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

(MIT Thesis Viva Voce 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 outperforming RoBERTa.

Outline

- Introduction
- Problem Statement
- Objectives
- Literature Review
- Methodology
- Dataset Description
- Data Preprocessing
- Description of Algorithms
- Implementation Details
- Result Analysis
- Conclusion
- Future Recommendation
- 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

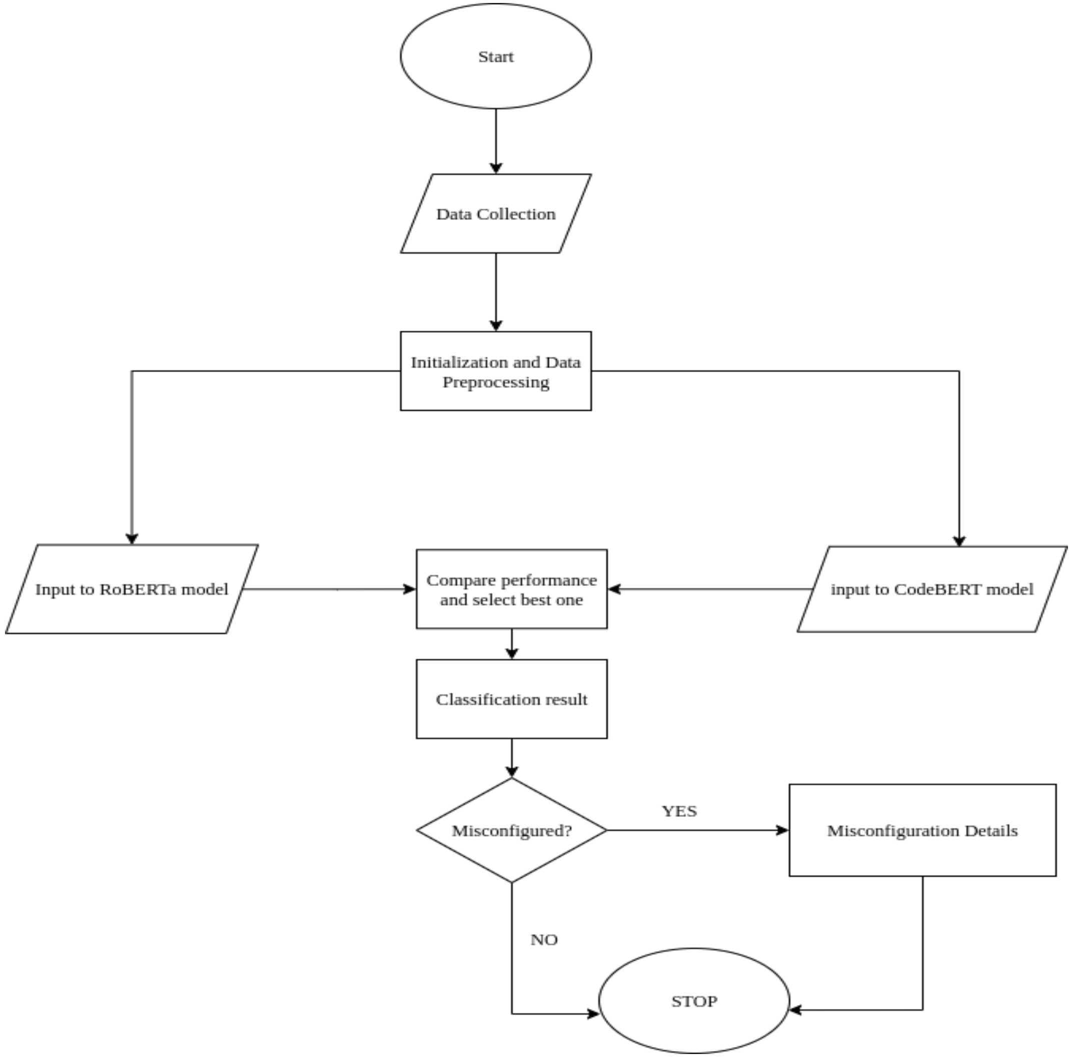
- To design and develop automated detection framework using RoBERTa and CodeBERT
- To evaluate and compare the performance of RoBERTa and CodeBERT for automated misconfiguration detection in Dockerfiles, using metrics such as accuracy, precision, recall, F1-score, and AUC-ROC

