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## A User-centred Evaluation of DisCERN: Discovering Counterfactuals for Code Vulnerability Detection and Correction

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#### Abstract

Counterfactual explanations highlight *actionable knowledge* which helps to understand how a machine learning model outcome could be altered to a more favourable outcome. Understanding *actionable* corrections in source code analysis can be critical to proactively mitigate security attacks that are caused by known vulnerabilities. In this paper, we present the Dis-CERN explainer for discovering counterfactuals for code vulnerability correction. Given a vulnerable code segment. DisCERN finds counterfactual (i.e. non-vulnerable) code segments and recommends actionable corrections. Dis-CERN uses feature attribution knowledge to identify potentially vulnerable code statements. Subsequently, it applies a substitution-focused correction, suggesting suitable fixes by analysing the nearest-unlike neighbour. Overall, DisCERN aims to identify vulnerabilities and correct them while preserving both the code syntax and the original functionality of the code. A user study evaluated the utility of counterfactuals for vulnerability detection and correction compared to more commonly used feature attribution explainers. The study revealed that counterfactuals foster positive shifts in mental models, effectively guiding users toward making vulnerability corrections. Furthermore, counterfactuals significantly reduced the cognitive load when detecting and correcting vulnerabilities in complex code segments. Despite these benefits, the user study showed that feature attribution explanations are still more widely accepted than counterfactuals, possibly due to the greater familiarity with the former and the novelty of the latter. These findings encourage further research and development into counterfactual explanations, as they demonstrate the potential for acceptability over time among developers as a reliable resource for both coding and training.

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*Keywords:* Counterfactual Explanations, Vulnerability Detection, Explainable AI

#### 1 1. Introduction

Security attacks that exploit hidden software code flaws pose serious risks 2 that compromise system performance and services. Therefore the ability to 3 detect these vulnerabilities in a timely manner as well as being able to de-4 tect potential flaws is a desirable feature that can help to avoid financial 5 and societal consequences. Application of AI for data-driven vulnerability 6 detection has increased significantly in recent years [1, 2]. This is mainly 7 due to the availability of large amounts of open-source code needed for train-8 ing vulnerability detection models. Traditional classifiers such as SVM and 9 Naive Bayes [3], as well as neural architectures for sequence modelling (e.g. 10 LSTMs), have been successfully used for code vulnerability classification [4]. 11 Given the structured textual nature of the data; these classifiers make use 12 of text representation methods from information retrieval [3] as well as deep 13 embedding techniques to represent software code [5]. 14

Once vulnerabilities are detected or classified into flaw categories, the 15 software needs to be fixed. Feature attribution methods enhance the trans-16 parency of AI model decisions by revealing the underlying reasoning for clas-17 sifying a code segment as vulnerable. It assigns a weight to each token of 18 the code which indicates how much it contributed to the AI model predic-19 tion (See examples in Figure 5). For example, authors of [1] used the feature 20 activation map of their convolutional neural model to highlight parts of the 21 code that contributed most to the AI model decision. Similarly authors of [6] 22 used LIME to highlight the contribution of code tokens towards vulnerabil-23 ity. The methods introduced in this paper address a gap in the current 24 approaches by focusing not only on identifying vulnerabilities but also on 25 providing corrections as a solution. Here we demonstrate how research in 26 counterfactual explanations can be conveniently adapted to generate code 27 correction operators to guide the fixing of vulnerable code segments that are 28 detected by a classification model. 29

Counterfactual Explanations for AI have accrued benefits from counterfactual thinking research from Psychology and GDPR guidelines for AI [7]. Counterfactuals reason with the inputs, the outputs, and the relationships between these to formulate a locally relevant explanation to convey how a

better or more desirable output (AI model decision) could have been achieved 34 by minimally changing the inputs. Questions concerning which part of the 35 input to modify and the appropriate methods for implementing such changes 36 to rectify code vulnerabilities are addressed in this paper. Here the input 37 is code segments and the proposed change relates to the code correction 38 operation. We present the DisCERN [8] algorithm, to locate the specific 39 area of vulnerability in a code segment, and to generate statement-level cor-40 rections using substitution operations. In contrast to previous work where 41 DisCERN was employed for identifying substitutions using similarity calcu-42 lations on tabular data, in this paper, substitutions are derived from code 43 snippets deemed similar but *non-vulnerable*. This is achieved by exploiting 44 similarity-driven pattern matching of pairs of code segments. 45

The utility of explanations in code vulnerability detection and correction 46 is best evaluated by the target users (i.e. developers). Accordingly, a user 47 study is performed to compare the effectiveness of counterfactuals from Dis-48 CERN in comparison to feature attribution explanations from LIME. The 49 goal is to understand how counterfactuals and feature attributions differ in 50 the application of code vulnerability detection and correction in terms of 51 shaping mental models, affecting cognitive load and explanation goodness 52 and acceptability. 53

<sup>54</sup> This paper makes the following contributions:

introduces the DisCERN Counterfactual Explainer as a tool for code vulnerability correction leveraging knowledge from feature attribution explainers and pattern matching to make correction recommendations (Section4);

demonstrates the generalisability of DisCERN across multiple programming languages in terms of validity and sparsity metrics (Section 5); and

establishes the effectiveness of counterfactuals compared to feature at tribution explanations for vulnerability detection and correction in a
 user study (Section 6).

The rest of the paper is organised as follows. Section 2 discusses the related work on vulnerability detection as a Machine Learning (ML) task and correction from the view of XAI. The introduction of the NIST Datasets and detection of code vulnerabilities using ML methods is presented in Section 3. Section 4 presents the DisCERN algorithm which discovers counterfactuals for vulnerable code segments and thereby guides the user to correct these vulnerabilities. The empirical evaluation and performance metrics with quantitative and qualitative results are presented in Section 5. Section 6 presents the user study that compares the utility of counterfactual vs feature attribution explanations. Finally, we draw conclusions in Section 7.

#### 75 2. Related Work

#### 76 2.1. Code Vulnerability Detection

The conventional approach to Code Vulnerability Detection (CVD) in-77 volved software and security experts auditing a software system for potential 78 security defects, bugs and weaknesses all of which are referred to as vul-79 nerabilities [9]. Automation of vulnerability detection of code is an active 80 applied research area where ML techniques are used for CVD [10, 11]. Early 81 ML methods for CVD focused on optimising feature extraction techniques 82 while neural network-based methods were used to learn semantic knowledge 83 from unstructured code to detect vulnerabilities [11]. Most recently, recur-84 rent networks [12], graph neural networks [13] and transformer-based lan-85 guage models [14, 15, 16] have been used for learning feature embeddings 86 from code for CVD. Many reviews in this research area provide comprehen-87 sive overviews of ML techniques for CVD while emphasising the scarcity of 88 explainability approaches [10, 17]. XAI can be harnessed to support CVD in 89 multiple ways. For instance, it can help explain how the model works, iden-90 tify the key features or variables that contribute to the detection process, 91 and provide insights into how to improve code and reduce vulnerabilities by 92 engaging humans in the loop. In this paper, we propose using the DisCERN 93 algorithm as a credible approach to address these issues. 94

#### 95 2.2. Code Vulnerability Correction

The conventional approaches to providing users with corrective feedback include rule-based [18, 19] and template-based approaches [20, 21]. Authors of [18] proposed to pre-configure corrections for specific vulnerabilities and reuse them as vulnerabilities are detected by their ensemble model in PHP code. Similarly, authors of [19] use pre-configured vulnerability matching rules and correction patterns for Java cryptography API code. Alternatively, sequence-to-sequence models have been trained to generate corrections [22].

<sup>103</sup> However, they are limited to a single programming language (C/C++) and <sup>104</sup> a vulnerability group (Buffer-overflow).

