Quantum Machine Learning for HEP Detector Simulations

FSP CMS Workshop 2021

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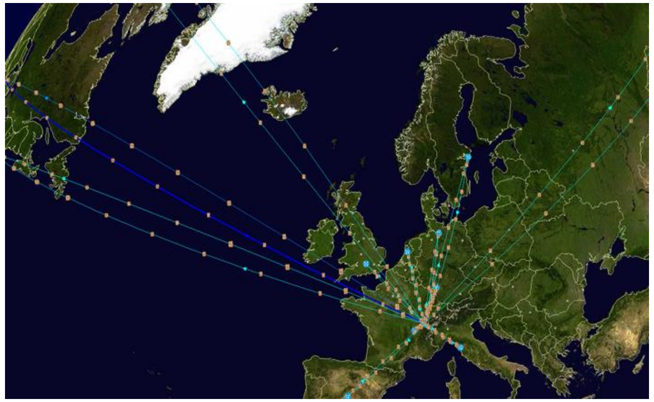
Calorimeter Simulations

- Calorimeter simulations are based on Geant4
- Simulations use about 50% of the resources of the worldwide LHC grid
- LHC high luminosity phase requires 100 times more simulated data*

→ **Develop a new approach which occupies less resources**

→ **Employ deep learning**

→ **Already done: We reached a 150 000x speed-up using GANs**



*A Roadmap for HEP Software and Computing R&D for the 2020s https://doi.org/10.1007/s41781-018-0018-8

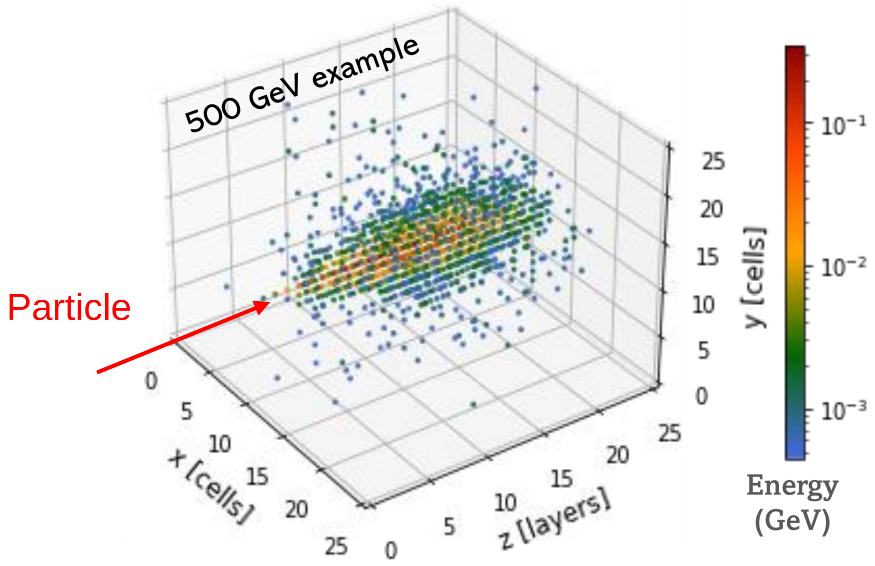
Now: Quantum Computing

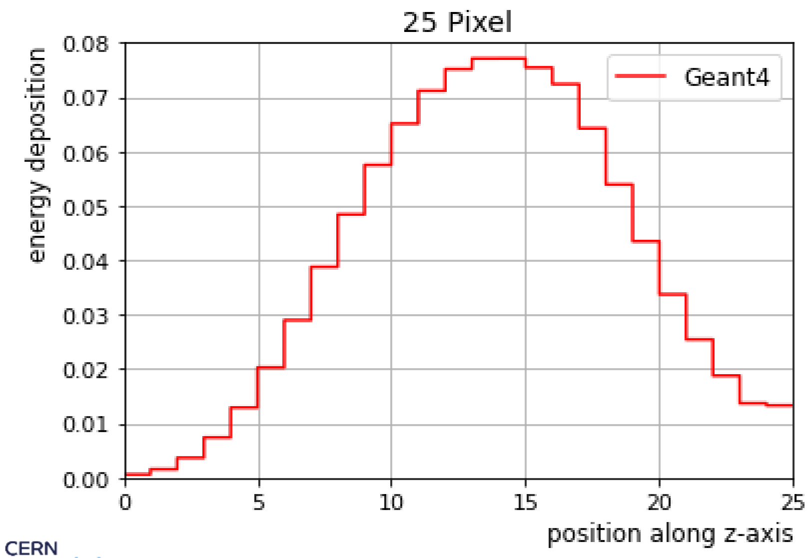
- **Explore potential of quantum computing**
  - Make use of quantum properties (entanglement, superposition)
  - Hope to solve problems faster and / or more accurately
  - "Quantum Advantage" not yet reached → only initial investigations
    - Understanding advantages and challenges

