Womanium Quantum + AI Project 2024
Fraunhofer ITWM
Quantum Machine learning for Conspicuity detection in production

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Outline

Section 1 - Introduction

       The project focuses on identifying Weld defects using non destructive testing (NDT). The Tungsten inert gas (TIG) [1] welding is an arc welding process which is mainly used in joining high value precision components together.It is traditionally a manually implemented process, capable of achieving higher quality weldments in comparison with other arc processes. However, it currently has many limitations, because of its manual process. Furthermore, it also lacks the flexibility to perform the welding of complex geometries.

The automation of the TIG welding process is crucial for overcoming its current limitations. To ensure high-quality, consistent, and repeatable results, it is essential to implement effective monitoring and control systems for the weld pool throughout the automated process. So, to incorporate automation in the quality analysis process, Computer Vision (CV) methodologies are used to find out whether the welded item is perfect for production or needs to be scraped using high dynamic range (HDR) cameras.

We will be using this dataset of images collected and preprocessed by Kaggle [2] and are available open source to train Deep learning and Quantum Machine learning models capable of identifying Weld defects in an automated, fast and less error prone manner. The model is trained to detect these 6 types of defects with significant accuracy.

1. good weld
2. burn through
3. contamination
4. lack of fusion
5. misalignment
6. lack of penetration

We treat this as a classification problem containing 6 different classes.

Section 2 - Classical Modeling

       In this section, the deep learning models which are used for this classification purpose are analyzed and compared based on the performance. The key idea in using Deep learning based approach is that, there is no need for manual feature detection which can be passed to a model for training. The deep learning algorithm learns to find out the necessary features which are required for providing a better classification result.

Section 2.1 - Binary class classification

       As a first step, starting from lower complexity, we train the model to perform just the binary classification. The model is trained to identify between a good weld and defective weld.

**Section 2.1.1 - Resnet18 - Weighted loss function**

The Resnet 18 [3] model which uses Convolutional Neural Networks followed by feedthrough layers for preventing the vanishing and restoring gradients problem is used to perform the classification. The model is trained using the Cross entropy loss function and Adam optimizer for 8 epochs in batches of 32.

The model performs well with a test accuracy of 97% in classifying images which are not used in training.
Train Accuracy - 99.49%
Validation Accuracy - 100 %
Test Accuracy - 97%
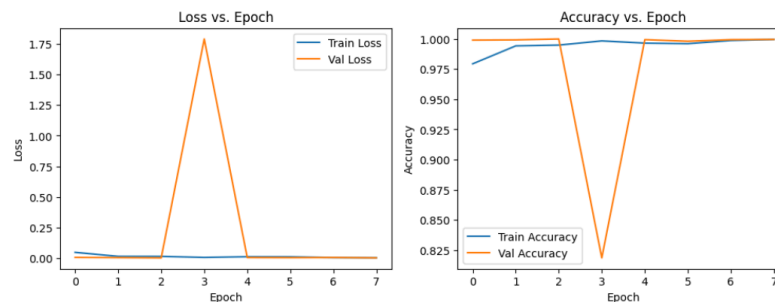
Section 2.2 - Multi class classification

Next, we try to perform classification to categorize the images in the corresponding buckets instead of just predicting whether the welding is good or not. The model is trained for 6 different classes and performance is analyzed.

Section 2.2.1 - Resnet18

In this section, we will explore using the same Resnet18 model to perform classification into 6 different buckets. The model is trained using Cross entropy and Stochastic gradient descent optimizer for 5 epochs in batches of 32.

Train Accuracy - 99.87%
Validation Accuracy - 99.98%
Test Accuracy - 67%
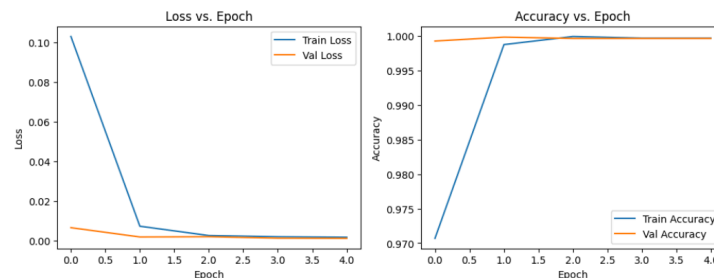
It can be noted that there is a significant drop in accuracy in the test image set because of the fact that the images in various training buckets are imbalanced. So to solve that, we will be using a weighted cross entropy loss function based on the number of images in various training buckets.