Our method is more closely related to work in [20] and [21] where the 105 methodology makes use of vulnerable and non-vulnerable code pairs to find 106 exemplar corrections. For each vulnerability in the code pair, they calcu-107 late edit operations and cluster them to find correction patterns. Discovered 108 patterns are saved as templates to reuse on new vulnerable code segments. 109 Their method captures a wider variety of corrections by identifying multiple 110 correction patterns per vulnerability group. These methods share the same 111 challenge as DisCERN which is once a correction example (in DisCERN) 112 or a template( others) is found, how to adapt it to match the target code. 113 DisCERN addresses this by selecting the corrections from the nearest unlike 114 neighbour, which does not always guarantee perfect adaptation. Template-115 based methods apply knowledge-intensive post-processing steps (such as cor-116 recting variable names to match target code) that are not generalisable to 117 different languages and vulnerabilities. 118

The main difference between existing work and ours is that DisCERN is 119 generating the corrections to explain the prediction of an AI model (ex-120 plaining the decision). Conversely, previous methods consider correction 121 generation to be an independent task and require a detection model that 122 classifies the exact vulnerability group. The difference is that DisCERN cor-123 rections are guided by the knowledge encapsulated in the AI model such as 124 what features/tokens contributed to the decision. DisCERN is also not re-125 liant on expert knowledge and heavily data-driven making it agnostic to the 126 detection-model and the programming-language. It also simplifies the task of 127 the detection AI model from a multi-class classification (up to 100+ classes) 128 problem to a binary-classification problem as the explainer does not require 129 the exact vulnerability group. 130

#### 131 2.3. Explainable AI in Vulnerability Detection

Research literature and regulatory guidelines emphasise the necessity for explanations of ML model decisions, as ML methods have increasingly become more opaque and difficult to interpret [23, 24]. This applies to code vulnerability detection and specifically towards prevention and or mitigation. Feature attribution explainers have been explored as a way to pinpoint code lines or segments that may have contributed to a *vulnerable* prediction by an ML algorithm. Authors of [25] describe the design of a human-in-the-loop

XAI system for vulnerability mitigation, whereby model predictions are ex-139 plained to forensic experts by way of feature attributions to enable them to 140 make necessary corrections. Authors of [26] explore the explanation needs 141 of target user groups of a code analyser to recognise two: a global expla-142 nation where the common behaviours of the tool are explained; and a local 143 explanation where feature attribution explains why a specific code snippet is 144 predicted to be vulnerable. Both explanations are targeted towards a knowl-145 edgeable audience of ML engineers. There are other works in similar areas 146 such as malware labelling in Android applications [27] and predicting phish-147 ing URLs [28] that also make use of feature attribution explanations. Authors 148 of [6] used LIME to explain vulnerability detection in C/C++ code when us-149 ing the Bidirectional LSTM model named VulDeePecker [12]. This paper 150 addresses a key gap in the literature by proposing the use of counterfactuals 151 not only for explaining detection but also for correcting vulnerabilities. Ac-152 cordingly, [6] is the most directly linked previous work we compared against 153 DisCERN in our user study. 154

#### 155 2.4. Explainable AI Techniques

Although there exists a broad range of explanation techniques and types [29] 156 our main emphasis is on factual and counterfactual explanations. The fac-157 tual explanation often answers the "what" or "why" questions by providing 158 empirical evidence to support a particular AI model outcome based on the 159 input provided [30]. This evidence can take the form of feature attribution 160 where each input feature is assigned an attribution towards the outcome or 161 example-based explanations where nearest neighbours are used to support 162 the outcome. In contrast, counterfactuals answer "Why-not" or "How-to" 163 questions by formulating a hypothetical scenario that has a *more desirable* 164 outcome [30]. In code vulnerability detection and correction, a factual expla-165 nation would highlight where the vulnerabilities exist within the code, while 166 a counterfactual explanation would help to demonstrate how to correct said 167 vulnerabilities. In this study, we investigate the use of the DisCERN algo-168 rithm for discovering counterfactual explanations and evaluate its effective-169 ness through a user study. The user study involves participants with varying 170 levels of expertise in code vulnerability detection and correction, allowing us 171 to assess the utility of the algorithm in a range of contexts. 172

```
public void method()
                                                      public void method()
Ł
                                                      ł
    int data;
                                                           int data;
    /* comment */
                                                           /* comment */
    data = (new SecureRandom()).nextInt();
                                                          data = 2:
    /* comment */
                                                           /* comment */
    int array[] = \{0, 1, 2, 3, 4\};
                                                          int array[] = { 0, 1, 2, 3, 4 };
    /* comment */
                                                           /* comment */
    if (data >= 0)
                                                           if (data >= 0 && data < array.length)</pre>
    {
                                                          ł
        IO.writeLine(array[data]);
                                                               I0.writeLine(array[data]);
    7
                                                          }
    else
                                                          else
    {
                                                           {
        IO.writeLine("Array index out of bounds"):
                                                               IO.writeLine("Array index out of bounds");
    }
                                                          }
}
                                                      }
                                                                   (b) Label: Non-vulnerable
               (a) Label: Vulnerable
```

Figure 1: Pre-processed code segments from the Java dataset

#### 173 3. Vulnerability Detection with NIST SAR Datasets

NIST Software Assurance Reference Dataset (SARD) Project promotes 174 the detection and correction of known security flaws in programming code. 175 The project maintains a publicly available repository of datasets from dif-176 ferent programming languages that are labelled for flaws and possible cor-177 rections. The flaws are standardised by the Common Weakness Enumera-178 tion (CWE) list which consists of software and hardware weaknesses. In this 179 work, we consider three datasets in Java, C and C# programming languages 180 from the NIST test suite <sup>1</sup>. 181

#### <sup>182</sup> 3.1. Preprocessing and Dataset Creation

In each dataset, code files are grouped under their CWE code and each file contains one or more functions (or methods in Java and C#). One function is *vulnerable* and often the remaining function is a proposed correction (i.e. non-vulnerable). We apply the following pre-processing steps to prepare each dataset for a binary-classification task:

 Split functions in a file that are *vulnerable* and those *non-vulnerable* into individual data instances. An instance (i.e. function) was labelled

<sup>1</sup>https://samate.nist.gov/SARD/testsuite.php



Figure 2: Java dataset statistics

*vulnerable* if it contains one or more comments that start with either *FLAW* or *POTENTIAL FLAW* and labelled as *non-vulnerable* if only contains comments that start with *FIX*.

Apply the following entity obfuscation steps to each function with the
 aim to prevent target leakage:

194 195

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192

(a) replace all comments with /\*comment\*/; and

196

(b) change all function signatures to public void method() (or language appropriate alternative).

Figure 1 presents two code segments from the Java dataset that were similar, one labelled as vulnerable and the other as non-vulnerable.

We present a detailed analysis of the class distribution of each dataset in Figures 2, 3 and 4. The left figure (Figure *a*) of each dataset shows that there are more *non-vulnerable* instances compared to *vulnerable* instances. Figure *b* on the right provides further analysis, examining the most frequent CWE codes (top 15) and the proportion of *vulnerable* and *non-vulnerable* instances for each code. Notably, there are no *non-vulnerable* examples for some CWE codes (example C# codes CWE313 and CWE94).

#### 207 3.2. Vulnerability Classification

Code data can be seen as a text that follows grammar rules defined by the respective Compiler. The most common Machine Learning (ML) pipeline for classification with text data is to use a Tokenizer (t) to transform the text data into a vector representation and then apply a classification algorithm (f)to learn from labelled data. In this work, we consider several standard vector representations and classifier combinations to compare the performance



Figure 4: C# dataset statistics

of commonly used black box models that detect vulnerabilities in code segments. We use 75/25 class stratified split to create 4 folds. For each fold, we train the model with 75% of the data and test with the remaining 25%. Table 1 presents the mean F1-score averaged across the four folds.

Overall we observe that BoW + Random Forest achieves the best perfor-218 mance for Java and C# datasets while CodeBERT classifier performs best 219 for the C dataset. It is noteworthy that the contributions of this paper are 220 model-agnostic, meaning that any combination of t and f should work with 221 DisCERN, including the most recent encoders such as CodeBERT [31]. Ac-222 cordingly, the focus of the paper is not on identifying the best classification 223 model, but rather to identify a model that performs well for experimental 224 purposes. Accordingly, XAI evaluations in Section 5 used the BoW + Ran-225 dom Forest as the detection pipeline for all three datasets. This allowed for 226 fairness and consistency across experiments and helped to observe the impact 227

Table 1: Class	affication Algorithms and	Performanc	e	
Tokenizer	Classifier	Dataset		
(t)	(f)	Java	С	C#
	Naive Bayes	0.7206	0.7284	0.7783
Tfjdf	kNN	0.9387	0.8457	0.9494
11-101	SVM	0.9574	0.8839	0.9723
	Random Forest	0.9722	0.8734	0.9844
BoW	Random Forest	0.9761	0.8790	0.9889
CodeBERT-base Tokerniser	CodeBERT classifier	0.9469	0.9484	0.9880

<sup>228</sup> of classification performance on the counterfactual generation.