Literature Review

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

Data Preprocessing

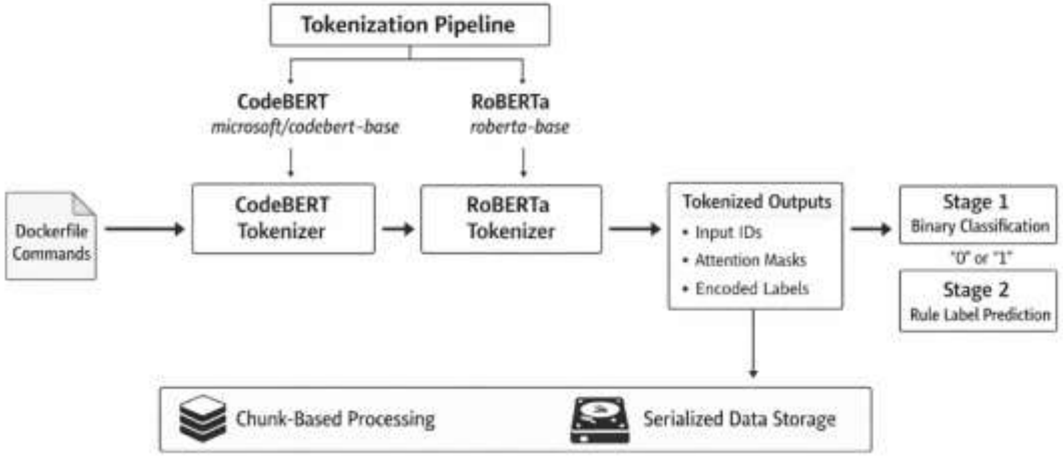
Data splitting

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

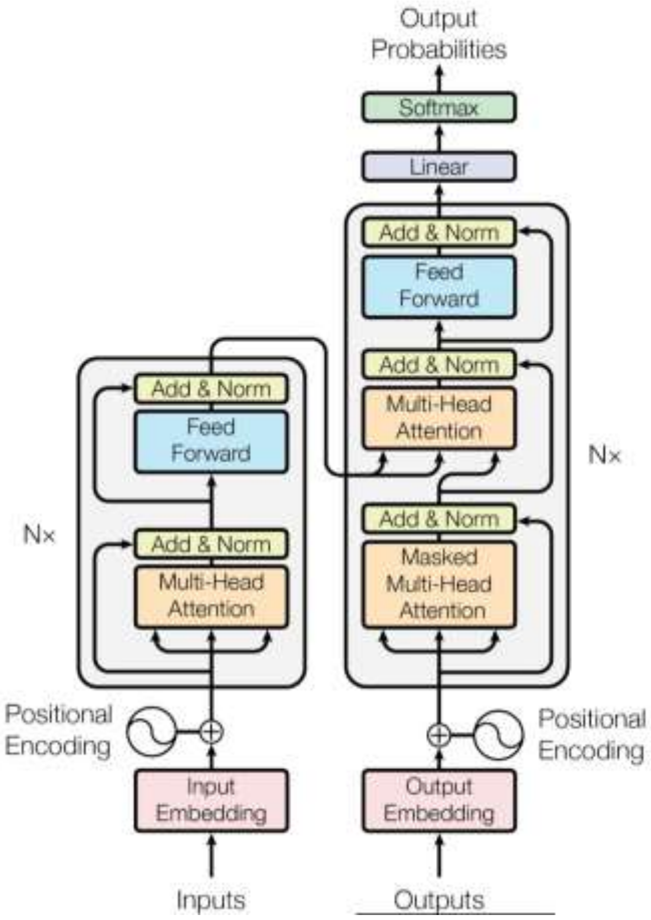


Data Preprocessing

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

