Explainable AI for Pre-Trained Code Models: 
What Do They Learn? When They Do Not Work? 

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Abstract In recent years, there has been a wide interest in designing deep neural network-based models that automate downstream software engineering tasks, such as program document generation, code search, and program repair. Although the main objective of these studies is to improve the effectiveness of the downstream task, many studies only attempt to employ the next best neural network model, without a proper in-depth analysis of why a particular solution works or does not, on particular tasks or scenarios. In this paper, using an eXplainable AI (XAI) method (attention mechanism), we study state-of-the-art Transformer-based models (CodeBERT and GraphCodeBERT) on a set of software engineering downstream tasks: code document generation (CDG), code refinement (CR), and code translation (CT). We first evaluate the validity of the attention mechanism on each particular task. Then, through quantitative and qualitative studies, we identify what CodeBERT and GraphCodeBERT learn (put the highest attention on, in terms of source code token types), on these tasks. Finally, we show some of the common patterns when the model does not work as expected (perform poorly while the problem in hand is easy) and suggest recommendations that may alleviate the observed challenges.

Keywords Explainable AI (XAI) · Interpretable machine learning · Attention · Transformer · CodeBERT · GraphCodeBERT

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1 Introduction

Pre-trained code models are proposed to analyze the big corpora of source code and natural languages collected from open-source platforms (e.g., GitHub and StackOverflow). Such pre-trained code models have been used to automate various software engineering tasks, e.g., code understanding, code generation, code clone detection (Shobha et al., 2021), defect detection (Pornprasit et al., 2021a; Humphreys and Dam, 2019), and code summarization (LeClair et al., 2020). Automating such software engineering tasks has been shown to greatly improve software developers’ productivity and reduce the costs of software development.

Recent studies proposed Transformer-based pre-trained code models, e.g., CodeBERT (Feng et al., 2020), GraphCodeBERT (Guo et al., 2020), CodeGPT (Lu et al., 2021), CodeT5 (Wang et al., 2021). However, most of these studies often focus on improving its accuracy—without considering its explainability aspect. Thus, when deploying such models in practice, practitioners still do not know why such models provide a given recommendation or suggestion.

Let’s consider a given Python code snippet of a bubble sort algorithm. A code summarization model may be able to correctly summarize that the given code snippet is a bubble sort algorithm. However, developers may not trust the models if the models correctly generate the natural text based on indentation, white spaces, or parenthesis of the Python code snippet, instead of the meaningful semantic information (i.e., bubble sort). Thus, the correct predictions generated by the models do not guarantee that the models are learned correctly. Therefore, a lack of explainability of the large and complex pre-trained code models could lead to a lack of adoption in practice.

In this paper, we conduct an empirical study to analyze the pre-trained code models through the lens of Explainable AI. Particularly, we focus on the two state-of-the-art pre-trained code models, i.e., CodeBERT and GraphCodeBERT with the three understanding & generation-specific downstream tasks, i.e., Code Summarization (Code→Text), Code Transformation (Code→Code), and Code Translation (Code→Code) tasks. To explain the predictions of these models, we leverage an attention mechanism inside the Transformer architecture, which is an intrinsic Explainable AI approach. The attention mechanism allows us to understand what are the most important tokens in the input sequence that contribute the most to the tokens in the output sequences. In particular, we aim to address the following three research questions:

(RQ1) Is the attention mechanism suitable to explain the pre-trained code models?

Results. The results show that in a notable proportion of the outputs generated by the models, the chosen token already exists in the input and it has a high attention score. As the average “normalized attention rank” of the chosen token in the last layers of the model is less than 3%, 4%, and 13% for code translation, code refinement,
and code document generation, respectively. We conclude that the attention mechanism has a considerable weight in the model’s decision making and hence, it can be a good suitable tool to explain it.

(RQ2) **What do the pre-trained code models learn?**

**Results.** Analyzing attention scores and their distribution over different token types shows that the models learn to focus on specific types of tokens for each downstream task. In CDG, the models learn to focus on the methods signatures (i.e., method name and input arguments). While in CT, syntax, that is tokens related to the programming language, attract more attention. CR has a middle ground compared to the other two tasks and has a more balanced distribution of attention. Also, it is shown that GraphCodeBERT pays more attention to the structural parts of the source code, rather than CodeBERT, which likely is the result of the additional step of GraphCodeBERT for parsing the code and leveraging the code’s data flow. These observations are inline with what is expected from a code model which led us to conclude that the two studied models are indeed learning (in most cases) what they are supposed to.

(RQ3) **When do the pre-trained code models not work?**

**Results.** Our finding shows that there are certain situations that cause the models to perform poorly across different tasks. For instance, the models don’t work well with samples having long or complex source code and/or long expected answers (model outputs). We also showed that poor performance of the model is usually projected in its attention distribution. In other words, whenever the model fails to achieve a good output for a model, it also has failed to pay enough attention to the corresponding token types for the respective downstream task. We have also provided some recommendations on how to potentially alleviate these weaknesses in the paper.

These findings lead us to conclude that even though pre-trained models have shown great results on software engineering tasks; none of them can be considered a closed problem and there are certain aspects of these models that need more focus through further studies. Explaining these models can shed light on their weaknesses and provide directions for future research.

**Contributions.** Contributions of this paper are as follows:

- We empirically study the suitability of the attention mechanism as an XAI method to explain Transformer-based models.
- Analyzing the attention scores, we found interesting insights into models’ decision-making for different tasks.
- We provide explanations on several scenarios, where CodeBERT and GraphCodeBERT under-perform.
- We offer some actionable recommendations on how to improve the models, in the future, to potentially alleviate the observed weaknesses.
Open Science. To foster the open science initiative, we made the replication package publicly-available at GitHub.\footnote{https://github.com/Ahmad535353/XAI-for-transformer-models}

**Paper Organization.** In the rest of this paper, in Section 2, we briefly introduce the background and related work on Transformer-based code models and XAI in software engineering. In Section 3, we provide motivating examples about some observed weaknesses in code models that could use some explanation. Section 4 explains our research method by going through the objectives and design details and finally Section 5 demonstrates and discusses the results of our experiments and Section 6 explains the possible limitations of this work that may get improved in the future works and finally Section 7 concludes the paper.

## 2 Background & Related Work

In this section, we present background knowledge and related work on the Transformer-based Pre-trained code models and Explainable AI in software engineering.

### 2.1 Transformer-based Pre-Trained Code Models

*Pre-training.* Pre-trained code models are deep learning models (such as transformers) which are trained on a large dataset (e.g., GitHub and StackOverflow) to perform specific source code understanding and generation tasks. Pre-trained code models (aka. language models of code) are normally trained in a self-supervision fashion using various model architectures (e.g., BERT) with various learning techniques. For example, Masked Language Modeling (MLM) and Next Sentence Prediction (NSP). When the pre-trained code models are trained on a large corpus, it allows them to learn the universal representations of source code and natural languages specific to programming. The development of such pre-trained code models is very beneficial for various downstream tasks, thus avoiding training a new code model from scratch, and making the code models more reusable.

Recently researchers developed pre-trained code models using various types of Transformer architecture (e.g., CodeBERT, GraphCodeBERT, CodeGPT, and CodeT5). CodeBERT (Feng et al., 2020) is a pre-trained code model that is trained on a BERT architecture (i.e., Bidirectional Encoder Representations from Transformers) (Devlin et al., 2018). It is trained on MLM and NSP tasks using NL-PL pairs in 6 programming languages (Python, Java, JavaScript, PHP, Ruby, Go).

GraphCodeBERT is similar to CodeBERT, but it considers the structure of the code by utilizing its data flow as well for pre-training. It uses MLM, Edge Prediction and Node Alignment as pre-training tasks. CodeGPT is another Transformer-based model but it’s pre-trained only on a programming language...
with tasks similar to GPT-2 [Radford et al., 2019] CodeT5 is also a pre-trained encoder-decoder model which utilizes token-type information written in code. It is pre-trained on Masked Span Prediction (MSP), identifier tagging, Masked Identifier Prediction (MIP), and bimodal dual generation which are designed to help the model understand token type information.

