Quantum Machine Learning for Particle Physics and Beyond

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Computing and Data Science Directorate

Outline

- Quantum Machine Learning for Particle Physics
- Quantum Deep Learning
  - QCNN, QGCNN, QLSTM, QRL
- Quantum Noise and Related Learning
  - Quantum Architecture Search
  - Differential Privacy, Federated Learning
  - qGradCam, Transfer Learning
  - Learning to Measure QNN
- Quantum Computing Forecast

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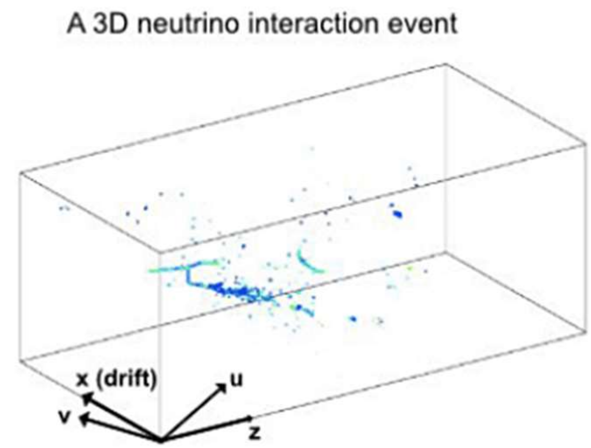
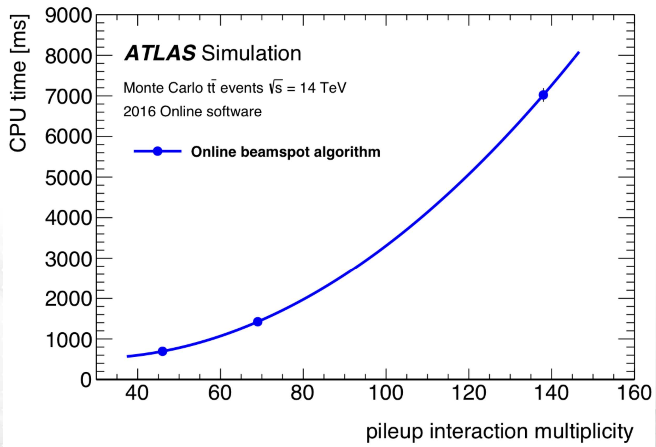
Quantum Machine Learning for Particle Physics

- Particle Physics (PP) pose an extreme scale data challenges
  - PP data (DUNE, LHC, e-RHIC, etc) are extremely sparse
  - Increased computational complexities (i.e. HL-LHC to reconstruction using MC simulation)
- Our project targets to develop the best quantum deep learning algorithms for event detection and reconstruction on PP data challenges



(top) Neutrino interaction events are characterized by extremely sparse data, as can be seen in the above 3-D image reconstruction from 2-D measurements.



(left) The ATLAS trigger track reconstruction time (quadratic time complexity) for the beamspot reconstruction algorithm for 14 TeV $t\bar{t}$ Monte Carlo simulated with 46, 69 and 138 interactions per bunch crossing, measured on a 2.4 GHz Intel Xeon CPU.

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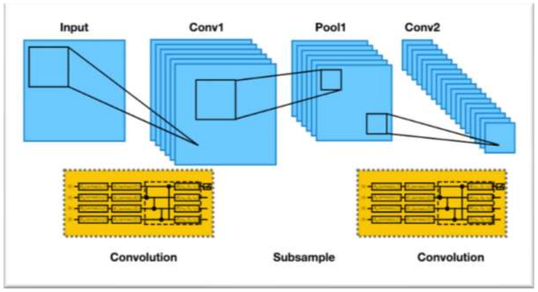
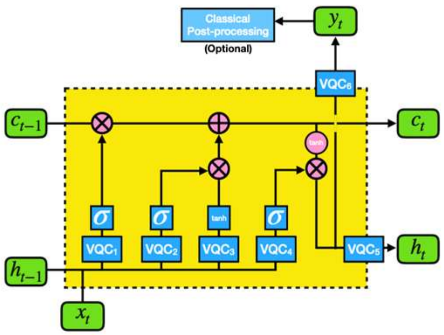
Quantum ML

