 (0.98) | -       | -       | 96.19   | 97.77 (1.58) | 96.42   | 97.98 (1.56) |

6 Limitations

The effect of each distribution shift is tested on 3 datasets, which is the main limitation. Especially, Java250-S and Python800-S are built on a smaller size of raw data than Python75. However, we believe the conclusions will remain the same when using larger datasets. For example, Table 3 shows that the shift degree by the task distribution shift on Java250-S and Python800-S is smaller than on Python75. If the raw data size of Java250-S and Python800-S is larger, the difference in data features (e.g., programmers, code representations) will increases. Accordingly, the shift effect will be greater.

7 Conclusion

This paper proposed CodeS, the first distribution shift benchmark dataset that supports two programming languages and both natural and representation-based distribution shifts. We evaluated the effectiveness of existing OOD detectors, the shift degree introduced by different shift types, and the generalization ability of famous code classification models based on CodeS. We found that the well-designed OOD detectors cannot be generalized to code data and representation-based distribution shifts are more challenging than natural distribution shifts. CodeS provides the stage for future study of source code learning, including OOD detection, model robustness enhancement, and more.

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Organization of the supplementary material. Section A presents the details of our artifacts. Section B introduces the information of the raw data of Python75. In Section C, we give examples of the data splitting based Token and CST-based distribution shift. Section D introduces the definitions and parameters of our used OOD detectors. Section E and Section F present our experiment details (computing resources) and additional results.

A Artifacts

All our artifacts (datasets, models, and OOD detectors) are released under an MIT license and archived on GitHub: https://github.com/testing-cs/CodeS.git

Datasets & Docs The online resource includes our crawled raw data from AtCoder, the original datasets of Java250 and Python800 downloaded from the Project CodeNet [13] and data descriptions. We also release the corresponding datasets (source code files and tokens) with distribution shifts of Python75, Java250, and Python800. The token representations are generated using the tokenizer tool\(^3\) provided by Puri et al. [13].

Model training/fine-tuning CNN (Sequence) and MLP (Bag) are trained using the implementation\(^4\) by Project CodeNet with the same parameters (e.g., random seed, dropout rate). The training set and ID test are involved in the training procedure for training and validation, respectively. The epoch number is set to 100. All the trained CNNs are released on GitHub. Pre-trained models are fine-tuned using the implementation\(^5\) with the same parameters.

OOD detectors & Code We modify the original implementations of the ODIN\(^6\) and Mahalanobis\(^7\), detectors to fit for the TensorFlow framework. The OE detectors have the same DNN architectures and we take the loss function from the original implementation\(^8\). The implementations of MSP, ODIN, Mahalanobis, and all the OE detectors are released on GitHub.

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\(^3\)https://github.com/IBM/Project_CodeNet/tree/main/tools/tokenizer
\(^4\)https://github.com/IBM/Project_CodeNet
\(^5\)https://github.com/microsoft/CodeXGLUE/tree/main/Code-Code/Defect-detection
\(^6\)https://github.com/facebookresearch/odin
\(^7\)https://github.com/pokaxpoka/deep_Mahalanobis_detector
\(^8\)https://github.com/hendrycks/outlier-exposure
B Raw data from AtCoder

Figure 3 shows a screenshot of the submissions to AtCoder Beginner Contest 044. The task distribution shift, time distribution shift and programmer distribution shift are prepared based on the tags "Task", "Submission Time", and "User". Table 7 shows the details of crawled data (the raw data of Python75) from AtCoder.

