Exploring transformers for multi-label classification of Java vulnerabilities

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Society is becoming **more dependent on technology**

Companies must develop code ASAP without compromising security

How can we do that?

Static analysis

Dynamic analysis

Pattern matching

(...)

- Too time-consuming
- High False Positive rate
- Applied by experts

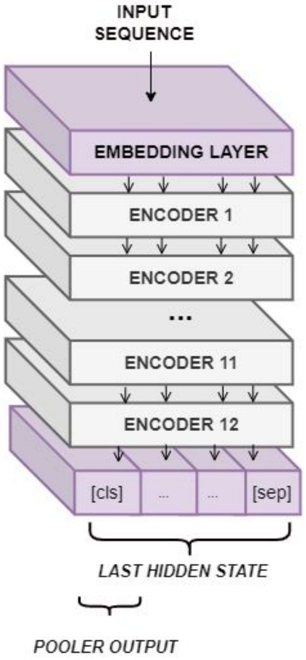
Machine learning

TRANSFORMERS

- Handle long range dependencies
- Transfer learning mechanism
- SOTA results for vulnerability detection

JavaBERT

CodeBERT



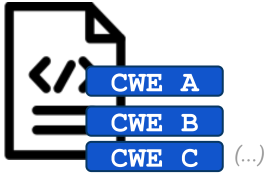
What about the data ?

- Using synthetic samples from the Juliet Test Suite
- Function-level granularity
- 113 898 methods (70% non-vulnerable; 30% vulnerable)
- 20 CWES

MULTILABEL: WHY?

Research focus on **binary** or **multi-class** classification:

Binary classification



Multi class classification

Both classifications lack information. For example:

```
public void action(byte data) throws Throwable {

    /* POTENTIAL FLAW: data == Byte.MAX_VALUE */
    byte result = (byte)(++data);

    IO.writeLine("result: " + result);
}
```

Binary: UNSAFE

What problem will you solve?

Multi-class: CWE-190

Is the code truly vulnerable?

Multi-label: UNSAFE CWE-190

Multilabel helps developers speed up software development by helping them in decision-making.

```
public void action(byte data) throws Throwable {
    /* POTENTIAL FLAW: data == Byte.MAX_VALUE */
    byte result = (byte)(++data);

    IO.writeLine("result: " + result);
}

/* (...) */
/* Restriction on the value of data */
    if( data < Byte.MAX_VALUE) {
        action(data);
    }
```