**Fine-tuning.** The existing pre-trained code models have been used for various downstream software engineering tasks, which can be categorized into four types: (1) Text→Text (e.g., language translation of code documentation [Lu et al., 2021], query reformulation [Cao et al., 2021]); (2) Text→Code (e.g., code search [Gu et al., 2018; Nguyen et al., 2016]); (3) Code→Text (e.g., code summarization [Haque et al., 2020], commit message generation [Jiang et al., 2017; Liu et al., 2018]); and (4) Code→Code (e.g., automated program repair [Jiang et al., 2021; Li et al., 2020; Chen et al., 2019], programming language translation [Roziere et al., 2020], code completion [Svyatkovskiy et al., 2020]).

Below, we provide the definition of the three selected downstream tasks.

**Code Summarization** (Code→Text) is an NLP task designed to generate natural language comments for a given source code, which could help developers to better understand codes in software projects with wrong or missing comments and decrease the extra time that should be spent on reading the source code. For example, given a Python method ("def sum(x,y): ..."), the NLP model will generate natural language comments as ("This is a summation function").

Currently, Transformer-based models proved to be state-of-the-art due to their capability at considering long dependencies for longer texts and source codes [Li et al., 2022].

**Code Refinement** (Code→Code) is an NLP task designed to generate refined source code (e.g., a fixed version) for a given source code (e.g., a buggy version). Code refinement has been widely studied in the context of code review [Tufano et al., 2022; Thongtanunam et al., 2022; Liu et al., 2022], helping developers automatically receive refined code that is likely to be approved without waiting for reviewers' feedback.

**Code Translation** (Code→Code) is an NLP task designed to generate source code in one language (e.g., Java) for a given source code in another language (e.g., C#).

### 2.2 Explainable AI for Software Engineering (XAI4SE)

Explainability is now becoming a critical concern in software engineering. Many researchers often employed AI/ML techniques for defect prediction, malware detection, and effort estimation. While these AI/ML techniques can greatly improve developers’ productivity, software quality, and end-user experience, practitioners still do not understand why such AI/ML models made those predictions [Tantithamthavorn et al., 2021; 2020; Jiarpakdee et al., 2021; 2020; Rajapaksha et al., 2021; Pornprasit et al., 2021b]. To address this chal-
(1) Global explanations can be generated using interpretable machine learning techniques (e.g., decision tree, decision rules, and logistic regression techniques) or intrinsic model-specific techniques (e.g., ANOVA, variable importance) so the entire predictions and recommendations process are transparent and comprehensible. However, such intrinsic model-specific techniques aim to provide global explainability, without providing explanations to individual predictions.

(2) Local explanations, on the other hand, can be generated using model-agnostic techniques (e.g., LIME, SHAP) to explain the predictions of complex black-box AI/ML models (e.g., neural network, random forest). Such model-agnostic techniques can provide an explanation for each individual prediction (i.e., an instance to be explained), allowing users to better understand why the prediction is made by the AI/ML models.

In software engineering, explainable AI has been recently studied in the domain of defect prediction (i.e., a classification model to predict if a file/class/method will be defective in the future or not). In particular, the survey study by Jiarpakdee et al. (Jiarpakdee et al., 2021) found that explaining the predictions is as equally important and useful as improving the accuracy of defect prediction. However, their literature review found that 91% (81/96) of the defect prediction studies only focus on improving the predictive accuracy, without considering explaining the predictions, while only 4% of these 96 studies focus on explaining the predictions.

Although XAI is still a very under-researched topic within the software engineering community, very few existing XAI studies have shown some successful usages e.g., in defect prediction. In one example, Wattanakriengkrai et al. (Wattanakriengkrai et al., 2020) and Pornprasit and Tantithamthavorn (Pornprasit and Tantithamthavorn, 2021) employed model-agnostic techniques (e.g., LIME) for line-level defect prediction (e.g., predicting which lines will be defective in the future), helping developers to localize defective lines in a cost-effective manner. In another example, Jiarpakdee et al. (Jiarpakdee et al., 2020) and Khanan et al. (Khanan et al., 2020) employed model-agnostic techniques (e.g., LIME) for explaining defect prediction models, helping developers better understand why a file is predicted as defective. Rajapaksha et al. (Rajapaksha et al., 2021) and Pornprasit et al. (Pornprasit and Tantithamthavorn, 2021) proposed local rule-based model-agnostic techniques to generate actionable guidance to help managers chart the most effective quality improvement plans.

2.3 Research Gaps

While there exist research efforts on the explainability of classification tasks in SE domains (e.g., defect prediction), little research is focused on transformer-based pre-trained code models. Particularly, practitioners often raised concerns e.g., why this source code is generated? why this code token is modified?. A lack
of explainability of code models could lead to a lack of trust, hindering the adoption in practice.

To address this challenge, prior studies in the software engineering domain have employed various Explainable AI approaches on transformer-based code models (Kenny and Keane, 2021; Mohankumar et al., 2020; Kobayashi et al., 2020; Liu et al., 2021). For example, Cito et al. (Cito et al., 2021a) proposed an approach to generate a global explanation to understand the weaknesses of the code models. Cito et al. (Cito et al., 2021b) proposed an approach to generate counterfactual explanations to explain the model’s behavior by letting the end user know if the source code had been changed in a specific way, how the model’s prediction would be. This will help the users to have a more specific answer, when asking the model to do a task like security vulnerability detection.

Also, another research using probing tasks has surprisingly claimed that CodeBERT and GraphCodeBERT which are trained on codes have a very slim difference in code understanding, compared to an NL model such as BERT (Karmakar and Robbes, 2021). Another work has replicated an NLP study (Clark et al., 2019) on BERT, but using codes as their training benchmark. They focused on the self-attention mechanism of BERT and compared the attention behavior of the model in NLP and code. However, no efforts have been made to study the different ways that each code model learns to perceive the source codes when doing different downstream tasks. Do they learn to focus on different parts of the code based on their given and fine-tuned tasks? Are there meaningful differences between similar code models understanding of the code, doing the exact same task?

Novelty & Contributions. To the best of our knowledge, this paper is the first to discover hidden patterns in different code models while they’re performing certain downstream tasks and how their way of learning and understanding the codes differ, according to the tasks they are fine-tuned to do. Also, comparisons between similar code models have been made to better understand their strengths and weaknesses objectively or compared to each other.

3 Motivating Analysis

In this section, we present some motivating examples to show the importance of explainability analysis in our case.

Example 1: CodeBERT correctly generates meaningful documents, which do not exactly match with the ground-truth. Fig. 1 presents two sample input methods (i.e., \texttt{f_translate_key()} and \texttt{equal_values()}). For the method \texttt{f_translate_key()}, we found that the generated document (“Translate a key”) is incorrect when compared to the ground-truth (“Translates integer indices into appropriate names”), but semantically conveys the same message. Similarly, the generated document for method \texttt{equal_values()}, (“Compare two arrays”), does not match with the ground-truth (“Checks if the parameter considers two values as equals”), but describes the same functionality. This
def _equal_values(self, val1, val2):
    if self.f_supports(val1) != self.f_supports(val2):
        return False
    if not self.f_supports(val1) and not self.f_supports(val2):
        raise TypeError('I do not support the types of both inputs (' +
                        str(type(val1)) + ' and ' +
                        str(type(val2)) + '), therefore I cannot judge whether
                        the two are equal. %',
                        str(comparisons.nested_equal(val1, val2)))
    if not self._values_of_same_type(val1, val2):
        return False
    return comparisons.nested_equal(val1, val2)

Gold document: Checks if the parameter considers two values as equal.
Best prediction: Compare two arrays.

def f_translate_key(self, key):
    if isinstance(key, int):
        if key == 0:
            key = self.v_name
        else:
            key = self.v_name + '_%d' % key
    return key

Gold document: Translates integer indices into the appropriate names
Best prediction: Translate a key.

Fig. 1: Two code snippets with their original and the CodeBERT’s predicted documents, where the prediction is good.

motivating example indicates that one explanation for CodeBERT’s weak performance may just be an inappropriate evaluation metric. This is a common problem with an automated metric-based evaluation of tasks that contain generating new sentences. Although it is common to use text similarity-based metrics such as BLEU (Papineni et al., 2002) to evaluate a Transformer for text generation, an XAI method can help distinguish between cases where the scores are low because the model is poor and the cases where the scores are low because the evaluation metric is not well suited for the task/data under study, such as this example.