| Contest ID | Tasks | Data sizes | Contest ID | Tasks | Data sizes |
|------------|-------|------------|------------|-------|------------|
| 044        | A, B  | 2579, 2683  | 057        | A, B, C| 3207, 2691, 3543 |
| 045        | A, B, C| 3130, 2740, 2104 | 058 | A, B, C| 2708, 2981, 2002 |
| 046        | A      | 3149, 3354  | 059        | A, B, C| 2722, 2900, 1304 |
| 047        | A, B, C| 3026, 2738, 2130 | 060 | A, B, C| 2865, 3358, 1557 |
| 048        | A, B, C| 3288, 3235, 1716 | 061 | A, B, C, D| 2874, 2992, 2444, 1043 |
| 049        | A, B, C| 3119, 2727, 3716 | 062 | A      | 2535, 2547 |
| 050        | A, B, C| 2991, 2768, 1270 | 063 | A, B, C| 2825, 2983, 2277 |
| 051        | A, B, C| 3711, 5071, 2195 | 064 | A, B, C, D| 3781, 2546, 2679, 1580 |
| 052        | A, B, C| 2920, 2908, 1395 | 065 | A, B, C, D| 2472, 3438, 2016, 1017 |
| 053        | A, B, C| 2877, 3426, 1370 | 066 | A, B, C| 2806, 2944, 2287 |
| 054        | A, B, C| 2811, 2389, 2899 | 067 | A, B, C| 2516, 2950, 2079 |
| 055        | A, B, C| 3092, 3837, 1446 | 068 | A, B, C| 2651, 4076, 2438 |
| 056        | A, B, C| 2795, 2167, 2056 | 069 | A, B, C| 2795, 2167, 2056 |
|           |       | **In total** | 75          |       | **200462** |

C Examples of Token and CST splitting

Here, in addition to Section 3.2 in the main paper, we present more splitting information about the token and CST distribution shifts. Figure 4 shows examples of the splitting by the frequency of tokens based on the density distribution. By comparison, the ID and OOD codes have very different token distributions. Figures 5 - 8 show the CST representations of 4 submissions. The distance between the first two and last two are 121 and 90, respectively.

D OOD detector

Here, we introduce the definitions of our used OOD detectors in the experiments. Let $f$ be a $N$-class classifier and $(x, y)$ be an sample with its true label $y$. Given $x$, $f$ predicts a label $\hat{y} = \text{arg max} \{ S_i(x), 1 \leq i \leq N \}$ which indicates that $x$ is most likely to belong to the $\hat{y}$ class. Here, $S_i(x)$ is the softmax output computed by:

$$
S_i(x) = \frac{\exp f_i(x)}{\sum_{j=1}^{N} \exp f_j(x)}
$$

(1)
Figure 4: Density distribution of ID and OOD code tokens. Each subfigure corresponds to token representations of two code files in a given task (caption of the subfigure). $x$–axis: ID code tokens. $y$–axis: OOD code tokens. First row: Python75. Second row: Java250-S. Last row: Python800-S.

$f_i(x)$ is the raw prediction (also named as logits in the literature) of $x$ belonging to the $i$th class predicted by $f$. In [21], $S_y = \max_i \{S_i(x), 1 \leq i \leq N\}$ is also named as the maximum softmax probability and softmax score. $\{S_i(x), 1 \leq i \leq N\}$ is the softmax distribution of $x$ generated by $f$.

- **MSP** The Maximum Softmax Probability is a baseline method proposed by Hendrycks and Gimpel [20] to detect wrongly classified and OOD samples. The intuition behind MSP is that a model tends to be rather confident (have a high softmax score) on correctly classified data. In concrete, given the softmax distribution of a model’s prediction on a test sample, MSP identifies the data as ID if the softmax score is greater than a threshold and vice versa.

- **ODIN** Similar to MSP, the Out-of-Distribution detector for Neural networks proposed by Liang et al. [21] also takes advantage of the softmax distribution. It points out that by adding slight perturbations to samples, the gap of softmax score between wrongly and correctly classified samples becomes larger. Compared to MSP that directly uses the original data to obtain the softmax score, ODIN first preprocesses the data by adding a perturbation $\epsilon$ and then scales the softmax output (Equation (1)) by:

$$S_i(x) = \frac{\exp f_i(x)/T}{\sum_{j=1}^{N} \exp f_j(x)/T}$$ (2)
Figure 5: CST representation of submission 1.
Figure 6: CST representation of submission 2.
Figure 7: CST representation of submission 3.
where $T$ is the temperature scaling parameter. Following the original implementation\(^9\), we use different perturbation magnitudes ($\epsilon = 0, 0.0005, 0.001, 0.0014, 0.002, 0.0024, 0.005, 0.01, 0.05, 0.1, 0.2$) and set $T = 1000$.