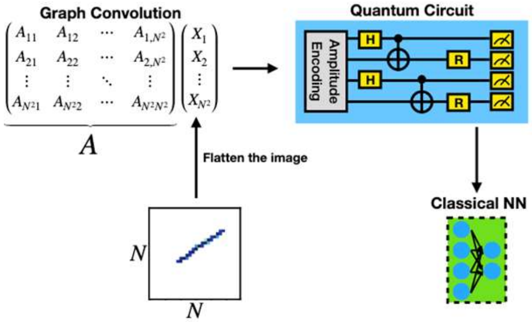
Quantum CNN



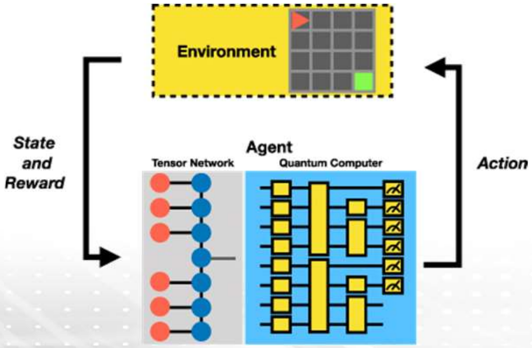
Quantum LSTM



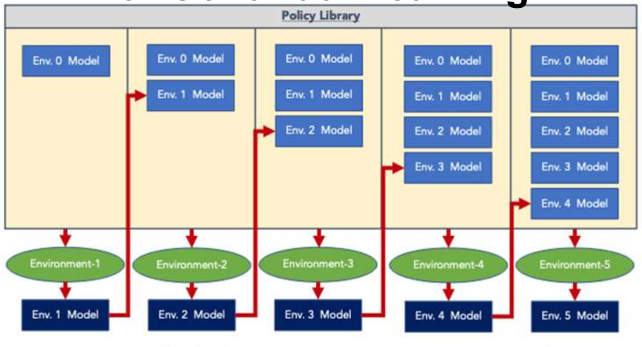
Quantum Graph NN



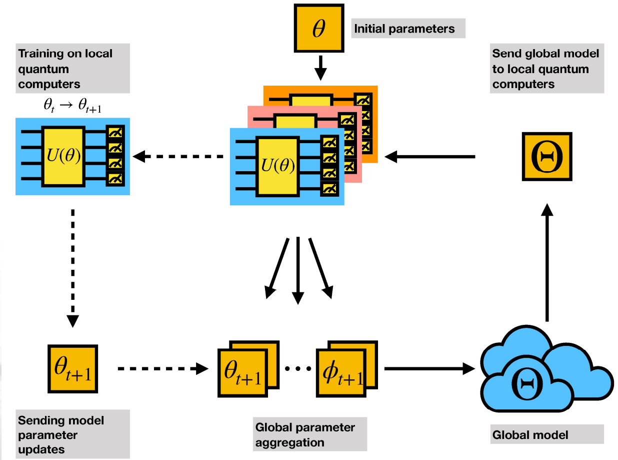
Quantum Tensor Network



Quantum Architecture Search with Continual Learning



Quantum Federated Learning

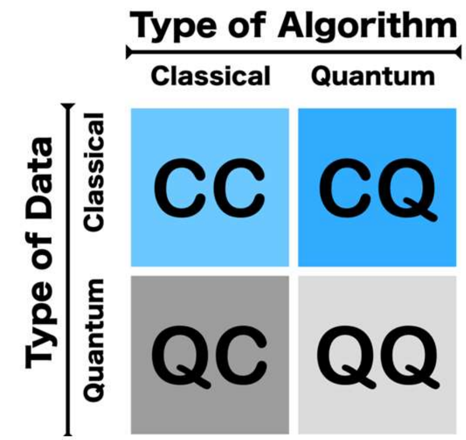


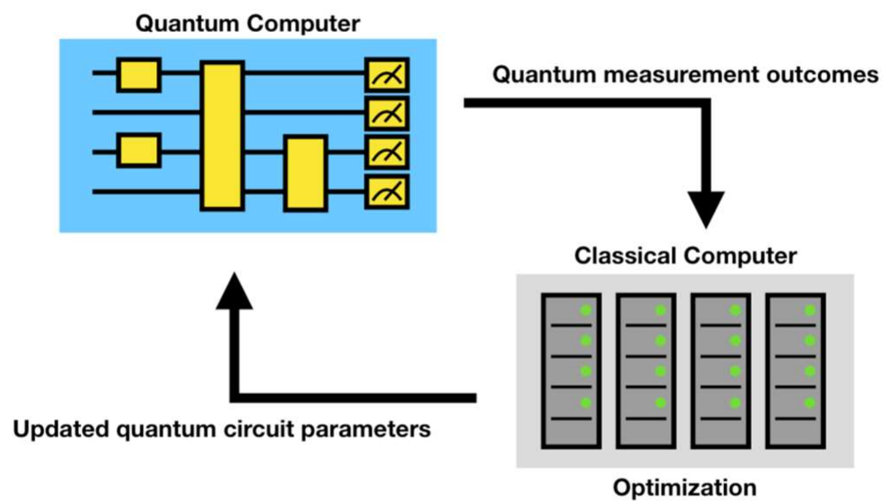
Variational Quantum Circuits (VQC)

Hybrid paradigm to leverage both quantum and classical computing.

Certain computations are carried out on quantum computers.

Others (e.g., calculating new parameters) are done on classical computers.





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Quantum CNN Learning for High Energy Physics Data Analytics

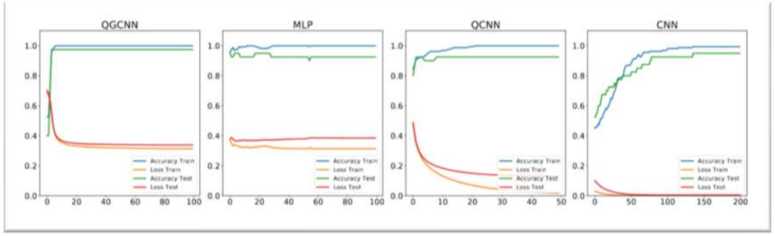
Motivation: Various experimentation/simulations have spatial correlations, but existing quantum classifiers cannot capture spatial relationships well.

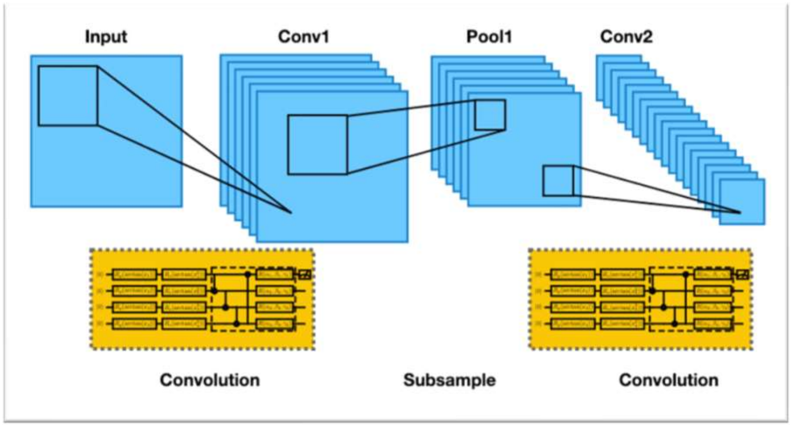
Approach:

Adapt convolutional neural network (CNN) algorithm, one of the most popular deep learning architectures in computer vision, to a Variational Quantum Classifier (VQC).

Demonstrated on a Deep Underground Neutrino Experiment dataset.

Impact: Quantum Advantage is confirmed: QCNN **converges faster** than classical CNN and reaches higher accuracies when the number of parameters are similar.

