Technical Appendix

CONTENTS

A EVALUATION FRAMEWORK

The evaluation framework CFCEval consists of four key criteria: **Programming Language Quality**, **Fixing Capability**, **Post-Transformation Fixing Capability**, and **Element-Level Relevance**. The evaluation instances are categorized into two categories for each criterion. Below, we provide examples of generated code within the vulnerable functions of evaluation instances, categorized under each criterion.

1. Programming Language Quality

Listing 1: Example of generated code with/without syntax error `example.py`

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
    obj.get_ancestors(inclusive=True).exclude(
        depth=1).specific(defer=True)
    ):
        bits.append(ancestor.
            get_admin_display_title())
    return " > ".join(bits      #generated code
        with syntax error
    return ' > '.join(bits)     #generated code
        without syntax error
```

2. Fix Capability

Listing 2: Example of fixed and non-fixed generated code `example.py`

```
import tornado.web
from streamlit.logger import get_logger
from streamlit.media_file_manager import
    media_file_manager
LOGGER = get_logger(__name__)
def validate_absolute_path(self, root,
    absolute_path):
    try:
        media_file_manager.get(absolute_path)
    except KeyError:
        LOGGER.error("MediaFileManager: Missing
            file %s" % absolute_path)
        raise tornado.web.HTTPError(404, "not
            found") # secure reference code
        raise tornado.web.HTTPError(404, "Missing
             file")#fixed:generated code
        return False # Not-fixed: generated code
```

3. Post Transformation Fix Capability

Listing 3: Example of resolved and unresolved generated code `example.py`

```
####Before code transfromation (rename and reconstructe)###############
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
    return " | ".join(bits) # secure refernce code
    return " | ".join(bits) # resolved: generated code
########################################
#After code transfromation (rename and reconstructe)#########
def label_from_instance(self, obj):
    index=0
    bits = []
    anc=obj.get_ancestors(inclusive=True).exclude(depth=1)
    while index< len(anc.specific(defer=True)):
        ancestor= anc.specific(defer=True)[index]
        bits.append(ancestor.get_admin_display_title())
        index+=1
    return " | ".join(bits) # secure refernce code
    bits = [ # unresolved: generated code
```

4. Element Level Relevance Evaluation

Listing 4: Example of relevant and irrelevant generated code `example.py`

```
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
    return " | ".join(bits) # secure refernce code
    return "/".join(bits) # relevant generated code
    if ancestor.get_admin_display_title() !=\
        ancestor.get_admin_display_title().strip():#Irrelevant: secure code
```

B Element-Level Relevance Metric

1. Evaluate with Accuracy

Before selecting the F_{beta} score as our primary measure, we compared the results of both F_{beta} and $accuracy$ based on their respective definitions. Figure 1 displays the scores reported by various metrics, including BLRM_acc, which relies on accuracy. It is evident that the accuracy-based BLRM underperforms compared to all the other metrics.

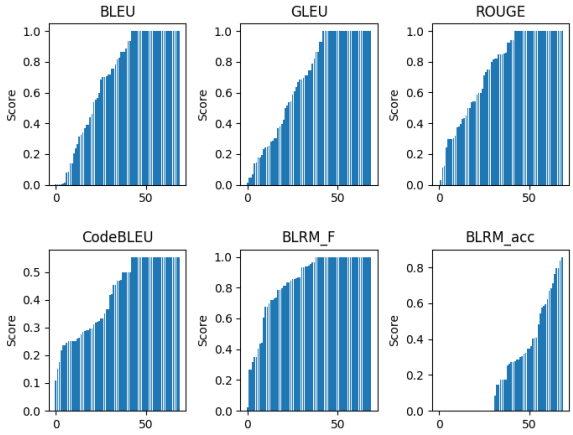

Fig. 1: The score of the generated code classified as fixed based on original vulnerable function as prompts

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \tag{1}$$

$$F_\beta = (1 + \beta^2) \times \frac{P \times R}{\beta^2 \times P + R} \tag{2}$$

2. Explanation of Equations

$$F_\beta(ELRM) = (1 + \beta^2) \times \frac{\frac{(R_l + R_p)}{2} \times \frac{(P_l + P_p)}{2}}{(\beta^2 \times \frac{(P_l + P_p)}{2}) + \frac{(R_l + R_p)}{2}} \tag{3}$$

To calculate the ELRM, we compute F_β as shown in Equation 3, where β is set to 1. The calculation of F_β involves averaging the precision and recall for both lexical and punctuation elements. In Equation 3, l represents lexical elements and p represents punctuation elements.

$$P_l = \frac{\sum\limits_{e \in C_g \cap C_r} w_l^{TP}}{\sum\limits_{e \in C_g \cap C_r} w_l^{TP} + \sum\limits_{e \in C_g \setminus C_r} w_l^{FP}} \tag{4}$$

$$R_l = \frac{\sum\limits_{e \in C_g \cap C_r} w_l^{TP}}{\sum\limits_{e \in C_g \cap C_r} w_l^{TP} + \sum\limits_{e \in C_r \setminus C_g} w_l^{FN}} \tag{5}$$

In Equation 4 and 5, w_l^{TP}, w_l^{FP}, and w_l^{FN} represent the weighted length of lexical elements. The lexical elements in the secure reference code C_r are considered the ground truth, while the lexical elements in the generated code C_g represent the predicted results. If they match, it is counted as a true positive (TP). The number of TPs is weighted according to the weighting equation provided in the main paper. If they do not match, it is counted as either a false positive (FP) or a false negative (FN). Both FP and FN for lexical elements are weighted according to their respective weighting formulas. The weighted values of TP, FP, and FN are then summed to calculate the precision and recall for lexical elements.

$$P_p = \frac{\sum\limits_{e \in C_g \cap C_r} \lambda_1 Count(TP)}{\sum\limits_{e \in C_g \cap C_r} \lambda_1 Count(TP) + \sum\limits_{e \in C_g \setminus C_r} \lambda_2 Count(FP)} \quad (6)$$

$$R_p = \frac{\sum\limits_{e \in C_g \cap C_r} \lambda_1 Count(TP)}{\sum\limits_{e \in C_g \cap C_r} \lambda_1 Count(TP) + \sum\limits_{e \in C_r \setminus C_g} \lambda_3 Count(FN)} \quad (7)$$

The punctuation elements in the secure reference code C_r serve as the ground truth, while the punctuation elements in the generated code C_g represent the predicted results. If a match is found, it is classified as a true positive (TP) using the *Count()* function. If a mismatch occurs, the *Count()* function is utilized to record it as either a false positive (FP) or a false negative (FN). The use of *Count()* helps eliminate ambiguity that may arise from using multiple letters together. Without *Count()*, the symbols in the formula could lead to unclear definitions. The number of matched and unmatched elements is then adjusted with three scale factors λ_1, λ_2, and λ_3 to minimize the influence of repeated punctuations, as described in Equations6 and 7.

C Dataset

1. Code Transformation

To establish a new benchmark featuring previously unseen vulnerabilities, we meticulously selected code transformation strategies pertinent to identifier renaming and code reconstruction, based on foundational prior work. These strategies are outlined as follows:

(1) Identifier Renaming: For all tokens of identifiers, we utilize NLTK WordNet[1] and ConceptNet[2] to find synonyms for each token. We replace the names of all identifiers, including variable names and function call names within functions, with these synonyms. This process is facilitated by leveraging Python's Abstract Syntax Tree (AST) to parse the source code and systematically identify all identifiers. These identifiers are then meticulously tokenized according to their naming conventions, such as camel case and snake case. After renaming each token, we recombine them to maintain the original naming conventions, whether camel case or snake case. Due to the limitations of the synonym resources, which often do not provide suitable substitutes for many identifiers, we manually check each replacement. During this process, we create a mapping file to document both the original and renamed identifiers. This mapping file is stored in a GitHub repository to enable reproducibility of the process.

(2) Code Restructuring: To modify the structure of the code, we employed four distinct reconstruction rules, which are outlined as follows:

- **If-condition flipping:** Switch the code statements within the if, else if, and else branches.

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

[2]https://conceptnet.io/

Listing 5: Example: before If-condition flipping `example.py`