# 4. DisCERN Counterfactuals for Vulnerability Detection and Cor rection

Code vulnerability detection decisions can be explained using different 231 types of explanations. As discussed in Section 2, it is commonly explained 232 using a factual explanation that uses feature attributions to explain the de-233 cision and it is often targeted to knowledgeable users. Given a code segment 234 that is labelled *vulnerable*, a factual explanation will point to the part of the 235 code segment which led the AI model to label it as *vulnerable*. An exam-236 ple factual explanation is shown in Figure 5a where text highlights indicate 237 vulnerable and non-vulnerable tokens in a Blue to Orange heat map scale. 238 For an expert, this type of explanation should be sufficient as they have the 239 knowledge to correct the vulnerability. In contrast, a counterfactual expla-240 nation in Figure 5b will compare the given code segment with a similar yet 241 non-vulnerable code segment and make recommendations on how to correct 242 the vulnerability. Accordingly we argue that counterfactual explanations are 243 more informative for both expert and non-expert users, and in support of 244 this claim, we present the DisCERN algorithm for generating counterfactual 245 explanations specifically for code vulnerability correction. 246

#### 247 4.1. Problem Definition

<sup>248</sup> Consider a query code segment x, with m number of statements where the <sup>249</sup>  $i^{th}$  statement is denoted by  $s_i$ . If the vulnerability detection pipeline used to



Figure 5: Examples of feature attribution and counterfactual explanations

predict the code vulnerability consists of a Tokeniser, t, and a classification model, f, the decision predicted for x is y.

For a given query x, having prediction, y = vulnerable, there are four steps to discovering *non-vulnerable* counterfactuals with DisCERN:

- 1. find the Nearest Unlike Neighbour (NUN),  $\hat{x}$  from the train dataset  $\mathcal{X}$ ;
- 255 2. for each token z in x, find the attribution weights, using a feature attri-256 bution explainer (in this work we use LIME);
- 257 3. given a vulnerable token, z, in x, find statements pairs for correction, 258 i.e. a list of statements in x and a list of candidate statements in  $\hat{x}$  as 259 a potential vulnerability correction;
- 4. create an updated code segment, x', by adapting the vulnerability correction and check x' for decision change using the vulnerability detection pipeline; and
- 5. repeat steps 3 and 4 until the detection pipeline predicts *non-vulnerable*.

Once the adapted code segment achieves the desired decision (i.e. nonvulnerable), it is identified as the counterfactual of the query. Next, we will explore each of these steps in detail.

#### 267 4.2. Finding the Nearest Unlike Neighbour

Given a query x, the NUN,  $\hat{x}$ , is the nearest instance found in the train 268 data with a different decision or label. In the context of counterfactual dis-269 covery, our query x is *vulnerable*. Selecting the NUN as the starting point, we 270 expect 1) to minimise the actionable changes needed to flip the prediction i.e. 271 with as few changes as possible; and 2) to preserve the original functionality 272 of the code segment while correcting vulnerabilities. As in Equation 2,  $\hat{x}$  has 273 n number of statements and the prediction is  $\hat{y}$ . Importantly,  $\hat{x}$  and x can 274 have different number of statements (i.e.  $n \neq m$ ) and should have different 275 decisions (i.e.  $\hat{y} \neq y$ ). 276

$$\hat{x} = [\hat{s}_1, \hat{s}_2, ..., \hat{s}_n] 
\hat{y} = f(t(\hat{x})) \mid \hat{y} \neq y$$
(2)

To find the NUN by similarity, it is necessary to use an encoder (E) to 277 transform code segments into a vector representation. This work used Code-278 BERT [31] to encode code segments. CodeBERT is based on the BERT [32] 279 architecture and is state-of-the-art for natural language code search and code 280 generation. It supports multiple programming languages making it most 281 suited for this task. More specifically, we use the pre-trained weights from 282 *codebert-base* shared in the Hugging Face repository  $^2$  which is trained using 283 bi-modal data (consisting of the code and its natural language description as 284 two modalities) from CodeSearchNet. 285

Given a code query, x, the encoder E generates a vector representation, 286 v, where the standard *codebert-base* encoding length, l, is 768 (Equation 3). 287 From the train data set  $\mathcal{X}$ , we filter data instances for which  $y_i \neq y$  and 288 create the subset  $\mathcal{X}'$ .  $\mathcal{X}'$  represents all the *non-vulnerable* code segments 289 that can be used to find a nearest-unlike-neighbour for x. Each data instance 290 in  $\mathcal{X}'$  is encoded using the encoder E to obtain the set of vectors  $\mathcal{V}'$ . We 291 use cosine similarity to find the NUN due to its robustness in comparing 292 high-dimensional data, and its output range of -1 to 1 allows for a clear 293 interpretation of similarity scores. We compute the cosine similarity between 294 the query x, and any other instance,  $x_i$  as in Equation 3. 295

<sup>&</sup>lt;sup>2</sup>https://huggingface.co/microsoft/codebert-base

$$v = E(x) \text{ and } v \in \mathbb{R}^{l}$$

$$cosine(x, x_{i}) = \frac{\sum_{j=1}^{l} v_{ij} v_{j}}{\sqrt{\sum_{j=1}^{l} v_{ij}} \sqrt{\sum_{j=1}^{l} v_{j}}}$$
(3)

Once the pair-wise similarity is computed (between x and each  $x_i$  in  $\mathcal{X}'$ ), we select the train instance  $x_i$  from the pair with the highest similarity as the NUN of x. In the rest of this paper, this function is referred to as nnwhich given, query, x, train subset,  $\mathcal{X}'$  and the similarity metric, returns the NUN,  $\hat{x}$ .

#### 301 4.3. Finding Feature Attribution Weights

Building upon counterfactual reasoning, DisCERN uses feature attribu-302 tion to reveal the most important code tokens or segments that contribute 303 to an outcome of *vulnerable*. By selectively substituting only these segments, 304 DisCERN can then identify the minimum changes needed to reverse that de-305 cision. The feature attribution explainers can provide the knowledge needed 306 for identifying the code segments that need to be substituted. Accordingly, 307 without loss of generalisability, this section describes the use of LIME ex-308 plainer to find feature attributions of the query to identify which parts of the 309 code had contributed to it being labelled as vulnerable. 310

LIME is a model-agnostic feature attribution explainer that creates an 311 interpretable model around a data instance to estimate how each feature 312 contributed to the black-box model outcome [33]. LIME creates a set of 313 perturbations within the query neighbourhood and labels them using the 314 black-box model. This newly labelled dataset is used to create a linear in-315 terpretable model (e.g. a linear regression model). The resulting surrogate 316 model is interpretable and only locally faithful to the black-box model (i.e. 317 correctly classifies the input instance, but not all data instances outside its 318 immediate neighbourhood). The new interpretable model is used to explain 319 the black-box model outcome of the query. The explanation is formed by 320 obtaining the linear model coefficients that indicate how each feature con-321 tributed to the outcome. 322

Our selection of LIME as the feature attribution explainer is motivated by the evidence from the literature. Authors of [6] proposed the use of LIME in the code vulnerability detection domain. Their evaluation demonstrated that the attributions correctly identify tokens that cause vulnerabilities. When

applying LIME in the context of code segment data, the *features* are the tokens identified by the Tokenizer, t, in the vulnerability detection pipeline. Accordingly, LIME can be used to understand the outcome of f(t(x)), by assigning an attribution, w, to each token which indicates how much the token contributes to the outcome.

$$LIME(x,t,f) \to \{w(z) \mid w(z) \in \mathbb{R}, z \in Z\}$$
(4)

If the vocabulary of code segments is Z, LIME assigns a weight w for each token  $z \in Z$  (Equation 4). A positive weight ( $w \ge 0$ ) indicates that the corresponding token contributes positively and a negative weight (w < 0) contributes negatively towards the outcome. We sort the weights using the partial order condition,  $\mathcal{R}$ , in Equation 5 to obtain the sorted list of tokens ordered from highest to lowest contribution towards the *vulnerable* outcome as Z'.

$$z_i \preceq_{\mathcal{R}} z_j \iff \mathcal{R} :: w(z_i) \ge w(z_j) \tag{5}$$

#### 339 4.4. Substitution Algorithm

Given a token, z, in the query code segment, the goal of the substi-340 tution algorithm is to find a matching list of statements in the query and 341 respective matches in the NUN to adapt the query such that it leads to a 342 changed decision (i.e. vulnerable to non-vulnerable). To the best of our 343 knowledge, existing feature attribution explainers identify the importance of 344 tokens instead of code statements or segments. Instead of modifying the 345 generic feature attribution explainers to operate at the statement level, we 346 use a post-processing step to find the matching statements in the query that 347 contains the token z, followed by a Pattern Matching (pm) algorithm to find 348 matching lists of statements as presented in Algorithm 1. This allows for 349 flexibility and compatibility of DisCERN with various existing attribution 350 explainers. 351