- Use case: calorimeter simulations
  - Using simplified models

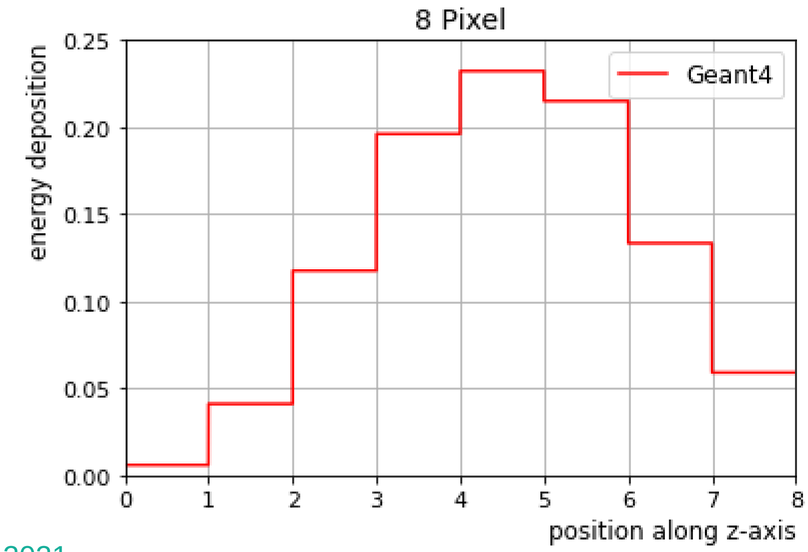
Training Data

- 3D particle shower images
- Average the image over z-axis → 1D image
- Down sample to only 8 pixel
- Average all of input energies
  → Only one distribution