Example 2: CodeBERT incorrectly generates documents for a simple method. Fig. 2 presents a sample code snippet, the file() method, which is short and easy to understand. In this example, we found that the generated document (“Write a file”) does not match the ground-truth (“Reads the body to match from a disk file”), but both sentences share some vocabulary (the word “file”). Based on the generated document, it seems that CodeBERT model is able to understand that this method aims to apply an operation on a file, but it fails to determine whether the operation is read or write. Although “read()” is called in the source code and there is no token to misguide the model to choose “write()”, CodeBERT is still incorrectly generated the document. This motivating example indicates that CodeBERT may generate incorrect
Fig. 2: An example of a simple method that CodeBERT fails to predict correctly.

program documents for even simple codes. Yet, little is known about why it fails in such scenarios.

**Example 3: GraphCodeBERT incorrectly translates a simple one-line method.** Fig. 3 presents an example input method, `getBeginIndex()`, which is a one-line simple method. In this example, the source code (in Java) is valid in the target language (C#) as is, and doesn’t need any change. However, we can see that the model makes an incorrect change by adding the virtual keyword. Also, it is interesting that the model understands the different naming conventions of Java and C# and capitalizes the first letter of the method name. According to this motivational example, we can see that even though the general accuracy of the model is good (in terms of BLEU score), it may be unable to translate the simplest of codes and the reason is unknown to us.

Prior studies in other fields such as image classification, pointed out that attention mechanisms can be used to understand or compare the models. Sometimes, two different models may predict the correct answer in a sample, but have a totally different focus and attention patterns. In this situation, providing an explanation for the decision-making process of the models may help the users to better compare their quality, or to trust them.

The above three examples suggest that there are serious ambiguities about the decision-making process of CodeBERT and GraphCodeBERT, such as the problem with some very simple codes, despite the good overall accuracy of the model. We believe explaining CodeBERT and GraphCodeBERT can potentially be beneficial to understanding the underlying reasons behind a poor quality output that potentially results in alternatives to improve the models.

### 4 Research Methodology

In this section, we explain CodeBERT and GraphCodeBERT which are used as pre-trained code models in this study (step 1). Then we describe how we have fine-tuned and used them for each task (step 2) and finally demonstrate the attention scores and how we attained them from the models (step 3). Fig. 4 illustrates an overview of the process and the following subsections present the details per step.
Source code:
public int getBeginIndex() { return start; }

Target code:
public int getBeginIndex() { return start; }

Generated code:
public virtual int GetBeginIndex(){
    return start;
}

Fig. 3: An example of a simple method that needs no change, but GraphCodeBERT fails to translate correctly.

Fig. 4: An overview of the experiments.

4.1 Collecting pre-trained code models (Step 1)

In this step, we simply download the pre-trained encoders of two transformer-based models, CodeBERT and GraphCodeBERT that will be our base models for fine-tuning.

4.1.1 CodeBERT

CodeBERT [Feng et al. 2020] is a bimodal multi-lingual pre-trained model for programming language (PL) and natural language (NL). It has a multi-layer Transformer encoder, trained on Masked Language Modeling (MLM) and Replaced Token Detection (RTD) with both NL and PL as inputs. The model has a similar architecture as BERT [Devlin et al. 2018] and showed
promising results on multiple downstream tasks such as Code Translation, Clone Detection, Defect Detection, etc (Feng et al., 2020).

4.1.2 GraphCodeBERT

GraphCodeBERT (Guo et al., 2020) is a pre-trained model similar to CodeBERT that considers the semantic-level structure of the code as well. It uses data-flow in the pre-training stage and uses MLM, alongside Edge Prediction and Node Alignment as pre-training tasks. Having this feature included, the model is able to improve the results on its benchmark tasks comparing to CodeBERT, but as we will show in our experiments, in tasks like Code Document Generation, it shows a great drawback.

4.2 Fine-tuning models (Step 2)

For CodeBERT experiments, we use the pipeline provided by the CodeXGLUE (Lu et al., 2021) benchmark. This model has a six-layer Transformer decoder on top of the pre-trained CodeBERT encoder, followed by a dense layer to generate the output token-by-token. For the GraphCodeBERT model, again we stick to the default settings of the model to replicate the reported results.

During training, we use default values as follows: max source length of 256 and max target length of 128 with the learning rate of 5e-4, with 16 as batch size and training it for 100 epoches.

Both models follow the same steps to generate the output. After training a model on a downstream task on the respective training dataset, the model generates the output for each test data item, token by token. That is, in the inference time, in each step, some tokens (depending on the beam size, set in the model) are being chosen from the potential predicted candidates, and this process is repeated (new tokens are added to the candidate output string) until the model generates the end-of-sentence token, which indicates the end of prediction.

**Downstream tasks**

In this study, we choose three different downstream tasks which are: Code Document Generation (CDG), Code Refinement (CR), and Code Translation (CT). Having three generation-based tasks, consisting of a uni-lingual (CR) and a bi-lingual (CT) code-to-code and also a code-to-NL (CDG) downstream task under experiment, we believe this research covers a diverse set of common CodeBERT and GraphCodeBERT applications.

4.2.1 Code document generation

CDG as our first downstream task is generating natural language comments for a given method’s source code. For this task, CodeBERT achieves an overall BLEU score of 17.83 (19.06 and 17.65 per Python and Java, respectively).
Table 1: Dataset statistics

| Task               | Input\Output Languages | Training | Validation | Test    | Total  |
|--------------------|------------------------|----------|------------|---------|--------|
| Code Translation   | Java\C#                | 10,300   | 500        | 1,000   | 11,800 |
| Code Document      | Java\NL                | 164,923  | 5,183      | 10,955  | 181,061|
| Generation         | Python\NL              | 251,820  | 13,914     | 14,918  | 280,652|
| Code Refinement    | Java\Java              | 52,364   | 6,545      | 6,545   | 65,454 |

As we mentioned in 4.1.2, GraphCodeBERT did not have this task on its benchmark, so we implemented the model and fine-tuned it for this task. The BLEU scores that model achieved for this task are 5.3 and 4.21 for Java and Python, respectively. These results are interestingly lower than CodeBERT.

We use the preprocessed and filtered Python and Java dataset of the CodeSearchNet [Husain et al., 2019] for this task. In this dataset, examples that can not be parsed into an AST, or have documents that are not in English or have some special tokens (e.g. `<img ...>` or https:...) or are shorter than 3 or longer than 256 tokens, are filtered. This dataset contains 280,652 samples of Python code from 12,361 unique repositories and 35,170 samples of Java code, from 4,123 unique repositories.

Each sample contains one method, with its actual documentation, the “docstring” description of the method, that we call the “gold document” in this paper, its repository, path, and the method name.

4.2.2 Code Refinement

The goal of this task is to automatically fix the bugs in a given faulty source code. The input is a buggy Java function and the output is the fixed code. We use the medium dataset from a previous work [Tufano et al., 2019] which contains 65,454 buggy Java functions with their fixed versions. In this dataset, all function and variable names have been normalized. BLEU scores for this task are 91.07 and 91.31 and exact match accuracies are 5.16 and 9.1 for CodeBERT and GraphCodeBERT, respectively.

4.2.3 Code Translation

This task aims to migrate source codes from a programming language to another one. We use CodeXGLUE dataset which is collected from multiple public resources with 11,800 samples of Java and C# functions mapped to each other. We take Java as our source language and C# as the destination. The BLEU score and exact match accuracy for CodeBERT on Java to C# task are 79.92 and 59.0, respectively. GraphCodeBERT however, achieves better results with 80.58 and 59.4 as BLEU score and exact match accuracy.
4.3 Extracting the attention scores (Step 3)

Transformer models are able to comprehend long dependencies among words in a sentence (or tokens in a code snippet) by benefiting from the attention mechanism. As it is shown in the following formula, an attention mechanism basically works with a key \((k)\), query \((q)\), and value \((v)\), and \(d_k\) denotes the dimensionality of the key. In its simplest form, it calculates the similarity between the query and key-values as:

\[
\text{Attention}(q, k, v) = \text{softmax}\left(\frac{qk^T}{\sqrt{d_k}}\right) V
\]

Where keys and queries are the elements in the sequence. Calculating all the dot products of \(q_i.k_j\) will result in a matrix where each row represents the attention weight for a specific element \(i\) to all other elements in the sequence. Afterward, a softmax layer and multiplication with the value vector will be applied to the matrix to obtain the weighted mean. This means every dependency between each two elements will be considered in the final output.