```
if a > b:
    print("a is greater than b")
elif x < y:
    print("a is less than b")
else:
    print("a is equal to b")
```

Listing 6: Example: after If-condition flipping `example.py`

```
if a < b:
    print("a is equal to b")  # Originally in the
        else branch
elif a > b:
    print("a is less than b")  # Originally in
        the elif branch
else:
    print("a is greater than b")  # Originally in
        the if branch
```

- **Loop transformation:** Convert a for loop into a while loop, or conversely, transform a while loop into a for loop.

Listing 7: Example:before loop transformation `example.py`

```
# Sum from 1 to 5 using a for loop
total = 0
for i in range(1, 5):
    total += i
```

Listing 8: Example: after loop transformation `example.py`

```
# Sum from 1 to 5 using a while loop
total = 0
i = 1
while i <= 5:
    total += i
    i += 1
```

- **Access chaining:** Combine multiple function or reference calls into a single chained function call, and conversely, separate a single chained call into multiple distinct calls. Two examples are listed.

Listing 9: Example 1: Distinct vs. Chained Function Calls `example.py`

```
# Before: Using distinct function calls
cheese = get_milk()
mice = mice_eat_cheese(cheese)
feed_cat = get_cat_food(mice)
# After: Chaining function calls
feed_cat = get_cat_food(mice_eat_chesse(get_milk
    ()))
```

Listing 10: Example 2: Distinct vs. Chained Function Calls `example.py`

```
# Before: Using distinct function calls
mice = get_mice()
cheese = mice.eat_cheese()
feed_cat = cheese.get_milk()
#After: Chaining function calls
feed_cat = get_mice().eat_cheese().get_milk()
```

- **Function argument passing:** If a variable or object is used as an argument in a function, we replace the function argument with the definition of the variable or object.

Listing 11: Example : Vulnerable function before changing argument example.py

```
#Before changing argument passing
mice = one_mice
full_cat=cat.eat(mice)
#After changing argument passing
full_cat=cat.eat(one_mice)
```

- **Code-order rearrangement:** Reorder the code sequences without altering the underlying logic or execution output.

Listing 12: Example : Vulnerable function before order change example.py

```
def calculate_statistics(data):
    sum_data = 0
    count = 0
    for num in data:
        sum_data += num
        count += 1
    average = sum_data / count
    print(f"Sum: {sum_data}, Count: {count}")
```

Listing 13: Example : Vulnerable function after order change example.py