Section 2.2.2 - Resnet18 - Weighted loss function

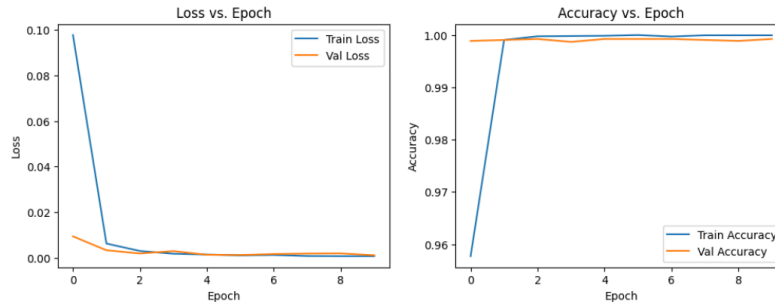In this section, we will train the Resnet18 model with a weighted cross entropy loss function for 10 epochs.
Train Accuracy - 99.99%
Validation Accuracy - 99.92%
Test Accuracy - 79%

It can be seen here that the test accuracy significantly improved over the previous case because of the weighted training. Even Though, the test accuracy is improved it is still less for highly critical application.If we take a closer look in the results, we can find that the train and validation accuracy seems pretty high but not the testing accuracy.

One possible reason is overfitting. Due to the large number of parameters in the Resnet18 model, it is prone to overfit with the training data. So, to solve this, we use a slightly smaller mode - VGG19

Section 2.2.3 - VGG19 - Weighted loss function
In this section, we will explore the VGG19 model as a solution to overfitting in the previous case. The model is trained for 10 epochs with weighted loss function.
Train Accuracy - 100%
Validation Accuracy - 99.96%
Test Accuracy - 82%
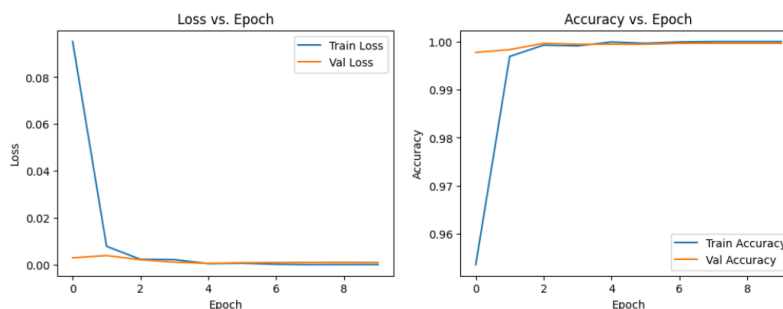
Now, we can see that the test accuracy improved to above 80%. But still there is room for improvement. Several Data Augmentation techniques can be used to create more training samples to increase the number of images from each bucket for getting better test results. This is the future scope of the project.

Section 3 - Task 4

In this section, we will be exploring Quantum Machine learning techniques and workflow for approximating a sine wave function. We will create a dataset of 1000 points between 0 and 2pi.

The Quantum Machine learning model has 4 modules.
- Initial state
- State preparation
- Ansatz
- Measurement

We set all 0's as the initial state in this example but there are other initialization strategies as well. Next, we use the amplitude embedding approach to prepare quantum states from the classical data followed by an basic entangler ansatz. Finally, we perform measurement over the Z axis (compute expectation) and readout the classification results.

Section 3.1 - State preparation

The initial state is set as |0> is passed to the quantum model and the classical data is mapped into the Hilbert space using the Angle Embedding State preparation. The x values are mapped into the Angles of the Rx rotation gates.

Section 3.2 - Ansatz

We will be using a basic entangler based ansatz. The ansatz contains 3 rotation gates in X, Y, Z followed by linear entanglement using CNOT gates. We will be using 4 qubit to have a large number of training parameters even though the input feature is 1.

Section 3.3 - Optimization and Results

A gradient free optimization process is performed for 100 iterations and the model is trained. Here, the optimization is treated as a regression problem with Mean squared error loss function and Adam optimization. The final results obtained are as below.
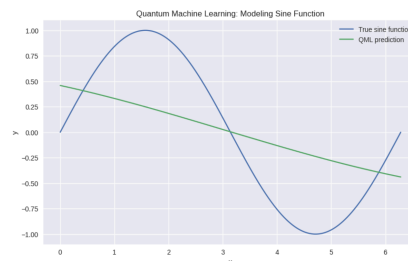
Section 4 - Quantum Modeling

In this section, we will explore the use of Quantum Machine learning [8] based models for performing Weld defect classification. The advantage of using quantum computing is the large dimension of the Hilbert space available to perform computation and gate based manipulation on any qubits will update the remaining qubits implicity without any separate gate application.