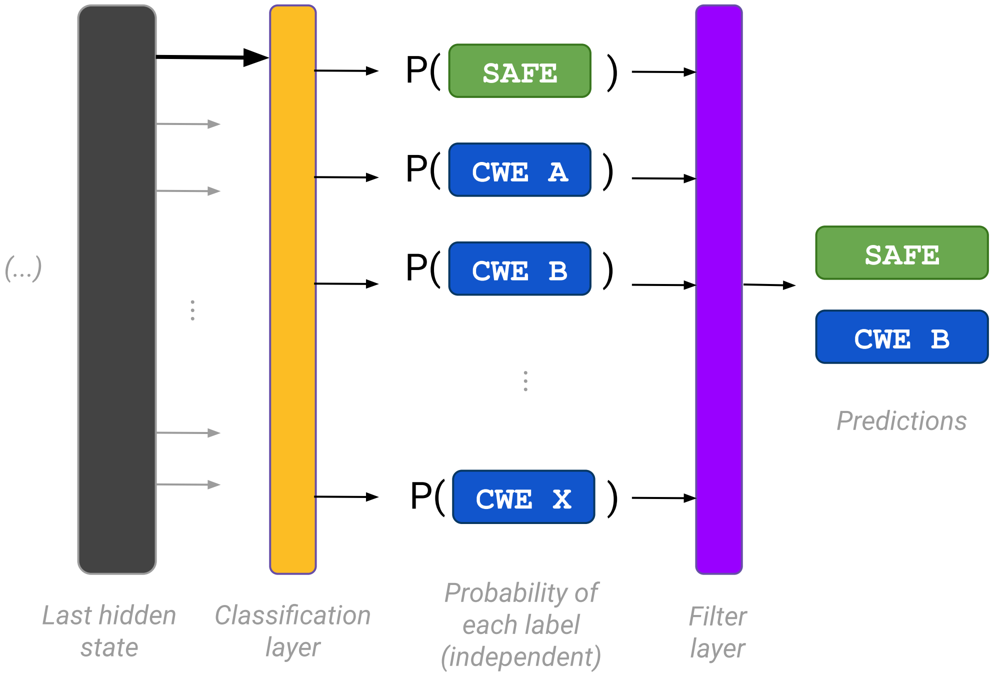
Multi-label: SAFE CWE-190

- **Threshold selection** to solve the problem of multi-label [1]
- **Threshold = 0.5** to filter the labels
- Theoretically, we can discover ≥ 1 CWE

  (no data to properly test this theory)

MULTILABEL: HOW?

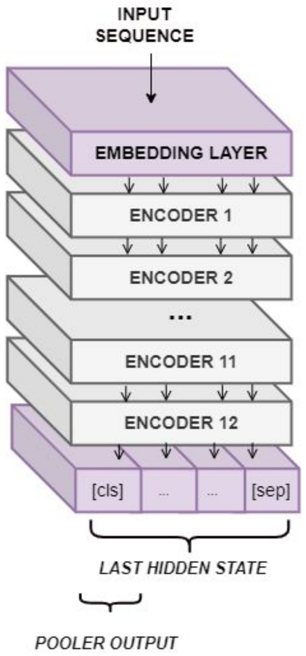
For example:

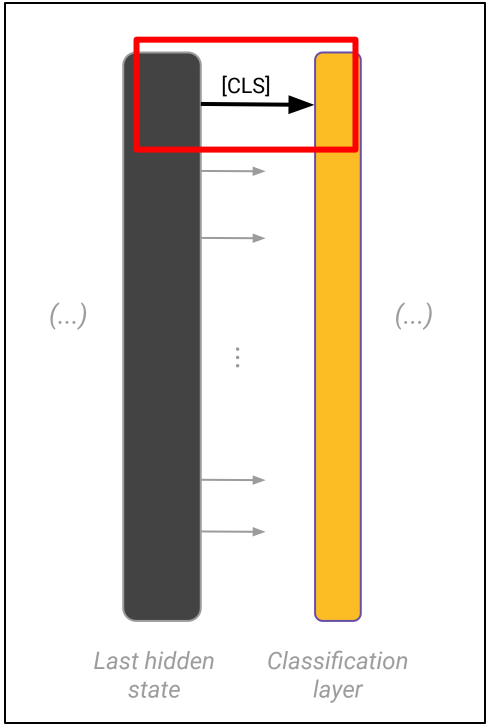


[2] H. Fallah *et al.* Adapting transformers for multi-label text classification. In *CIRCLE'22*

RQ 1 | How do different output configurations impact the learning of BERT-based models?

BERT-based model architecture



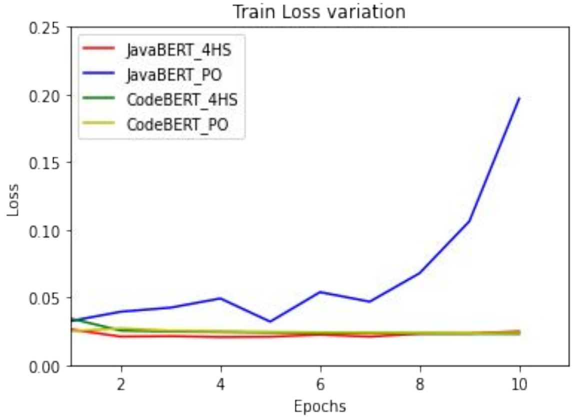


How to improve the representation of the [CLS] token?

Configurations:

- Pooler output (default in most libraries) 🤗
- Concatenation of the [CLS] tokens of the last 4 hidden states

RQ 1 | How do different output configurations impact the learning of BERT-based models?