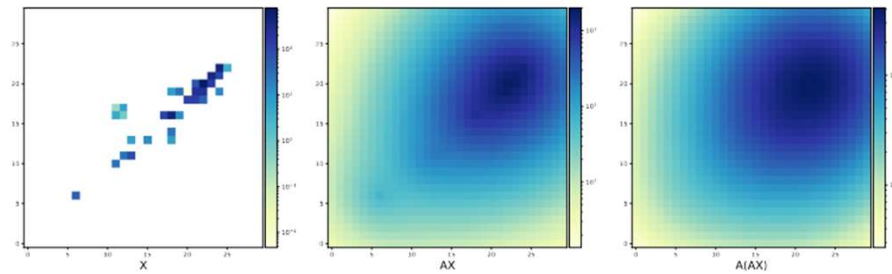


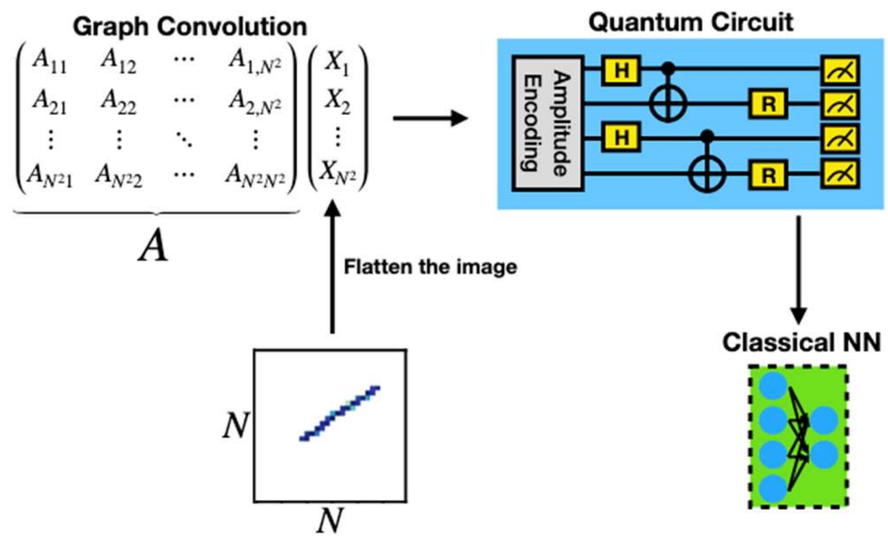


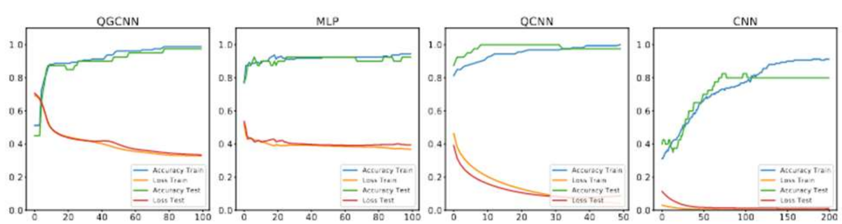
Chen, S. Y. C., Wei, T. C., Zhang, C., Yu, H., & Yoo, S. (2022). Quantum convolutional neural networks for high energy physics data analysis. Physical Review Research, 4(1), 013231.

Maintaining Quantum Advantage for Sparse Data

- **Approach**: Combining graph convolutional operation and quantum amplitude encoding on Variational Quantum Circuits.
- **Test Case**: Demonstrated on simulated DUNE dataset.
- **Result**: QGCNN **converges faster** than classical CNN, and quantum CNN reaches higher accuracies when the number of parameters are similar.







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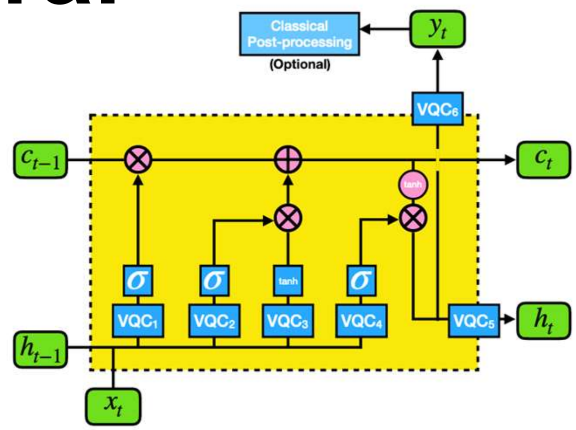
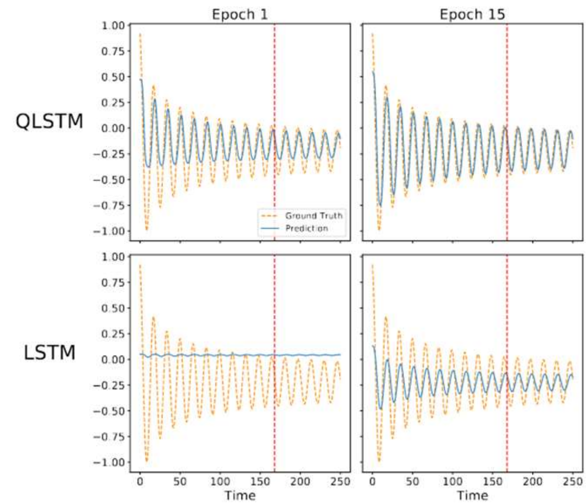
Chen, S.Y.C.; Wei, T.C.; Zhang, C.; Yu, H.; Yoo, S. Hybrid Quantum-Classical Graph Convolutional Network. arXiv 2021, arXiv:2101.06189

Capturing Long-Term Temporal Dependencies with QML

- **Challenge**: Existing quantum time series models cannot capture longer-term temporal dependencies.
- **Approach**: Develop Long Short-Term Memory (LSTM) neural network algorithm on Variational Quantum Circuits.
- **Test Case**: Demonstrated on periodical functions and quantum dynamics (delayed quantum feedback, population inversion).
- **Result**: QLSTM **converges faster** than classical LSTM when the number of parameters are similar.





Chen, S.Y.C.; Yoo, S.; Fang, Y.L.L. Quantum Long Short-Term Memory. ICASSP 2022.