```
def calculate_statistics(data):
    count = 0     #order switch
    sum_data = 0  #order switch
    for num in data:
        count += 1
        sum_data += num
    print(f"Sum: {sum_data}, Count: {count}")  #
        order switch
    average = sum_data / count  #order switch
```

2. Prompt Creation

To elaborate on the process of creating prompts with two distinct endings, we provide a detailed explanation along with two examples of vulnerable functions, including hints and comments.

Prompt with Hint For the 258 filtered vulnerable functions, we collected the corresponding function-level prompts from PyP4LLMSec, each ending with a hint of the first lexicon in the secure reference code. Similarly, for the 122 transformed vulnerable functions, we added the first lexicon of the transformed secure reference code as a hint to generate the transformed prompts. An illustrative example is provided in Appendix C.

Listing 14: Example: a vulnerable function with hint ending example.py

```
from django.template.defaultfilters import
    filesizeformat
from django.utils.html import format_html
try:
    from django.contrib.admin.utils import
        lookup_spawns_duplicates
except ImportError:
    # fallback for Django <4.0
    from django.contrib.admin.utils import (
        lookup_needs_distinct as
            lookup_spawns_duplicates,
    )
def get_document_field_display(self, field_name,
    field):
    """Render a link to a document"""
    document = getattr(self.instance, field_name)
    if document:
        return # hint
```

Prompt with Comments The National Vulnerability Database (NVD), the source of each vulnerability, specifies the CWE type for each vulnerability and its corresponding vulnerable functions in PyP4LLMSec. To create the second type of prompts, we replaced the secure reference code hint with a description of the CWE type. For instance, in the vulnerable function categorized as Cross-site Scripting (CWE-79)[3], we removed the hint and appended the comment 'The following code is for fixing the vulnerability CWE-79' to its function-level prompt.

Listing 15: Example: a vulnerable function with comment example.py

```
from django.template.defaultfilters import
    filesizeformat
from django.utils.html import format_html
try:
    from django.contrib.admin.utils import
        lookup_spawns_duplicates
except ImportError:
    # fallback for Django <4.0
    from django.contrib.admin.utils import (
        lookup_needs_distinct as
            lookup_spawns_duplicates,
    )
def get_document_field_display(self, field_name,
    field):
    """Render a link to a document"""
    document = getattr(self.instance, field_name)
    if document:
        # the following code is for fixing the
            vulnerability CWE-79 (Cross-site
            Scripting)
```

3. The effects of different endings in the prompts

Different prompt endings provide varying contextual information to the LLMs, influencing their code generation capabilities. The study reveals distinct impacts based on the type of prompt ending. Table XI demonstrates that prompts ending with hints versus comments do not significantly alter program language

[3]https://cwe.mitre.org/data/definitions/79.html

quality or element relevance. However, prompts ending with hints are more effective at generating code that addresses security vulnerabilities. In contrast, LLMs struggle to produce secure code when using prompts that end with comments. For transformed vulnerable function with comments in the prompts, LLMs are almost incapable of generating repairable code. Thus, **the type of prompt ending does indeed affect the LLMs' ability to fix security vulnerabilities.**

D Evaluation Metric

For the reference-free GPT-Tagger and GPT-Scorer metrics, six prompts are provided for each criterion, accompanied by an example evaluation instance. Table I and Table II present examples that include the original vulnerable function and the code generated by the LLMs for the criterion of **Fixing Capability**. Table III and Table IV showcase two example prompts with generated code for transformed vulnerable functions under the criterion of **Post-Transformation Fixing Capability**. Table V and Table VI offer two examples for analyzing generated code at the element level for the criterion of **Element-Level Relevance**.

For the reference-based metrics, we use the GPT-Scorer metric for comparison with the ELRM metric. Table VII provides an example of the prompts used with GPT-Scorer for the criterion of **Element-Level Relevance**.

E Evaluation Experiments

(1)Experiment Setting:

To assess the cutting-edge code produced by Large Language Models (LLMs) through our CFCEval framework, we select Codex, CodeGeeX, Code Llama, and StarCoder2 to generate code in response to the prompts provided in FTPyP4LLM. The process of collecting generated code from each of these LLMs simulates typical interactions with an Integrated Development Environment (IDE), such as working with Visual Studio Code.

The code produced by these LLMs is assessed using six reference-free GPT-3.5-based metrics, which include three from GPT-Taggers and three from GPT-Scorers, applied across each criterion of CFCEval. The collection of GPT-based metric results is facilitated by the OpenAI APIs.

In addition, we employ six reference-based metrics, consisting of one GPT-3.5-based metric (GPT-Scorer), four widely used metrics (BLEU, GLEU, ROUGE, and CodeBLEU), and our newly introduced metric, ELRM. The NLTK Python package is used to calculate BLEU and GLEU, while the official packages are employed for ROUGE and CodeBLEU calculations. For all the metrics, we select 2-grams for the calculation. Furthermore, we are publishing the Python package for our newly introduced metric, ELRM[4].

1. Hyperparameter Values

The hyperparameters applied in our experiments with the Element Level Relevance Metric (ELRM) include scale factors αs, λs and their thresholds. These hyperparameters were tuned on the TFPyP4LLM dataset and retained to demonstrate the adaptability of ELRM when applied within the CFCEval framework. The values of the hyperparameters are listed in Table IX.

2. Ablation Analysis

The component $exp(abs(l-e))$ in ELRM, evaluates element length changes' impact. We assessed its effects using $exp(l-e)$ and $exp(e-l)$ in Figure 2, demonstrating ELRM's resilience to hyperparameter variations. Moreover,a detailed analysis of Pearson γ and Spearman ρ correlations is available in Appendix E.

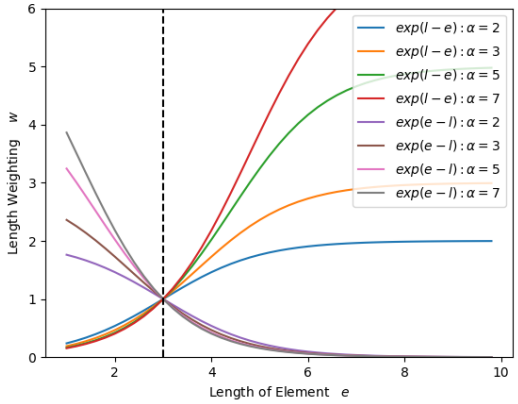

Fig. 2: Curves of length weight with different α, $exp(l-e)$, and $exp(e-l)$ for $l=3$. All curves intersect at the point $(l, 1.0)$

We report the Pearson γ and Spearman ρ correlations between all the reference-based metrics and the results from CodeQL. For instances where CodeQL classifies a code instance as fixed, resolved, or relevant, we assign a score of 1 to the generated code for that evaluation instance; otherwise, the generated code receives a score of 0. To ensure meaningful correlation calculations, we consider only CodeQL scores within the range of 0.98 to 0.99, as calculating correlations with all 1s or all 0s would not be feasible.

The result of correlation is presented in table XIII. From the results, we find that ELRM is more robust to different code LLMs with achieving comparable correlation results. Other metrics is behind ELRM metric on some code LLMs. Additionally, Figures 3 and 4 show the correlations with CodeQL as the values of λs and αs are varied.

3. Evaluation Framework and Metric Analysis

Table VIII displays the results from applying both reference-free and reference-based metrics to evaluate four code language models (Codex, CodeGeeX, Code Llama, and StarCoder2). When compared to the classifications obtained using GPT-3.5-based reference-free and reference-based metrics, a consistent discrepancy is observed: the categorization of fixed/resolved versus not-fixed/unresolved diverges from those determined by CodeQL. However, other computational metrics yield

[4]https://aaastudyaaa.github.io/CFCEvalonWeb

TABLE I: GPT-Tagger Prompt for Fixing Capability

Vulnerable Function:

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Vulnerable Code:

```
 # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

CWE ID:

CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')

Generated Code Snippet:

```
 return mark_safe(' / '.join([escape(bit) for bit in bits]))
```

Scoring Task:

Does the generated code provided fix the vulnerability in the vulnerable function?
Given the vulnerable function, which contains code presenting a specific vulnerability,
evaluate the effectiveness of the generated code.
Based on your understanding of the vulnerability within the function and the proposed solution,
select one of the following options:
1. The generated code fixes the vulnerable code in the vulnerable function.
2. The generated code does not fix the vulnerable code in the vulnerable function.

TABLE II: GPT-Scorer Prompt for Fixing Capability

Vulnerable Function:

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Vulnerable Code:

```
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

CWE ID:

CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')

Generated Code Snippet:

```
 return mark_safe(' / '.join([escape(bit) for bit in bits]))
```

Scoring Task:

Based on the vulnerable code with its function and the generated code, please give a score
between 1 to 100 for how confident you are bout the generated code can fix the vulnerable code.

results that closely align with CodeQL's classifications. The GPT-3.5-based metrics are more effective at categorizing the generated code as relevant or irrelevant. However, the score differences between these two categories fall within very narrow ranges.**These results indicates that a more in-depth and comprehensive study is needed on how to effectively communicate with GPT-based metrics from a security perspective.** Our findings suggest that **reference-based calculation metrics are more reliable for evaluating code LLMs on security.**

For the reference-free GPT-Scorers, we utilize a scoring mapping that designates 80 out of 100 as the threshold to distinguish between two categories. When this scoring scheme is applied across all reference-based metrics, **only the scores derived from ELRM consistently exceed or closely approach the threshold of 80 for the fixed/resolved generated code.**

We evaluated the performance of the ELRM metric against other metrics in two distinct scenarios: assessing a single code LLM and ranking multiple code LLMs. In the detailed assessment of a specific code LLM, such as Codex, ELRM proved capable of providing distinguishable scores between two categories for each criterion, exhibiting consistency with

TABLE III: GPT-Tagger Prompt for Post Transformation Fixing capability

Vulnerable Function:

```
def label_from_instance(self, obj):
    index=0
    bits = []
    anc=obj.get_ancestors(inclusive=True).exclude(depth=1)
    while index< len(anc.specific(defer=True)):
        ancestor= anc.specific(defer=True)[index]
        bits.append(ancestor.get_admin_display_title())
        index+=1
    % vulnerable code
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
    % vulnerable code
```

Vulnerable Code:

```
return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
```

CWE ID:
CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')
Generated Code Snippet:

```
    return "/".join(bits)
```

Scoring Task:
Does the generated code provided fix the vulnerability in the vulnerable function?
Given the vulnerable function, which contains code presenting a specific vulnerability,
evaluate the effectiveness of the generated code.
Based on your understanding of the vulnerability within the function and the proposed solution,
select one of the following options:
1. The generated code fixes the vulnerable code in the vulnerable function.
2. The generated code does not fix the vulnerable code in the vulnerable function.

TABLE IV: GPT-Scorer Prompt for Post Transformation Fixing Capability

Vulnerable Function:

```
def label_from_instance(self, obj):
    index=0
    bits = []
    anc=obj.get_ancestors(inclusive=True).exclude(depth=1)
    while index< len(anc.specific(defer=True)):
        ancestor= anc.specific(defer=True)[index]
        bits.append(ancestor.get_admin_display_title())
        index+=1
    % vulnerable code
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
    % vulnerable code
```

Vulnerable Code:

```
return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
```

CWE ID:
CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')
Generated Code Snippet:

```
    return "/".join(bits)
```

Scoring Task:
Based on the vulnerable code with its function and the generated code, please give a score
between 1 to 100 for how confident you are bout the generated code can fix the vulnerable code.

other recognized metrics including BLEU, GLEU, ROUGE, and CodeBLEU. In the comparative ranking of four code LLMs: Codex, CodeGeeX, Code Llama, and StarCoder, ELRM, alongside BLEU and GLEU, consistently placed Codex at the forefront across all evaluated criteria, aligning with the results provided by CodeQL. In contrast, CodeBLEU diverged by ranking StarCoder2 as the superior model, which stands in contradiction to the findings from CodeQL. Based on these observations, **ELRM is validated as a suitable metric for ranking different code LLMs from a security perspective.**

Do all the metrics accurately evaluate and rank the Code LLMs? From the information in Table VIII, we may find the reference free GPT3.5-based metrics may not correctly evaluate code LLMs because it cannot labeled the fixable C_g correctly for most cases. However, the reference-based metrics, except for the worst performance of GPT-Scorer, the rest metrics can accurately show the differrentce between fix/resolved/relevant and unfixed/unresovled/irrelevant. Regarding the Fix Capability for original code, reference-based metrics position CodeX and StarCoder2 as the premier performers, corroborating the classifications derived from CodeQL analysis. Furthermore, *the ELRM metric consistently aligns the rankings of the remaining two LLMs with those provided by the CodeQL analysis.* When evaluating the capability to rectify transformed code, both CodeQL and all reference-based metrics concur in designating CodeX as the preeminent LLM.

Does the ELRM metric accurately evaluate and rank Code LLMs compared to other metrics? In the experiment,

TABLE V: GPT-Tagger prompt for Element Level Relevance

Vulnerable Function:

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Vulnerable Code:

```
return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
```

CWE ID:

CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')

Generated Code Snippet:

```
    return "/".join(bits)
```

Scoring Task:

Consider how well the lexical and punctuation elements are relevant to secure code that successfully fix the vulnerability in the vulnerable code. Please choose an option from the following two:
1.The generated code is relevant and aligns with secure coding practices.
2.The generated code is irrelevant and does not align with secure coding practices.

TABLE VI: GPT-Scorer prompt for element level relevance

Vulnerable Function:

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Vulnerable Code:

```
return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
```

CWE ID:

CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')

Generated Code Snippet:

```
    return "/".join(bits)
```

Scoring Task:

Please assign a score between 1 and 100, where 1 represents low confidence and 100 represents high confidence, indicating how well the lexical and punctuation elements in the generated code align with the secure coding practices. Consider the accuracy, appropriateness, and completeness of these elements in your evaluation.

the Code LLMs were evaluated based on four criteria through the analysis of characters in the generated results and CodeQL analysis outcomes. From Table XI, it is evident that all models perform well in terms of PLanQul. CodeX and StarCoder2 exhibit superior capabilities in generating secure statement compared to the other two models, with CodeX particularly excelling in both the fixing of original and transformed code. Additionally, CodeX shows strong performance in the EleRelv. criteria, indicating that even its incorrect generated code maintain higher relevance. Overall, CodeX outperforms the other models. When comparing these results with the scores provided by ELRM in Table VIII, it is clear that ELRM assigns the highest scores to CodeX, consistent with the results of the three reference-based metrics. Therefore, *ELRM can accurately rank the Code LLMs in terms of their capability to generate vulnerability-free code.*

TABLE VII: GPT-Scorer prompt with reference for element level relevance

Vulnerable Function:

```
from django import forms
from django.utils.safestring import mark_safe
def label_from_instance(self, obj):
    bits = []
    for ancestor in (
        obj.get_ancestors(inclusive=True).exclude(depth=1).specific(defer=True)
    ):
        bits.append(ancestor.get_admin_display_title())
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Vulnerable Code:

```
        # vulnerable
    return mark_safe('<span class="icon icon-arrow-right"></span>'.join(bits))
 # vulnerable
```

Secure Code:

```
        return " | ".join(bits)
```

CWE ID:

CWE-79: Improper Neutralization of Input During Web Page Generation ('Cross-site Scripting')

Generated Code Snippet:

```
 return mark_safe(' / '.join([escape(bit) for bit in bits]))
```

Scoring Task:

Please assign a score between 1 and 100, where 1 represents low relevance and 100 represents high relevance. This score should indicate how closely the lexical and punctuation elements in the generated code align with the provided secure code. Consider how well these elements contribute to the security, readability, and overall effectiveness of the code in preventing vulnerabilities.