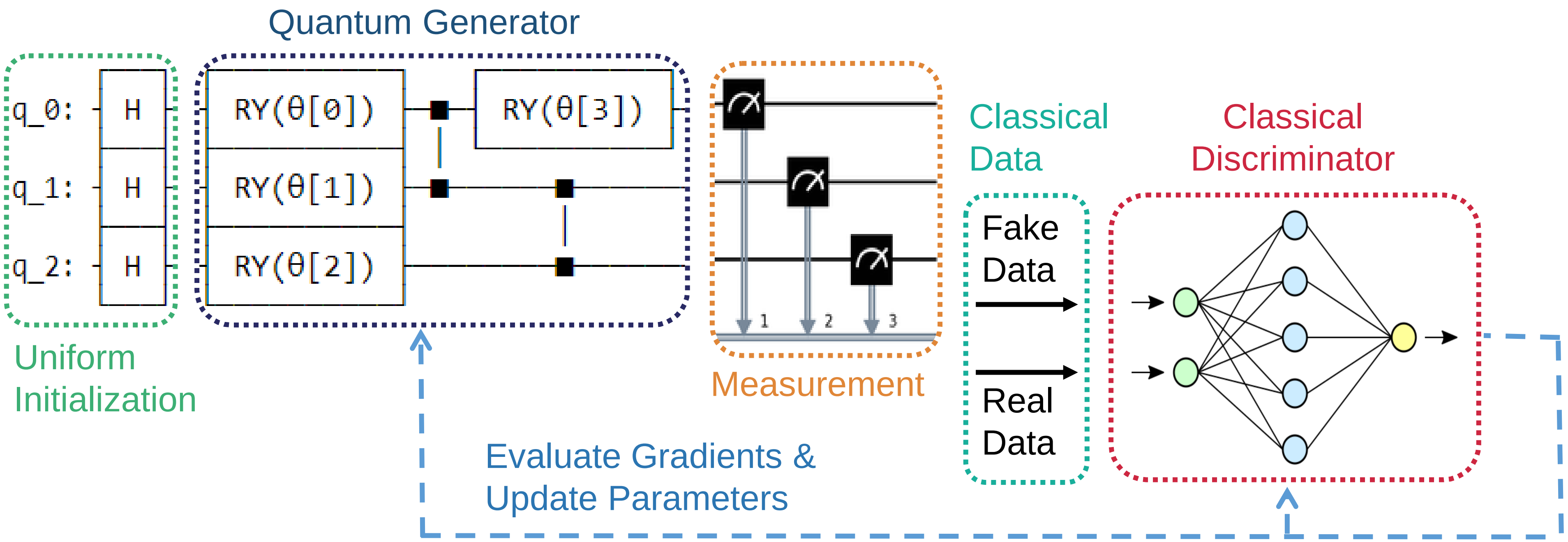
down sampling



Hybrid qGAN

Quantum Generative Adversarial Networks

- Hybrid quantum – classical ansatz



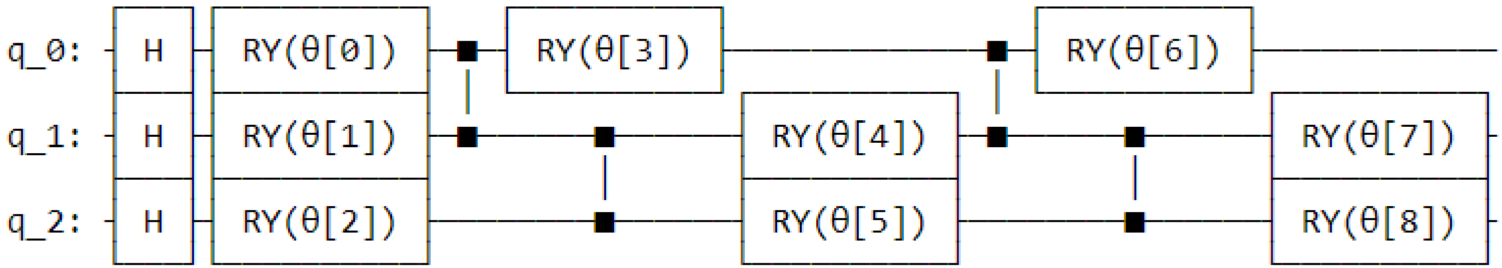
1D Quantum GAN

1D Quantum Generator Circuit

- Only 1D 8-pixel images
  - 3 qubits ($2^3 = 8$) in quantum generator circuit
    - 8 quantum states: $|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle$
- Modified a Qiskit qGAN model developed by IBM*

* https://qiskit.org/documentation/machine-learning/tutorials/04_qgans_for_loading_random_distributions.html

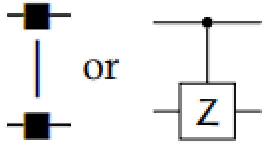
Quantum Generator Circuit:



Gates:

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$$

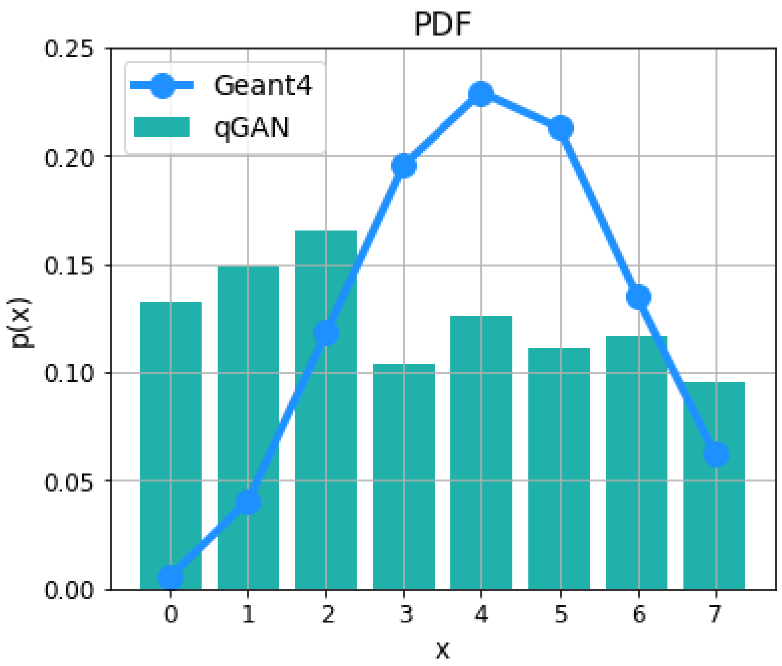
$$R_y(\theta) = \begin{pmatrix}\cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right)\\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right)\end{pmatrix}$$



