Comparative Analysis of RoBERTa and CodeBERT for Automated Misconfiguration Detection in Dockerfiles

(MIT Thesis Viva Voice Examination)

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ABSTRACT

- This thesis explores automated detection of Dockerfile misconfigurations using transformer-based NLP models.
- A two-stage framework is proposed for binary and rule-specific misconfiguration classification.
- The models are evaluated on a dataset of public Dockerfiles.
- Results show high detection accuracy, with CodeBERT slightly outperforming RoBERTa.

Outline

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- Conclusion
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- References

Introduction

- Docker is a core technology in modern DevOps for building and deploying applications
- Dockerfiles define container build processes but are complex and under-analyzed
- Misconfigurations in Dockerfiles can cause security vulnerabilities and build failures
- Existing tools detect rule violations but fail to generalize to complex patterns
- This research evaluates transformer-based NLP models to improve Dockerfile misconfiguration detection

This naturally leads to the problem addressed in this thesis.

Problem Statement

- Public Dockerfiles frequently violate best practices and contain security risks
- Many engineers lack deep security expertise when writing Dockerfiles
- Existing tools are rule based and limited to predefined checks which fail to detect unseen patterns
- NLP/AI for Dockerfiles is still underexplored

Problem Statement

traefik:latest [v2.11.34]

- Traefik http router rule

traefik.http.routers.${PROJECT}.rule=Host(`api.${DOMAIN}`) || (HostRegexp(`{subdomain:(app)}.${DOMAIN}`) && PathPrefix(`/api/`))

traefik:latest [v3.6.6]

- Traefik http router rule

traefik.http.routers.${PROJECT}.rule=Host(`api.${DOMAIN}`) || (HostRegexp(`{subdomain:(app)}.${DOMAIN}`) && PathPrefix(`/api/`))

traefik.http.routers.${PROJECT}.rule=Host(`api.${DOMAIN}`) || ((Host(`app.${DOMAIN}`) && PathPrefix(`/api`))

Objectives

- To design and develop automated detection framework using either RoBERTa or CodeBERT, and find out which one has better performance
- To evaluate and compare the performance of RoBERTa and CodeBERT for automated misconfiguration detection in Dockerfiles, using metrics such as accuracy, precision, recall, F1-score, and AUC-ROC