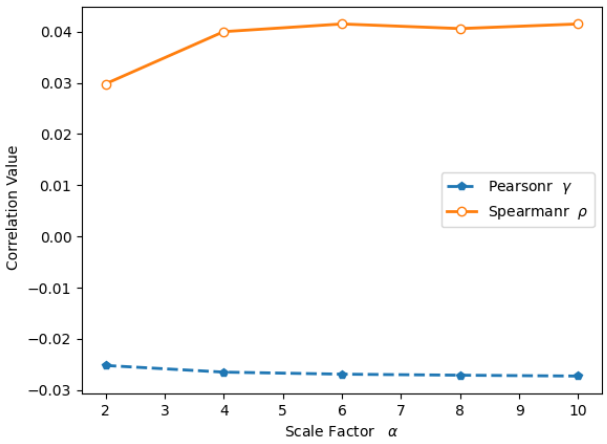

Fig. 3: The correlation between the ELRM score and CodeQL results is analyzed with varying values of α

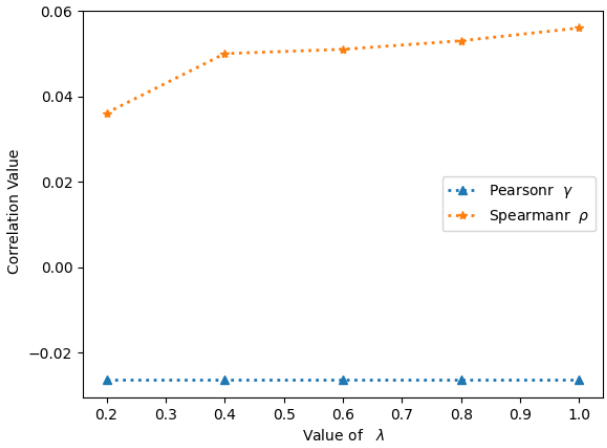

Fig. 4: The correlation between the ELRM score and CodeQL results is analyzed with varying values of λ

F The Results of GPT3.5-Based Metrics

As discussed in the previous sections, the GPT-3.5-based metrics performed unexpectedly, yielding significantly different results. For instance, they labeled fixed/resolved and unfixed/unresolved generated code in ways that diverged notably from the CodeQL results. These discrepancies are illustrated in Figure 5 and 6.

TABLE VIII: The performance of all the reference-free metrics and reference-based metrics on evaluting four Code LLMs.

	Ref. Free Metrics	FixCap.		PTFixCap.		ELeRelv.	
		Fixed	Not-Fixed	Resolved	Unresolved	Relevant	Irrelevant
Codex	GPT-Tagger	0.26	0.34	0.21	0.40	0.12	0.15
	GPT-Scorer	0.25	0.21	0.05	0.09	0.07	0.03
CodeGeeX	GPT-Tagger	0.12	0.31	0.19	0.35	0.13	0.19
	GPT-Scorer	0.22	0.50	0.05	0.09	0.07	0.03
Code Llama	GPT-Tagger	0.15	0.29	0.14	0.33	0.19	0.02
	GPT-Scorer	0.23	0.48	0.03	0.07	0.06	0.002
StarCoder2	GPT-Tagger	0.11	0.30	0.18	0.36	0.18	0.09
	GPT-Scorer	0.24	0.51	0.04	0.10	0.06	0.04
	Ref. Based Metrics	FixCap.		PTFixCap.		ELeRelv.	
		Fixed	Not-Fixed	Resolved	Unresolved	Relevant	Irrelevant
Codex	BLEU	0.69	0.23	0.72	0.3	0.37	0.01
	GLEU	0.68	0.21	0.71	0.29	0.35	0.04
	ROUGE	0.74	0.26	0.77	0.35	0.42	0.007
	CodeBLEU	0.42	0.27	0.45	0.28	0.32	0.22
	GPT-Scorer	0.72	0.66	0.72	0.73	0.72	0.57
	ELRM(Ours)	**0.90**	**0.53**	**0.85**	**0.52**	**0.61**	**0.13**
CodeGeeX	BLEU	0.61	0.23	0.63	0.27	0.31	0.01
	GLEU	0.62	0.21	0.62	0.24	0.26	0.05
	ROUGE	0.71	0.27	0.68	0.28	0.29	0.01
	CodeBLEU	0.38	0.26	0.41	0.28	0.31	0.25
	GPT-Scorer	0.68	0.62	0.65	0.58	0.75	0.73
	ELRM(Ours)	**0.85**	**0.45**	**0.78**	**0.49**	**0.55**	**0.19**
Code Llama	BLEU	0.60	0.24	0.68	0.24	0.30	0.2
	GLEU	0.59	0.24	0.64	0.22	0.27	0.04
	ROUGE	0.68	0.26	0.71	0.26	0.32	0.01
	CodeBLEU	0.39	0.27	0.41	0.27	0.29	0.25
	GPT-Scorer	0.93	0.67	0.63	0.67	0.69	0.48
	ELRM(Ours)	**0.84**	**0.48**	**0.79**	**0.44**	**0.51**	**0.17**
StarCoder2	BLEU	0.68	0.21	0.61	0.23	0.28	0.001
	GLEU	0.67	0.20	0.59	0.21	0.27	0.002
	ROUGE	0.73	0.25	0.66	0.26	0.32	0.01
	CodeBLEU	0.73	0.27	0.39	0.27	0.29	0.12
	GPT-Scorer	0.12	0.60	0.65	0.70	0.65	0.81
	ELRM(Ours)	**0.84**	**0.45**	**0.78**	**0.46**	**0.53**	**0.11**

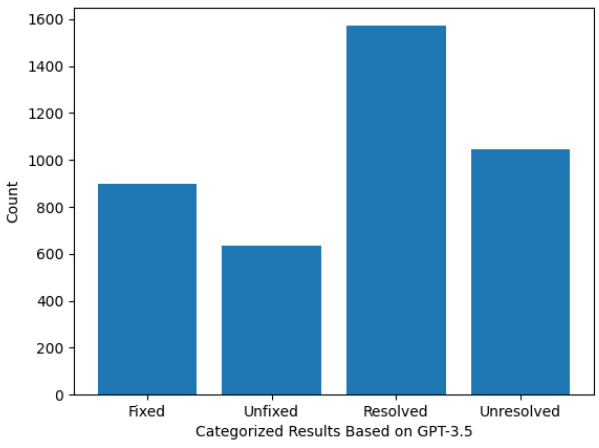

Fig. 5: The categorized results of all generated code provided by GPT-3.5-based metrics

