# Accomplishments

**Major Activities: (no more than 6,000 characters)**

Our efforts this year were primarily concentrated on an extensive exploration of quantum machine learning (QML) techniques, focusing on their potential to complement and possibly surpass classical machine learning methods. In the last few years, there has been a large number of seminal publications analyzing the impact of quantum computing on machine learning. Recent theoretical work even offers mathematical proofs that quantum approaches should not improve machine learning performance. Recent experimental work has proposed a wide variety of new architectures (e.g., quantum gates) that claim to offer significant advantages over conventional computing.

While quantum computing has demonstrated success on a series of problems involving what might be described as search of combinatorial spaces (e.g., prime numbers), the impact on machine learning has been minimal. We spent significant time this year studying the literature in this area and developing an understanding of why this might be. We have implemented a range of quantum versions of these algorithms and compared their performance. We specifically investigated three quantum computing paradigms: (1) quantum annealing-based Restricted Boltzmann Machines (QRBM) using D-Wave systems, (2) variational quantum machine learning algorithm using IBM quantum platform, and (3) quantum entanglement to improve correlation measurement within machine learning tasks.

**Specific Objectives: (no more than 6,000 characters)**

Objective 1: Confirm the Behavior of D-Wave for More Complex Graphs and Datasets

Task 1 (Completed): Utilize D-Wave to identify unfamiliar local valleys that would be

elusive even to an impractically lengthy classical search.

Task 2 (Completed): Discern the most promising local valleys through statistical analysis

using a predefined set of criteria.

Task 3 (Continued): Statistically compare the basins of attraction for otherwise similar

local valleys concerning their relative sizes.

Objective 2: Develop a Hybrid Classical Quantum (HCQ) Sampling Algorithm for RBM

Training

Task 1 (Completed): Develop an approach for embedding larger graphs within the QAC

hardware.

Task 2 (Completed): Develop an Approach for Embedding Deep Graphical

Models (DGMs) within the QAC Hardware.

Task 3 (Completed): Develop the Training Algorithm for Restricted Boltzman Machines (RBMs).

Objective 3: Apply Quantum Annealing Computing to Contemporary Machine Learning

Problems

D-Wave’s adiabatic quantum computing and quantum annealing effectively solve specific optimization problems but lack flexibility for broader machine learning tasks. Variational quantum machine learning (VQML) algorithms, which use parameterized quantum circuits (“ansatz”) optimized by classical computers, are favored for their adaptability to various data-driven tasks by the research community. We implemented several VQML algorithms, including Quantum Support Vector Machines (QSVM), Quantum Neural Networks (QNN), and Quantum Vision Transformer (QViT). We generated synthetic vector datasets (Gaussian, overlapping Gaussian, Yin-Yang, Toroidal) with binary classes and features using IMLD tools. To evaluate QViT, we use a small subset of images from the Temple University Hospital Digital Pathology Breast Tissue Subset (TUBR) to classify five labels. All quantum-based experiments were conducted using local simulation.

QSVM adapts the classical SVM for quantum computers by encoding the classical data into quantum states using quantum circuits (e.g., ZZFeatureMap). The encoded data is then processed in a quantum circuit involving several quantum gates to compute the decision boundaries.

QNN is the quantum analog of classical neural networks, where parameterized quantum gates form the “layers,” and classical inputs are embedded via angle encoding (e.g., RX, RY, or RZ gates). The circuit is trained using a classical optimizer, minimizing a loss function as in classical networks.

QViT follows the Vision Transformer (ViT) architecture but replaces classical self-attention with a quantum circuit using angle encoding. We analyzed its classification performance on the TUBR dataset using an off-the-shelf QViT model.

Quantum entanglement is a physical phenomenon where the pair or group of particles remain connected so that the quantum states of each particle cannot describe independently of the other. Entangled particles have non-local correlation between them, which makes them different than the classical correlation measure. We can quantify the quantum entanglement between parts of a system using entanglement entropy, specifically von Neumann entanglement entropy. It is a quantum generalization of the classical Shannon entropy which captures both classical and quantum correlations between subsystems of a quantum system. So, it provides strictly more information than classical measure.

In machine learning, with a large amount of data, we want to capture the correlation between the data and its label. The transformer model is dominating the field because it is a better correlation learning machine, which was trained with billions of parameters. In quantum machine learning literature suggests that if we have N qubits and all of them are entangled, only one training sample is needed to get an accurate classification score. Quantum entanglement is the currency of QML, similar to how data is the main resource for performance in classical ML. We are now focused on exploring its value in machine learning as a replacement for conventional correlation.