Scope and Limitation

⚡ **Models compared:** RoBERTa & CodeBERT

🛠️ **Objective:** Automated detection of Dockerfile misconfigurations

📄 **Analysis type:** Static, NLP-based evaluation

📊 **Performance metrics:** Accuracy | Precision | Recall | F1-score | AUC-ROC

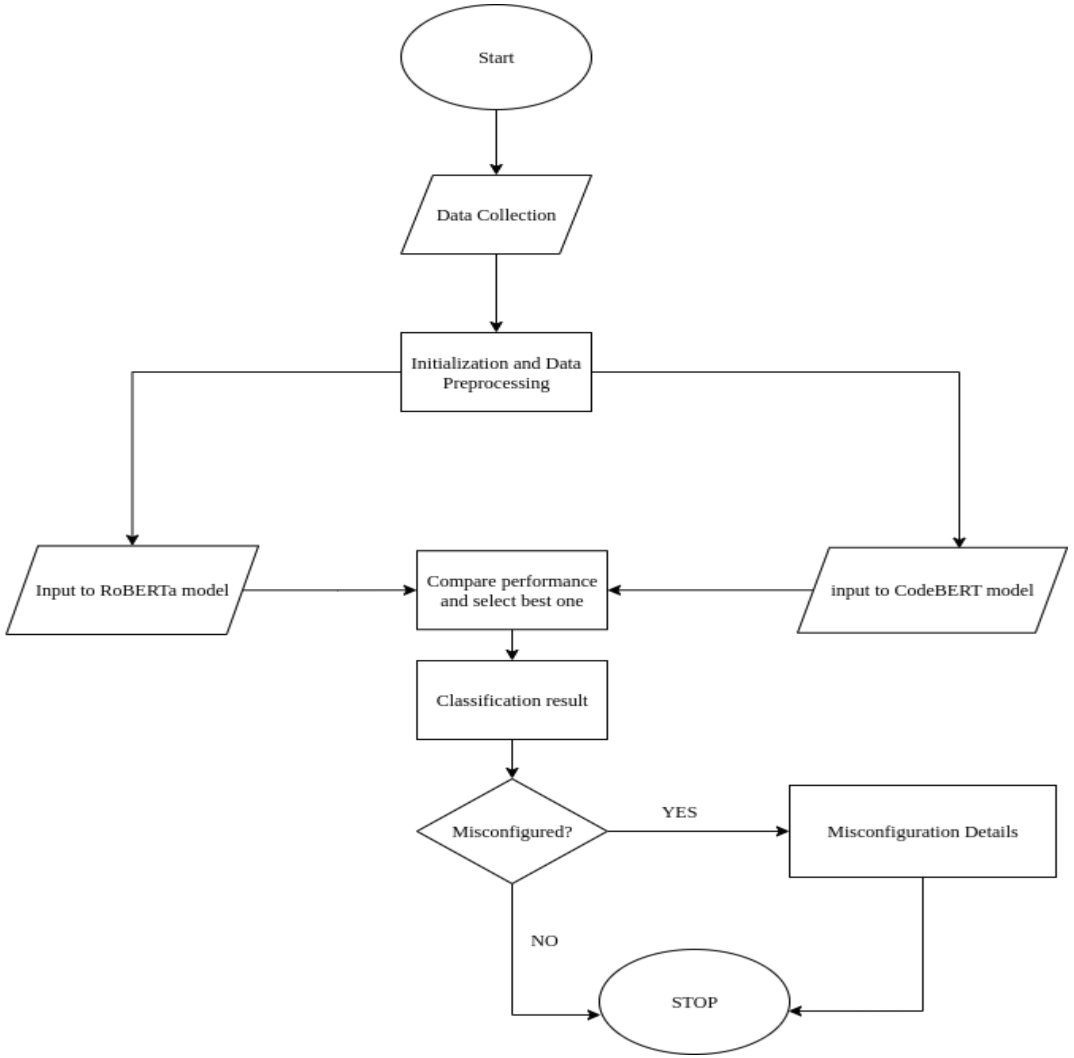
- 🐳 **Scope:** Only Dockerfiles
- 📁 **Dataset:** Publicly available Dockerfiels
- ⚡ **Models:** Only RoBERTa and CodeBERT
- 💻 **Resources:** Limited computational power may affect experiments and tuning

Literature Review

Study	Dataset	Key findings	Research gap
Learning from, DevOps Artifacts	Expert & non-expert Dockerfiles	Non-expert Dockerfiles violate best practices ~6× more; IDE integration suggested	Needs adaptive AI methods for complex misconfigs
Shipwright	Faulty Dockerfiles	Automated repair suggestions; Improves build correctness	Focus on build failure, not misconfiguration
Dockerfile Flakiness	Flaky Dockerfiles	Characterizes flakiness; Improves repair success	No line-level security detection
Dockerfile Linting	Docker Workflows	Ensures consistent quality via linting	No AI/NLP misconfiguration detection
Not all Dockerfile Smells are the Same	39,000 Dockerfiles	Experts overlook smells; Validates linting	No AI/NLP detection explored
DRIVE: Rule Mining	Dockerfiles	Identifies semantic & syntactic rules; Improves quality	Focus on static rules, not AI/NLP

Methodology

System flow chart



Dataset Description

- Source: Publicly available Dockerfiles from GitHub
- Primary Corpus: Henkel et al. Dockerfile corpus (ICSE 2020)
    - ~178,000 real-world Dockerfiles
- Extended data: Additional Dockerfiles collected via GitHub Search API
- Processing and labels: Dockerfiles parsed line by line; each instruction (e.g., FROM, RUN, COPY) labeled as correct or wrong for training and evaluation of NLP models.
- Dataset Size:
    - ~178,800 Dockerfiles
    - ~1.6 million Dockerfile instructions

Data Preprocessing

Model training strategy

- Stage 1: Binary misconfiguration classification
  - Correct vs wrong
- Stage 2: Rule-specific misconfiguration classification
  - Misconfigured instructions with rule id

Data Preprocessing

Data splitting

- Stratified splitting into:
    - Training: 80%
    - Validation: 10%
    - Test: 10%
- Separate strategies for stage 1 and stage 2
- Due to computational resource constraints, a representative subset of the dataset was used for training and evaluation.