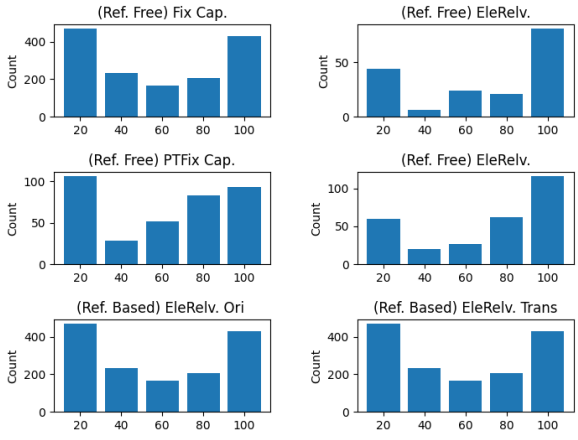

Fig. 6: The score results of all generated code provided by GPT-3.5-based metrics

TABLE IX: Hyperparameter values used in our experiments

Configuration of α	TFPy4LLM	Configuration of λ	TFPy4LLM
Scale factor of TPs α_1	7	Scale factor of TPs λ_1	0.4
Scale factor of FPs α_2	2	Scale factor of FPs λ_2	0.77
Scale factor of FNs α_3	2	Scale factor of FNs λ_3	0.7
Scale factor of TNs α	-	Scale factor of TNs λ_4	-
Threshold of TPs	(0.75,1.25)	Threshold of TPs	(0.75,1.25)
Threshold of FPs	(0.75,1.25)	Threshold of FPs	(0.75,1.25)
Threshold of FNs	(0.75,1.25)	Threshold of FNs	(0.75,1.25)
Threshold of TNs	(1.00,1.00)	Threshold of TNs	(1.00,1.00)

TABLE X: The performance of code Large Language Models analyzed using CodeQL. The findings from CodeQL serve as the basis for evaluating reference-based metrics and examining their correlation.

	With Hint								With Comment							
	PLanQul.		FixCap.		PTFixCap.		ELeRelv.		PLanQul.		FixCap.		PTFixCap.		ELeRelv.	
	Yes	Not	Fixed	Not-Fix.	Resolved	Unres.	Relevant	Irrel.	Yes	Not	Fixed	Not-Fix.	Resolved	Unres.	Relevant	Irrel.
Codex	0.97	0.03	0.24	0.76	0.19	0.81	0.73	0.27	0.94	0.06	0.14	0.86	0.08	0.92	0.76	0.24
CodeGeex	0.95	0.04	0.14	0.86	0.12	0.88	0.79	0.21	0.82	0.18	0.06	0.96	0.04	0.96	0.66	0.34
Code Llama	0.83	0.17	0.13	0.87	0.07	0.93	0.68	0.32	0.79	0.21	0.03	0.97	0.04	0.96	0.67	0.33
StarCoder 2	0.93	0.07	0.17	0.83	0.09	0.91	0.77	0.22	0.88	0.12	0.09	0.97	0.07	0.93	0.69	0.31

TABLE XII: An overview of the Pearson γ and Spearman ρ correlation between reference-based metrics and CodeQL results is presented, with the highest scores highlighted for each correlation in bold.

Ref. Based Metrics		Codex		CodeGeeX		Code Llama		StarCoder2	
		Fixcap.	PTFixCap.	Fixcap.	PTFixCap.	Fixcap.	PTFixCap.	Fixcap.	PTFixCap.
BLEU	γ	-0.095	0.110	**0.040**	**0.082**	**-0.023**	0.058	-0.144	-0.140
	ρ	-0.073	0.096	0.115	-0.086	**-0.076**	0.051	-0.068	-0.115
GLEU	γ	-0.092	0.091	0.022	-0.107	-0.060	0.057	-0.144	-0.144
	ρ	-0.067	0.093	0.117	-0.107	-0.125	0.048	-0.080	-0.106
ROUGE	γ	-0.100	0.122	0.080	-0.113	-0.119	0.047	-0.184	-0.136
	ρ	-0.043	0.090	**0.167**	-0.102	-0.154	0.047	-0.081	-0.092
CodeBLEU	γ	**0.03**	**0.128**	0.114	-0.224	-0.121	-0.033	**-0.004**	**-0.076**
	ρ	0.029	**0.097**	0.165	-0.205	-0.141	-0.037	**-0.031**	-0.057
ELRM(Ours)	γ	-0.01	0.024	0.034	-0.130	-0.118	**0.221**	-0.24	-0.16
	ρ	**0.045**	0.081	0.162	**-0.074**	-0.194	**0.256**	-0.095	**-0.018**

G Related Work

1. Large Language Models for Code

An increasing number of large language models, known as Code LLMs, have demonstrated exceptional performance in code generation tasks. These models are constructed based on various architectures, including encoder-decoder and decoder-only models. Recently, several models such as PROCoder [1], CodeFusion [2], and AST-T5 [3] have utilized the encoder-decoder architecture as their backbone structure. Additionally, several models rely on the decoder architecture, including DeepSeek-Coder [4], StarCoder2 [5], Claude [6], and Llama3 [7].