Using the principles of superposition, interference and entanglement, the Quantum Machine learning models provide a better enhancement feature to classical deep learning models.

We will be mainly exploring hybrid quantum models instead of pure quantum models as the pure quantum models are linear and it is not possible to model non-linear dataset using pure quantum models with much accuracy. Also, pure quantum models are prone to Barren plateau issues as the depth and number of qubits are increased, it becomes nearly impossible to converge to global minima.

These Hybrid models having a Classical deep neural network feature extractor followed by a linear quantum model solves the above problems. The Classical model can tune the features based on the functioning of the quantum model learnt through the backpropagation of the loss.

Section 4.1 - Binary classification
We will start with the Binary classification of the welded items as good weld or defective items. The Pennylane [4] library along with Pytroch [5] library is used for the training process.
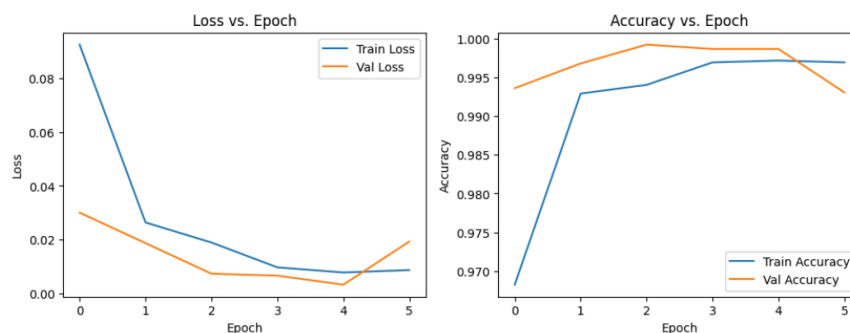
Section 4.1.1 - Hybrid - Resnet18 and VQC (4 qubits)(depth 4)(angle embedding)(Basic entangled)
In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 4 qubits, angle embedding, basic entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.
Train Accuracy - 99.40%
Validation Accuracy - 99.92%
Test Accuracy - 92%

It can be seen that the model neatly converges and has a good test accuracy of 92%.

Section 4.2 - Multi class classification
Next, we will train the hybrid quantum machine learning model (QML) to classify the weld defects into various buckets. This is treated as a multi class classification problem.
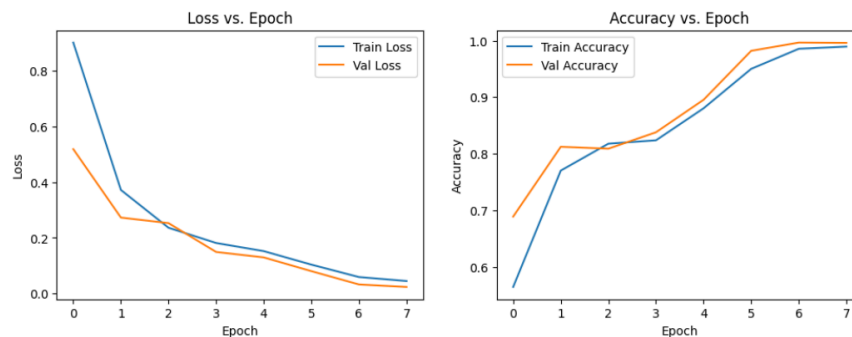
Section 4.2.1 - Hybrid - Resnet18 and VQC (4 qubits)(depth 4)(angle embedding)(Basic entangled)

In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 4 qubits, angle embedding, basic entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.

Train Accuracy - 98.58%
Validation Accuracy - 99.68%
Test Accuracy - 58%

It can be seen that the hybrid QML model has a good learning curve and it was able to achieve 99% validation accuracy. Unfortunately, it suffers from overfitting and was not able to be recovered even using a weighted loss function for unknown images.