As explained in Section 2.1, attention is a reasonable XAI method to explain CodeBERT and GraphCodeBERT. To calculate the attention per token, we need the weights for the encoder-decoder attention layers. Since we have six Transformer decoder layers stacked up, we have six attention layers. Rather than somehow aggregating these 6 layers’ attention values into one metric, we decided to keep all layers’ data and analyze the different layers’ roles in explaining the outputs. The attention weights are available inside the model, but the Transformers library that is used by CodeBERT and GraphCodeBERT, doesn’t provide them by default. Hence, we changed the model’s implementation to collect them, as well.

As we mentioned before, the model has an encoder-decoder attention mechanism and output tokens are generated one by one. So basically for each generated output, we have an attention vector, distributed over all of the input tokens.

The attention weight for each token is the output of a softmax layer, therefore it has a value between 0 and 1. However, in practice, most attention scores are in a much smaller range. So for the sake of visualization and only in our visualized examples, we normalize the scores in each sample, to a zero-to-one range. We represent each attention value as the token’s background color opacity.

**Preprocessing.** The pre-trained CodeBERT model uses the "Roberta-base" tokenizer and the GraphCodeBERT model, use "Microsoft/graphcodebert-base" tokenizer, and both tokenizers are not code-specific. So as shown in Fig. 5 example, the actual "code tokens" may be broken into smaller pieces, each considered one token, having its own attention score. For example, as you can see in Fig. 5, the model tokenizes the name of the method, which is "delete_function" (a single token, tokenized by python interpreter), as three different tokens of "delete", ", " function" and this means it generates three different attention scores for it.
Fig. 5: An example of the model’s tokenization and the attention assignments, per token.

This is not ideal for our analysis because we care about the code tokens as a whole and their roles (e.g., keyword, variable name, method name, etc). To handle this discrepancy, we use Tree-sitter to parse our source codes to get the actual “code tokens”. Then for each token, we consider the mean of its component’s attention as the final attention for that token. From now on, when we talk about tokens, we mean code tokens.

4.4 Evaluating the models (Step 4)

To evaluate the CDG downstream task, we use smoothed BLEU-4 score that is used in CodeBERT’s original study (Feng et al., 2020) and is commonly used by baseline document generation techniques (Hu et al., 2018). For other tasks, we use simple BLEU-4 score. The BLEU-4 is the only evaluation metric we use in this paper and from now on, unless we explicitly say otherwise, when we use BLEU score we are referring to BLEU-4 score.

In our study, BLEU score (Papineni et al., 2002) calculates the n-gram overlap of the prediction and the gold document or code snippet, for all n-gram orders up to four. In other words, it counts the number of all n-gram (from one to four) sub-sequences of the predicted output that are also in the gold string and it gives all n-gram scores an equal weight to calculate the final score. Since in CDG, the generated sentences are usually short, and the higher-level n-gram are not likely to have an overlap, CodeBERT uses a smoothed version (Lin and Och, 2004) that compensates it, by giving additional counts to higher-level n-gram overlaps.

Gold document: Deletes the specified Cloud Function.
Best prediction: Deletes a function.
BLEU score: 0.27
Overlap: 0.20

\(2\) https://github.com/tree-sitter/tree-sitter
5 Research questions

The primary goal of this paper is to explain in which scenarios a pre-trained code model works well and in which cases it may not do well. So that the research community can adjust their effort to designing better models for the software engineering tasks that benefit from a pre-trained code model. The motivation behind this goal is that embedding models are usually complex and applying them on a software downstream task such as CDG, CT, and CR sometimes creates nice outputs and sometimes disappoints. Now the question is can an XAI method such as “attention mechanism” help us shed light on the limitations and strengths of code embedding? To achieve this goal, we focus on two state-of-the-art neural program embedding models (CodeBERT and GraphCodeBERT) and borrow techniques from XAI to explain the underlying decisions made by these models. Among the existing XAI methods, in this paper, we study the attention mechanism, as it is one of the main approaches in XAI and is indeed already a part of some of the mainstream neural code embedding techniques. Therefore, our empirical study targets the following research questions:

(RQ1) Is the attention mechanism suitable to explain the pre-trained code models?

Motivation. Prior studies pointed out that attention mechanisms can be used to understand which tokens contribute to predictions of attention-based models [Danilevsky et al. 2020, Wiegreffe and Pinter 2019]. However, some studies also argued against it [Jain and Wallace 2019]. They claim that in many situations, there is no correlation between the attention weights and other methods like gradient-based feature importance analysis. These studies have also observed that in some cases, input samples with different attention distributions have ended up with equal outcome. In this RQ, we want to justify the use of attention as our XAI method. We specifically want to know if attention outputs on CodeBERT and GraphCodeBERT, provide any meaningful information that helps explain (and potentially improve) these models. To do so, the hypothesis to test is that “attention has a significant contribution in the final decision of the model” and thus studying the attention values will shed light on why certain decisions have been made. We expect that when the model generates a token X in the output, if X or a token similar to X (with a specific definition of similarity) exists in the input, then the model focuses its attention on X more than other tokens.

Design. In order to find out if attention is a suitable mechanism to explain CodeBERT and GraphCodeBERT, we need to inspect if attention weights have a relatively direct and strong relationship with the model’s output and we expect such a dependency to exist. That will mean analyzing and explaining the attention score, will be a good representation of the model.

To evaluate this relationship between attention scores and model’s outputs, we take two different approaches, one for the CDG task which has NL output, and another for CT and CR. Both approaches share the same idea (examining
Fig. 6: An example of the attention impact calculated for an example input and output with attention weights. Each column in the table is the attention scores for the output token, distribution over different input tokens. Blue cells show top-3 attentions in each column. If one of the top-3 tokens in each column corresponds to a row with identical (or similar) token, we count that as a hit.

The impact of attention weights on the model’s outputs, but are different in implementation, to adjust to their corresponding task’s input/output type.

As we mentioned in 4.1, in our generation-based tasks, the models generate the outputs in multiple steps token by token, and for each step, we have the respective attention weights. Therefore, we analyze the attention scores in each step.

To test our hypothesis in this RQ (“Are source code words that are used in the output among the high attention ones?”), in each step that one output token is generated, we look for its equivalent (case insensitive equal) token in the input and its attention rank, compared to others in the sample. If there is no such token, we ignore it. For instance, when a “for” token is generated by the model as an output token, we look at the attentions on input tokens and sort them based on their attention score. If there is no “for” token, in the input, then it’s a new token that was generated (and not being copied) and we skip it. But if there is one, then we record its rank.

It is worth mentioning that our experiment design is a bit conservative, since we ignore the potential indirect impact of attention scores on output. For example, assume a new token “C” is generated in the output (chosen from the vocabulary). Although there is no equivalent token to “C” in the input
but the model may have chosen “C” partly because of high attention to other tokens “A” and “B”, where they are always in the same context as “C” in the training phase. This means that the actual contribution of the attention mechanism to the model’s decision can be higher than what our experiments will suggest.

For instance in Fig. 6, each column and row represent an output and input token, respectively. The first column is the first step in output generation, where the model has generated the token “public”. Now each row for this column shows the attention of each input token for “public”.

In this example, we can see that the input token “public” has the highest attention score among input tokens for output token “public”. Similarly, studying the attention scores for the generated token “clone”; the similar token “clone” has the second rank after “record”. We then repeat this process for every generated token by the model to see whether we can find a pattern between generating a token in the output and its corresponding input token’s high attention score or not.

We use the rank rather than the raw scores, since even though the attention score range is always between 0 and 1, it may vary a lot between different samples. In addition, the tokens in one code snippet may have very close attention scores. Therefore, in order to compare the token’s attention scores, we sort the tokens based on their attention score in their respective code snippet and ignore the absolute values.

Furthermore, using absolute ranks we be deceiving when input length is variable, in different samples. For instance, while having the rank 9 among 100 input tokens is good, having the same rank among 12 inputs is not. Therefore, we are reporting the normalized rank of the tokens between 0 and 100. So a rank less than 1 means the token was among the top 1% attention scores.

A final design decision for RQ1 is that we have multiple layers in our decoder, each having its own attention weight vector. Since each layer would have its unique attention focus mechanism (e.g., one layer maybe focusing on names and another one focusing on syntax, etc.), we apply the analysis per layer and report them all.

