Google Summer of Code 2025

Quantum Representations of Classical HEP Data with Contrastive Learning

Details:

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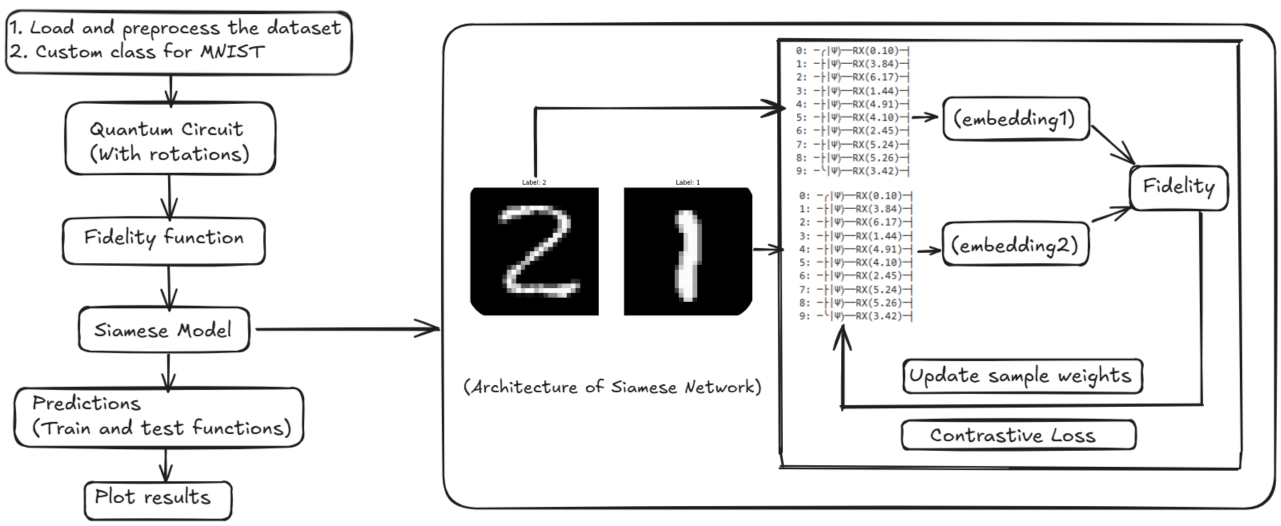


2. Goals and Deliverables

2.1. Deliverables

1. Start with a function that converts HEP dataset images into quantum states.
2. Experiment with different circuits, each yielding different quantum embeddings and fidelity results.
3. Compare each quantum model with its previous versions to evaluate performance improvements.
4. Compare the representation spaces of quantum encoding models and classical encoding models.

2.2. Prerequisite Tests

The solutions to common and specific tasks I have completed can be found here:
`https://github.com/KushalTrivedi19032005/QMLHEP`

2.3. Implemented Work and Observations

As mentioned in Task VI of the QMLPHEP document, I began my work by creating a simple function that takes an image from the MNIST dataset (which had been loaded and pre-processed earlier) and returns the quantum state (which was later extended to include two images as arguments too).

There are primarily three ways of encoding the data of image pixels into quantum information: Amplitude Encoding, Angle Encoding, and Basis Encoding.

For amplitude encoding, we first normalize the pixel values, and then we map this normalized pixel vector to quantum states. Mathematically,

$$\mathbf{p} = \left[\frac{p_1}{\sum p_i}, \frac{p_2}{\sum p_i}, \dots, \frac{p_N}{\sum p_i}\right]$$

$$|\psi\rangle = \textstyle\sum_{i=1}^{N} \alpha_i |i\rangle$$

where,

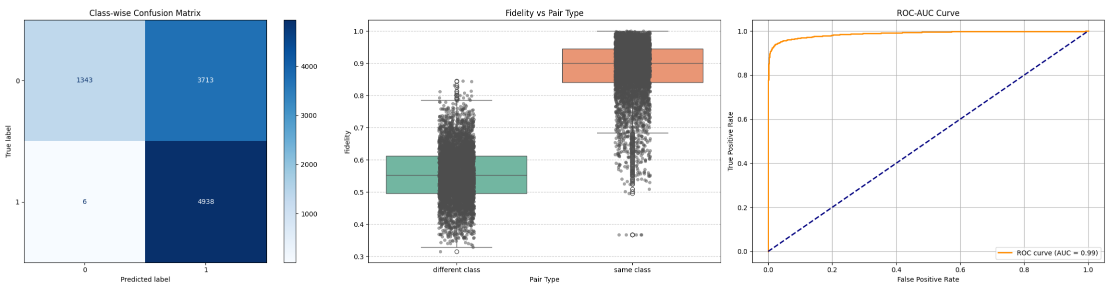
- $\alpha_i = \sqrt{\frac{p_i}{\sum p_i}}$ are the amplitudes, and
- $|i\rangle$ are the computational basis states.