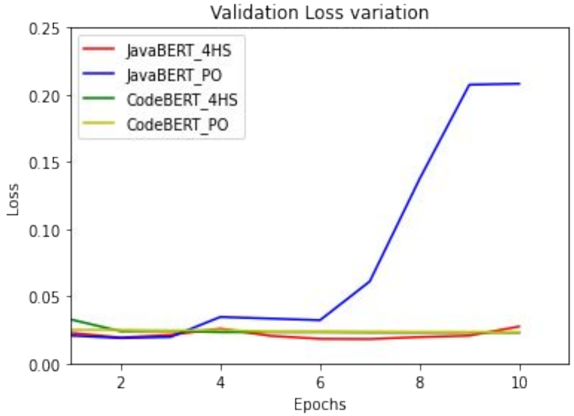


Figure | Learning curves (loss variations) during training (left) and validation (right) for all models.

Finding 1

The pooler output configuration compromises the transfer learning capabilities of JavaBERT.

RQ 2 | Which BERT-based model configuration achieves better vulnerability identifications?

Model	#Epoch	Accuracy	$\overline{wF1}$	$\overline{wPrecision}$	$\overline{wRecall}$	$\overline{FNR}$	$\overline{FPR}$
JavaBERT_4HS	8	98.90%	94.0%	95.0%	93.0%	7.12%	0.98%
CodeBERT_4HS	10	98.68%	93.0%	95.0%	91.0%	12.28%	1.02%
CodeBERT_PO	9	98.67%	93.0%	95.0%	91.0%	12.39%	1.06%

Table | Performance results for JavaBERT and CodeBERT with different model configurations

Finding 2

Combining the outputs of the last four hidden layers yields more accurate predictions.

RQ 3 | To what extent does implicit bias in datasets affect the ability of the model to learn?

- Find **problematic tokens** in datasets
- **Our hypothesis:**
  Problematic tokens are most likely over represented, causing the model to make wrong predictions.

POINTWISE MUTUAL INFORMATION

Class	Token	PMI
Unsafe or vulnerable	##ad	0.98
	bad	0.88
Safe or non-vulnerable	good	1
	##BS	1
CWE-15	##15	1
CWE-23	##23	1

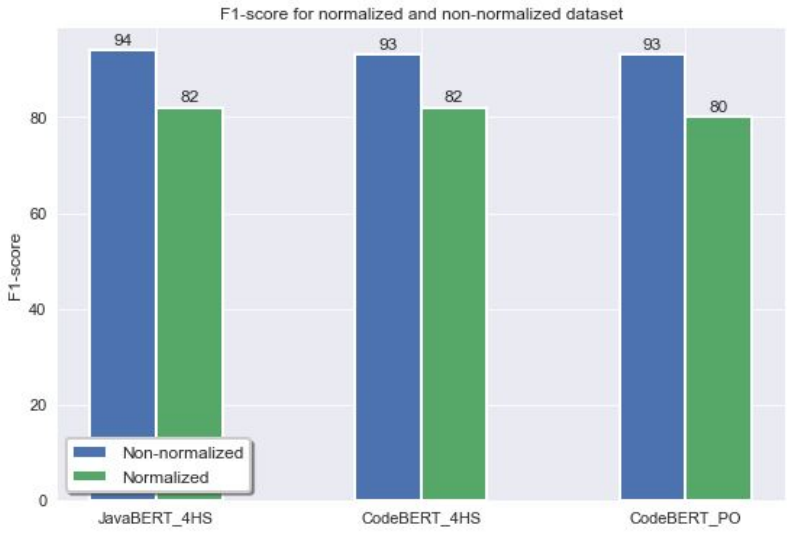
Table | Top PMI scores for some labels

RQ 3 | To what extent does implicit bias in datasets affect the ability of the model to learn?

Original dataset normalized method and variable names

Missing: exceptions, some method calls and global variables

Replace problematic tokens with random strings (of the same size). Repeat training.



Findings 3 and 4

We can use the Pointwise Mutual Score (PMI) to identify problematic tokens in code.

Removing token that bias the model substantially reduces the f1 score (up to 12%).