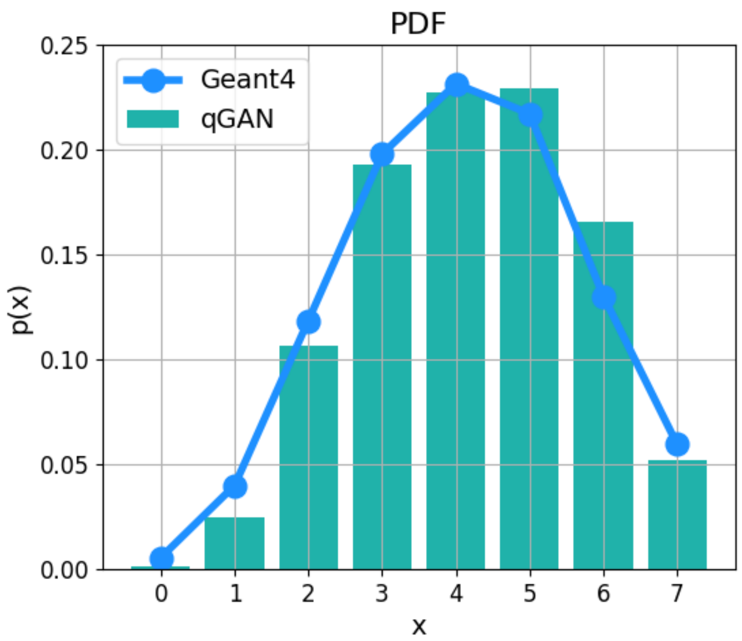
$$= CZ = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}$$

