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INAÊ SOARES DE FIGUEIREDO

Code Quality Metrics for Circuit Optimization in a Quantum Anomaly Detection Context

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Inaê Soares de Figueiredo

Code Quality Metrics for Circuit Optimization in a Quantum Anomaly Detection Context

Dissertação, apresentada à Universidade Estadual Paulista (UNESP), Faculdade de Ciências, Bauru, para obtenção do título de Mestrado em Ciência da Computação.

Orientador: Prof^o Dr. Kelton Augusto Pontara da Costa

Coorientador: Prof^o Dr. Higor Amario de Souza

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ATA DA DEFESA PÚBLICA DA DISSERTAÇÃO DE MESTRADO DE INAÊ SOARES DE FIGUEIREDO, DISCENTE DO PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIA DA COMPUTAÇÃO, DA FACULDADE DE CIÊNCIAS - CÂMPUS DE BAURU.

Aos 05 de dezembro de 2025, às 10h, por meio de Videoconferência, realizou-se a defesa de DISSERTAÇÃO DE MESTRADO de INAÊ SOARES DE FIGUEIREDO, intitulada **Code Quality Metrics for Circuit Optimization in a Quantum Anomaly Detection Context**. A Comissão Examinadora foi constituída pelos seguintes membros: Professor Doutor KELTON AUGUSTO PONTARA DA COSTA (Orientador(a) - Participação Virtual) do(a) Departamento de Computação / UNESP / Câmpus de Bauru - FC, Prof. Dr. FELIPE FERNANDES FANCHINI (Participação Virtual) do(a) Departamento de Física e Meteorologia / UNESP / Câmpus de Bauru - FC, Professor Doutor RONALDO MARTINS DA COSTA (Participação Virtual) do(a) Instituto de Informática / UNIVERSIDADE FEDERAL DE GOIAS, Após a exposição pela mestrandia e arguição pelos membros da Comissão Examinadora que participaram do ato, de forma presencial e/ou virtual, a discente recebeu o conceito final APROVADO. Nada mais havendo, foi lavrada a presente ata, que após lida e aprovada, foi assinada pelo(a) Presidente(a) da Comissão Examinadora.

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Dissertação apresentado(a) à Universidade Estadual Paulista (UNESP), Faculdade de Ciências,
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RESUMO

A cibersegurança é uma preocupação crescente, sendo a privacidade e a proteção contra ataques pontos de discórdia importantes entre organizações e clientes. A aplicação de tecnologias modernas, como modelos de aprendizado de máquina para detecção de anomalias, pode ser eficaz para a privacidade e a segurança, e há uma urgência em compreender como a aplicação de tecnologias modernas, como computadores quânticos, pode trazer ainda mais avanços para essas aplicações. A computação quântica encontra-se atualmente em uma era de ruído, na qual os computadores quânticos existentes não conseguem executar tarefas sem gerar quantidades consideráveis de erros.

Este projeto de pesquisa visa analisar o desempenho de um modelo de Rede Neural Quântica quando aplicado a tarefas de detecção de anomalias usando os conjuntos de dados UNSW-NB15 e CSE-CIC-IDS2018. Além disso, avaliará como a remoção de "code smells" quânticos impacta as simulações e o desempenho do modelo. O modelo é reproduzido usando simulações com e sem ruído, e o impacto da otimização na redução de ruído também será avaliado.

Palavras-Chave: Computação Quântica, Detecção de anomalias, Aprendizado de máquina quântico, Engenharia de *software* quântica.

ABSTRACT

Cybersecurity is a growing concern, with privacy and protection against attacks being important contention points between organizations and customers. The application of modern technologies, such as machine learning models for anomaly detection, can be effective for privacy and security, and there is an urgency to understand how the application of modern technologies, like quantum computers, can bring even more advancements to these applications. Quantum computing is currently in a noisy era where the existing quantum computers cannot perform tasks without generating considerable amounts of error.

This research project aims to analyze the performance of a Quantum Neural Network model when applied to anomaly detection tasks using the UNSW-NB15 and CSE-CIC-IDS2018 datasets. Furthermore, it will evaluate how the removal of quantum code smells impacts the simulations and performance of the model. The model is reproduced using noisy and noiseless simulation, and the impact of the optimization on noise reduction will also be evaluated.

Keywords: Quantum computing, Anomaly detection, Quantum machine learning, Quantum software engineering.