Data Preprocessing

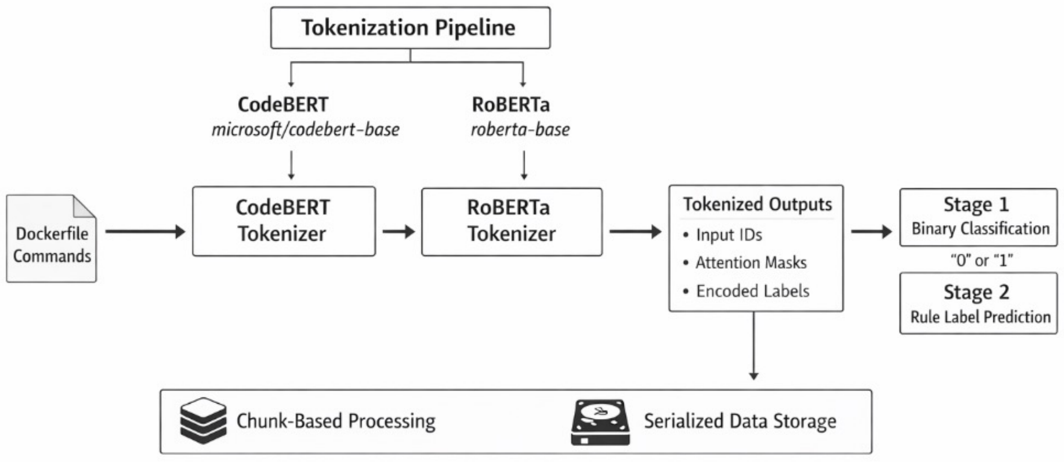
Data splitting

Aspect	**Stage 1: Binary classification**	**Stage 2: Rule-level classification**
Task	Correct vs Wrong	Rule-level misconfiguration classification
Initial data	~1.6M instructions	Misconfigured instructions only
Data reduction and balancing method	Downsampled and selected 200K samples per class	Rare rules removed (<200 samples) and capped dominant rules (<=5K)
Final split	80% / 10% / 10% (stratified)	80% / 10% / 10% (rule-stratified)
Motivation	Computational feasibility	Fair multi-class learning and fair cimputational feasibility

Data Preprocessing

Tokenization and encoding

- Unified subword tokenization applied for both learning stages
- Fixed input length of 256 tokens with truncation and padding
- Training set only label encoding, with pre-tokenized inputs stored for efficient reuse