**Results.** As we said earlier, we are interested in tokens that appear in the output and also exist in the input. These are basically the situations where the model has decided to copy a token directly from input, instead of choosing one from the vocabulary. We analyzed our test dataset to analyze the frequency of such decisions.

As in Table 2, for the CR task, more than 94% and 99% of the output tokens are available in the input for GraphCodeBERT and CodeBERT, respectively. This ratio drops to 52% and 70% in CT for GraphCodeBERT and CodeBERT, respectively; which is expected because of the uncommon tokens between the source and destination languages. For the CDG task, this ratio is between 30% and 40% for different languages and models. This is an anticipated fall since the output for this task is natural language and therefore, there are lots of NL tokens in the output to form a meaningful sentence. The models learn to rely less on copying mechanism, and rather focus on generat-
Table 2: The proportion of the tokens that appear in the output and also exist in the input for each sample

| Task              | Model        | % of repeated tokens |
|-------------------|--------------|----------------------|
| Code Translation  | CodeXGLUE    | 70.55%               |
|                   | GraphCodeBERT| 52.53%               |
| CDG _java_        | CodeXGLUE    | 35.50%               |
|                   | GraphCodeBERT| 30.45%               |
| CDG _python_      | CodeXGLUE    | 40.63%               |
|                   | GraphCodeBERT| 31.76%               |
| Code Refinement   | CodeXGLUE    | 99.97%               |
|                   | GraphCodeBERT| 94.72%               |

ing tokens. Even in cases that the model decides to use a word from the input code, it’s expected that its form would be changed to be suitable for a human readable sentence (e.g. tenses in verbs).

It’s noteworthy that the ratio of newly generated tokens for GraphCodeBERT is always higher than in CodeBERT for all tasks. This means GraphCodeBERT tends to be more generative and less prone to copy the same tokens from the input for the output.

Fig. 7 shows the average normalized rank for an input token X based on its attention score, whenever the model have generated a token equivalent to X (case insensitive equal), as output. As we mentioned earlier in the design section, we only considered the output tokens that their equivalent token also existed in the input. This means if a new token is generated (not available in the input), we have skipped it (and reported them separately, see Table 2).

An interesting pattern is the decrease of the described rank throughout the layers. In all tasks and models, the last three layers have a much smaller average normalized rank compared to the first layers. This means that tokens with high attention scores in the last layers, have a greater chance of ending up as the output token.

In general, these results show the significant influence of attention scores on the final output, especially in CR and CT tasks. For example, in CT with both models, in the last three attention layers as in Fig. 7a the average normalized rank of the token is less than 2% in CodeBERT and less than 3% for GraphCodeBERT. Also, further experiments showed that more than 80% of the times, the rank is less than 3 in both models. The code refinement task also shows a similar result in Fig. 7d where the average normalized rank for the last three layers is always less than 4%. Also, our analysis shows that almost 70% of these tokens are among top-3.

Code document generation, however, has a larger average normalized rank, since the task has different types of input and output. As in Fig. 7c and Fig. 7b, The source codes are much longer than the NL outputs so there is a less one-to-one correspondence between output and input tokens. Meaning for each
As a final answer to our RQ1, even though we can not claim causality, we can assert that the attention mechanism’s focus on tokens, has a considerable correlation with the model’s decision. We only considered the more direct and obvious kind of impact, but the total contribution of the attention mechanism is definitely higher than what is reported here. We also observe that, this direct effect is higher in tasks with the same types of input and output (code-to-code). This justifies the attention mechanism’s suitability as an explanation method for the Transformer-based models.
**Answer to RQ1:** Our findings show that in CT, more than 80% of the tokens that are generated by the model as the output, and also are available in the input, have one of the top-3 attention scores in their corresponding step in last three layers. While the average normalized rank is less than 3% for those layers.

The average normalized rank for CR is also less than 4% for last layers. For CDG it’s less than 10% for GraphCodeBERT and less than 13% for CodeBERT which is expected, since CDG has different types of input and output.

Therefore, we conclude that the attention mechanism has a considerable impact on the model’s output and hence, it is a suitable XAI method to explain the strengths and weaknesses of our code models under study, in the next RQs.

**(RQ2) What do the pre-trained code models learn?**

**Motivation.** Applying a Transformer-based model on a source code, for any downstream task, accepts the source code snippets as sequences of tokens. Yet, little is known about what the code models learn from that code snippets. For example, what kinds of code tokens are often highlighted by the model in the learning process and whether such highlighted tokens are semantically important or not. In general, knowing what has been learnt is important from two perspectives: (1) Trust: depending on what tokens are impacting the output one can rely more or less on the recommendations. For example, if XAI reveals that a model makes its decision mainly based on parentheses and indentations in the source code, the user will not (and should not) trust its recommendations. (2) Debugging: knowing which tokens have the highest influence on a generated wrong output, one can devise mechanisms to change the training data, models, or the training process to fix the issue.

Therefore, in this RQ, we study the attention weights of different token types provided by CodeBERT and GraphCodeBERT’s internal layers, to see which kind of source code tokens have the highest influence on each generated output, for a given downstream task. This helps us understand whether these models’ success and failure are related to focusing on the right/wrong tokens or whether the highlighted tokens are reasonable and the potential problems’ root causes are somewhere else (e.g., inappropriate evaluation metrics).

**Design.** As discussed, in [3] to explain the models, we analyze the attention weights per token type and not individual tokens. To do so, we first need to define a list of token types. This is a subjective decision on what tokens types are of interest for our study. We opt for a set of seven token types that cover all tokens and group them according to their semantic relevance, as follows:

**Method name:** The method under study’s name can be one of the main decision factors on perceiving what a method does which is a very important step for the model, specially in some tasks such as CDG. This only includes the main method’s name in each sample (reminder that each input sample is the source code for one method) and not the methods called within the main method’s body.
Table 3: Control flow command tokens for Java and Python.

| Language | Tokens |
|----------|--------|
| Python   | False, None, True, and, as, assert, async, await, break, class, continue, def, del, else, except, finally, for, from, global, if, import, in, is, lambda, nonlocal, not, or, pass, raise, return, try, while, with, yield |
| Java     | if, else, switch, case, while, class, enum, interface, annotation, public, protected, private, static, abstract, final, native, synchronized, transient, volatile, strictfp, assert, return, throw, try, catch, finally, default, super, do, for, break, continue, super, void, import, extends, implements, import, instanceof, new, null, package, this, throws |

**Type identifiers:** This category represents all the keywords that are used for identifying token types in our source languages Python and Java. For more information on these tokens, look at “type_identifier” and “*type” node types in tree-sitter for each language.

**Language keywords:** Control flow command tokens are all bundled together for each language in this category. These tokens can be found in Table 3.

**Method calls:** This category includes all the tokens that are the name of methods invoked within the body of the method under study. These method calls can also be instrumental in describing what the method is doing and may contain bugs to fix.

**Local variables:** Here we consider all variables that are used only in the body of the method under study. That is, the input arguments of the method are excluded.

**Input variables:** This category only contains the input arguments of the method under study. We have separated it from the Local variables category.

**Others:** This category represents all the tokens that are not included in any of the categories above. Mostly tokens like punctuation, constant values, parentheses, etc.

Note that although these token types are chosen subjectively, the results will show that they are among the most important tokens and not many contributing tokens are left for the “Others” category. We should also emphasize that the level of abstraction on what constitutes a “token category” is up to the XAI user. For instance, we decided to separate the Input Arguments category from the Variable Names category, to better analyze their effects individually, but merging the two categories is a valid design choice as well (just in different level of abstraction).

In RQ2, for each sample in test data, we follow these steps to find the distribution of attention scores over different categories:
Table 4: Number of tokens in each category for each task

| Method | Input variables | Method call | Variable identifier | Language keywords | Others | Total |
|--------|----------------|-------------|---------------------|------------------|--------|-------|
| CT     | 1,033          | 2,859       | 2,065               | 4,289            | 2,815  | 21,731|
| CDG_Java | 12,991         | 44,175      | 42,285              | 101,352          | 63,143 | 784,009|
| CDG_Python | 16,633         | 110,630     | 19,567              | 197,878          | 0      | 910,230|
| CR     | 7,761          | 19,316      | 33,717              | 70,750           | 52,966 | 319,544|

For each generated token (each step), we take its attention weights toward the input tokens and find their corresponding type. Then, we accumulate the attention scores of all the tokens in each category to get a total score for that category in that sample. Our categories cover all tokens so the sum of all scores for each step is equal to one. We go through the same process for all output tokens in all code snippets of the testing dataset and gather the accumulation of attention scores for each category.