- **Mahalanobis**  
  Lee et al. \([22]\) proposed the Mahalanobis detector that learns a Gaussian distribution for each class. Then the detector calculates a confidence score for a test sample by measuring the Mahalanobis distance between the sample and the closest class-conditional Gaussian distribution. The test data is ID if its confidence score is greater than a threshold and vice versa. Similar to ODIN, this detector also preprocesses the test samples with a perturbation $\epsilon$. Following the original implementation\(^9\), we use different perturbation magnitudes ($\epsilon = 0, 0.0005, 0.001, 0.0014, 0.002, 0.0024, 0.005, 0.01, 0.05, 0.1, 0.2$).

- **OE**  
  Different from the above three detectors, Hendrycks et al. \([23]\) proposed to train a neural network named Outlier Exposure to detect OOD data by using available ID and OOD data. Remarkably, the OOD data for training is not necessarily to include the distribution of test OOD data, which makes the OE detector more practical to generalize to unseen distributions.

### E Experiment details

**Computing infrastructure**  
All CNN (Sequence) and MLP (Bag) relevant experiments were conducted on a 3.00 GHz Intel Xeon Gold 5217 CPU with two RTX 8000 GPUs. The implementation was based on the Tensorflow 2.5.1 framework. All pre-trained language model-based experiments were performed on a high-performance computer cluster consisting of Dell C4140, 6 GPU nodes x 4 Nvidia V100 SXM2 32GB. We implemented the related experiments based on the PyTorch 1.6.0 framework.

**F Additional results**

In addition to Table 4 in the main paper, we present Table 8 and Table 9 to show the AUROC scores of ODIN and Mahalanobis, respectively, with different parameter settings. Recall that ODIN includes the perturbation magnitude $\epsilon$ and temperature $T$. Mahalanobis only includes $\epsilon$.

Table 8 lists the AUROC scores measured by ODIN with different perturbation magnitudes. We also conducted experiments using different temperatures $T = 1, 10, 100, 1000$ and got the same results, hence, the results are not listed here. In general, changing the perturbation magnitude gives the same conclusion compared to Table 4 in the main paper. Additionally, using a different magnitude may result in a very different AUROC score. For example, in Python75, the scores on the token distribution shift are 77.39 and 71.12, respectively, when using $\epsilon = 0.2$ and $\epsilon = 71.12$.

Table 9 lists the AUROC scores measured by the Mahalanobis detector with different perturbation magnitudes. Compared to Table 8, the result varies more than the ODIN detector and the standard deviation ranges from 0.77 to 4.35. For example, in Python75, the AUROC scores are 78.28 and 69.20 when using $\epsilon = 0.001$ and $\epsilon = 0.005$, respectively. However, in most cases, we can still draw the conclusion that the task difference introduces the greatest distribution shift to the dataset.

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\(\text{https://github.com/facebookresearch/odin}\)  
\(\text{https://github.com/pokaxpoka/deep_Mahalanobis_detector}\)
Table 8: AUROC results by the ODIN detector with different perturbation magnitudes ($\epsilon$). The highlighted column $\epsilon = 0.0014$ is the same as Table 4 in the main paper. $T = 1000$. Min: minimum. Max: maximum. Std: standard deviation.

| Shift type | Magnitude | Statistics |
|------------|-----------|------------|
|            | 0 | 0.0005 | 0.001 | 0.0014 | 0.002 | 0.005 | Min | Max | Average | Std |
| Python75   | Random | 49.69 | 49.70 | 49.85 | 50.00 | 50.27 | 49.69 | 50.27 | 49.79 | 0.19 |
|            | Task | 44.86 | 44.84 | 44.84 | 44.81 | 44.76 | 44.30 | 43.61 | 41.87 | 44.40 | 0.92 |
|            | User | 49.38 | 49.36 | 49.35 | 49.32 | 49.25 | 48.71 | 48.12 | 47.17 | 49.38 | 0.98 |
|            | Token | 52.32 | 52.26 | 52.25 | 52.19 | 52.06 | 51.06 | 49.92 | 47.91 | 49.71 | 0.25 |
|            | CST | 41.90 | 41.85 | 41.83 | 41.72 | 41.54 | 40.11 | 38.38 | 35.33 | 35.33 | 0.16 |
| Java250    | Random | 37.64 | 37.62 | 37.59 | 37.55 | 37.20 | 36.73 | 35.73 | 35.73 | 37.64 | 0.60 |
|            | Task | 13.12 | 13.13 | 13.13 | 13.14 | 13.16 | 13.19 | 13.43 | 13.63 | 13.74 | 0.23 |
|            | User | 46.34 | 46.34 | 46.34 | 46.34 | 46.34 | 46.34 | 46.34 | 46.22 | 45.92 | 0.13 |
|            | Token | 39.23 | 39.24 | 39.24 | 39.25 | 39.27 | 39.35 | 39.30 | 38.74 | 38.74 | 0.16 |
|            | CST | 48.04 | 48.01 | 47.95 | 47.86 | 47.16 | 46.38 | 45.12 | 45.12 | 48.04 | 0.95 |