**Significant Results: (no more than 6,000 characters)**

Objective 2:

We implemented two variants of QRBM: a standalone QRBM as a classifier, and QRBM as a feature detector with K-Nearest Neighbour (KNN) as a classifier. Table 1 presents a quantitative comparison of error rates (lower is better) for classical and quantum RBM, evaluated across three synthetic datasets (set-08, set-09, and set-10). Our experiments show that the quantum variants achieve a better error rate when the number of training samples is small ($N \leq 50$). This suggests that QRBM is a viable alternative to classical RBM when data is scarce.

We also analyzed the performance of quantum RBM models to classical RBM as a function of the number of training samples in Figure 1. We concluded that quantum models do not benefit as much from larger training sets. Adding a KNN layer to QRBM slightly improves performance over standalone QRBM, particularly on eval splits of set-09 and set-10, but not enough to close the gap with classical approach.

Objective 3:

We compared the error rates of classical and VQML algorithms. For the Toroidal dataset shown in Figure 2, both QSVM and QNN achieve very low error rates, sometimes matching or surpassing classical neural networks, likely due to the dataset’s inherent periodicity or symmetry. This suggests quantum circuits can exploit certain structural features more efficiently than classical models. For many other typical datasets (e.g., Gaussians with/without overlap and Yin Yang), QSVM and QNN did not outperform their classical counterparts.

We can visualize the decision boundaries of QSVM and SVM on the four datasets as shown in Figure 2. The plots indicate stripe-like patterns for QSVM instead of the smooth decision boundary found in SVM. ZZFeatureMap encodes classical data into quantum states through rotations with a period of $2π$. The periodic nature of quantum rotations naturally creates stripe-like patterns. Recent literature also confirms such decision boundaries. To enable a smoother decision boundary, there is a need for better quantum feature encoding algorithms.

In Figure 3, we compare the performance of SVM with quantum and classical kernel in terms of error rate, number of support vectors, training and evaluation time as a function of number of samples. We show results for a typical dataset, Yin Yang, that requires a nonlinear decision surface. We have analyzed performance for a wide range of these kinds of representative datasets, and observed that with increasing number of samples, QSVM does not improve its performance. When $N \leq 100$, the performance of QSVM is similar to or better than its classical counterpart, which also indicates that when there is data scarcity, the quantum algorithm can provide better performance. Our experimentation also supports the recent literature, which concludes that quantum classification algorithms do not give better performance or outperform their classical counterparts.

We have also analyzed performance of a fairly new algorithm, ViT. We have a quantum and non-quantum implementation of this. The ViT model outperforms the QViT model on a breast cancer detection task from tissue images. We used 8 qubits, resized the original 1024x1024 pixel image to 224x224, and it took around 3 hours for each epoch using a single GPU-accelerated quantum simulator. We need to perform more rigorous analysis to understand QViT’s capability.

Overall, our findings highlight a current performance gap for VQML on typical ML tasks, emphasizing the need for further advancements in quantum circuit and feature map design before achieving practical quantum advantage in machine learning.

To test quantum entanglement’s utility, we conducted a preliminary experiment comparing error rates of three feature extraction methods on highly complex, noisy binary datasets generated by IMLD (70% noise, significant class overlap). The three methods evaluated are (i) cosine similarity between data and weight vectors and linear classifier, (ii) MLP, and (iii) quantum entanglement entropy (Q-Ent), where feature and weight vectors are fully entangled in a quantum circuit and the entanglement entropy is measured as a non-classical feature representation.

We systematically varied the number of samples (from 10 to 10,000) and features (from 10 to 5,000) to investigate each method’s robustness. For larger sample sizes and higher feature dimensions, the Q-Ent method often matches or outperforms the classical methods (e.g., at 10,000 samples and 1,000 features, Q-Ent achieves the lowest error rate). Although preliminary and requiring more runs for statistical significance, the Q-Ent method demonstrates competitive or superior results in several scenarios, suggesting that quantum-inspired entanglement features may capture relationships missed by classical techniques.

**Key Outcomes: (no more than 6,000 characters)**

We have integrated our QRBM, QNN and QSVM models into our well-known machine learning teaching tool (IMLD). This makes it very easy to do back-to-back comparisons between quantum algorithms and their classical counterparts. Unfortunately, the quantum algorithms are extremely computationally expensive on conventional processors, so only small data sets can be run. Nevertheless, it is very useful to be able to compare conventional and quantum algorithms from a common framework.

We developed the computing infrastructure in Python, enabling local experimentation through the simulation environment (CPU and GPU) compatible with both D-Wave and IBM quantum computing systems. We also established an end-to-end workflow to submit and manage computational tasks on cloud-based quantum platforms provided by D-Wave and IBM. Our infrastructure ensures reliable simulated experimentation as well as easy integration to the real quantum hardware, enhancing our ability to validate QML algorithms effectively.