Evolutionary Quantum Machine Learning with Tensor Networks

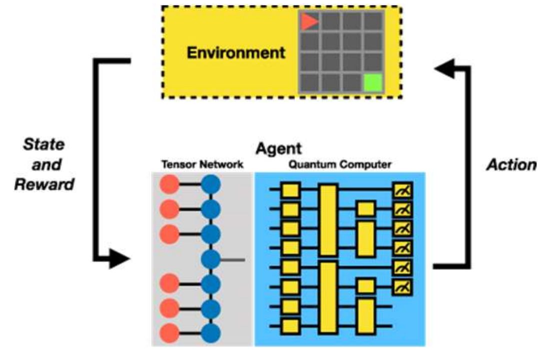
Motivation: Without certain preprocessing, quantum reinforcement learning (RL) cannot deal with complex sequential decision problems.

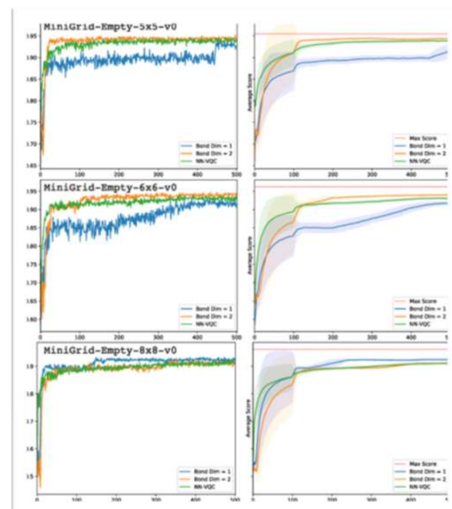
Approach:

Adapting quantum-inspired architectures, such as tensor network and evolutionary optimization algorithms, to solve quantum RL problems.

Demonstrated on a maze navigation problem.

Impact: Hybrid tensor network-variational quantum circuit (TN-VQC) architecture can exceed the classical neural network models when both models are of similar size (number of parameters).





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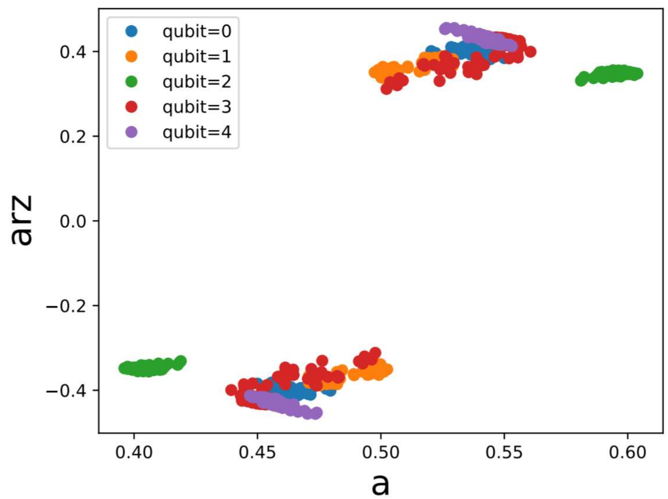
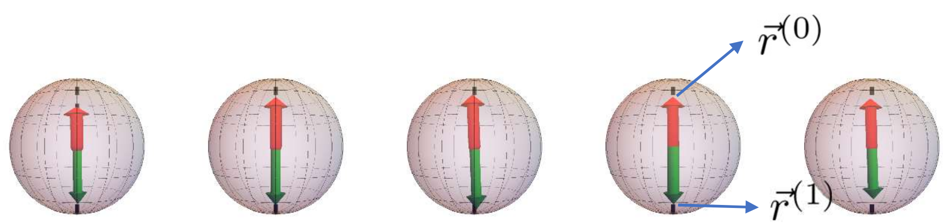
Chen, S. Y. C., Huang, C. M., Hsing, C. W., Goan, H. S., & Kao, Y. J. (2022). Variational quantum reinforcement learning via evolutionary optimization. Machine Learning: Science and Technology, 3(1), 015025.

Quantum Error Characterization [1]

- Utilizing Quantum Detector Tomography to characterize and compare the quantum error behavior of different quantum computers on IBM Q 5 Tenerife and IBM Q 5 Yorktown
  - The characterized detector model deviates from the ideal projectors by a few percent
  - Observed crosstalk across qubits (qubit operations influencing each other)
  - Consistent error behavior out of multiple measurements shows the possible approach to estimate ideal detection distribution
- Gradual distribution shift suggested the continual alignment needs



(top) Showing consistent error behavior out of multiple measurements, which shows the possibilities to estimate ideal detection distribution.



(left) IBM QX4 (5qubit) measured individually, deviate from perfect detectors (vectors pointing to north & south poles)

[1] Chen, Yanzhu, Maziar Farahzad, Shinjae Yoo, and Tzu-Chieh Wei. "Detector tomography on IBM quantum computers and mitigation of an imperfect measurement." *Physical Review A* 100, no. 5 (2019): 052315.

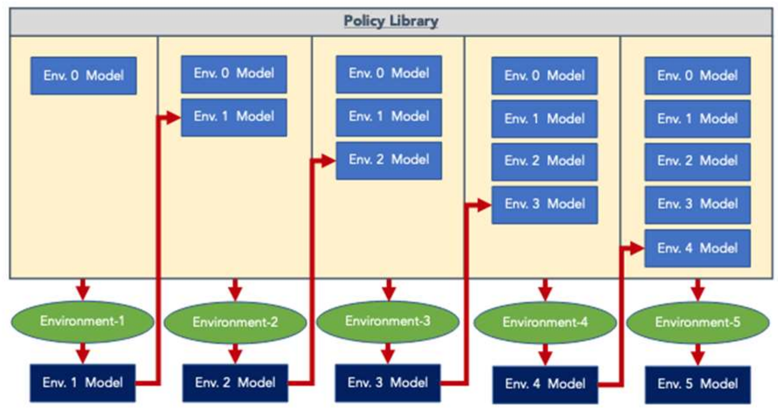
Quantum Architecture Search via Continual Reinforcement Learning

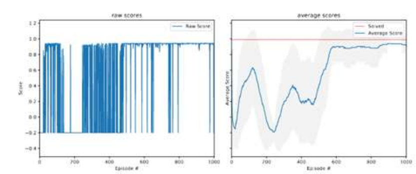
Motivation: Existing quantum architecture search schemes assume some prior knowledge of quantum circuits, are sampling from a set of potential circuits, and cannot automatically reuse previously learned policy.