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LIST OF ABBREVIATIONS AND ACRONYMS

AD	Anomaly Detection
ADS	Anomaly Detection System
alap	As late as possible
API	Application Programming Interface
asap	As soon as possible
CIC	Canadian Institute for Cybersecurity
CPU	Central Processing Unit
CSE	Communications Security Establishment
DDoS	Distributed Denial of Service
DoS	Denial of Service
DT	Decision Tree
FFT	Fast Fourier Transform
FM	Feature Map
FN	False Negative
FP	False Positive
FS	Feature Selection
GPU	Graphic Processing Unit
IDE	Integrated Development Environment
IDS	Intrusion Detection System
QaaS	Quantum as a Service
QADS	Quantum Anomaly Detection System
QC	Quantum computing
QDT	Quantum Decision Tree
QML	Quantum Machine Learning

QNN	Quantum Neural Network
QP	Quantum Program
QPU	Quantum Processing Unit
QSE	Quantum Software Engineering
QSVM	Quantum Support Vector Machine
ML	Machine Learning
NaN	Not a Number
NISQ	Noise Intermediate Scale Quantum
NN	Neural Network
NNC	Neural Network Classifier
OS	Operational Service
RAM	Random Access Memory
SDK	Software Development Kit
SVM	Support Vector Machine
TN	True Negative
TP	True Positive
UN	United Nations
VQA	Variational Quantum Algorithm

LIST OF SYMBOLS

$ x\rangle$	Ket notation, represents a quantum state
$\langle x $	Bra notation, represents the transposed conjugate of a quantum state
$ x\rangle\langle x $	KetBra notation, represents the external product, or vector product, of a quantum state
$\langle x x\rangle$	BraKet notation, represents the internal product of a quantum state
$ \psi\rangle$	General state of a qubit
α	Alpha
β	Beta
γ	Gamma
ϵ	Epsilon
$ \alpha ^2$	Module of α squared
\otimes	Tensor product
\mathbb{H}	Hilbert Space
\in	Included in
\mathbb{C}	Complex numbers set
\dagger	Dagger, represents the transposed conjugate of a vector or matrix
us	microsecond, 10^{-6} s
ns	nanosecond, 10^{-9} s

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A INTRODUCTION

Quantum computing, an area that has been studied for decades, finds itself in the middle of a boom of interest, investments, discoveries, and advancements. Part of the current excitement with the area comes from the fact that 2025 has been declared by the United Nations (UN) the International Year of Quantum Science and Technology (IYQ) (IWQ, 2025). Adding to the expectations that are being directed towards quantum technology developments, big companies that have spent years investing in quantum research have been announcing and making available more advanced resources.

IBM started their Quantum platform offering to the free plan users access to their 5 and 7 qubit quantum processing units (QPUs), but in less than 2 years made the 127 QPUs available. In the beginning of 2025, the company announced more changes to its platform, including making the Heron QPU (156 qubits) available in the free use plan (Roberts et al., 2025). By the end of 2024, Google unveiled its newest quantum chip, Willow, with the promise that it reduces error exponentially as more qubits are used (Neven, 2024). Microsoft recently presented the Majorana 1 topological chip, declaring that it paves the way for quantum chips with millions of qubits (Bolgar, 2025).

In the first months of 2025, Amazon Web Services scientist also announced a new quantum chip that has integrated error correction (Brandão; Painter, 2025). They propose that it makes the step of correction more efficient and less expensive in terms of energy and resources it requires to be implemented. Error reduction, or noise reduction, is another important research topic related to the necessity to minimize the amount of error that quantum computers generate to a point where it is no longer necessary to factor it in the evaluation of quantum programs.

Parallel to the advancements in quantum hardware development, research into other topics such as quantum networks, communication and data transference have gained traction, with promises that quantum computing could be the solution for safer network communications and better cryptography protocols (Hannover, 2025). In 2024, a group of scientist carried out the first demonstration of quantum teleportation using optical fibers carrying conventional telecommunications traffic (Thomas et al., 2024) and another group proposed a method for automatic polarization compensation, which is important to maintain the quantum information being transferred intact (Chapman et al., 2024). There is even research being conducted on the future of the Internet and the impacts of quantum computing on the safety and protection of data being shared over it, already considering the attacks that may be directed towards a quantum Internet and all the classical encrypted data that is shared today. To that extent, some researchers aim to find ways to transfer data that is more secure against interception (Kashi; Kues, 2025), and others focus on developing safer communication protocols (Hassani et al., 2025). The QIY institutions is also supporting events that promote discussions about cybersecurity in the quantum era, such as Quantum Safe: Quantum Communication for Data Security, a discussion panel set

to happen later this year (QuIN, 2025).

Another application for which quantum computers have been greatly applied is Quantum Machine Learning (QML). Many different models have been developed, considered equivalent to their classical counterparts, but most times they are unable to reach the same good results. Some of these models aim to implement Quantum Anomaly Detection ((Gouveia; Correia, 2020; Chen; Liu, 2022; Deng; Wan; Guo, 2022; Huang et al., 2017)), considering that the classical Anomaly Detection research would be greatly advanced by any application that could present high-quality real-time predictions and that could be possible with noise-free QC.