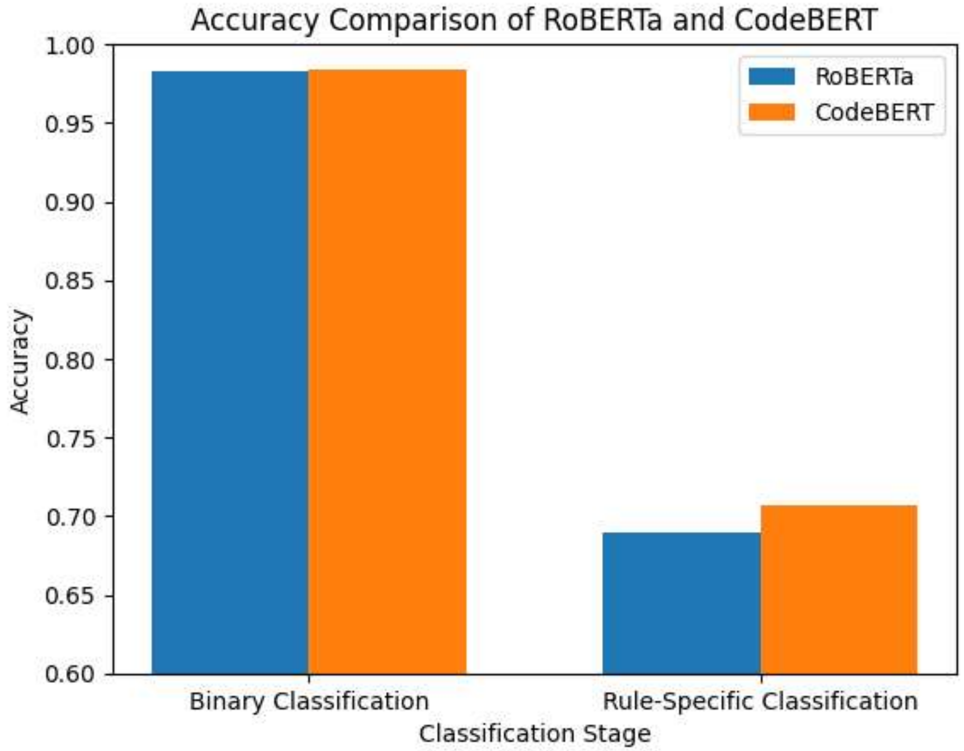
Model persistence:

- Epoch-wise checkpointing for reproducibility

Result Analysis

Accuracy

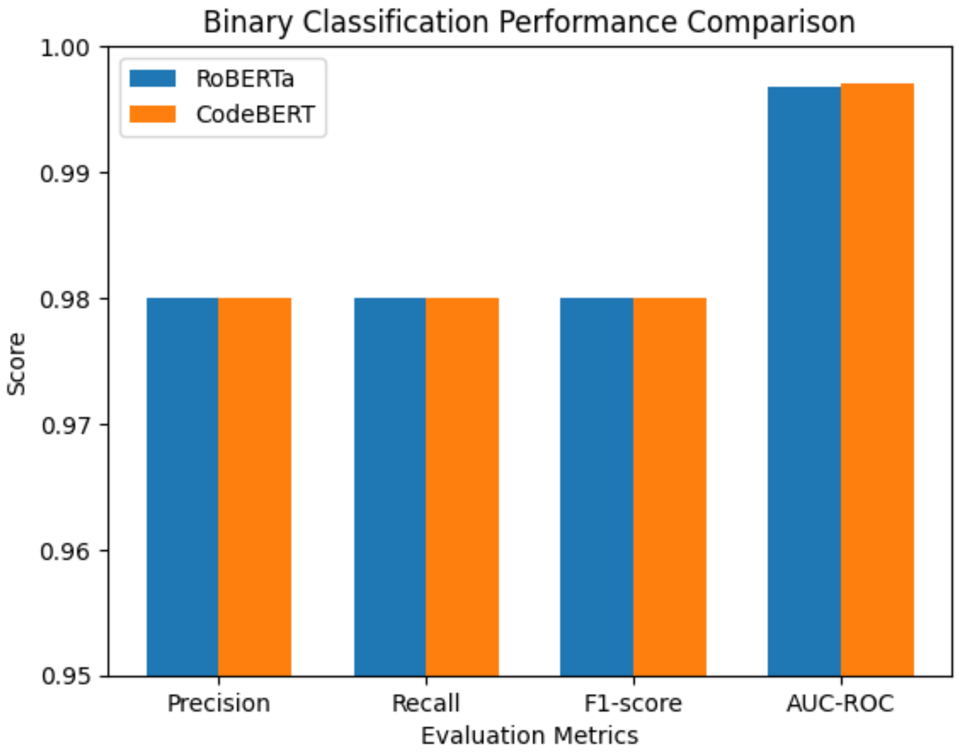
Models Stages	RoBERTa	CodeBERT	Diff
Binary classification	0.98	0.98	-
Multi class classification	0.7048	0.7070	+0.31%