Further, I implemented the SWAP test and functions for calculating fidelity, creating quantum embeddings using the above circuit, and defining the class for contrastive loss.

I also implemented a custom class to obtain pairwise images from the MNIST dataset—positive pairs (images from the same class) and negative pairs (images from different classes).

The main task was to implement the Siamese model. It flattens the images from a pair, calls the quantum embeddings function, and compares them. After each epoch, the sample weights (which are parameters of the model) are updated during backpropagation, and the loss value is updated.

Note : Since no pre-processing was applied, the training time per epoch was long. Therefore, the model was trained for just five epochs.



A few important observations from these plots are :

- The high number of False Positives (3713) suggests that the model tends to predict class 1 more often, potentially leading to a high recall but lower precision for class 1.
- For different-class pairs, median fidelity score is around 0.55, and for same-class pairs it is around 0.90. Some overlap might suggest misclassifications.
- AUC = 0.99 is an excellent measure.

2.4. Future Research Directions for GSoC

- After training the model, it was observed that the loss started saturating earlier than expected. Experimenting with hyperparameters such as the margin parameter and replacing the simple learning rate with learning rate schedulers could yield interesting results.

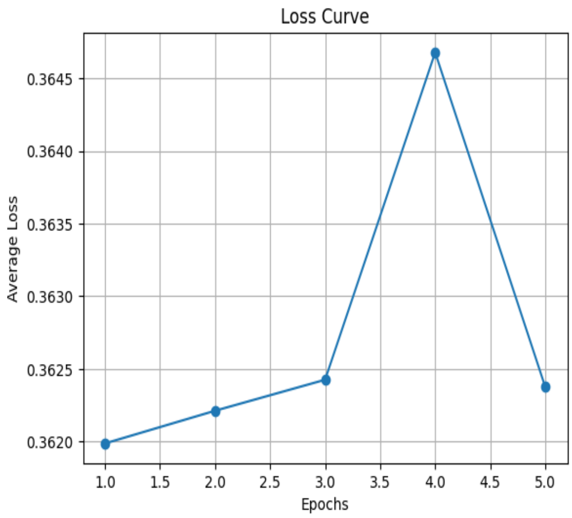


Figure 2.1: Loss curve for the Siamese network with Contrastive loss

- Pre-processing MNIST images could reduce computational costs. Since no pre-processing was applied and all 28×28 pixels were processed directly in the model, a future direction could involve methods such as Principal Component Analysis (PCA).
- Amplitude encoding is difficult to scale for large images, so trying angle encoding in the quantum circuit and comparing performances could be beneficial.
- Visualizing both quantum and classical embeddings in a low-dimensional t-SNE space could provide deeper insights.

3. Schedule of Deliverables

3.1. Application Review Period

(8th April - 8th May): During this assessment period, I will further enhance my programming skills in PennyLane and the necessary libraries for the QKANs project. Additionally, I will use this one-month period to deepen my theoretical understanding of QKANs and explore potential experimental ideas that could be implemented during the coding phase.

3.2. Community Bonding Period

(8th May - 1st June): During this period, I will focus on getting to know the mentors, thoroughly reading the project documentation, and familiarizing myself with the details, especially since this project is being introduced for the first time in ML4SCI. This is expected to take some time. Afterward, I will discuss ideas with the mentors, gather feedback, finalize the datasets, iterate on improvements, and ultimately begin working once all conditions are deemed satisfactory.

3.3. Programming Period

Phase 1 (2nd June - 14th July):

- **Week 1: Classical KAN Model Implementation**
  - Set up the project environment for training and testing (including necessary libraries/tools).
  - Implement the classical KAN model as a baseline on the new HEP dataset.
  - Identify strengths and weaknesses of the classical KAN model.
- **Week 2 and Week 3: Implementing QKAN Model**
  - Research and implement the Quantum Kolmogorov-Arnold Network (QKAN) model.
  - Train and test the QKAN model on HEP dataset.
  - Compare the performance of the QKAN model with the classical KAN model.
- **Week 4: Performance Metrics and Evaluation**
  - Define performance metrics (e.g., accuracy, loss, training time).
  - Evaluate both the classical KAN and QKAN models using these metrics.
  - Document findings and identify areas for further research and improvements.

Phase 2 (14th July - 1st September):

- **Week 5: QKAN Model Refinement**
  - Complete any incomplete work related to the QKAN model.