It’s noteworthy that the size of token categories is quite imbalanced. For example, there is only one method name for each sample but many tokens in the “others” category. Therefore, we normalize the total score of each category, according to its population as in Table 4. This gives us the attention score per token for each category. Finally, we normalized scores of all categories, between 0 and 100 for the purpose of easier comparison.

Among these defined categories, “Method name”, “Input variables”, and “Local variables” are more representative of the naming aspects of a source code. So we group them in a higher-level category of “Naming”, while “Method calls”, “Type identifiers”, and “Language keywords” are more related to the structure of the code. Thus, we consider them as the higher-level category of “Structure”. Also note that we only report the average score of all six layers for each task and model here, since reporting all results per layer would be too lengthy and also this RQ results were quite similar over different layers.

Results. In the three downstream tasks under study, we expect different normalized attention scores per high-level category, as follows: (a) CT is a task that heavily relies on the structure, since the model must learn the source language structure, and generate the equivalent structure in the target language. (b) In CDG, the structure is less important (nested blocks and syntax trees have less to do with the output document). On the other hand, names are very important in this task, since they basically describe the functionality of the source code. (c) Finally, we expect code refinement to be in the middle of these two ends, since both names and the structure are important in debugging a code.

Table 5 shows the normalized total attention score of each high-level category and validates our hypothesis. Code Document Generation, as a task that heavily relies on naming, has a considerably high normalized attention score of over 63% for the Naming category, while it pays much less attention to the Structural token types category, compared to other tasks. It has also a
Table 5: Normalized attention score of the two high-level categories of tokens, for different code models and tasks. The results are the average of all six layers for each task.

| Task             | Model     | Naming | Structural | Others |
|------------------|-----------|--------|------------|--------|
| Code Translation | CodeXGLUE | 42.36% | 51.38%     | 6.27%  |
|                  | GraphCodeBERT | 42.60% | 51.30%     | 6.09%  |
| CDG_java         | CodeXGLUE | 63.31% | 29.19%     | 7.50%  |
|                  | GraphCodeBERT | 64.51% | 28.19%     | 7.30%  |
| CDG_python       | CodeXGLUE | 67.97% | 23.75%     | 8.28%  |
|                  | GraphCodeBERT | 74.63% | 17.83%     | 7.54%  |
| Code Refinement  | CodeXGLUE | 56.46% | 37.96%     | 5.58%  |
|                  | GraphCodeBERT | 55.49% | 38.86%     | 5.65%  |

higher number for the Other category which can be understandable considering the fact that NL comments in the code are also part of this category. Code Translation, on the other hand, is the only task that has more than 50% normalized attention score for Structural tokens and less than any task for the Naming category. Code Refinement in this comparison holds the middle ground between the two mentioned tasks in both categories.

In Table 6, we have a more detailed analysis for each of our categories. We saw that both models pay more attention to the structural tokens for CT. Getting into more details, the results show that this attention is more focused on Method calls, and Type identifiers rather than Language keywords, roughly having only 6% of the normalized score. It is very interesting that studying individually, the Method name category has the second highest score after Method calls. Even though in translating a code, the method name is usually unchanged, this shows that the models considerably utilize the name of the method to understand its functionality.

In the CDG task, we observed a great reliance on Naming categories, the results show that the Method name category plays the most significant role. It always has a normalized score of close to 40% or higher. In the absence of Type identifiers, in GraphCodeBERT CDG_python, this category has the highest score ever among all the token types across all tasks/models. Intuitively, this amount of importance is justifiable, given that even humans rely a lot on the method names to understand their functionality. In addition, in three out of four different experiments for this task, the Input variables have the second highest normalized attention score (between 11% to 16%). This basically means that the models have learned that while generating document for a method, the main and most interesting part is the signature of the method and not the body.

Code Refinement which holds a middle ground between two other tasks has a very close score for four categories of Method name, Input variable, Method call, and Variable. Since in this task the model is supposed to look for bugs
Table 6: Normalized attention score of different token types, for different code models and tasks. The results are the average of all six layers for each task.

| Task | Model  | Method name | Input variables | Method call | Variable | Type identifier | Language keywords | Others |
|------|--------|-------------|-----------------|-------------|----------|-----------------|-------------------|--------|
|      | Code   | XGLUE       | 21.36%          | 9.63%       | 24.26%   | 11.36%          | 20.67%            | 6.45%  |
|      |        | CodeBERT    | 22.78%          | 7.89%       | 23.46%   | 11.93%          | 21.66%            | 6.18%  |
| CDG_java | Code   | XGLUE       | 39.44%          | 13.88%      | 10.49%   | 10.00%          | 13.07%            | 5.63%  |
|       |        | CodeBERT    | 41.04%          | 15.10%      | 8.44%    | 8.38%           | 13.13%            | 6.62%  |
| CDG_python | Code   | XGLUE       | 46.17%          | 11.96%      | 16.00%   | 9.83%           | 0.00%             | 7.76%  |
|      |        | CodeBERT    | 54.21%          | 12.79%      | 10.79%   | 7.64%           | 0.00%             | 7.03%  |
|      | Code   | XGLUE       | 22.01%          | 16.60%      | 20.33%   | 17.83%          | 9.82%             | 7.81%  |
|      |        | CodeBERT    | 19.36%          | 17.19%      | 21.15%   | 18.93%          | 10.02%            | 7.69%  |

and try to fix them, it seems that the models have learned that fewer bugs happen in categories like Type identifier, Language keywords, and Others. This makes sense because we know that databases for this task are gathered from public projects and they probably don’t have syntactical errors. The method name is also less likely to have a bug, but as we saw in other tasks, this category always has a minimum appeal for the models.

It is interesting that according to the table, Type identifiers which is a category purely related to the syntax of the code and don’t include any naming, have the most contribution to CT with a gap compared to others. It has a score of 20.67% and 21.66% for CodeBERT and GraphCodeBERT respectively while its score in other categories is below 14%. Also, it is worth mentioning that GraphCodeBERT which uses the dataflow of the code in order to capture its structure; always has a higher score for this category compared to CodeBERT.

The same patterns appear to be valid for Variable names and for CR. The score of this category for CR is 17.85% and 18.93%, while in other tasks the score is always below 12%.

Similarly, the Method name category has a harshly higher score in CDG. For this task in python, this category has a score of 39.44% and 41.04%, and in Java, it has 46.17% and 54.21% for CodeBERT and GraphCodeBERT, respectively.
**Answer to RQ2:** Having all these observations, we can see a pattern of importance comparing different tasks together. The method name and input variable (basically the first line of the code samples) are the most important categories for CDG; Method calls and local variables play the most significant role on code refinement, alongside the method name with slightly lower importance. On the other hand, code translation is concerned with type identifiers and language keywords, more than any other task, while still caring about some naming categories, as well. In Table 3, we have aggregated the numbers for our two main categories and we can see a pattern that we expected. Naming tokens are important for all tasks, but less for code translation which alternatively, cares more about structural tokens compared to other tasks.

(RQ3) When do the pre-trained code models not work?

**Motivation.** In RQ1, we made sure attention is a reasonable tool to explain CodeBERT and GraphCodeBERT, and in RQ2 we show that the tokens are mostly picked up correctly by the model, so the models learn the right tokens per task, in most cases. In this RQ, we delve deeper and explore the scenarios where the code models did not perform well but the problem at hand was not that difficult. Answering this question will help understand what should be done to make the model at least perform consistently well, on simple data items.

**Design.** To provide explanations on when CodeBERT and GraphCodeBert perform well and when they fail, in this RQ, we start by a qualitative analysis of some sample predictions. Then we make hypotheses based on our observations and finally verify them quantitatively on the whole dataset. To define the strong and weak performances of the models, we cannot simply rely on the absolute values of the evaluation metric (BLEU). Since the magnitude of the BLEU score partially depends on how difficult or easy the document generation task is, per sample code. Therefore, we need to somehow measure the difficulty level of the document generation task, given a source code.

To achieve our purpose in this RQ, firstly, we need to define a few metrics that can represent the easiness/difficulty of a specific sample, and secondly, evaluate the model’s performance on that sample.