We use a simple lookup function to identify all code statements (S')352 in the (adapted) query x', that contain the token z (Line 1). The next 353 steps (Lines 2-5) of finding the vulnerable statements and their replace-354 ments from NUN are based on the hypothesis that if a statement  $s_i$  in S' is 355 vulnerable, it must be corrected in the NUN. Accordingly, for a statement, 356  $s_j$ , in S', first, we use a Pattern Matching algorithm to find a matching 357 list of statements  $s'_{[i:i]}$  from x' and  $\hat{s}_{[v:w]}$  from  $\hat{x}$ . Here, the subscripts indi-358 cate the start and end indices of the list of statements and  $s_i$  is found within 359

Algorithm 1 substitute	
<b>Require:</b> $x' = [s'_1, s'_2,, s'_m]$ : (adapted)	query
<b>Require:</b> $\hat{x} = [\hat{s}_1, \hat{s}_2,, \hat{s}_n]$ : NUN as a l	ist of statements
<b>Require:</b> $z$ : token in the query	
1: $S' \leftarrow [s \in x' \mid z \in s]  \triangleright \text{ find the list}$	t of statements in $x'$ that include $z$
2: for $s_j \in S'$ do	
3: $s'_{[i:k]}, \hat{s}_{[v:w]} \leftarrow pm(s_j, [s'_1, s'_2,, s'_m])$	$, [\hat{s}_1, \hat{s}_2,, \hat{s}_n])$
4: $c_j = cosine(E(s'_{[i:k]}), E(\hat{s}_{[v:w]}))$	$\triangleright$ calculate similarity
5: end for	
6: $(s', \hat{s}) \leftarrow \arg \max c_j$	$\triangleright$ select maximum similarity pair
$(s'_{[i:k]}, \hat{s}_{[v:w]})$	
7: $x' \leftarrow replace(x', s', \hat{s})$	$\triangleright$ replace $s'$ in $x'$ with $\hat{s}'$
8: return <i>x</i> ′	$\triangleright$ return the newly adapted query

 $s'_{[i:k]}$  (Line 3). A pattern-matching algorithm like the Gestalt Pattern Matching or Levenshtein Edit Distance can find the changes required to transform one string to another where the types of edits are *replace*, *delete* and *insert*. This paper used the Gestalt Pattern Matching algorithm implemented by cdifflib Python package <sup>3</sup>. We consider consecutive lists of statements rather than individual statements to preserve the grammatical structure of the programming language as closely as possible.

Next, we calculate the similarity between the two lists of statements using 367 Cosine similarity (Line 4). Similar to Section 4.2 we use the *codebert-base* 368 encoder to transform the list of statements to a vector representation and 369 calculate the cosine similarity. Once we have all the  $(s'_{[i:k]}, \hat{s}_{[v:w]})$  pairs, and 370 their similarities,  $c_i$ , we select the pair,  $(s', \hat{s})$ , that has the maximum sim-371 ilarity (Line 6). We assume a vulnerable code segment and its corrected 372 counterpart are different yet carry some similarities. Accordingly, by select-373 ing the pair with the highest similarity from the remaining, we expect to 374 discard those suggested by pm that are not vulnerability corrections. Note 375 that pm only returns edit operations, not exact matches, hence the similarity 376 score between a pair is always < 1. Finally, in Line 7 we replace the list of 377 statements s' in x' with the list of statement  $\hat{s}$  to return the new adapted 378 query. 379

<sup>3</sup>https://github.com/mduggan/cdifflib

#### 380 4.5. DisCERN Algorithm

#### Algorithm 2 DisCERN Algorithm

**Require:**  $x = [s_1, s_2, ..., s_m]$ : query as a list of statements **Require:** f(t(.)): vulnerability detection pipeline **Require:** sim: similarity metric, default is cosine similarity **Require:**  $\mathcal{X}$ : train dataset **Require:** y = f(t(x)): black-box prediction for the query 1:  $\mathcal{X}' \leftarrow \{x_i \in \mathcal{X} \mid y_i \neq y\}$  $\triangleright$  filter the train dataset 2:  $\hat{x} \leftarrow nn(x, \mathcal{X}', sim)$  $\triangleright$  find the NUN 3:  $\{w(z)\} \leftarrow LIME(x, t, f)$ ▷ feature attributions 4:  $Z' \leftarrow \mathcal{R}(\{w(z)\})$  $\triangleright$  tokens sorted by  $\mathcal{R}$ 5: Initialise x' = x and y' = yfor  $z \in Z'$  do  $\triangleright$  for each token in the sorted list 6:  $x' \leftarrow substitute(x', \hat{x}, z)$  $\triangleright$  Algorithm 1 7: y' = f(t(x')) $\triangleright$  predict decision for the adapted query x'8: 9: if  $y' \neq y$  then  $\triangleright$  check if the decision is changed 10:Break  $\triangleright$  stop substitutions if decision is changed end if 11: 12: end for 13: return x' $\triangleright$  return the adapted query as the counterfactual

DisCERN (Algorithm 2) brings together Sections 4.2 to 4.4 to discover 381 counterfactuals for vulnerable code. Given the query x, and the train dataset 382  $\mathcal{X}$ , in Lines 1 and 2 we find the NUN as discussed in Section 4.2. Next, 383 we find the LIME feature weights for the query and sort it to obtain the 384 list of tokens that indicate which parts of the code contributed to the cur-385 rent decision (Line 3 and 4, Section 4.3). We iterate over the sorted list of 386 tokens where for each token we find corresponding statements and substi-387 tutions (from Algorithm 1) until the prediction is changed (Line 8). Here 388 the prediction for the adapted query x' is obtained using the original clas-389 sification pipeline f(t(.)). The iteration is terminated when a prediction is 390 changed and the algorithm returns the adapted query x' as the counterfac-391 tual for the query x. Compared to DisCERN for tabular data [8] the key 392 novelty is the substitution algorithm that aims to preserve programme lan-393 guage syntax and original functionality while correcting the vulnerabilities. 394 However, the outcome of, the substitution algorithm is dependent on the 395

Nearest-Unlike-Neighbour and does not always guarantee to find a counterfactual from the NUN. Accordingly, in the worst-case scenario, DisCERN iterates through all tokens in Z' and may fail to lead to a desirable decision change (of *non-vulnerable*) even after all corrections are actioned on the query.

#### 401 5. Evaluation

This section presents the evaluation of the counterfactual DisCERN algorithm for vulnerable code correction. To the best of our knowledge, there are no existing algorithms in the literature for counterfactual discovery in the code vulnerability correction domain to compare performance with other methods.

407 5.1. Performance Metrics

DisCERN algorithm is evaluated using the three NIST datasets (Section 3); in each dataset, we only use *vulnerable* test data instances for the XAI evaluations. The following metrics are used to measure the performance.

• Validity measures the percentage of data for which the algorithm successfully finds a counterfactual [34, 35, 8]. At this stage, the requirement for a counterfactual discovered by an algorithm is to achieve a *positive* change of decision <sup>4</sup>. Given the set of test instances that were predicted *vulnerable* are  $X_v$ , and the subset for which the algorithm found a counterfactual is  $X_v^c$ , the validity is calculated as in Equation 6. A higher percentage of validity is desirable.

$$Validity = \frac{|X_v^c|}{|X_v|} \times 100 \tag{6}$$

• Sparsity measures the mean number of statements that were changed (i.e. (i.e. cost) for a change in decision [34, 35, 8]. Given the cost for each test instance in  $X_v^c$  is  $[r_1, r_2, ..., r_N]$ , where  $N = |X_v^c|$ , the sparsity is calculated as in Equation 7. In Algorithm 1, the number of statements changed for replace, delete and insert operations are calculated as max(k-i, w-v),

<sup>&</sup>lt;sup>4</sup>A more stringent metric would be to evaluate if the change conforms to grammar rules of the Language Compiler, which we will explore in future work.

k-i and w-v respectively. As such, the cost of a test instance is determined by aggregating the number of statement changes that correspond to the applied operations. In other domains, lower sparsity is preferred, however, in this domain, we hypothesise sparsity is not directly correlated to the algorithm performance as a vulnerability correction could require adding more statements. This will be discussed further with empirical results in Section 5.2.

$$Sparsity = \frac{1}{N} \sum_{j=1}^{N} r_j \tag{7}$$

There are other metrics used in counterfactual evaluations such as proximity (measures the difference between the original and the substitution code segments) [34, 35, 8] and diversity (measures the difference between multiple counterfactuals) [34] which we did not find to be transferable to the code vulnerability correction domain.

435 5.2. Results

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Table 2 presents the performance evaluation results of DisCERN using the three NIST datasets. In addition to performance metrics, we also measure the mean number of statements in a query, nearest-unlike-neighbour and counterfactual which we found useful when discussing the performance of DisCERN.