1D Quantum Simulator

Without Noise



Uniform Initialization



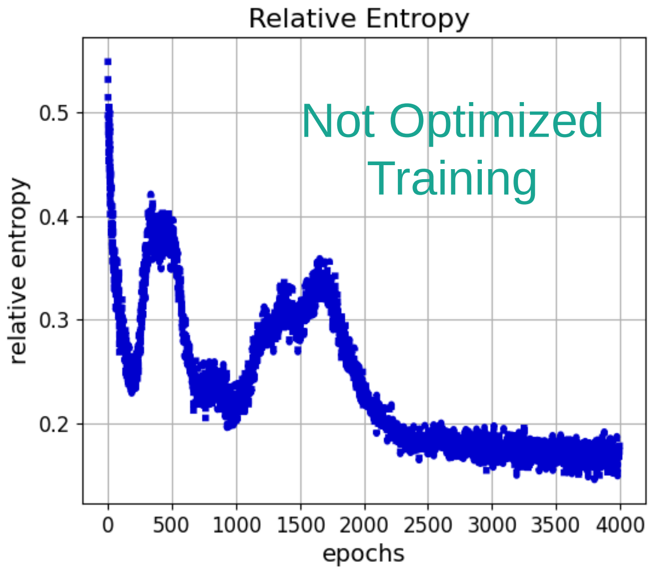
Trained Model

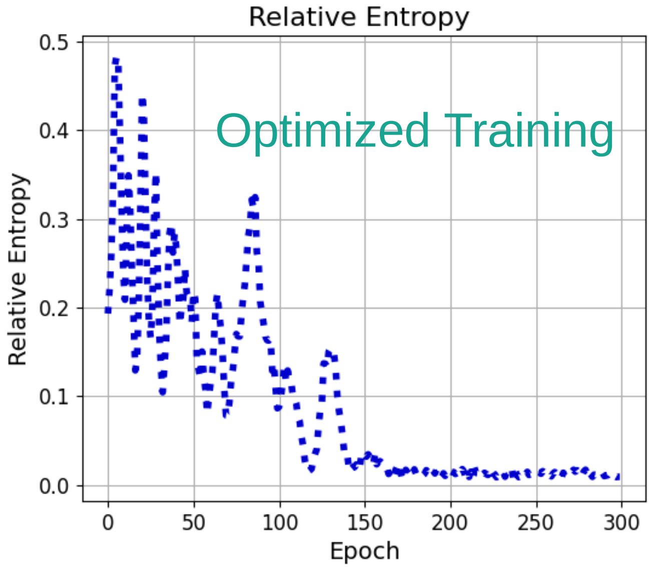
→ Good results

1D qGAN

Optimize Training

- Training time ~ 1 day for 3000 epochs
  - → speeding training up
- Hyperparameter optimizations:
  - Higher learning rate
  - Implement exponential learning rate decay
  - Different generator and discriminator learning rate
  - Train discriminator more often than generator
- Results:
  - **10x speed up** in training time
    → Only ~300 epochs instead of > 3000