Table 9: AUROC results by the Mahalanobis detector with different perturbation magnitudes ($\epsilon$). The highlighted column $\epsilon = 0.0014$ is the same as Table 4. DNN: CNN (sequence). Min: minimum. Max: maximum. Std: standard deviation.

| Shift type | Magnitude | Statistics |
|------------|-----------|------------|
|            | 0 | 0.01 | 0.005 | 0.002 | 0.0014 | 0.001 | 0.0005 | Min | Max | Average | Std |
| Python75   | Random | 51.78 | 47.83 | 49.77 | 50.04 | 49.07 | 47.32 | 48.12 | 47.32 | 51.78 | 49.13 | 1.54 |
|            | Task | 71.31 | 75.82 | 69.20 | 76.16 | 70.54 | 78.28 | 72.04 | 69.20 | 78.28 | 73.34 | 3.40 |
|            | User | 54.31 | 50.21 | 48.92 | 49.56 | 50.21 | 45.85 | 40.40 | 40.40 | 54.31 | 48.49 | 4.35 |
|            | Time | 54.88 | 53.18 | 52.83 | 49.79 | 50.00 | 48.65 | 48.33 | 48.33 | 54.88 | 51.10 | 2.52 |
|            | Token | 59.91 | 59.63 | 55.89 | 52.08 | 56.70 | 56.06 | 54.59 | 52.08 | 59.91 | 56.41 | 2.74 |
|            | CST | 58.28 | 59.32 | 63.24 | 56.92 | 57.84 | 61.38 | 59.89 | 56.92 | 63.24 | 59.55 | 2.18 |
| Java250    | Random | 49.58 | 51.88 | 50.77 | 48.27 | 52.25 | 49.95 | 49.27 | 48.27 | 52.25 | 50.28 | 1.43 |
|            | Task | 72.36 | 73.03 | 71.15 | 74.45 | 70.78 | 71.80 | 71.37 | 70.78 | 73.03 | 71.71 | 0.77 |
|            | User | 51.65 | 50.40 | 51.06 | 50.96 | 46.33 | 50.05 | 48.23 | 46.33 | 51.65 | 49.81 | 1.88 |
|            | Token | 48.40 | 52.66 | 48.28 | 48.01 | 49.47 | 50.57 | 48.02 | 48.01 | 52.66 | 49.35 | 1.74 |
|            | CST | 46.88 | 51.03 | 50.17 | 47.88 | 50.98 | 51.64 | 47.66 | 46.88 | 51.64 | 49.46 | 1.93 |

| Python800  | Random | 49.55 | 51.85 | 53.23 | 47.22 | 48.55 | 47.41 | 52.63 | 47.22 | 53.23 | 50.06 | 2.50 |
|            | Task | 51.21 | 49.26 | 51.82 | 51.34 | 51.82 | 48.23 | 54.79 | 51.47 | 51.47 | 2.22 |
|            | User | 50.09 | 53.81 | 56.32 | 55.45 | 54.30 | 53.55 | 54.43 | 50.09 | 56.32 | 53.99 | 1.97 |
|            | Token | 47.04 | 55.76 | 50.18 | 46.91 | 50.52 | 48.40 | 48.23 | 46.91 | 55.76 | 49.58 | 3.06 |
|            | CST | 49.91 | 50.12 | 52.17 | 47.95 | 48.26 | 51.45 | 50.82 | 47.95 | 52.17 | 50.10 | 1.56 |