In recent years there have been a number of wide-ranging studies that have suggested quantum approaches do not provide improved performance. We have added to this impressive body of literature by calibrating these results as a function of complexity and the amount of training data. We have also shown that quantum entanglement offers a potential for better machine learning algorithms for certain types of data. Explorations of this are on-going.

**Training Opportunities:**

All our students are trained on the three key parts of machine learning: data, programming and machine learning experiments. Since data development is a large part of our mission, they learn how to manage and manipulate big data sets in Linux. This involves scripting and learning how to create complex Linux commands using pipes.

Students are also exposed to a very strict software engineering process. We have been doing this for over 40 years, so we are very experienced at how to train students to become good, disciplined programmers. We follow a strict design, implementation and testing process. The code we produce is widely regarded as being well designed and documented.

We also train them on how to script experiments that run on CPUs, GPUs, and new to this project, the DWAVE and IBM quantum computers. They typically program in Python and learn how to manage jobs across our heterogenous compute cluster.

The combination of these skills makes our students very valuable when seeking full-time employment after graduation.

**Dissemination:**

As has been our practice for the past 40 years, all of our data and results are publicly available from our web site. The landing page for this project is here: *https://isip.piconepress.com/projects/nsf\_fet\_quantum/html/about.shtml*. The data sets described in this report are available from this site as well. Interim project presentations and related documents are also made available as well.

**Plans for the next reporting period: (no more than 6,000 characters)**

For the upcoming reporting period, our primary goal is to advance Objective 3, specifically T3 (optimization of training) and T4 (experiments on EEG and DPATH). Our efforts will focus on developing and evaluating lightweight quantum self-attention mechanism using a quantum linear algebraic approach, which is more suitable for current Noisy Intermediate-Scale Quantum (NISQ) quantum computing era. The primary applications are DPATH and EEG data segmentation and classification.

We aim to design a scalable and efficient quantum self-attention mechanism based on quantum linear algebra algorithms. This approach will directly leverage quantum primitives such as quantum state preparation, quantum matrix multiplication, and quantum inner product estimation. The goal is to overcome the inefficiencies of VQML algorithms and instead exploit the well-established speedups provided by quantum linear algebra, especially in correlation measures central to the self-attention mechanism. Our focus will be on (i) high-resolution digital pathology images and (ii) multichannel time-series EEG signals.

For DPATH, we will select a representative subset of WSIs (e.g., TUBR dataset), preprocess into smaller patches (e.g., 16×16 or 32×32), and map their features into quantum states. For EEG systems, multichannel datasets will be segmented into short-time channels will be encoded as quantum states. Then we will compute query-key similarity, attention weights, and context vectors by exploiting quantum entanglement entropy. We will benchmark performance against classical and quantum baselines, including linear ResNet, ViT, and QViT models. All development will be performed in quantum simulators, allowing detailed analysis of circuit depth, memory requirements, and computational complexity.

We have developed a modified version of the DICE measure that compares the degree of overlap between two comparable patches in the reference and hypothesized annotations. This scoring system is available as part of our open source digital pathology tools. We refer to this modified DICE score as MDICE. We will assess the segmentation performance using MDICE for both DPATH and EEG tasks. Model efficiency will be measured by quantum circuit depth, gate count, runtime and memory requirements, benchmarking quantum linear algebra methods against variational and classical approaches. We will also assess the interpretability of quantum-derived attention patterns in the context of tissue regions and EEG channel relevance.

By the end of the next period, we expect to deliver a validated prototype of a lightweight quantum self-attention module based on linear algebra, with benchmarking against classical and variational quantum approaches for DPATH and EEG datasets. The work will provide new insights into the practicality of quantum linear algebra for real-world ML tasks and help guide further algorithmic and hardware development for QML in medical applications.

# Impact

***What is the impact on the development of the principal discipline(s) of the project?***

**The performance baselines we have established often demonstrate that many published results on quantum computing don’t hold up well under careful evaluation on realistic data. The performance gains of the algorithms we have tested based on external publications have not shown to hold on our EEG and digital pathology data sets.**

***What is the impact on other disciplines?***

**Our open source tools make it easy for other disciplines to come up to speed on quantum machine learning.**

***What is the impact on the development of human resources?***

We continue to train a significant number of undergraduates and high school students who would not normally get these opportunities.

***What was the impact on teaching and educational experiences?***

**Our ML application, IMLD, is used in our own machine learning course. The web version will make it easy for other to adopt this since they do not have to install any software.**

***What is the impact on physical resources that form infrastructure?***

***What is the impact on institutional resources that form infrastructure?***

***What is the impact on information resources that form infrastructure?***

**We provide a number of resources from our web site that are useful to ML and quantum computing researchers. Our software implementations make it easy to integrate these tools into existing research.**

***What is the impact on technology transfer?***

***What is the impact on society beyond science and technology?***