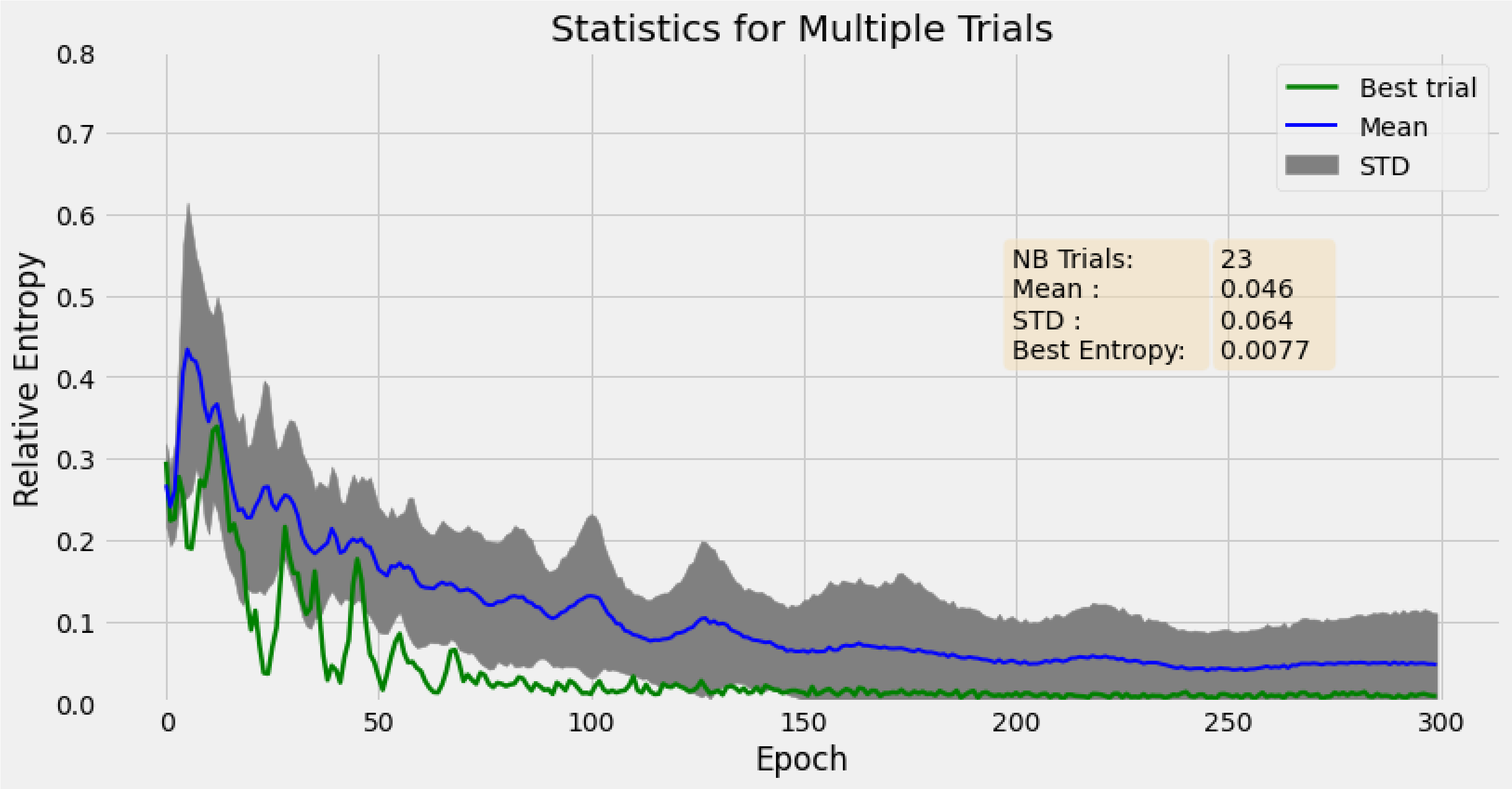


1D qGAN Robustness

- Run 23 trials with same hyperparameters

→ Stable training

→ On average good accuracy

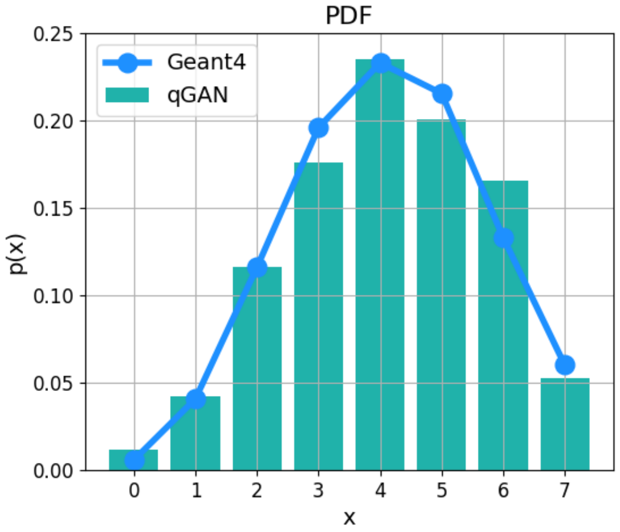


1D qGAN with Noise

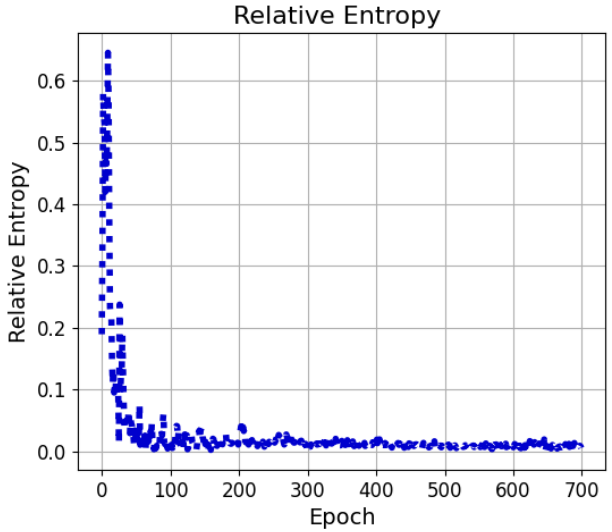
Readout Noise Only

- We applied readout noise to the qubit measurements
  - Noise model from IBMq belem quantum computer