Quantum computing research has shown great improvement in recent years, with the development of machine learning algorithms with the potential to be advantageous compared to their classical counterparts (Li; Deng, 2022), the development of many different quantum machine learning models (Li; Deng, 2022; Larocca et al., 2023), and the researches into quantum communications. But the quality of these applications and future advancements depend greatly on finding the best solutions for the removal or correction of error in quantum codes. In 2023, a group of researchers (Chen et al., 2023) presented eight code smells that are prevalent in quantum code, proposing that the removal of them could be metrics to evaluate code quality in quantum environments. Other more recent researches on the Quantum Software Engineering (QSE) field agree with Chen et al. (2023) and propose a great variety of techniques and tools for identifying and removing problems from quantum code.

One thing that greatly impacts the error rate in quantum programs is the size of the circuit used, since every quantum gate and operation can introduce noise into the system, and the longer the execution time, the more vulnerable the system is to suffering physical interferences. Taking this into consideration, this research proposes to evaluate how well adhering to the above mentioned code quality metrics affects the results of quantum machine learning algorithms aimed at anomaly detection. This evaluation regards both the predictive capabilities of the models as well as the circuit generated after transpilation. The lack of work published on these themes is a strong motivator for this research, as the author believes that any advancement can be of great contribution to the whole quantum computing field. The recent publications also highlight the perceived importance of the topic.

A.1 OBJECTIVES

The quantum computing field has seen many changes and advancements in the last two years. Some of those affected directly this research project, causing it to suffer some changes and evolve into something more relevant to the current quantum computing challenges. The main focus of the research remained the same: to understand and explain the impacts of applying code quality metrics and removing code smells on the results obtained by machine learning models trained for anomaly detection on simulators and real quantum computers. But some of the steps to get to the final result were changed.

J.2 CONCLUSION

Developing research in areas that are still developing is rewarding because there is still a lot to discover. But it is also a challenge to have to work with constantly adjusting tools and limited resources. Nevertheless, it is a great learning opportunity to be dealing with new discoveries and updates in real time.

The main focus of this Masters research project was to evaluate possible code optimization techniques with the expectations that, when applied to a quantum development environment, they would result in better transpiled circuits that could yield better results. In the end, it was verified that there are some steps that need to be taken when writing quantum circuits that will have this expected results, and these observations were validated by other researchers and by IBM Qiskit updates that reinforce the importance of well done pre-processing of the circuit before execution.

One innovative thing done in this project was testing different feature mapping techniques to find the one that generated the best data representation for the QAD problem at hand. It was observed that it varies depending on the dataset, as expected, and it does not generalize well from one to another in a noisy environment. The best results were obtained using the XY Pauli matrices.

The results from the various model configuration tests showed that each smell can affect the QNN's prediction capabilities in a higher or lower degree but they all change it in some way. Some effects were related more to longer training times than to actual metrics values, but that is also an important indicator to consider when choosing a learning model to train.

It is possible that the relatively small overall size of the circuit caused the interference of noise on results to be less pronounced, but it was still observable, indicating that having a code with too many smells is indeed detrimental to the development of good learning and classification models. Also, the chosen FM, the backend layout and the small number of qubits did not create the need for the inclusion of SWAP gates into the circuit, which is a gate that is known to add lots of noise to quantum circuits. The use of SWAP gates is a great exploration to be done in future work.

For cybersecurity applications a better QNN model would still need to be developed, or perhaps more qubits would need to be used. Either way, the metrics reached through the model trained for this research is far from the quality of state-of-the-art classical AD applications.

In relation to cybersecurity and the need for real time results, it needs to be considered that with the present model of quantum computing through online services this can not be achieved. For real-time applications, classical computation is still the only solution.

J.3 FUTURE WORK

The research conducted and presented in this document leaves many points to be explored with more time and resources. Some important topics for future work that the researcher would like to highlight are listed below:

- Execute and evaluate the developed and simulated codes on a real quantum computing backend;
- Test the effectiveness of the QNN Classifier on unbalanced datasets and other key cybersecurity datasets;
- Evaluate the effectiveness of other feature selection techniques;
- Implement different quantum circuit optimization methods proposed by authors in recent years;
- Compare other data encoding methods to the Feature Mapping technique evaluated in this research;
- Work with more data features and consequently with circuits composed of more qubits;
- Personalize the QNN Classifier, changing optimizers, loss functions and other parameters that can be modified;
- Try multi-threading techniques to try and overcome the hardware limitations that were encountered.

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