Dataset	Validity (%) Sparsity	Mean no of statements in the			
		Query	NUN	CF	
Java	96.49	13.88	44.62	51.81	50.93
С	85.50	8.40	24.78	28.26	26.08
С#	97.55	13.16	27.67	33.96	33.44

Table 2: Validity and Sparsity of DisCERN

We observe that the validity is consistently below 100% across all datasets. The validity for the C dataset is significantly lower which means the C dataset queries were not able to find counterfactuals using DisCERN. This can be linked to a high ( $\sim 21\%$ ) classification error seen in the vulnerability detection pipeline. For example, the query can be misclassified as vulnerable

<sup>446</sup> or the adapted query can be continuously misclassified as *vulnerable*. It is <sup>447</sup> further validated by the Java and C# datasets showing validity consistent <sup>448</sup> with their classification pipeline performance.

Sparsity is measured as the number of changes that were required to 449 get the decision changed from *vulnerable* to *non-vulnerable*. Considering the 450 mean number of statements in the query (column 4), Java and C datasets 451 make less number of changes compared to C#. It is noteworthy that these 452 changes include *deletion* operations, thus it is not an indication of the length 453 of the counterfactual. When generating counterfactuals for tabular data, a 454 common goal is to minimise sparsity. However, when discovering counter-455 factuals for correcting code vulnerabilities we argue that lower sparsity is 456 not always desirable. In general, correcting vulnerabilities can be costly; for 457 example in Java, adding a try-catch-finally block surrounding a vulnerable 458 statement can add up to 4-10 lines based on the formatting styles (Allman 459 vs K&R). 460

Further analysis of the number of statements between NUN and the counterfactual shows the effectiveness of the DisCERN algorithm. The mean number of statements in a CF is consistently lower than that in the NUN indicating that DisCERN is in fact finding meaningful corrections instead of completely converting the query into its NUN. The consistently higher number of statements in CF compared to the Query further indicates the increased cost of correcting code vulnerabilities.

#### 468 5.3. Qualitative Analysis

While DisCERN aims to maintain syntactic integrity and preserve the originally intended code functionality, sparsity, and validity metrics do not specifically measure these aspects. As a result, we examined a selection of the generated counterfactuals to determine whether the proposed code adaptations can effectively address code vulnerabilities and to what extent they implement reasonable modifications without compromising functionality.

Consider the two illustrative Java code examples in Figures 6a and 6b 475 which were counterfactuals discovered by the DisCERN algorithm. In each 476 figure, the first two columns indicate the line numbers of the query and the 477 counterfactual; the third column uses addition and subtraction signs to in-478 dicate adaptation operations. In example 1, a replacement is proposed (i.e. 479 replace query lines 5-6 with NUN lines 5-12). With Example 2, the coun-480 terfactual proposes an insertion (i.e. insert new lines 4-6) and a replacement 481 (i.e. replace query lines 6-7 with NUN lines 9-13). Both sets of adaptations 482



Figure 6: DisCERN Counterfactual Examples

have maintained the grammatical structure of the Java language, however,
Example 1 is better at preserving functionality, because it ensures that the
original functionality of writing an empty line (originally line 6) even after
having introduced an *if* condition. In Example 2, DisCERN fails to preserve
the intended functionality in the original query line 7 (by failing to treat *data*as an array).

Both examples corroborate findings in Table 2 that code vulnerability correction can increase sparsity due to the insertion of additional statements. Overall, both evaluations indicate that DisCERN is a promising approach to discovering counterfactuals, however, to ensure comprehensive validity, further adaptation heuristics are needed to verify counterfactuals maintain the original functionality (e.g., apply unit testing if available).

#### 495 6. User Evaluation

The primary objective of this user study is to assess the effectiveness 496 of factual and counterfactual explainers in addressing code vulnerabilities, 497 specifically examining their utility for both experienced and novice develop-498 ers. While existing literature [25, 26, 27] highlights a focus on factual ex-499 planations (such as feature attributions) for knowledgeable users in the XAI 500 research, our hypothesis posits that counterfactual explanations may prove 501 more informative for both skilled and trainee developers aiming to correct 502 code vulnerabilities. Table 3 presents the user study protocol; enumeration 503

indicates the order in which the questions were presented; Green colour indicates content presented to the participant (code segment or explanation) and the protocol is grouped by different intents (Blue). The questionnaire was prepared to capture users' mental models before and after receiving explanations, as well as to evaluate the quality and acceptability of the explanations provided by the system for detecting and correcting code vulnerabilities.

Present code snippet
A priori mental model for detecting code vulnerabilities
Q1. Do you think the code snippet contains code vulnerabili- ties? Yes, No, Maybe
A priori mental model for correcting code vulnerabilities
Q2. If you answered yes, which lines would you change to Free text correct code vulnerabilities?
Q3. If you listed any lines, why do you think these lines contain Free text code vulnerabilities?
Present explanation (annotated or modified code snippet)
A posterior mental model for correcting code vulnerabilities
Q4. After seeing the explanation, which lines would you change Free text to correct code vulnerabilities?
Q5. If you changed your answer from before viewing the explanation, please mention why?
Measure goodness of the explanation for detection and correction
Q6. Did the explanation help you detect vulnerabilities? Yes, No
Q7. Did the explanation help you to identify the lines you Yes, No would change to correct code vulnerabilities?
Measure acceptability of the explanation
Q8. Did the explainer correctly annotate the parts of the code Yes, No, Partially that contain vulnerabilities?

The questionnaire was repeated with three different code snippets of dif-510 ferent lengths (11, 33 and 21 lines of code) to minimise bias. Snippets were 511 selected from the Java dataset over C and C# languages considering the 512 wider usage and familiarity within the target user group. All snippets con-513 tained a variant of the CWE-191:Integer Underflow vulnerability. To priori-514 tise the evaluation of the explanation over participant proficiency in detecting 515 various types of vulnerabilities, only one type of vulnerability was included 516 in the user study. 517

The hypothesis was evaluated with independent groups of participants 518 recruited through Amazon Mechanical Turk. One group received the ques-519 tionnaire together with DisCERN counterfactual explanations and the other 520 with LIME feature attribution explanations. From here on we will refer to the 521 two groups as DisCERN and LIME. The inclusion criteria for recruitment 522 were set as Employment Industry is Software and/or IT Services and Job 523 function is Information Technology to ensure the participants have a working 524 knowledge of programming languages. In 40 days, 95 and 103 submissions 525 were received for DisCERN and LIME groups respectively from which 78 526 and 68 were accepted. These submissions met the minimum requirements 527 where they attempted to answer at least one free-text question in addition 528 to all multiple choice questions (There were only 9 and 12 submissions for 529 DisCERN and LIME groups where participants answered all questions). 530

#### 531 6.1. A priori mental model - detecting code vulnerabilities

Q1 measures the a priori mental model for understanding how to detect 532 code vulnerabilities. There are 438 responses (78 + 68 participants responded 533 to 3 code snippets each) considered in total. Figure 7a plots the percentage of 534 Yes, No and Maybe responses from the two groups. The percentages between 535 the groups are comparable which suggests that the a priori knowledge and 536 understanding levels are similar. However, the LIME group demonstrates 537 higher accuracy and more confidence in their decision choices evidenced by 538 the lower percentage in *Maybe* responses. 539

Figure 7b plots the percentage of responses received for each snippet. The DisCERN group identifies Snippet 2 as the most complex, as evidenced by their higher percentage of *Maybe* responses. Additionally, we observe that the high confidence of the LIME group stems from the least complex Snippet 1. Both observations imply that the responses are not arbitrary, lending credibility to the utilisation of Q1 responses as an indicator of the group's a priori mental model.

#### 547 6.2. A priori mental model - correcting code vulnerabilities

Q2 measures the a priori mental model for correcting code vulnerabilities. Participants answered Q2 with line numbers or code lines which they considered to be *vulnerable*. Few example responses were 3,4,5, *int data* = *method()*; and *3rd line*. After pre-processing, Table 4 plots the number of responses for the three snippets across the two groups against corresponding code lines. Here the number of responses relates to the number of times



Figure 7: Q1 analysis on a priori mental model - detecting code vulnerabilities

a specific line was identified as vulnerable. We then analyse these against the actual vulnerable lines (the ground truths). The plots use a two-way colour coding to distinguish between lines that are correctly identified as vulnerable (in blue) and those that are incorrectly identified as vulnerable (in red). Although we wouldn't anticipate participants who answered No (or to a lesser extent Maybe) in Q1 to respond to Q2, we have still included their Q2 responses in the graphs if they chose to provide them.