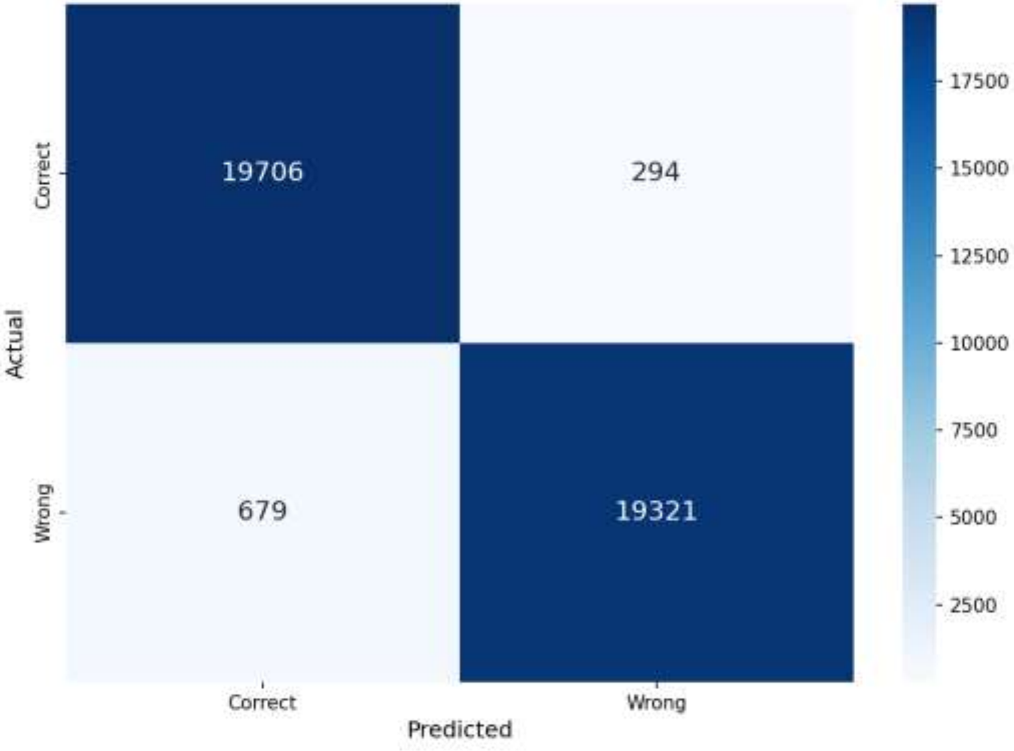
Result Analysis

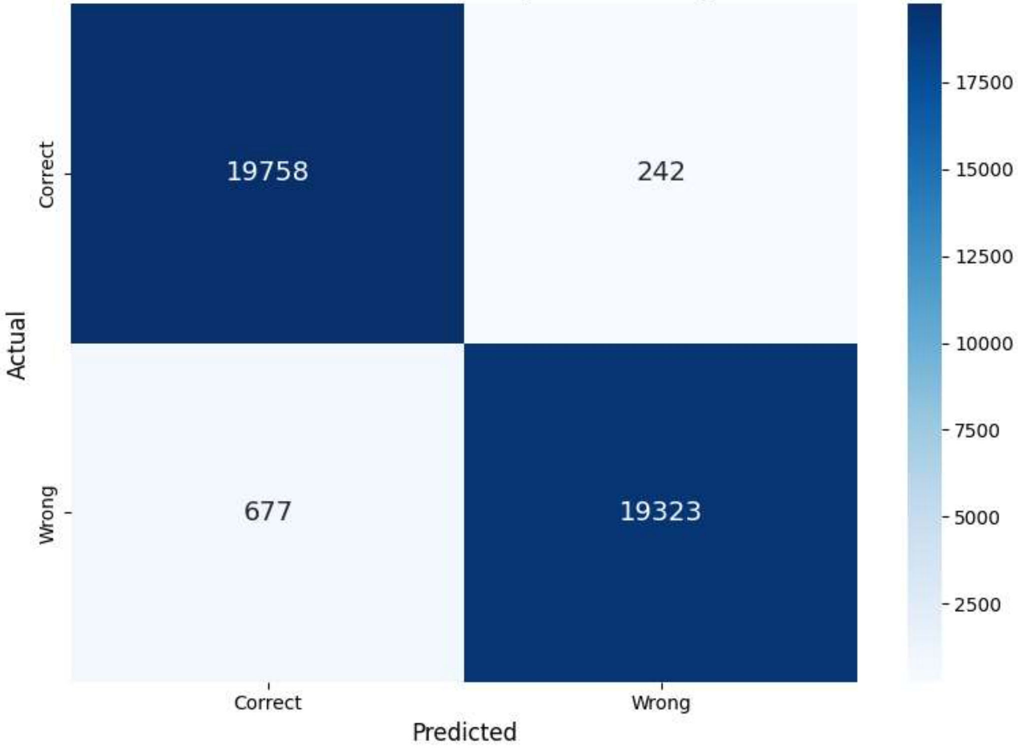
Binary classification performance

Models / Metrics	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


Confusion Matrix (RoBERTa)