If we print the confusion matrix, we can see that the model was unable to perform well for images samples with small training inputs.
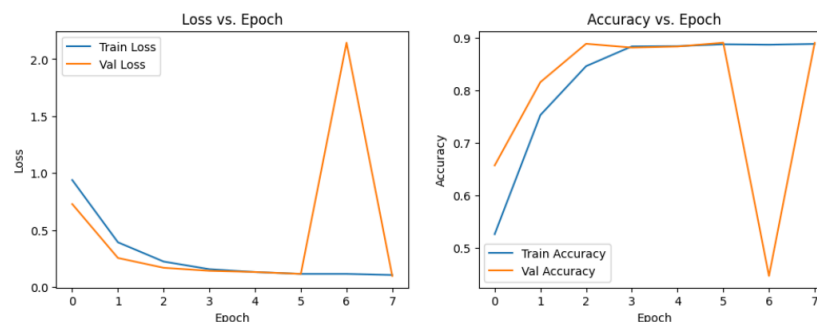
Section 4.2.2 - Hybrid - Resnet18 and VQC (4 qubits)(depth 4)(angle embedding)(Strongly entangled)
In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 4 qubits, angle embedding, strongly entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.

Train Accuracy - 88.84%
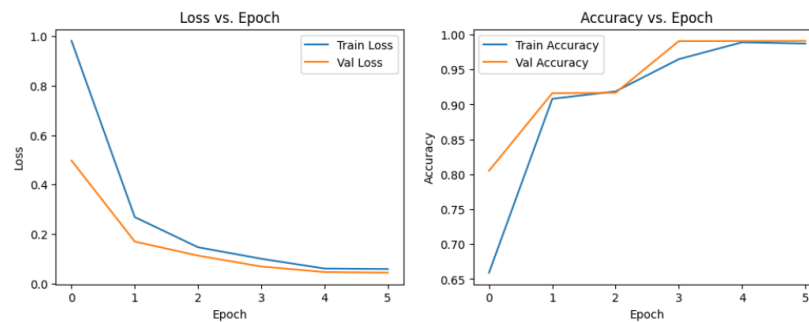Validation Accuracy - 89.14%
Test Accuracy - 59%

Section 4.2.3 - Hybrid - Resnet18 and VQC (4 qubits)(depth 8)(angle embedding)(Basic entangled)

In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 4 qubits, angle embedding, basic entangled ansatz and a ansatz repetition depth of 8. The model is trained for 10 epochs.

Train Accuracy - 98.70%
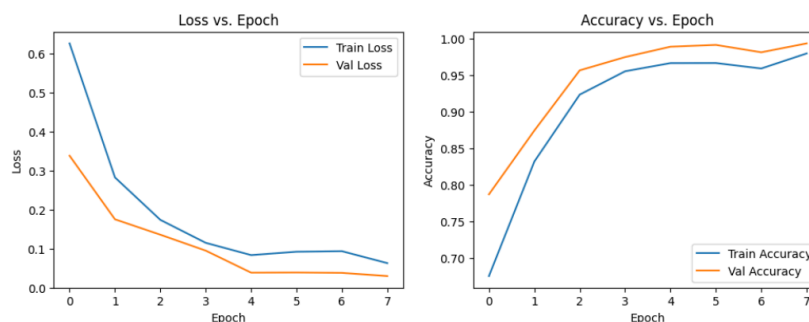Validation Accuracy - 99.08%
Test Accuracy - 56%

Section 4.2.4 - Hybrid - Resnet18 and VQC (10 qubits)(depth 4)(angle embedding)(basic entangler)

In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 10 qubits, angle embedding, basic entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.

Train Accuracy - 98.00%
Validation Accuracy - 99.38%
Test Accuracy - 58%

Section 4.2.5 - Hybrid - Resnet18 and VQC (4 qubits)(depth 4)(amplitude embedding)(basic entangler)

In this section, we will be using a Resnet18 based feature extraction followed by a Variational quantum circuit using 4 qubits, amplitude embedding [7], basic entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.

Section 4.2.6 - Hybrid - VGG19 and VQC (4 qubits)(depth 4)(angle embedding)(Basic entangled)

In this section, we will be using a VGG19 based feature extraction followed by a Variational quantum circuit using 4 qubits, angle embedding, basic entangled ansatz and a ansatz repetition depth of 4. The model is trained for 10 epochs.

Train Accuracy - 32.88%
Validation Accuracy - 32.70%
The VGG19 model due to less complexity was not able to produce good training results compared to Resnet18.

Section 4.2.7 - Comparison of models - Barren plateaus.