Approach: Offer a continual reinforcement learning (DRL) agent to generate desired quantum circuits without encoded physics knowledge that can reduce training episodes with previous learning knowledge.

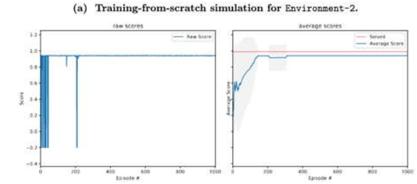
Results: The DRL agent can generate quantum circuits under the effects of noise and can learn quickly when device noise patterns change.

Impact: Results suggest the possibilities of building ML models to rewrite and update quantum AI.





(a) Training-from-scratch simulation for Environment-2.

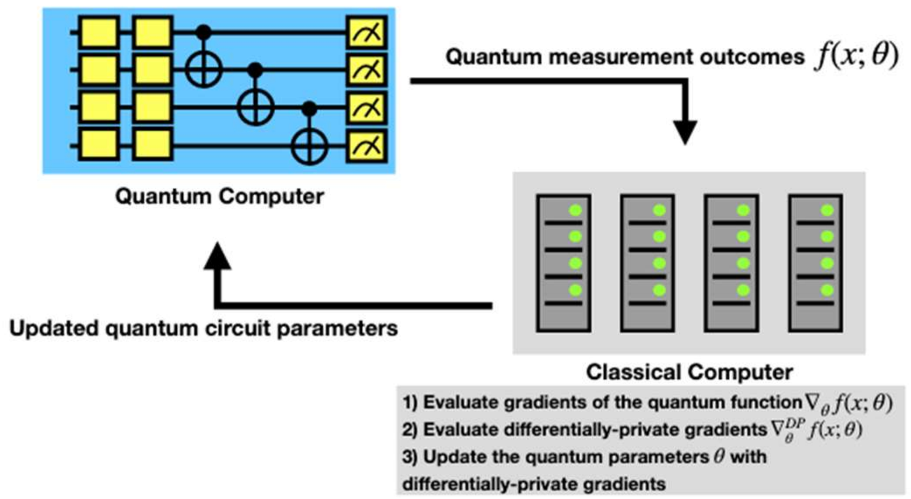


(b) Policy reuse simulation result for Environment-2.
Starting Policy Library: from Scratch - Environment-0, Policy Reuse - Environment-1.

Ye, E., & Chen, S. Y. C. (2021). Quantum Architecture Search via Continual Reinforcement Learning. arXiv preprint arXiv:2112.05779.

Differentially Private QML for Sensitive Data

- **Challenge**: Is it possible to train a QML model with good performance while simultaneously preserving privacy?
- **Approach**: Combining the differentially private (DP) optimization algorithm with optimized quantum circuit parameters.
- **Results**: Demonstrated the QML can be trained with DP algorithms and maintain performance (accuracy).
- **Impact**: Quantum advantage confirms that DP-QML **can reach comparable accuracies** to classical models while using fewer parameters.



Watkins, William M., Samuel Yen-Chi Chen, and Shinjae Yoo. "Quantum machine learning with differential privacy." Scientific Reports 13, no. 1 (2023): 2453.

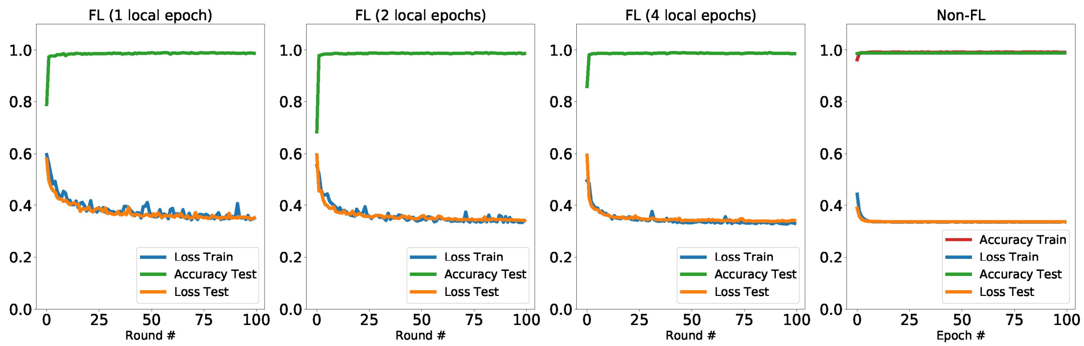
Federated Quantum Machine Learning

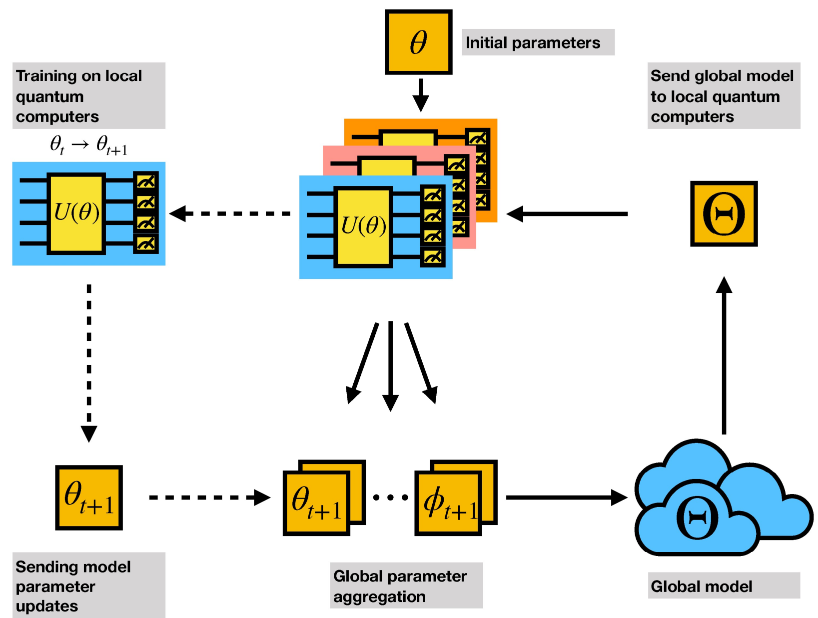
Challenge: Efficient Training of QML models on NISQ-era quantum computers.