- Test the performance of the QKAN model with different loss functions and optimizers.

- **Week 6: SineQKAN Extension**
  - Extend QKANs to SineQKANs as suggested in previous sections.
  - Implement and test the performance of SineQKAN.
- **Week 7 and Week 8: Hybrid KANs and Documentation**
  - Explore the possibility of a hybrid version of KANs, if feasible.
  - Thoroughl documentation of all work completed during Google Summer of Code (GSoC '25) in GitHub README files, Medium blog posts, and presentations for the end-term evaluations.
  - The documentation will cover:
    * Prior research and initial contributions before the cohort began.
    * Discussions and brainstorming sessions with mentors during the bonding period.
    * Final implementation of the models.

4. Biographical Infomation

4.1. Academic Details

I am Kushal Trivedi, a second-year undergraduate (sophomore) pursuing an Integrated B.Tech + M.Tech degree in Information Technology at the Atal Bihari Vajpayee Indian Institute of Information Technology and Management, Gwalior, India. Currently, I am in my fourth semester with a CGPA of 8.41 out of 10, placing me in the top 15% of my batch.

From 2021 to 2023, I prepared for the Joint Entrance Examination (JEE) Mains and Advanced, highly competitive entrance exams for admission to India's prestigious research and engineering institutes. I secured a rank in the top 1 percentile in both exams, which are taken by approximately 12–13 lakh students each year, leading to my admission to this institute.

Over the past two years, I have been actively practicing Machine Learning and Artificial Intelligence. I am familiar with Rust, Java, and C, and I consider myself proficient in C++ and Python.

Alongside my passion for computer science, I have always been deeply interested in the natural sciences, particularly Physics and Mathematics. My fascination with particle physics began in middle school after reading the globally renowned book *A Brief History of Time* by *Stephen Hawking*. More recently, attending the International Conference on Applied AI and Scientific Machine Learning provided me with further insights into the intersection of physics and programming.

Beyond my academic pursuits, I enjoy participating in nationwide hackathons. I was a winner of the Smart India Hackathon '24, a government-initiated competition aimed at developing hardware and software solutions to real-world challenges. In this event, my team developed a multimodal chatbot for Bharat Electronics Limited, a major public-sector organization supplying defense utilities to the Indian Army. Additionally, I have participated in several other hackathons, including IIT Roorkee's TechFest Hackathon, Convolve 3.0, and more.

4.2. Motivation for Quantum Machine Learning

Simply put, I truly value the opportunity provided by Google and ML4SCI QML-HEP. My passion for quantum physics dates back to my school days when I had little knowledge of advanced sciences. However, as I started preparing for the JEE and later took it as a course in college, I began to understand it piece by piece, admiring both its complexity and its real-world applications. Last summer, I started studying Quantum Computing using textbooks and online resources.

However, there was no way to apply the knowledge or gain experience since it is still a niche field with limited opportunities. Therefore, this initiative is the perfect platform to connect with like-minded individuals, further hone my skills, and also provide me with a pathway to pursue my postgraduate studies in the subject.

5. Availability Schedule

5.1. Working Hours

I can commit the required time for the project to achieve the timely deliverables as outlined below:

- **Working Timimgs for Weekdays :**
  Preferred Timings: Between 8 p.m. to 2 a.m. IST
- **Working Timings for Weekends :**
  Preferred Timings: Between 10 a.m.to 1 p.m. IST and/or 4 p.m. to 8 p.m.

I have summer holidays from May 4 to July 28, which allows me to work flexibly according to the needs of the project, as directed by the mentors. After the summer break, I have college classes scheduled from 9 a.m. to 5 p.m. (with some free slots), which will allow me to work comfortably in the late evenings or nights, from 8 p.m. to 2 a.m., depending on the project requirements.

As additional information, I am also actively seeking research internship opportunities. Should I be selected for one, I assure you that it will not delay the project's progress. In such a case, I will be able to work more comfortably in the late evenings onwards.

5.2. Mentor-Mentee Meetings and Updates

I can assure you that I will work in the following manner:

- Weekly meetings with mentors (preferably on Google Meet/Zoom, but I'm flexible with any platform) to discuss new progress, including both theoretical ideas and code implementations.
- Pushing the code to GitHub repositories after seeking feedback, and correcting the code if negative feedback is received, as well as proper documentation of every step.
- Finalizing the current steps and creating a list of the next achievable tasks.

5.3. Post Google Summer of Code '25

I believe that open-source initiatives are not limited to the timespan of the program; contributions beyond that period also matter. I would love to continue working on these projects after GSoC and certainly apply as a mentee next year, or perhaps even as a mentor!

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