We calculate response accuracy as a percentage of correct responses com-561 pared to ground truth. DisCERN group demonstrated 37.8%, 18.9%, 53.1% 562 response accuracy while LIME group achieves 35.0%, 16.7%, 38.3%. Overall 563 accuracy for DisCERN and LIME groups were 36.6% and 30.0%. Snippet 564 2 was the most challenging for both groups indicated by the lowest accu-565 racy, The wide variety of responses suggests that the increased complexity 566 made participants uncertain and led to guessing. Overall, guessing or ran-567 dom responses are expected from those who did not detect vulnerability in 568 Q1. 569

We observe that the code segment length has some correlation to the 570 number of errors. Accordingly, we further normalise the accuracy values by 571 the "difficulty of predicting vulnerable code lines in a code segment" using 572 inspirations from document length normalisation which alleviates the "term-573 frequency-bias". Given the number of lines of code in the segment is  $\alpha$  out 574 of which  $\beta$  number of lines are vulnerable, the difficulty is calculated as 575  $1 - \beta/\alpha$ . If all lines were vulnerable  $\beta = \alpha$  then difficulty = 0 and vice 576 versa. The weighted accuracy values are 20.4%, 17.8% and 45.6% for Dis-577 CERN group (mean is 27.93%) and 18.9%, 15.7% and 32.9% for the LIME 578



group(mean is 22.5%). The difference between the two groups is influenced by 579 two factors: the number of responses for Snippet 2 from the DisCERN group 580 was significantly lower than LIME group (37 vs 54) which contributed to the 581 2.1% difference, and for Snippet 3 DisCERN group responses were signifi-582 cantly more accurate (45.6% over 32.9%) although the number of responses 583 was comparable (49 vs 47). This analysis aids in determining the groups' 584 initial mental models, which is valuable for assessing the subsequent changes 585 in their mental models a posteriori. We recognise the marginally higher (ap-586 proximately 5%) performance of the DisCERN cohort and will consider this 587

in our subsequent analysis when we focus on a posteriori evaluations.

<sup>589</sup> 6.3. A posteriori mental model for correcting code vulnerabilities

Q4 measures the a posteriori mental model for addressing vulnerabilities 590 after participants have been exposed to the explanation. This implies that 591 participants have been informed about the snippet's vulnerability and are 592 presented with an explanation—either a counterfactual from DisCERN or 593 feature attribution from LIME. The explanations were presented as code-diff 594 for DisCERN and heat maps for LIME. To minimise the possibility of misin-595 terpretations, we have provided supporting text alongside both explanations, 596 detailing how to interpret them effectively. 597

Following pre-processing of the participants' responses, we analysed any 598 changes in knowledge among each user group after exposure to the explana-599 tion for the three code snippets, as shown in Table 5. Here, we anticipate 600 that changes to their mental model will be evident in at least two ways: 1) 601 withdrawing their belief for lines that were incorrectly identified as vulner-602 able in  $Q_{2}$ , and 2) recognising new lines that are necessary to address the 603 vulnerability having seen the explanation in Q4. For example, if the change 604 in response for a code line is denoted by -3, it means that the number of 605 responses for that line after participants saw the explanation (Q4) decreased 606 by three compared to before (Q2), indicating a shift in their belief about 607 the vulnerability of that line. Here, the reductions observed with the Orange 608 lines represent a positive change that was achieved a posterori. Unlike LIME, 609 DisCERN not only identifies vulnerabilities but also provides hints on how 610 to correct them by displaying counterfactuals. As a result, participants can 611 access additional lines from the counterfactual that were not available in Q2. 612 This is seen in Table 5 for DisCERN, where a relatively larger number of 613 blue lines can be observed on the x-axis, indicating a notable difference. 614

Overall Table 5 observations strongly indicate that participants found 615 counterfactuals more informative to correct vulnerabilities compared to fea-616 ture attributions. The DisCERN group exhibited some errors, as misiden-617 tified lines on either side of the vulnerability boundary were observed. For 618 instance, in Snippet 2, lines 28 and 39 were considered worthy of change, 619 despite not being vulnerable. Similarly, in Snippet 3, lines 18 and 19 were 620 not recognised as vulnerable, representing another error. The boundary cases 621 observed with DisCERN and the errors observed with the LIME group both 622 suggest that some participants are likely to either misinterpret or disagree 623 with the explanations. 624



Table 5: Q4 analysis on a posterior mental model - correcting code vulnerabilities

625 6.4. Goodness of explanations for vulnerability detection and correction

Q6 and Q7 aim to measure the overall goodness of the explanation to detect and correct vulnerabilities. Both questions are further analysed in relation to Q1 to examine the utility of the explanations to different cohorts: knowledgeable participants who responded *Yes* in Q1; and trainee participants who responded *No* or *Maybe* in Q1.

Q6 results across the two groups are plotted in Figure 8. The positive response rate from DisCERN and LIME groups were 66.7% and 62.7% respectively when asked about the utility of explanations for vulnerability

detection. This indicates a slight preference towards counterfactual explanations. Furthermore, Figure 8b indicates that the counterfactual explanations were found to be useful for more complex snippets (2 and 3) and feature attributions useful for the smallest snippet (1). This suggests that using counterfactual explanations may result in a lower cognitive load for detecting errors when compared to feature attributions.



Figure 8: Q6 analysis on the goodness of explanations - detecting code vulnerabilities

Figures 9a and 9b present an in-depth analysis of the Q6 responses with 640 respect to Q1. Figure 9a shows that participants with prior knowledge of 641 vulnerability detection found both types of explanations useful. The im-642 proved positive response rates of 83.61% and 77.56% from their baselines 643 for DisCERN and LIME indicate that knowledgeable users found both types 644 of explanations helpful. However, counterfactuals have been significantly 645 more helpful than feature attributions, especially for complex code snippets. 646 Figure 9b shows that trainee cohorts struggle with types of explanations. 647 It is indicated by the decreased positive response rate from their baselines 648 to 53.7% and 50.2% for DisCERN and LIME groups. However, trainee co-649 horts found counterfactuals significantly helpful for the most complex snippet 650 whereas feature attribution helped with the simplest snippet. These obser-651 vations further verify that counterfactuals reduced the cognitive burden of 652 vulnerability detection in complex code snippets. 653

Q7 measures the utility of the explanation to **correct** vulnerabilities and we plot similar graphs to Q6. Figure 10a shows that the overall positive response rates from DisCERN and LIME groups were 66.24% and 63.24% respectively. Similar to detection (Q6), the responses for Q7 indicate a preference for the counterfactuals for more complex snippets. In contrast to



Figure 9: Q6 analysis on the goodness of explanations - detecting code vulnerabilities by knowledgeable and trainee cohorts

detection, counterfactuals are found to be comparably helpful for the correc tion of vulnerabilities in simpler snippets which evidence an overall preference
 towards counterfactual explanations.



Figure 10: Q7 analysis on the goodness of Explanations - correcting code vulnerabilities

Figure 11 presents the analysis of the Q7 response with respect to cohorts 662 identified in Q1. Similar to Q6, the positive response rate for both explana-663 tions have improved from the knowledgeable cohort and decreased from the 664 trainee cohort. The preference for counterfactuals over feature attributions 665 by both cohorts for complex snippets remains significant for vulnerability cor-666 rection. While trainee cohorts consistently find counterfactuals to be more 667 helpful, knowledgeable cohorts find feature attributions are sufficient for cor-668 recting vulnerabilities in simple snippets. 669



Figure 11: Q7 analysis on the goodness of explanations - correcting code vulnerabilities by knowledgeable and trainee cohorts

We acknowledge that a significant number of trainee users did not find 670 either type of explanation helpful for both detection and correction. This was 671 clearly seen from responses to both Q6 and Q7 having less than 50% positive 672 responses for Snippets 2,3 in the LIME group and Snippet 3 in DisCERN 673 group. However, the overall preference was for DisCERN counterfactuals. 674 This feedback is useful for future research to further improve counterfactual 675 explanations to assist trainee developers to learn about vulnerability detec-676 tion and correction. 677

#### 678 6.5. Acceptability of the explanations

Q8 is aimed to measure the acceptability of the explanations. Similar to 679 Q6 and Q7 we plot overall responses and responses by snippets in Figure 12. 680 In both groups, approximately 60% of the participants agreed with the ex-681 planations provided. However, the disagreement is significantly lower in the 682 DisCERN group where 3% more partially accepted the counterfactual ex-683 planation. Figure <u>12b</u> shows that the acceptability of LIME is significantly 684 lower for Snippet 3 which has affected the overall acceptance. Otherwise, 685 agreement with feature attributions is similar to or greater than that of coun-686 terfactuals which is inconsistent with the previous observations on change in 687 mental model and goodness. LIME is a well-established explanation method 688 in various domains for several years, which may have influenced the observed 689 results, to further verify, we perform a more in-depth analysis. 690