Confusion Matrix (CodeBERT)

Result Analysis

Rule(Multi) classification performance (Overall)

Models Metrics	RoBERTa	CodeBERT	Diff
Macro-averaged F1	0.7055	0.7136	+1.15%
Weighted-averaged F1	0.7013	0.7040	+0.38%
Top-1 accuracy	0.7048	0.7070	+0.31%
Top-3 accuracy	0.8901	0.8938	+0.42%

Result Analysis

Per class rule(multi) classification performance

Models Metrics	RoBERTa	CodeBERT
Total number of rules	63	63
Average F1-score	0.7055	0.7136 (+1.15%)
Number of rules with F1 > 0.8	21	21
Number of rules with F1 < 0.5	11	11

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 outperformed RoBERTa, demonstrating its stronger ability to capture Dockerfile-specific and semantic patterns.
- Although RoBERTa has nearly three times more parameters, its general text pretraining limits its effectiveness for code analysis, while CodeBERT's code centric training enables better rule specific detection.
- Both models are suitable for large-scale binary detection, but CodeBERT is the more effective choice for detailed rule-level analysis due to its code-aware training.

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 detection framework as a pre-commit Git hook to provide instant feedback on misconfigurations and best practice violations.
- 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

References

- [1] S. Phillips, T. Zimmermann, and C. Bird, “Understanding and Improving Software Build Teams,” *Proc. - Int. Conf. Softw. Eng.*, May 2014, doi: 10.1145/2568225.2568274.
- [2] A. Vaswani et al., “Attention is All you Need,” in Neural Information Processing Systems, 2017. [Online]. Available: https://api.semanticscholar.org/CorpusID:13756489
- [3] J. Henkel, C. Bird, S. K. Lahiri, and T. Reps, “Learning from, Understanding, and Supporting DevOps Artifacts for Docker,” *2020 IEEE/ACM 42nd Int. Conf. Softw. Eng.*, pp. 38–49, 2020, [Online]. Available: https://api.semanticscholar.org/CorpusID:211069127

References

- [4] J. Henkel, D. Silva, L. Teixeira, M. d’Amorim, and T. Reps, “Shipwright: A Human-in- the-Loop System for Dockerfile Repair,” *2021 IEEE/ACM 43rd Int. Conf. Softw. Eng.*, pp. 1148–1160, 2021, [Online]. Available: https://api.semanticscholar.org/CorpusID:232045443
- [5] T. Shabani, N. Nashid, P. Alian, and A. Mesbah, “Dockerfile Flakiness: Characterization and Repair,” *2025 IEEE/ACM 47th Int. Conf. Softw. Eng.*, pp. 1793–1805, 2024, [Online]. Available: https://api.semanticscholar.org/CorpusID:271855816
- [6] D. W. Elliott, “Dockerfile Linting: Every time, Everywhere,” 2020, [Online]. Available: https://medium.com/@david.w.elliott/dockerfile-linting-every-time-everywhere-d8d271a1e650

References

- [7] G. Rosa, S. Scalabrino, G. Robles, and R. Oliveto, *Not all Dockerfile Smells are the Same: An Empirical Evaluation of Hadolint Writing Practices by Experts*. 2024. doi:10.1145/3643991.3644905.
- [8] Y. Zhou, W. Zhan, Z. Li, T. Han, T. Chen, and H. C. Gall, “DRIVE: Dockerfile Rule Mining and Violation Detection,” *ACM Trans. Softw. Eng. Methodol.*, vol. 33, pp. 1–23, 2022, [Online]. Available: https://api.semanticscholar.org/CorpusID:254564701
- [9] J. Henkel, C. Bird, S. K. Lahiri, and T. Reps, “ICSE 2020 Artifact for: Learning from, Understanding, and Supporting DevOps Artifacts for Docker.” Zenodo, 2020. doi: 10.5281/zenodo.3628771.

Thank you!!!