Approach: Create a Federated QML Training Framework executed on an array of quantum computers.

Results:

- Performance does not degrade, suggesting that distributed training of QML is possible.
- Opens the possibilities that training can be scaled up to large arrays of quantum





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Chen, S.Y.-C.; Yoo, S. Federated Quantum Machine Learning. Entropy 2021, 23, 460

Quantum Federated Learning with Quantum Networks

Achievements

Implementing quantum federated learning (QFL) with quantum networks (QNs) to enhance data transfer and data security

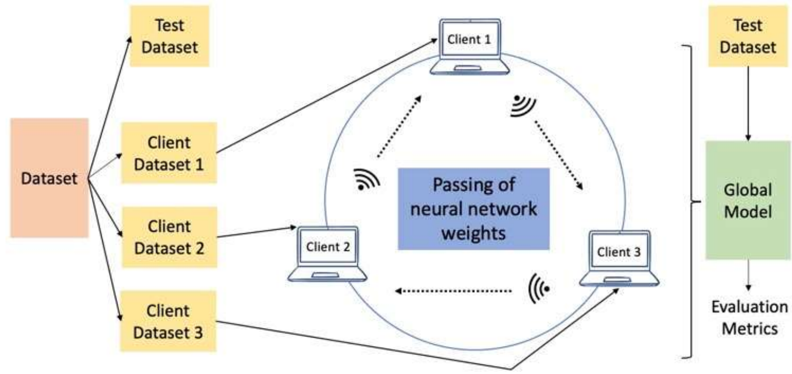
Using ring-topology structure to avoid centralized nodes and central data aggregation (no need for quantum memory)

Employing quantum teleportation in the QFL, quantum model (parameters) is free from leaking or eavesdropping.

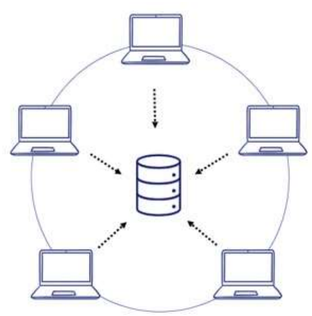
Future Work

Create Distributed Quantum Sensing using the developed QFL + QN without data gathering – more secure; less noise

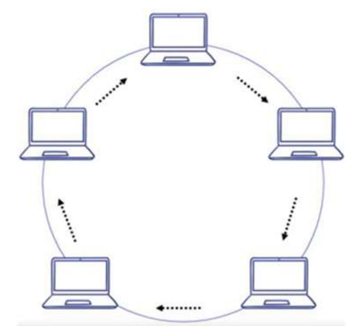
Apply to quantum astrometry for cosmology and dark matter detection via photon-entangled optical interferometry



Decentralized ring QFL framework: Data are divided between clients for training. Quantum models then update and pass weights to the next.



Hub-spoke topology (left) and Ring topology (right): (a) contains an extra central node to collect client models, while in (b) clients simply pass model parameters to the next.



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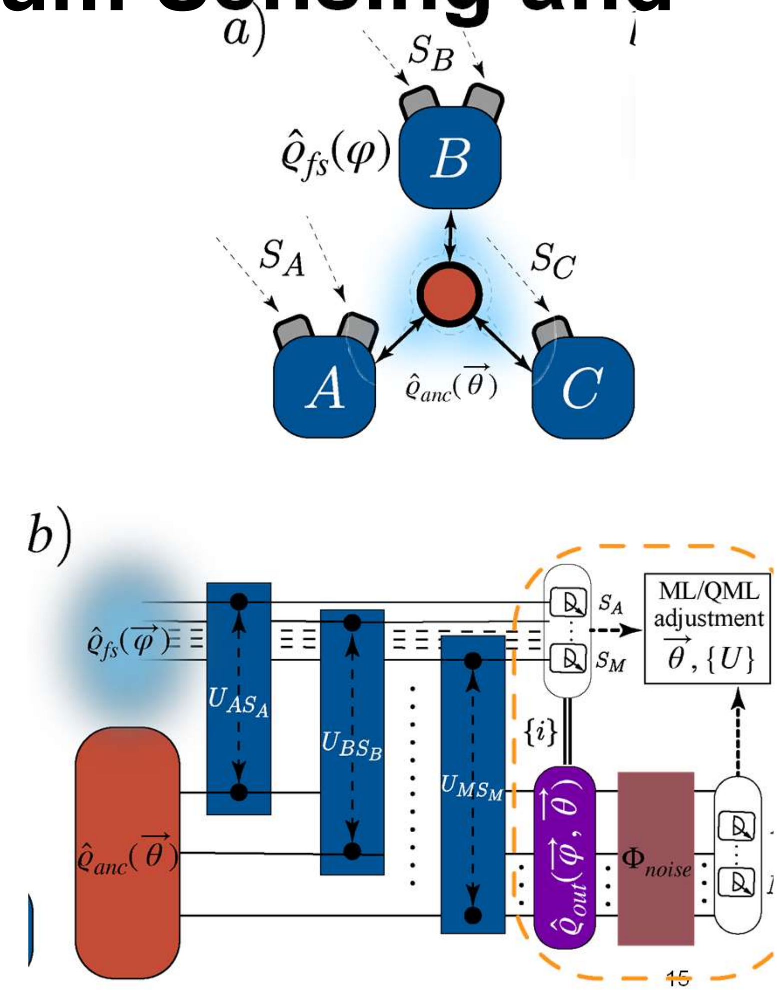
Staff: Shinjae Yoo; Huan-Hsin Tseng

Quantum federated learning with quantum networks. International Conference on Acoustics, Speech and Signal Processing (ICASSP). IEEE, 2024.