If we take a look at the graphs from **1) Section 4.2.1 - Hybrid - Resnet18 and VQC (4 qubits)(depth 4)(angle embedding)(Basic entangled), 2) Section 4.2.3 - Hybrid - Resnet18 and VQC (4 qubits)(depth 8)(angle embedding)(Basic entangled), 3) Section 4.2.4 - Hybrid - Resnet18 and VQC (10 qubits)(depth 4)(angle embedding)(basic entangler)**

We can note that convergence for the loss curve doesn't change that much with an increase in depth from 4 to 8 (Graph 1 and 2). This is due to the fact that, even though we have a large number of trainable parameters with increase in depth, due to the Barren plateauing effect [6] (where the optimization landscape becomes much flatter), we are not able to leverage the advantages of a large number of trainable parameters.

On the other hand, with an increase in the number of qubits from 4 to 8 (Graph 1 and 3) and having the same depth of 4, the convergence becomes faster. **So, we can note that having a large number of qubits with lesser depth is better than having a smaller number of qubits with large depth.**
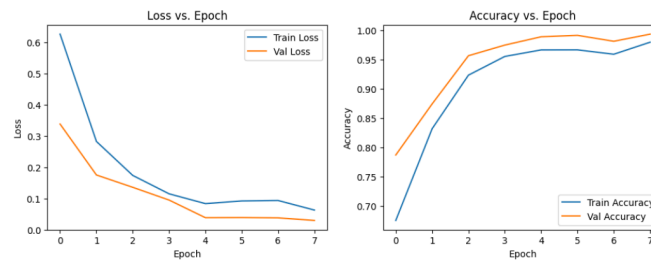
Graph 1)
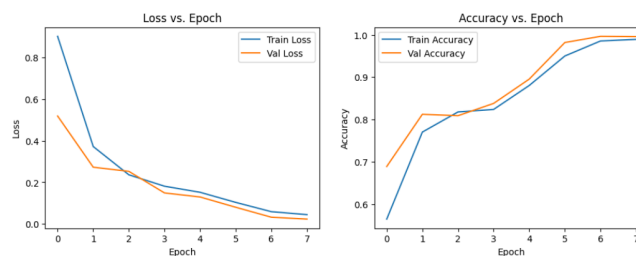
Graph 2)
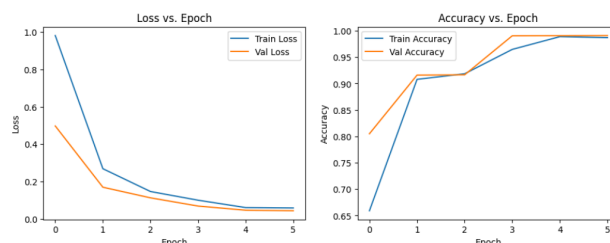
Graph 3)

Section 5 - References

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7. Mottonen, M., Vartiainen, J. J., Bergholm, V., & Salomaa, M. M. (2005). Transformation of quantum states using uniformly controlled rotations. Quantum Information and Computation, 5(6), 467–473. https://doi.org/10.26421/qic5.6-5.
8. Schuld, M., & Petruccione, F. (2019). Supervised learning with Quantum Computers. Springer.

Section 6 - Summary

In this project, we have explored the usage of Deep learning techniques and Quantum Machine learning (QML) techniques to perform classification of Welded structures whether it is a good weld or a defective item. We have also categorized the detective item into various buckets of the weld defects in an automated way.

In the case of the binary classification into good welds and defects, the classical deep learning (DL) model Resnet18 was able to achieve an accuracy of 97% while the hybrid QML model achieved 92%. It can be noted that the hybrid QML model was able to achieve good results like the DL model with a lesser number of parameters in the linear layer.

In the case of the multi class classification into good welds and also categorizing defects into various categories - burn through, contamination, lack of fusion, misalignment, lack of penetration, the classical deep learning model Resent18 was able to achieve 79% while the less complex DL model VGG19 was able to achieve 82%. This is due to the fact that an imbalanced dataset and complex model like Resnet18 are much prone to overfitting. On the other hand, the hybrid QML models were able to perform slightly less than the DL model with an accuracy of 59%. Even Though, we can see that the training and validation accuracies in hybrid QML models are more than 95%, it was not able to work well because of class imbalances, classical DL overfitting and Barren plateaus.

We can note that convergence for the loss curve doesn't change that much with an increase in depth from 4 to 8. This is due to the fact that, even though we have a large number of trainable parameters with increase in depth, due to the Barren plateauing effect (where the optimization landscape becomes much flatter), we are not able to leverage the advantages of a large number of trainable parameters.

On the other hand, with an increase in the number of qubits from 4 to 8 and having the same depth of 4, the convergence becomes faster. **So, we can note that having a large number of qubits with lesser depth is better than having a smaller number of qubits with large depth.**