As we said, in CR and CT, expectedly, the model is busy copying and inserting the same tokens from the input to output and doesn’t usually have to generate new tokens. Having this fact, we expect the Levenshtein Distance (LD) of the input, and their corresponding expected true output (let’s call it “gold output” from now on) as a suitable metric for the difficulty-level of that sample. So in CR and CT, for each task, we calculate the Levenshtein Distances for all samples in the dataset, and consider the first one-third samples with the least LDs as the easier targets.

For the CDG task, we keep the same general approach (that is considering the similarity of input and gold output), but since in this scenario, the output is in NL and the input is in PL, we define slightly different steps.
To define the difficulty-level for the CDG task, we use the intersection between the set of preprocessed tokens of the gold output document, per method, and the set of preprocessed tokens of the method’s source code.

To find the overlap between source code and output tokens, we follow these preprocessing steps: First, we remove punctuations and tokens shorter than three characters, in the output document. Then, lemmatize those tokens using the standard Wordnet \cite{Loper2002} lemmatizer, offered in the NLTK package. Next, we tokenize the source code using a parser for the respective language. Note that as explained in Section 4.3, due to CodeBERT and GraphCodeBERT’s tokenizations, which may split one meaningful word into multiple tokens, we don’t use their tokenization for this analysis. Finally, we create a set of case-insensitive tokens that fall at the intersection of processed output and source code tokens.

Now an easy/difficult document generation task is when the overlap between the two sets is high/low. Therefore, the same as the cut-offs for CR and CT, we consider the first one-third samples with the highest overlaps as easy, and the one-third cases with the least overlaps as hard problems, and ignore the rest (average difficulty-level).

The above process tells us which samples are considered hard and which ones are considered easy. Now we need to measure the performance of models. To do so, we use BLEU score since it is the most accepted and reliable score that is applied in these tasks in the literature. For the accuracy, we also take the one-third of the samples with the highest BLEU scores as \textit{High} and the samples with the one-third least BLEU scores as \textit{Low}.

Having these definitions, there will be four categories (for the tuples of \textit{<easiness level, model accuracy>}) as below:

\textbf{Easy} – \textbf{High}: This category contains test data items that are easy problems (meaning high similarity between the input and the gold data) that the models have achieved a High BLEU score on them.

\textbf{Hard} – \textbf{High}: This category contains the samples labeled as \textit{Difficult} and \textit{High}. This means even with the lack of common tokens, the model was able to achieve a satisfactory result in these cases.

\textbf{Hard} – \textbf{Low}: This category includes the cases that are \textit{difficult} again, and expectedly, end up with \textit{Low} accuracy for the model’s prediction.

\textbf{Easy} – \textbf{Low}: This category is the most interesting one in this paper, since it can show the potential weaknesses of the model and is very suitable for being analyzed and “explained”. Samples in this group, are among the samples with higher overlaps in their corresponding dataset that means that the model is having rather an easy job predicting. However, the BLEU score as our indicator of the model’s accuracy is showing poor performance comparing to other samples.

In order to perform our manual observation (qualitative study) for this RQ, after grouping our test dataset into these four categories, we randomly choose 100 samples from our target category (\textit{Easy} – \textit{Low}), and manually analyze their outputs and attention weights.
Table 7: The ratio of the Easy-Low category population to the whole dataset, for each task-model.

|            | CodeBERT | GraphCodeBERT |
|------------|----------|---------------|
| CT         | 11.70%   | 11.41%        |
| CDG / Java | 5.12%    | 5.59%         |
| CDG / Python| 5.87%   | 5.85%         |
| CR         | 2.49%    | 4.37%         |

For each sample, we record the most interesting findings to identify the most frequent patterns. This way we develop some hypotheses. Finally, we try to verify these hypotheses by quantitatively studying the whole test dataset, with respect to the hypotheses. The output of this quantitative phase is in the form of some descriptive statistics to either confirm or reject the observations made based on the 100 samples.

**Results.** Having the data divided according to the defined groups, Table 7 shows the ratio of the target category population to the whole dataset for each task-model and also, Fig. 11 and Fig. 12 show the distribution of the target category. Next, we will explain the observations from the manual analysis.

**Observation 1: The pre-trained code models don’t work well, when the output gold document is long.**

Our first observation regarding the CDG task is that in cases with long gold documents the BLEU scores tend to be low! We plotted the distribution of BLEU scores, according to the gold document’s length, in Fig. 8. According to the plot, most high BLEU scores happen when the length of the gold document is less than 50 characters.

In general, the idea of the BLEU score is about counting the number of n-grams that are common between the reference and the output. Model-generated documents are usually short so for longer sentences, there is less chance that the model chooses the same phrasing and words with the same order. Another plausible explanation for this observation is that a longer document means the method implements a more complex task and thus it is harder for the model to generate the right documentation for the complex method.

One potential solution for this problem is forcing the model to generate longer sequences as the output which will increase the chance of a high BLEU score, in cases with long reference documents. But obviously, since this is not actually the model’s fault and in these cases, a low BLEU score does not necessarily indicate a bad prediction (like the example shown in Fig. 9), the best way to handle this problem is considering other evaluation metrics and ideally more subjective ones.

**Observation 2: The pre-trained code models don’t work well, when the input source code is complex.**
Another interesting observation is about the length of the source code. The results show that in cases with longer code, the BLEU score is usually lower. We started the initial analysis with the CDG data and the results, which are summarized in Fig. 10, show a decreasing trend of BLEU scores, by the increase of the source code length. For example, the average BLEU score for cases shorter and longer than 300 tokens is 0.161 and 0.149, respectively.

There are two explanations for this observation. The first one is the fixed length of the inputs in models, which basically means if the source code’s length is higher than a fixed value (in our experiments, 256 tokens), then the input will be truncated. This means some tokens will not make it to the decoder, and thus we have a potential degradation in the final scores.

Another reason is the increased complexity of the code. Similar to Observation 1, longer source code means more complex logic, more objects, and functionalities to consider for the model that probably leads to a poorer results.

According to these reasons, two basic solutions can be suggested: (a) increasing the input threshold and (b) decreasing the input’s length. Input threshold can be easily modified in the training process of the model and only requires more resources. The second option, however, is a more complex solution that is already kind of naively implemented by the truncation. Another potential alternative is to refactor long methods to multiple smaller methods, then pass each method to the models to generate documents for, and finally merge all output documents as one document.

Next, to expand this observation on all tasks-models, and find more statistical results, we used some common code complexity metrics and conducted...
def parse_cache_control(self, headers):
    cc_header = 'Cache-Control' in headers
    if cc_header in headers:
        headers[cc_header] = split('', parts, with_args=[tuple(x.strip(), lower(x) for x in parts if -1 != part.find('=""'))])
    parts = [name.strip(), lower(x) for x in parts if x == name]
    parts = [name + args[1] + parts, wo + args]
    return ret_val

Gold document: Parse the cache control headers returning a dictionary with values for the different directives.

Best prediction: Parse a dict of headers

BLEU score: 0.08
Overlap: 0.54

Fig. 9: A sample method, broken into tokens, the gold document, the best prediction by CodeBERT, the BLEU score, and the amount of overlap between the method’s code and the gold document. The attention values of the last layer of CodeBERT executed on this code are also shown, as shades of blue (the darker, the higher). We used the attention scores of the last generated token (“headers” in this example), in the last layer, for the visualization.

an analysis on all 8 model-tasks to get a better understanding of the root cause of the poor results for long code snippets. We chose ‘number of tokens’, ‘cyclomatic complexity’, ‘nested block depth’, ‘number of variables’ as complexity metrics. To measure the difficulty of the task, we also included the same ‘Levenshtein distance’ for CT and CR and ‘overlap’ for CDG, in our analysis.

For each task-model, we have five different metrics to study, so we have one plot per metric. In each plot, the distribution of samples in the respective dataset, regarding that metric is shown with blue bars and the same distribution but only for the target category (Easy-Low) is shown by red. With this visualization, we can identify any difference in terms of trends on a specific metric in the target category vs. the whole dataset.