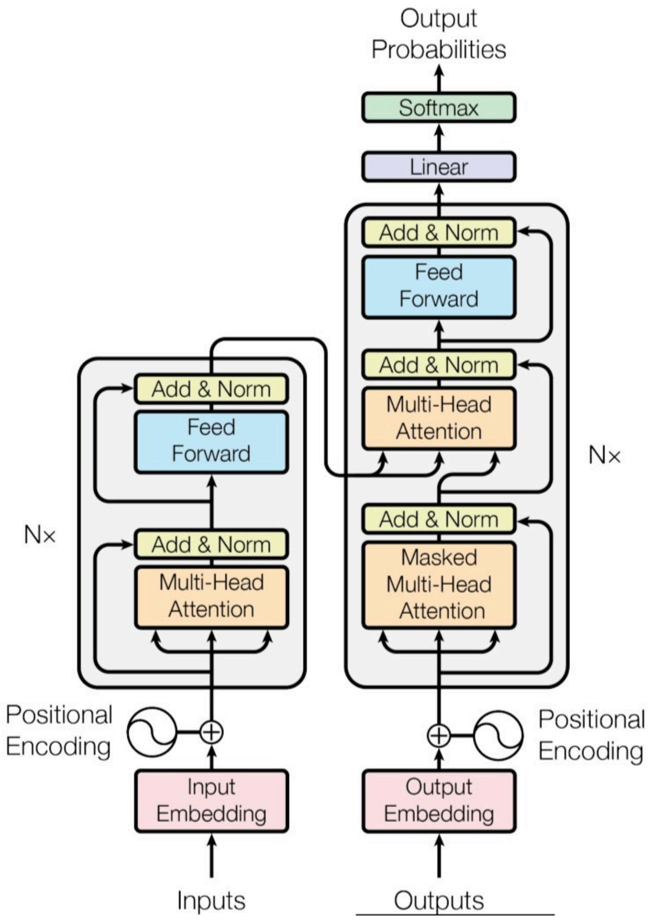


Data Preprocessing

Dataset summary

Aspect	**Stage 1: Binary classification**	**Stage 2: Rule-level classification**
Initial dataset	~1.6M instructions	Same dataset
Classes	2 (correct vs wrong)	63 rules
Class balance	2,00,000 per class	Filtered 200+ samples, capped at 5,000 per rule
Total samples used	4,00,000	1,73,297
Training set (80%)	3,20,000	1,38,637
Validation set (10%)	40,000	17,330
Test set (10%)	40,000	17,330
Purpose	Detect misconfiguration	Predict violated rule if misconfigured

Description of Algorithms



- Faster than RNNs/LSTMs: parallel training on large datasets
- Attention mechanism: focuses on most relevant words in context
- Encoder/Decoder: encoder for classification, both for translation
- Self-attention: captures dependencies even across distant words
- Positional encoding: keeps track of word order

Description of Algorithms

RoBERTa and CodeBERT

- Encoder only transformer architecture
- Optimized version of BERT with larger datasets and better training strategies
- Dynamic masking: different tokens are masked in each epoch

Description of algorithms

RoBERTa and CodeBERT

Transformer encoder

- Stack of self-attention layers producing contextualized token representations.
- Input tokens => embedding vectors => processed by encoder layers.

$$Attention\ (Q,K,V) = softmax(QK^T/\sqrt{d_k})V$$

- Where Q, K, V: query, key, value from embeddings and dk: dimension of key vectors

Classification head

- The [CLS] token embedding from the encoder is passed through a feed-forward layer to produce a probability distribution over class labels, enabling classification of Dockerfiles as correct or misconfigured.

$$y = softmax(W.\ hCLS + b)$$

- Where W,b = trainable parameters and y = probability distribution overs classes

Implementation Details

Model architecture and input processing

Pretrained models

- RoBERTa-base (text-oriented)
- CodeBERT-base (code-aware)

Tokenization

- Model-specific tokenizers
- Subword encoding
- Maximum sequence length: 256 tokens

Input granularity

- Dockerfile commands processed at line level

Output heads

- Binary classifier (Stage 1)
- Multi-class classifier (Stage 2)

Implementation Details

Training configuration and optimization

Optimizer: AdamW

Learning rate:

- Binary classification: $2 * 10^{-5}$
- Rule classfication: $5 * 10^{-5}$

Batch size: 32

Epochs: 3

Training strategy:

- Validation-based loss monitoring
- Gradient accumulation

Loss function:

- Binary classification: Cross-entropy loss
- Rule classification: Multi-class cross-entropy loss

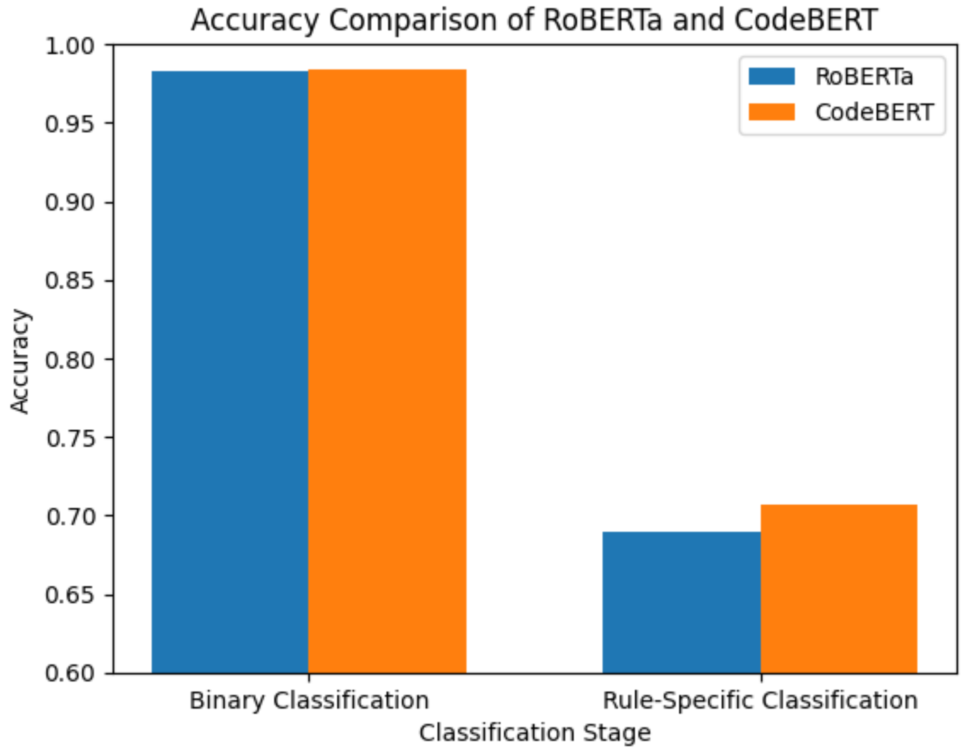
Model persistence:

- Epoch-wise checkpointing for reproducibility

Result Analysis

Accuracy

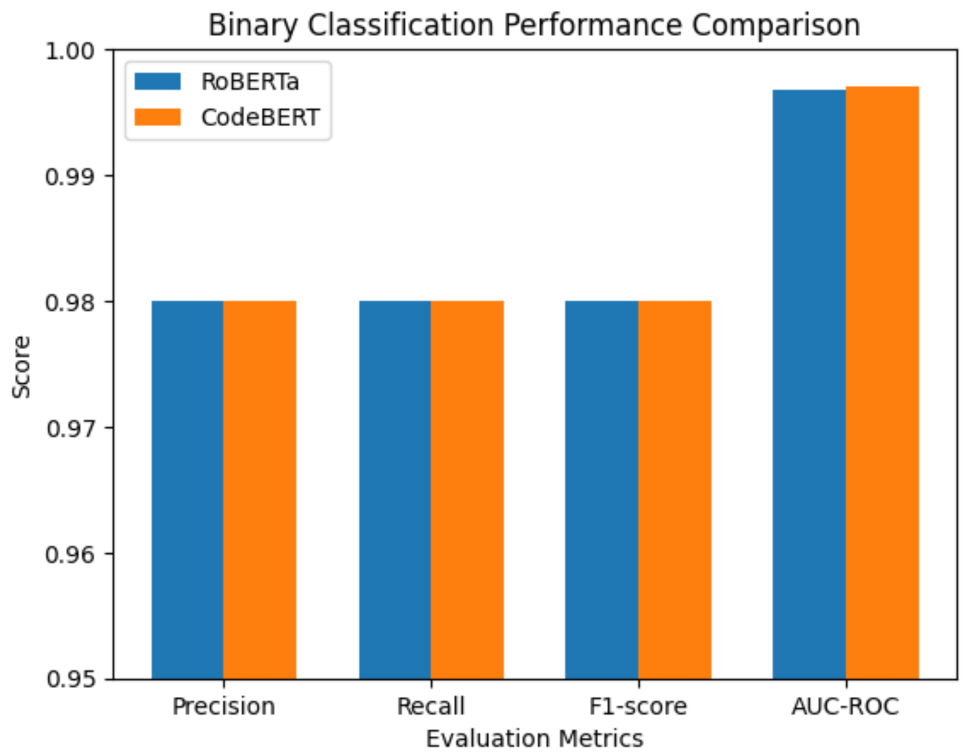
Stages \ Models	RoBERTa	CodeBERT
Binary classification	0.98	0.98
Multi class classification	0.7048	0.7070