The first analysis of acceptability is with respect to the cohorts recognised in Q1. Figure 13 plots the acceptability by knowledgeable and trainee co-



Figure 12: Q8 analysis on the acceptability of explanations

horts. The knowledgeable cohorts found counterfactuals more agreeable than 693 feature attributions, indicated by the accumulated positive response rates of 694 81.47% and 75.60%. The most significant difference is that the counterfac-695 tual explanation for the most complex snippet is found to be more agreeable 696 which aligns with previous observations. We failed to observe a majority of 697 trainee cohorts agreeing with either explanation, however, we observe partial 698 agreement rates of 63.70% and 62.20% respectively for DisCERN and LIME. 699 These findings reinforce the overall utility of counterfactuals over feature at-700 tribution and also highlight the need to improve the counterfactuals to build 701 trust among trainee developers as an effective learning tool. 702



Figure 13: Q8 analysis on the acceptability of explanations by knowledgeable and trainee cohorts

The second analysis of acceptability is with respect to the explanation goodness observed by Q6 and Q7. We recognise two cohorts from Q6 and

Q7, the ones who found explanations helpful and others who did not for both 705 vulnerability detection and correction. Figure 14a plots the Q8 responses for 706 those who found explanations helpful. Results show that the participants 707 who found feature attribution helpful overwhelmingly agreed with the expla-708 nation (0% no responses). However, not all who found counterfactuals use-709 ful agreed with it indicated by 2.11% disagreeing and 13.34% only partially 710 agreeing. Figure 14b plots the Q8 responses for those who found explana-711 tions not helpful. Those who found feature attribution not helpful for small 712 snippets completely disagreed with the explanation and those who found 713 counterfactuals not helpful for complex snippets, also completely disagreed 714 with the explanation. It is noteworthy that both of these cohorts are the 715 minority when determining goodness. Overall, 31.63% and 24.89% at least 716 partially agreed with counterfactuals and feature attributions respectively. 717

These observations conclude that the higher overall agreement with fea-718 ture attributions seen in Figure 12b for Snippets 1 and 2 is influenced by 719 the cohorts who found counterfactuals helpful (Q6 and Q7) but did not fully 720 agree with them. What is unknown and needs to be established in the long 721 term is if this acceptance of feature attribution is influenced by familiarity 722 with LIME explanations. The need for this is supported by the results in 723 Section 6.3 which clearly showed that counterfactuals influence a positive 724 mental model change compared to feature attributions. 725



Figure 14: Q8 analysis on the acceptability of explanations by goodness cohorts

#### 726 6.6. Implications and Limitations of the User Study

<sup>727</sup> Overall, counterfactual explanations encourage positive mental model <sup>728</sup> changes and were perceived as more helpful than feature attributions for

detecting and correcting code vulnerabilities. However, feature attributions
exhibit comparable or higher acceptability, possibly due to their widespread
use. These conclusions should be made with the limitations of the study in
mind. The key limitations of the above user study are three-fold: 1) incompleteness of heuristics used to identify the knowledgeable and trainee cohorts;
2) inclusion and exclusion criteria of participants; and 3) representations and
interpretation of explanations.

The a priori mental model for detecting vulnerabilities was based on Q1 736 which recognised two cohorts as knowledgeable and trainee. However, we did 737 not account for those who recognised the vulnerabilities incorrectly by col-738 lating them with answers to Q2. As seen in Section 6.2 only 36% and 30% of 739 the two groups identified the lines correctly and it includes all participants. 740 We found it challenging to filter participants by both Q1 and Q2 because 741 many of those who answered Yes in Q1 were able to partially identify vul-742 nerable lines. A more strict filter would have resulted in no knowledgeable 743 participants. Accordingly, we relied solely on Q1 to categorise participants 744 into the two cohorts. 745

The recruitment of participants for the user study was limited to Amazon Mechanical Turk (AMT), which placed constraints on the inclusion criteria. Accordingly, the inclusion criteria for selecting participants were constrained to those possible in the AMT platform. Ideally, a more comprehensive study would include participants in various career stages with Java software development skills.

The explanations generated by LIME and DisCERN are significantly dif-752 ferent in their presentation. LIME highlights the original query using a 753 heat-map scale and DisCERN presents counterfactual in a code-diff view. 754 With LIME explanations where the individual tokens are highlighted, it may 755 mislead the participants. An example scenario is if two tokens in a state-756 ment were highlighted as *vulnerable* and *non-vulnerable*, the participant can 757 consider the statement as vulnerable, non-vulnerable or have no impact on 758 the vulnerability detection. DisCERN code-diff view has two columns with 759 query line numbers and counterfactual line numbers. A participant who is 760 unfamiliar with code-diff may mistakenly use the line numbers from the in-761 appropriate column when responding to the questionnaire. 762

All three limitations are well-founded, however, they do not invalidate the findings, rather, they provide enhancing user studies in this particular domain and in Explainable AI in general.

The user study was conducted with three code segments, all of which be-

longed to the same vulnerability code (CWE-191). Our main reasoning was 767 to prioritise the evaluation of the utility of different types of explanation while 768 keeping other variables constant. Additionally, it allowed the user study not 769 to be biased by the proficiency of the participant in detecting various types of 770 vulnerabilities. However, there can be implications for this approach if some 771 vulnerabilities were better explained using feature attributions over counter-772 factuals. This can be linked to our observations in Section 6.4 where there 773 was no significant preference between feature attribution and counterfactual 774 explanations when the code segment was simple. The generalisability of Dis-775 CERN to different vulnerability classes and languages (as seen in Section 5) 776 provides an opportunity to evaluate this in the future. 777

#### 778 7. Conclusion

The DisCERN algorithm finds counterfactual explanations for correcting 779 code vulnerabilities using pattern matching to find corrections to a code seg-780 ment from its nearest-unlike neighbour. DisCERN was evaluated using three 781 NIST datasets in different programming languages and the results showed 782 that it finds counterfactuals in 85% - 96% of the cases with  $8 \sim 14$  statement 783 corrections needed. A qualitative analysis revealed that some of the counter-784 factuals generated by DisCERN did not preserve the original functionality of 785 the code. This highlights the need for comprehensive heuristics in the future 786 to ensure plausible code corrections. We conducted a user study to assess the 787 utility of counterfactual explanations compared to the more commonly used 788 feature attribution explanations for correcting vulnerabilities. The user study 789 showed that counterfactuals facilitated a positive mental model change to-790 wards correcting vulnerabilities. Counterfactuals were specifically preferred 791 over feature attributions when dealing with complex code segments, indi-792 cating a reduction in cognitive burden. However, despite being less helpful 793 for vulnerability correction, feature attribution explanations received higher 794 acceptance than counterfactuals, possibly due to the trust built around their 795 familiarity. These findings provide evidence for the utility of counterfactual 796 explanations over feature attribution explanations. Nonetheless, they also 797 emphasise the importance of conducting long-term evaluations to determine 798 if counterfactuals can establish trust with developers as a reliable tool for 799 vulnerability detection and correction. 800

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### <sup>805</sup> Appendix A. Code snippets from the user study

	p	ublic void method()		
{     int data = someMethod();				
		/*comment*/ data; int result = (int)(data);		
		IO.writeLine("result: " + result);		
	}			
Figu	ure 4	A.15: Snippet 1: LIME Explanation		
1	1	<pre>public void method()</pre>		
2	2	{		
3	-	<pre>int data = someMethod(); int data:</pre>		
4	3+	int data;		
4	4	/*comment*/		
6	_	data		
7	_	int result = (int)(data):		
	6+	data = $2;$		
	7+			
	8+	/*comment*/		
	9+	<pre>int result = (int)(data);</pre>		
8	10			
9	11	<pre>I0.writeLine("result: " + result);</pre>		
10	12			
11	13	}		



 $^{5} \rm https://isee4xai.com/\\ ^{6} \rm https://www.chistera.eu/projects/isee$ 







Figure A.18: Snippet 2: DisCERN Explanation



Figure A.19: Snippet 3: LIME Explanation



Figure A.20: Snippet 3: DisCERN Explanation

#### 806 References

[1] R. Russell, L. Kim, L. Hamilton, T. Lazovich, J. Harer, O. Ozdemir,
P. Ellingwood, M. McConley, Automated vulnerability detection in source code using deep representation learning, in: 2018 17th IEEE international conference on machine learning and applications (ICMLA),
IEEE, 2018, pp. 757–762.

[2] Z. Bilgin, M. A. Ersoy, E. U. Soykan, E. Tomur, P. Çomak, L. Karaçay,
Vulnerability prediction from source code using machine learning, IEEE
Access 8 (2020) 150672–150684.