RQ 4 | How do BERT-based models perform when exposed to real-world samples?

Synthetic data

- Similar to real-world data
- Programmatically generated
- Similar style and structure

  (particularly single-sourced synthetic samples)

Real-world data

- (Usually) no rules for naming vars/methods
- (Usually) no particular code structure

Original real-world dataset from T. Le *et al.* [2]

CVE → CWE

Filter the samples our models can identify (by CWE)

Final test set: **70 vulnerable samples** (targeting only **8 known CWEs**)

[2] T. Le and M. Babar. On the use of fine-grained vulnerable code statements for software vulnerability assessment models. In *MSR'22*

RQ 4 | How do BERT-based models perform when exposed to real-world samples?

Model	Accuracy	$\overline{wF1}$	$\overline{FNR}$	$\overline{FPR}$
JavaBERT_4HS	**90.06%** (-8.87%)	**44.0%** (-50%)	**36.03%** (+28.91%)	**4.12%** (+3.14%)
CodeBERT_4HS	**86.88%** (-11.8%)	**23.0%** (-70%)	**37.74%** (+24.46%)	**5.39%** (+4.37%)
CodeBERT_PO	**85.86%** (-12.81%)	**20.0%** (-73%)	**39.52%** (+27.13%)	**9.85%** (+8.79%)

Table | Performance results for models tested with real-world samples

Finding 5

Models trained on synthetic data have a tendency to identify true vulnerable samples as non-vulnerable.

RQ 5 | To what extent BERT-based models can predict unknown vulnerabilities?

“ (...) **generalizability** measures how applicable the results of a study are to a broader group.

In this context, a model is said to have good generalizability if it can be successfully applied to **identify unknown flaws.**”

Test with samples of unknown vulnerability types that are **related** to the ones the models know.

Software Fault Patterns

Test with samples of unknown vulnerability types that are **unrelated** to the ones the models know.

RQ 5 | To what extent BERT-based models can predict unknown vulnerabilities?

SFP Secondary Cluster	CWE	# samples (training set)
Glitch in computation	190, 191, 369, 197	12 020
Tainted input to command	89, 113, 134, 80, 78, 643, 90	6 569
Tainted input to variable	606, 15	960
Path traversal	23, 36	554

Not listed in the SFP view: 129, 789 and 690
1-to-1 mapping: 400, 470 and 319

Test set for unknown and related CWEs

1. CWE-611 and CWE-79 `ds_611_79`
   (Tainted Input to Command; 239 samples)
2. CWE-22 `ds_22`
   (Path Traversal; 179 samples)

Test set for unknown and unrelated CWEs

1. CWE-287 `ds_287`
   (Authentication Bypass; 159 samples)

RQ 5 | To what extent BERT-based models can predict unknown vulnerabilities?

"Vulnerable" class:

Model	Dataset	Accuracy	F1	FNR	FPR
JavaBERT_4hs	**ds_611_79**	**74.47%**	**85.37%**	**25.52%**	**0%**
	ds_22	55.86%	71.69%	44.13%	0%
	ds_287	38.36%	55.45%	61.63%	0%
CodeBERT_4hs (CodeBERT_PO behaves similarly)	ds_611_79	17.57%	29.89%	82.4%	0%
	ds_22	12.85%	22.77%	87.15%	0%
	ds_287	4.40%	8.43%	95.60%	0%

Findings 6 and 7

JavaBERT fine-tuned on synthetic data can successfully predict unknown and relatable vulnerabilities

BERT-based models fine-tuned on synthetic data cannot predict unknown and unrelated vulnerabilities.

THREATS TO VALIDITY

- Small and imbalanced datasets
- Not using cross-validation
- No preprocessing strategies (e.g.: sampling)
- Lack information regarding flaw location

FUTURE IMPROVEMENTS

- **More data (!!)**
  - Train with synthetic & real-world samples
  - Include non-vulnerable samples in the test set
  - Balance the dataset
- Explore the models' **ability to discover ≥ 1 CWE**

Code & datasets available: **https://github.com/TQRG/VDET-for-Java**