Fig. 13 and Fig. 14 show the results for code refinement (CR). As illustrated in the plots, the Easy-Low category has a very similar distribution to the whole dataset, except a slight increasing trend for some reported metrics like number of tokens and number of variables. This means that the model tends to make bad decisions, whenever the source code gets more complex in terms
of number of tokens and variables, even if the overlap of tokens is high. For instance, considering the number of tokens, as a measure of code complexity, the proportion of samples with more than 100 tokens is mostly higher in the Easy-Low category than the share of the same samples in total. It means that the samples with many tokens, are more likely to be assumed “Easy” in our categories (more overlaps between input and outputs) but in fact they are harder for the model to understand (given the long length of the code snippet).

Fig. 15 and Fig. 16 show the same results for code translation (CT). For this task, number of variables follow the same pattern as the CR task, that is Easy-Low category is harder based on those metrics. On the other hand, considering the number of tokens, nested block depth, and even cyclomatic complexity, there is a reversed connection. In other words, samples that have smaller values of these metrics, have higher density in Easy-Low category. For instance, in both models, samples with tokens less than 20, are around 50% of the target category population, even though they occupy a very small portion of the total dataset. One plausible explanation is that when the source code is too short (very small number of tokens and very few nested blocks), the model fails to translate it properly, due to the lack of enough information/context. Another explanation is the fact that it’s harder to maintain a high BLEU score when the input is very short.

Fig. 17, Fig. 18, Fig. 19, and Fig. 20 illustrate the same results this time for code document generation (CDG). In this downstream task, we can see patterns more dependent on the language, rather than the model. In all cases, the number of variables, number of tokens, and nested block depth follow the same general pattern.

In these experiments, we can see that both models struggle with samples with less complexity in Java and on the other hand, have problems figuring out the more complex samples in Python. For instance in Python, samples with more than 80 tokens or 8 variables, have always a higher density in the Easy-Low category compared to all of the dataset. Meanwhile, it’s interesting that considering the cyclomatic complexity, both models in both languages struggle with samples with higher complexity.

So all-in-all, one can conclude that code models perform poorly on the code snippets with extreme values of complexity-related metrics on either direction (i.e., both long code with many nested blocks and tokens and also very short code with only a few variables and tokens are hard for the models).

**Observation 3:** The pre-trained code models don’t work well, when the models fail to focus on important categories:

Finally, we analyzed the contribution of token categories similar to what we had in RQ2, but specifically for the target category of (Easy − Low). In Table 8 we have the normalized score of two main categories for the target samples. We were interested to compare the results for this category and the previous results for the whole test dataset. Hence, we calculated the difference between these two from Table 8 and Table 4 and the outcomes are shown in Table 9. The negative numbers in this table indicate a decrease in the target category.
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Fig. 10: Distribution of BLEU scores according to the source code length.

As the results show, there is a considerable decrease in the scores for the Structural category in CT. While answering to RQ2, we showed that this task mostly relied on this group of tokens. Likewise, we have a slighter decrease in the score of the Naming category in CDG while the naming category also proved to be the more important category for CDG.

Both of these clues lead us to the conclusion that the results are less satisfying whenever the model fails to pay enough attention to the corresponding important token category for a specific task. Based on this observation, potential research questions to investigate in the future are: “Will the model work better if we help it by tagging the token types? Can manually amplifying the attention scores of specific categories according to the task beneficial for the code models?”

6 Limitations

One limitation of this study is that our experiments only cover Java datasets in CT and CR and for CDG, it’s only Java and Python. Even though our experiments and conclusions are not bound to anything specific to one language; since we needed syntactic information on tokens (and for this purpose, parsing the test cases was required), we couldn’t run our experiments on the whole CodeSearchNet dataset for CDG. Other datasets for two other tasks also needed lots of pre-processing to become consistent with our designs and requirements. We plan to extend these analyses to other languages as well in the future.

Another limitation is we used the BLEU score as our evaluation metric for the accuracy of the model, which is commonly used in document generation
Fig. 11: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), based on the BLEU score and the Levenshtein distance of the input and gold output for CT and CR.

Table 8: Normalized attention score of the Easy-Low samples, in three general categories of tokens, for different code models and tasks. The results are the average of all six layers for each task.

| Task | Model     | Naming | Structural | Others |
|------|-----------|--------|------------|--------|
| CT   | CodeXGLUE | 48.85% | 44.51%     | 7.70%  |
|      | GraphCodeBERT | 49.51% | 43.49%     | 7.57%  |
| CDG_{java} | CodeXGLUE | 60.08% | 33.28%     | 8.89%  |
|      | GraphCodeBERT | 63.85% | 37.06%     | 7.43%  |
| CDG_{python} | CodeXGLUE | 66.37% | 29.14%     | 8.61%  |
|      | GraphCodeBERT | 73.68% | 24.16%     | 7.87%  |
| CR   | CodeXGLUE | 56.64% | 46.29%     | 5.63%  |
|      | GraphCodeBERT | 55.82% | 48.35%     | 5.62%  |
Fig. 12: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), based on the BLEU score and the Levenshtein distance of the input and gold output for CDG

Table 9: The difference of normalized attention scores for the Easy-Low samples and all samples, in two general categories of tokens, for different code models and tasks. The results are the average of all six layers for each task.

| Task   | Model       | Naming | Structural | Others |
|--------|-------------|--------|------------|--------|
| CT     | CodeXGLUE   | 6.49%  | -7.92%     | 1.43%  |
|        | GraphCodeBERT | 6.90%  | -8.38%     | 1.48%  |
| CDG_{java} | CodeXGLUE   | -3.24% | 1.85%      | 1.39%  |
|        | GraphCodeBERT | -0.66% | 0.53%      | 0.13%  |
| CDG_{python} | CodeXGLUE   | -1.59% | 1.27%      | 0.33%  |
|        | GraphCodeBERT | -0.96% | 0.63%      | 0.33%  |
| CR     | CodeXGLUE   | 0.18%  | -0.23%     | 0.06%  |
|        | GraphCodeBERT | 0.33%  | -0.30%     | -0.03% |
downstream tasks to reduce the subjectivity of the results. However, as we mentioned in the paper, it is not a comprehensive metric as it is unable to find rephrasings or cases that the prediction is not wrong, but doesn’t exactly match with the gold label.

The observations we made are also limited to the main patterns we have observed in the 100 samples, manually. Although we later quantitatively validate them, it is of course possible that there exist some other explanations as well that we have missed observing, due to the samples we have chosen.

We have also subjectively selected a set of six token types that we believed could have the highest impact on our models. Although, the RQ2 results showed that these categories actually contributed the most out of all tokens; the level of abstraction (grouping of tokens into categories) is a matter of design choice, which may reveal other findings (at different levels). In other words, although our observations in this level of abstraction are correct, they are not the only way to look at the tokens’ attention scores and other categorizations can be studied in the future.

Finally, the study is only limited to three downstream tasks (CT, CDG, and CR) and two code models (CodeBERT and GraphCodeBERT). More work is required to generalize the findings for other Transformer-based models, in the future.

7 Conclusion and future works

This paper proposes an approach for explaining pre-trained code models (e.g., CodeBert and GraphCodeBert), using their internal end-to-end attention mechanism, as the XAI method. Unlike most XAI research, where the explanation is applied to high-accuracy models to make sure the results are trustworthy, we have used XAI on both high (to find out what the models learn) and low-accuracy scenarios (to see when they do not perform well).

Our findings not only provide observations about what these state-of-the-art Transformer-based models learn in terms of token type categories and why they underperform in some scenarios, but also suggest actionable recommendations, such as using more subjective evaluation metrics for CGD task, giving token types as additional input to the model, and manually amplifying attention scores for specific token types.

In the future, we plan to extend this work by examining other downstream tasks, models, and XAI methods. In addition, we also plan to work on pre-trained code models by implementing the suggested recommendations from our observations.

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Appendix

Distribution of the whole dataset (displayed in blue) and the Easy-Low category (displayed in red), according to different code complexity metrics, for each task and model in RQ3.

Fig. 13: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code refinement on CodeBERT.
Fig. 14: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code refinement on GraphCodeBERT.
Fig. 15: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code translation on GraphCodeBERT
Fig. 16: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code translation on CodeBERT.
Fig. 17: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code document generation on CodeBERT on Java.
Fig. 18: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code document generation on CodeBERT on Python.
Fig. 19: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code document generation on GraphCodeBERT on Java.
Fig. 20: Distribution of the whole dataset (in blue) and the Easy-Low category (in red), according to code complexity metrics, for code document generation on GraphCodeBERT on Python.