[3] B. Chernis, R. Verma, Machine learning methods for software vulnerability detection, in: Proceedings of the Fourth ACM International Workshop on Security and Privacy Analytics, 2018, pp. 31–39.

[4] H. K. Dam, T. Tran, T. Pham, S. W. Ng, J. Grundy, A. Ghose,
 Automatic feature learning for vulnerability prediction, arXiv preprint
 arXiv:1708.02368 (2017).

[5] Z. Li, D. Zou, J. Tang, Z. Zhang, M. Sun, H. Jin, A comparative study
 of deep learning-based vulnerability detection system, IEEE Access 7
 (2019) 103184–103197.

[6] G. Tang, L. Zhang, F. Yang, L. Meng, W. Cao, M. Qiu, S. Ren, L. Yang,
H. Wang, Interpretation of learning-based automatic source code vulnerability detection model using lime, in: Knowledge Science, Engineering
and Management: 14th International Conference, KSEM 2021, Tokyo,
Japan, August 14–16, 2021, Proceedings, Part III, Springer, 2021, pp.
275–286.

[7] S. Wachter, B. Mittelstadt, C. Russell, Counterfactual explanations
without opening the black box: Automated decisions and the gdpr,
Harv. JL & Tech. 31 (2017) 841.

[8] A. Wijekoon, N. Wiratunga, I. Nkisi-Orji, C. Palihawadana, D. Corsar,
K. Martin, How close is too close? the role of feature attributions in
discovering counterfactual explanations, in: Case-Based Reasoning Research and Development: 30th International Conference, ICCBR 2022,
Nancy, France, September 12–15, 2022, Proceedings, Springer, 2022, pp.
33–47.

[9] D. Votipka, R. Stevens, E. Redmiles, J. Hu, M. Mazurek, Hackers vs. testers: A comparison of software vulnerability discovery processes, in: 2018 IEEE Symposium on Security and Privacy (SP), IEEE, 2018, pp. 374–391.

- [10] A. C. Eberendu, V. I. Udegbe, E. O. Ezennorom, A. C. Ibegbulam, T. I.
  Chinebu, et al., A systematic literature review of software vulnerability detection, European Journal of Computer Science and Information Technology 10 (1) (2022) 23–37.
- [11] S. M. Ghaffarian, H. R. Shahriari, Software vulnerability analysis and
   discovery using machine-learning and data-mining techniques: A survey,
   ACM Computing Surveys (CSUR) 50 (4) (2017) 1–36.
- [12] Z. Li, D. Zou, S. Xu, X. Ou, H. Jin, S. Wang, Z. Deng, Y. Zhong,
   Vuldeepecker: A deep learning-based system for vulnerability detection,
   arXiv preprint arXiv:1801.01681 (2018).
- Y. Zhou, S. Liu, J. Siow, X. Du, Y. Liu, Devign: Effective vulnerability
  identification by learning comprehensive program semantics via graph
  neural networks, Advances in neural information processing systems 32
  (2019).
- <sup>857</sup> [14] X. Yuan, G. Lin, Y. Tai, J. Zhang, Deep neural embedding for soft<sup>858</sup> ware vulnerability discovery: Comparison and optimization, Security
  <sup>859</sup> and Communication Networks 2022 (2022) 1–12.
- E. Mashhadi, H. Hemmati, Applying codebert for automated program
  repair of java simple bugs, in: 2021 IEEE/ACM 18th International Conference on Mining Software Repositories (MSR), IEEE, 2021, pp. 505–
  509.
- [16] N. Ziems, S. Wu, Security vulnerability detection using deep learning
  natural language processing, in: IEEE INFOCOM 2021-IEEE Conference on Computer Communications Workshops (INFOCOM WKSHPS),
  IEEE, 2021, pp. 1–6.
- <sup>866</sup> [17] J. Senanayake, H. Kalutarage, M. O. Al-Kadri, A. Petrovski, L. Piras,
  <sup>869</sup> Android source code vulnerability detection: a systematic literature re<sup>870</sup> view, ACM Computing Surveys 55 (9) (2023) 1–37.

- [18] I. Medeiros, N. Neves, M. Correia, Detecting and removing web application vulnerabilities with static analysis and data mining, IEEE Transactions on Reliability 65 (1) (2015) 54–69.
- [19] D. K. P. Newar, R. Zhao, H. Siy, L.-K. Soh, M. Song, Ssdtutor: A
  feedback-driven intelligent tutoring system for secure software development, Science of Computer Programming 227 (2023) 102933.
- [20] S. Ma, F. Thung, D. Lo, C. Sun, R. H. Deng, Vurle: Automatic vulnerability detection and repair by learning from examples, in: Computer Security–ESORICS 2017: 22nd European Symposium on Research in Computer Security, Oslo, Norway, September 11-15, 2017, Proceedings, Part II 22, Springer, 2017, pp. 229–246.
- Y. Zhang, Y. Xiao, M. M. A. Kabir, D. Yao, N. Meng, Example-based
  vulnerability detection and repair in java code, in: Proceedings of the
  30th IEEE/ACM International Conference on Program Comprehension,
  2022, pp. 190–201.
- [22] A. Savchenko, O. Fokin, A. Chernousov, O. Sinelnikova, S. Osadchyi,
   Deedp: vulnerability detection and patching based on deep learning,
   Theoretical and Applied Cybersecurity 2 (1) (2020).
- [23] D. Gunning, D. Aha, Darpa's explainable artificial intelligence (xai)
   program, AI magazine 40 (2) (2019) 44–58.
- [24] M. Ebers, Regulating explainable ai in the european union. an overview of the current legal framework (s), An Overview of the Current Legal Framework (s)(August 9, 2021). Liane Colonna/Stanley Greenstein (eds.), Nordic Yearbook of Law and Informatics (2020).
- <sup>895</sup> [25] T. N. Nguyen, R. Choo, Human-in-the-loop xai-enabled vulnerability
  <sup>896</sup> detection, investigation, and mitigation, in: 2021 36th IEEE/ACM
  <sup>897</sup> International Conference on Automated Software Engineering (ASE),
  <sup>898</sup> IEEE, 2021, pp. 1210–1212.
- [26] S. Höhn, N. Faradouris, What does it cost to deploy an xai system: A case study in legacy systems, in: Explainable and Transparent AI and Multi-Agent Systems: Third International Workshop, EXTRAA-MAS 2021, Virtual Event, May 3–7, 2021, Revised Selected Papers 3, Springer, 2021, pp. 173–186.

2

904 905 906	[27]	D. Arp, M. Spreitzenbarth, M. Hubner, H. Gascon, K. Rieck, C. Siemens, Drebin: Effective and explainable detection of android malware in your pocket., in: Ndss, Vol. 14, 2014, pp. 23–26.
907 908 909 910	[28]	V. J. Sudhakar, S. Mahalingam, V. Venkatesh, V. Vetriselvi, Phishing url detection and vulnerability assessment of web applications using ivs attributes with xai, in: ICT Analysis and Applications, Springer, 2022, pp. 933–944.
911 912 913	[29]	G. Schwalbe, B. Finzel, A comprehensive taxonomy for explainable ar- tificial intelligence: a systematic survey of surveys on methods and con- cepts, Data Mining and Knowledge Discovery (2023) 1–59.
914 915	[30]	T. Miller, Explanation in artificial intelligence: Insights from the social sciences, Artificial intelligence 267 (2019) 1–38.
916 917 918 919	[31]	Z. Feng, D. Guo, D. Tang, N. Duan, X. Feng, M. Gong, L. Shou, B. Qin, T. Liu, D. Jiang, et al., Codebert: A pre-trained model for programming and natural languages, in: Findings of the Association for Computational Linguistics: EMNLP 2020, 2020, pp. 1536–1547.
920 921 922	[32]	J. Devlin, MW. Chang, K. Lee, K. Toutanova, Bert: Pre-training of deep bidirectional transformers for language understanding, arXiv preprint arXiv:1810.04805 (2018).
923 924 925 926	[33]	M. T. Ribeiro, S. Singh, C. Guestrin, "why should i trust you?" explaining the predictions of any classifier, in: Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining, 2016, pp. 1135–1144.
927 928 929 930	[34]	R. K. Mothilal, A. Sharma, C. Tan, Explaining machine learning classifiers through diverse counterfactual explanations, in: Proceedings of the 2020 conference on fairness, accountability, and transparency, 2020, pp. 607–617.
931 932	[35]	D. Brughmans, P. Leyman, D. Martens, Nice: an algorithm for near- est instance counterfactual explanations, Data Mining and Knowledge

<sup>933</sup> Discovery (2023) 1–39.