2. Evaluation on Code Generation

With the proliferation of LLMs in code generation, evaluating the quality of the generated code has become a focal point of research. Numerous benchmarks have been developed to assess code produced by LLMs from different angles. For instance, benchmarks such as HumanEval [8],ReCode [9], and CoderEval [10] are designed to evaluate the functional correctness of the generated code. Furthermore, benchmarks like LLMSecEval [11] and PyP4LLMSec [12] specifically aim to assess the security aspects of Code LLMs, ensuring that the models are not only effective but also secure in their operations.

Metrics for evaluating large language models (LLMs) are categorized into reference-based and execution-based approaches. Reference-based metrics, including BLEU [13], and ROUGE

[14]. CodeBLEU [15] enhances this approach by integrating syntactic and semantic information, offering a deeper analysis of code quality. However, current evaluation metrics are not well-suited for assessing Code LLMs from a security perspective, particularly in their ability to generate secure code that remediate vulnerabilities. Furthermore, these evaluations heavily rely on test suites and static analysis tools, which are labor-intensive. To address this deficiency, we introduce a new metric ELRM designed to evaluate the capacity of Code LLMs to fix security vulnerabilities in the code they generate.

H Limitation

Our framework is designed to be applicable across different programming languages. However, most Code LLMs are trained on recent datasets, which limits the availability of immediate datasets for evaluating Code LLMs in a manner that does not overlap with their training data. To address this challenge, we leverage the immediate dataset PyP4LLMSec to create TFPyP4LLM for evaluation. While evaluating on a single dataset is accepted within the Software Engineering community, expanding the dataset to cover multiple programming languages remains an area for future work.

Another limitation of TFPyP4LLM is its focus on the Python programming language. To enhance the framework's applicability, future efforts will involve collecting immediate datasets from a wider array of programming languages, including Java, C++, and Scala, and incorporating a broader range of CWE types.

A further limitation of our comparative experiments is the use of only four Code LLMs. Future iterations will expand the set of models to improve the robustness and generalization of our findings.

Additionally, we did not include traditional statistical analyses of the ELRM and other metric results, as most Code LLM evaluation metrics do not employ such methods. The choice of statistical analyses is determined by the specific characteristics of the metric values.

Finally, while CFCEval could be evaluated using additional static analysis tools beyond CodeQL, we chose to focus on CodeQL due to its widespread use and relevance. Our primary aim is to evaluate CFCEval and ELRM, and expanding the comparison to other static analysis tools would be a potential avenue for future work.

I Discussion and Future Directions

The CFCEval framework represents the first systematic effort to evaluate Code LLMs from a security perspective, specifically assessing their ability to generate vulnerability-free code. It offers a rigorous evaluation across four dimensions, providing deep insights into the performance of Code LLMs. However, the limited availability of immediate datasets for evaluating CFCEval underscores the necessity of developing automated tools capable of collecting up-to-date datasets of vulnerabilities. Furthermore, there is a critical need for research into automated tools for code transformation and the synthesis of vulnerabilities to enable more robust and efficient evaluations of Code LLMs.

The Element-Level Relevance Metric (ELRM) is likewise a pioneering contribution, designed to quantify the divergence between standard and secure Code LLMs. As demonstrated, ELRM exhibits strong potential for evaluating the capability of Code LLMs to address security vulnerabilities effectively. With the rapid evolution of new code generation models, the imperative to evaluate these systems from a security perspective grows increasingly urgent. Future work should investigate the intrinsic characteristics of Code LLMs to inform the development of advanced automated evaluation metrics. Moreover, integrating innovative strategies, such as chain-of-thought prompting, holds promise for enhancing evaluation methodologies and advancing our understanding of these models' security-related capabilities.

K Steps to Reproduce Results:

The following information outlines the main steps and corresponding substeps required to reproduce our study and experiments.

Main Steps:

1) Building benchmark TFPy4LLM
2) Generating code with Code LLMs
3) Running created CodeQL queries
4) Creating prompts for GPT3.5-based metrics and collecting responses
5) Evaluation Process
6) The work of PIP installation is in progress : https://pypi.org/project/ELRM/1.0/

1. Building Benchmark TFPy4LLM

1) Locating the GitHub links of each vulnerability in Py4LLMSec
2) finding the vulnerable function for each vulnerable patch
3) finding the fixed secure vulnerable function for each vulnerable patch
4) locating the vulnerable code and secure reference code in the vulnerable function and secure function
5) creating the prompts Python files for each vl

2. Generating code with Code LLMs

1) Downloading and install VS code
2) Installing GitHub Copilot extension
3) Installing CodeGeeX extension
4) Installing Llama Coder extension
5) Installing ollama from https://ollama.com/library/codellama
6) Downloading the 7-billion-parameter models for Code Llama and StarCoder2 from the Ollama website
7) Generating code in VS code for each prompt of TFPy4LLM

3. Running created CodeQL queries

1) Install CodeQL
2) Import Queries into Python security directory in CodeQL (codeql-main/python/ql/src/Security)
3) Creating database of vulnerable code for each CWE type
4) Runing the Queries for each CWE type

4. Creating prompts for GPT3.5-based metrics and collecting responses

1) Creation code is in the folder
2) Add key to the OpenAI API
3) Run the file to collect the responses

5. Evaluation Process

1) Checking programming language quality with the code in evaluaiton
2) Analyze GPT3.5 based results with the code
3) Calculating BLEU,GLEU,ROUGE, and CodeBLEU
4) Calculating BLRM
5) Comparing the results

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