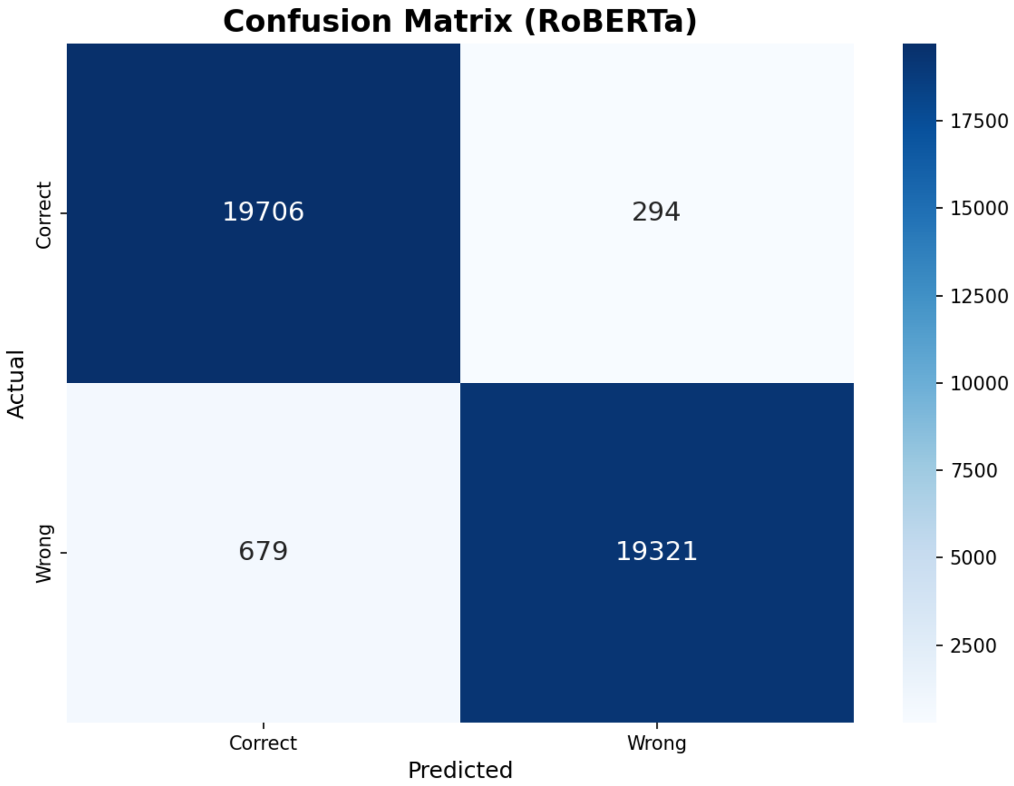
Result Analysis

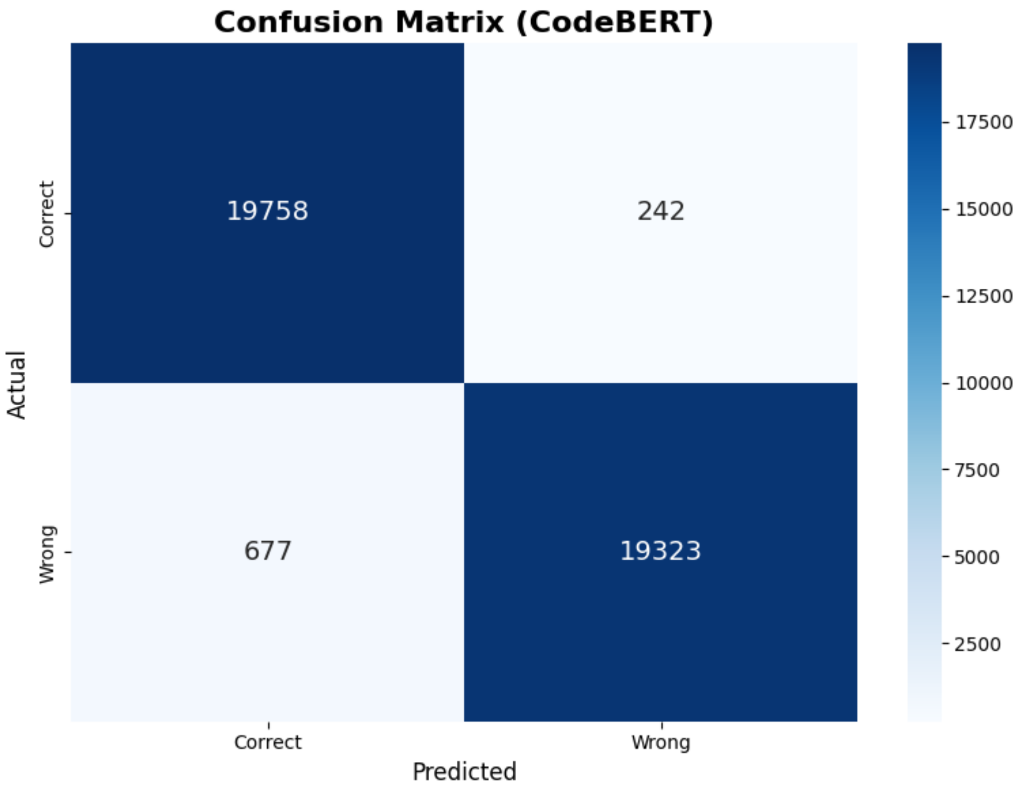
Binary classification performance

Metrics \ Models	RoBERTa	CodeBERT
Precision	0.98	0.98
Recall	0.98	0.98
F1 score	0.98	0.98
AUC-ROC	0.9968	0.9970