Upcoming Distributed Quantum Sensing and Machine Learning

- Distributed Reinforcement Learning
  - Quantum Sensor Network (A, B, …)
  - Tunable two-qubit (or two-mode) sets of gates described by quantum channels $\{U_{MS_M}\}$ or multi channels and qubit settings
  - Optimize the parameters of a quantum sensor network
    - choosing a particular set $\{U_{MS_M}\}$
    - tuning parameters of ancilla states $\hat{\varrho}_{anc}\,(\vec{\theta})$
    - applying the Distributed Quantum Machine Learning approach.



Quantum xAI

Motivation:

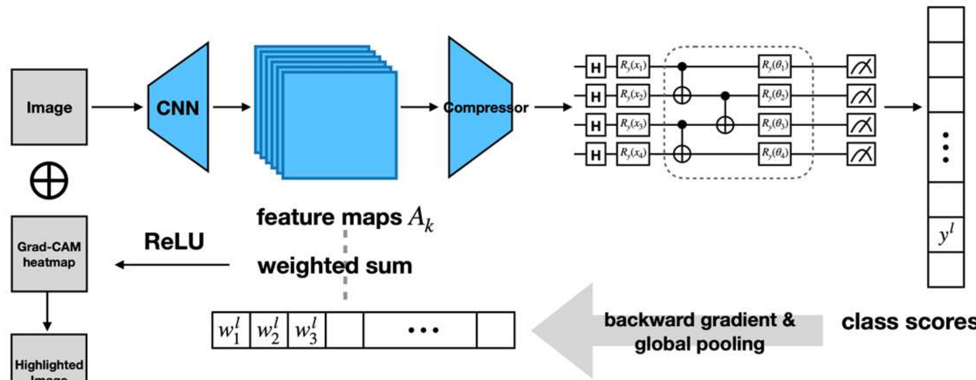
- AI is widely applied on various co-design and operation activities with the specified objective functions
- Next generation detector / accelerator / reactor design and operation
- Disruptive energy efficient computing is seriously required

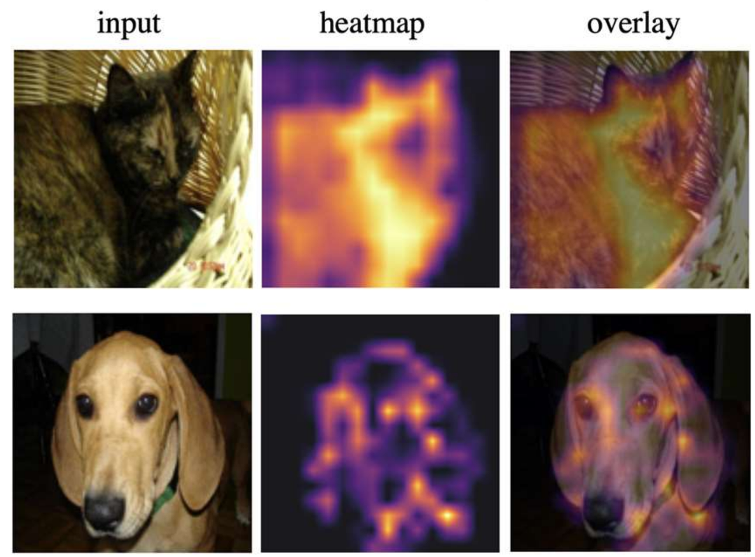
Challenges:

- Design and operation **competing objective** (energy vs accuracies vs noise)
- Algorithmic behavior understanding given the device condition

Related Work:

- QGrad-Cam for QML (IBM 100+ qubit test awards) [1]
- Causal Analysis for understanding entanglement, expressibility, etc. [2]





1. Lin, Hsin-Yi, Huan-Hsin Tseng, Samuel Yen-Chi Chen, and Shinjae Yoo. "Quantum Gradient Class Activation Map for Model Interpretability." In *2024 IEEE Workshop on Signal Processing Systems (SiPS)*, pp. 165-170. IEEE, 2024.
2. Park, Junghoon, Samuel Yen-Chi Chen, Shinjae Yoo, Huan-Hsin Tseng, and Wells Fargo. "Over the Quantum Rainbow: Explaining Hybrid Quantum Reinforcement Learning.", QCE 2024

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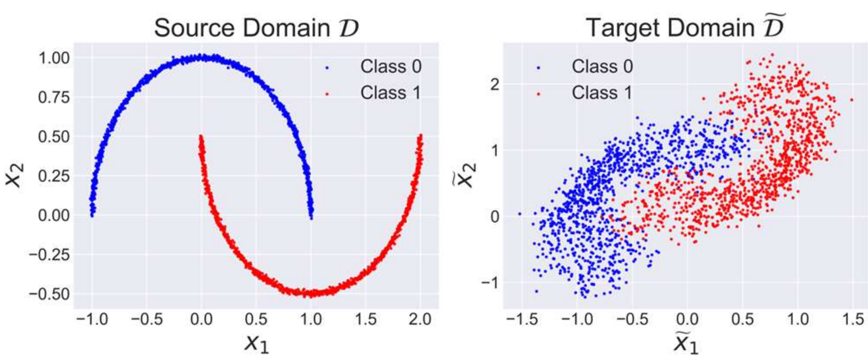
Quantum Transfer Learning

- **Motivation:** Transfer learning between two "make_moons" datasets $D \to \widetilde{D}$ (Fig. 1).
- **Approach:** Our One-shot fine-tuning (Quantum Variational Analysis, **QVA**) vs. Gradient Descent (**GD**).
- **Results:** QVA achieves 77.2% accuracy on the target domain immediately, competing with GD after 17 epochs.