Result Analysis





Result Analysis

Rule(Multi) classification performance (Overall)

Models / Metrics	RoBERTa	CodeBERT
Macro-averaged F1	0.7055	0.7136
Weighted-averaged F1	0.7013	0.7040
Top-1 accuracy	0.7048	0.7070
Top-3 accuracy	0.8901	0.8938

Result Analysis

Per class rule(multi) classification performance

Metrics \ Models	RoBERTa	CodeBERT
Total number of rules	63	63
Average F1-score	0.7055	0.7136
Number of rules with F1 > 0.8	21	21
Number of rules with F1 < 0.5	11	11

Inference

RoBERTa

```
================================================================================
RUNNING INFERENCE EXAMPLES ROBERTA
================================================================================

================================================================================
DOCKERFILE LINE ANALYSIS
================================================================================
Input: EXPOSE 8080
--------------------------------------------------------------------------------

[STAGE 1] Checking if configuration is correct...
  Prediction: ✅ CORRECT
  Confidence: 0.9996 (99.96%)
  Inference time: 171.94 ms

[STAGE 2] Skipped (configuration is correct)

--------------------------------------------------------------------------------
```

```
================================================================================
RUNNING INFERENCE EXAMPLES ROBERTA
================================================================================

================================================================================
DOCKERFILE LINE ANALYSIS
================================================================================
Input: RUN apt-get update && apt-get install -y python3
--------------------------------------------------------------------------------

[STAGE 1] Checking if configuration is correct...
  Prediction: ❌ WRONG
  Confidence: 0.9996 (99.96%)
  Inference time: 208.00 ms

[STAGE 2] Identifying violated rule...
  Violated Rule: DL3009
  Confidence: 0.4662 (46.62%)
  Inference time: 1297.62 ms

  Total inference time: 1505.62 ms

--------------------------------------------------------------------------------
```

Inference

CodeBERT

```
================================================================================
RUNNING INFERENCE EXAMPLES CODEBERT
================================================================================

================================================================================
DOCKERFILE LINE ANALYSIS
================================================================================
Input: EXPOSE 8080
--------------------------------------------------------------------------------

[STAGE 1] Checking if configuration is correct...
  Prediction: ✅ CORRECT
  Confidence: 0.9998 (99.98%)
  Inference time: 163.87 ms

[STAGE 2] Skipped (configuration is correct)

--------------------------------------------------------------------------------
```

```
================================================================================
RUNNING INFERENCE EXAMPLES CODEBERT
================================================================================

================================================================================
DOCKERFILE LINE ANALYSIS
================================================================================
Input: RUN apt-get update && apt-get install -y python3
--------------------------------------------------------------------------------

[STAGE 1] Checking if configuration is correct...
  Prediction: ❌ WRONG
  Confidence: 0.9996 (99.96%)
  Inference time: 164.99 ms

[STAGE 2] Identifying violated rule...
  Violated Rule: DL3009
  Confidence: 0.4786 (47.86%)
  Inference time: 177.43 ms

  Total inference time: 342.41 ms

--------------------------------------------------------------------------------
```

Conclusion

- For binary misconfiguration detection, both CodeBERT and RoBERTa achieve excellent and identical performance (≈98% accuracy), demonstrating strong and reliable classification capability.
- In rule-specific misconfiguration classification, CodeBERT performs slightly better than RoBERTa, indicating its stronger ability to capture Dockerfile-specific and semantic patterns.
- Model selection depends on application needs: both models are suitable for large-scale binary detection, while CodeBERT is more effective for detailed rule-level misconfiguration analysis.

Future Recommendation

- Improve rule-specific classification using larger and more diverse datasets, including data augmentation for rare rules
- Explore ensemble models or hybrid approaches combining transformers with rule-based heuristics
- Integrate the proposed models into CI/CD pipelines for real-time misconfiguration detection
- Extend the approach to other IaC technologies such as Terraform, CloudFormation, and Ansible

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Thank you!!!