QVA formula: $\delta\vartheta^* = (z^T \cdot z)^{-1}\, z^T \cdot q$ and $q_i = \underbrace{\delta y^{(i)} - \langle r, \delta x^{(i)} \rangle_{\mathbb{R}^d}}_{\text{domain mismatch}(\Delta)} + \overbrace{\langle H \rangle \left(x^{(i)}; \vartheta\right) - y^{(i)}}^{}_{\text{pretrain error}(\star)}$



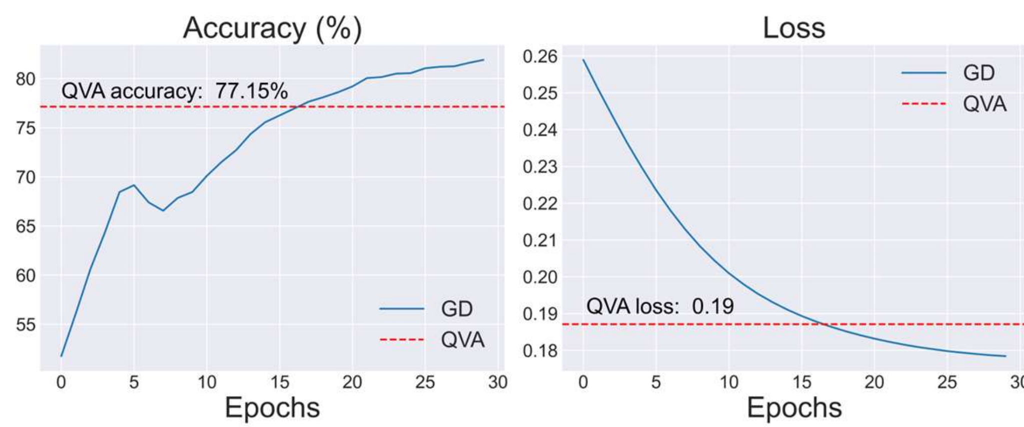


Fig.1 Transfer learning from $D \to \widetilde{D}$

Tseng, Huan-Hsin, Hsin-Yi Lin, Samuel Yen-Chi Chen, and Shinjae Yoo. "Transfer Learning Analysis of Variational Quantum Circuits." *arXiv preprint arXiv:2501.01507* (2025).

Quantum Learning to Measure Quantum Neural Networks

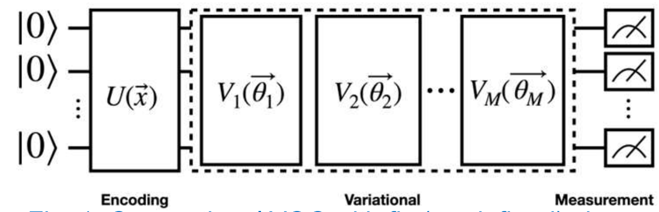


Fig. 1: Conventional VQC with fix (predefined) observables

- **Challenge**: Existing QML (VQC) models rely on fixed measurement observables (e.g., Fig. 1 with Pauli matrices), limiting flexibility and task-specific optimization.
- **Approach**: Learnable, parameterized observables Q for VQCs (Fig. 2).

$$\langle Q \rangle := \langle \psi_0 | V^\dagger(x_j) \boxed{U^\dagger(\theta)} \boxed{Q} \boxed{U(\theta)} V(x_j) | \psi_0 \rangle \in \mathbb{R}$$

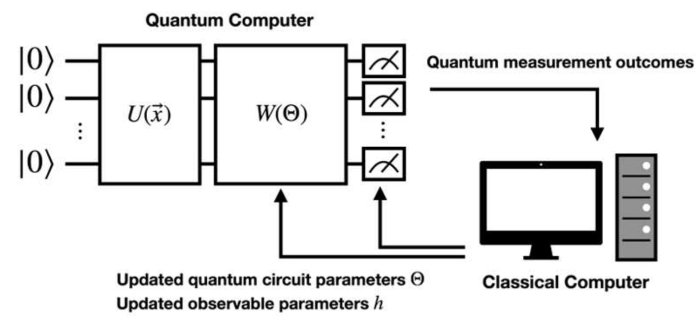
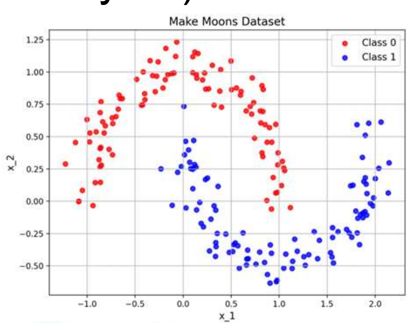
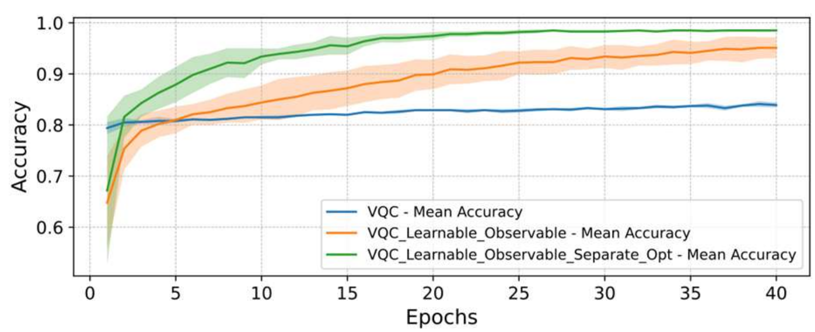


Fig. 2: VQC with learnable observables (Hermitians)

$$\begin{tikzcd} \mathcal{H} \arrow[r, "\boxed{U(\theta)}"] & \mathcal{H} \arrow[d, "\boxed{<\cdot|Q|\cdot>}"] \\ \mathbb{R}^n \arrow[u, "V(x_j)"] \arrow[r, dashed, "f_{\mathrm{VQC}}"] & \mathbb{R}^m \end{tikzcd}$$

- **Results**: Demonstrated QNN (make moon, 4 qubit, 2 layers)





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Samuel Yen-Chi Chen, Huan-Hsin Tseng, Hsin-Yi Lin, Shinjae Yoo, "Learning to Measure Quantum Neural Networks", arXiv:2501.05663 (2025)

Acknowledgement

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- Samuel Yen-Chi Chen (Wells Fargo)
- Junghoon Park, Jiook Cha (Seoul National University)

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- DOE Office of Electricity QIS Award
- C2QA (Center for Quantum Advantage)

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