Qubit Number	0	1	2
Readout Error	3.6%	4.7%	9.6%



→ No decrease in accuracy

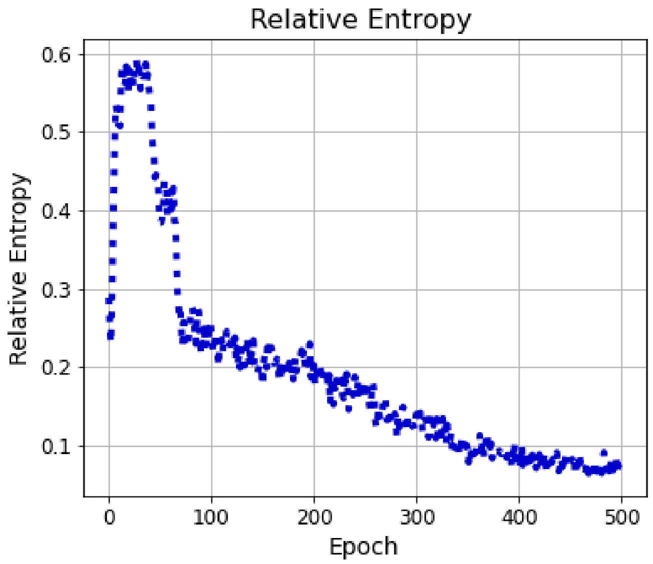


→ Fast convergence

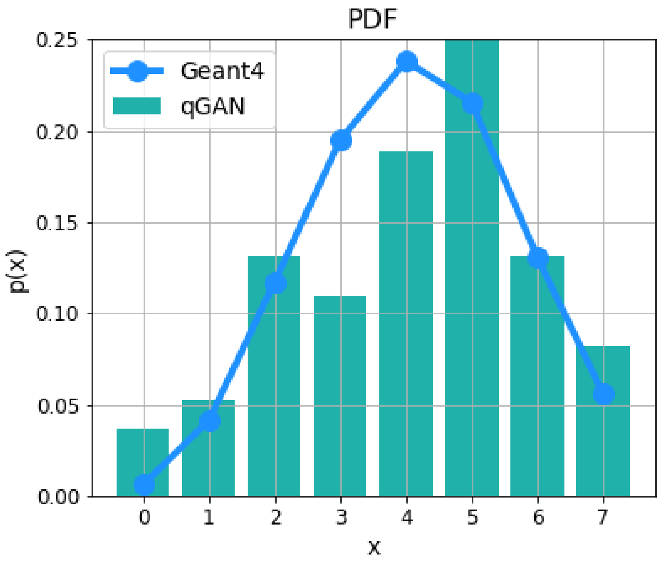
1D qGAN with Noise

Full Noise Model

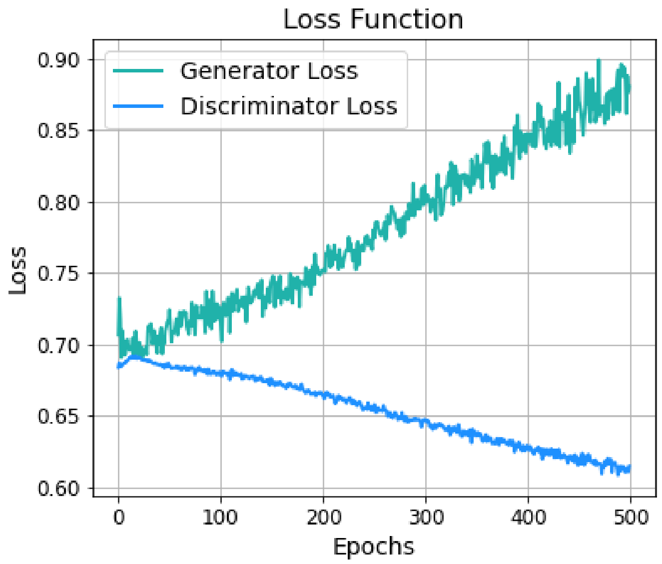
- We applied noise to the qubit gates (readout noise + gate level noise)
  - Noise model from IBMq belem quantum computer
  - Average gate level noise: 4.32%



→ Good entropy



→ Lower accuracy



→ Non-converging losses

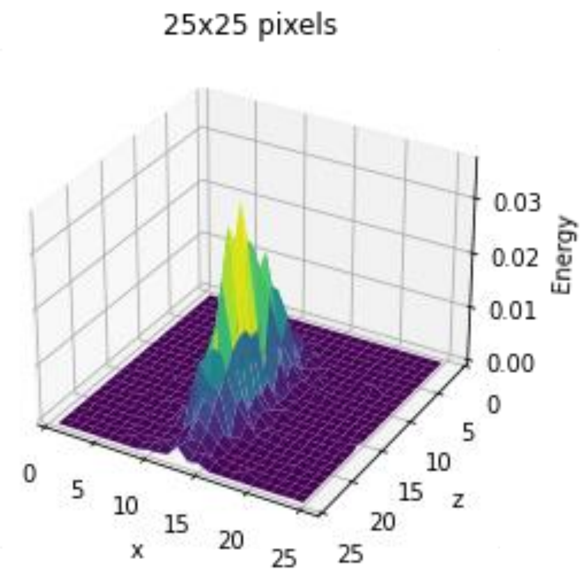
2D Quantum GAN

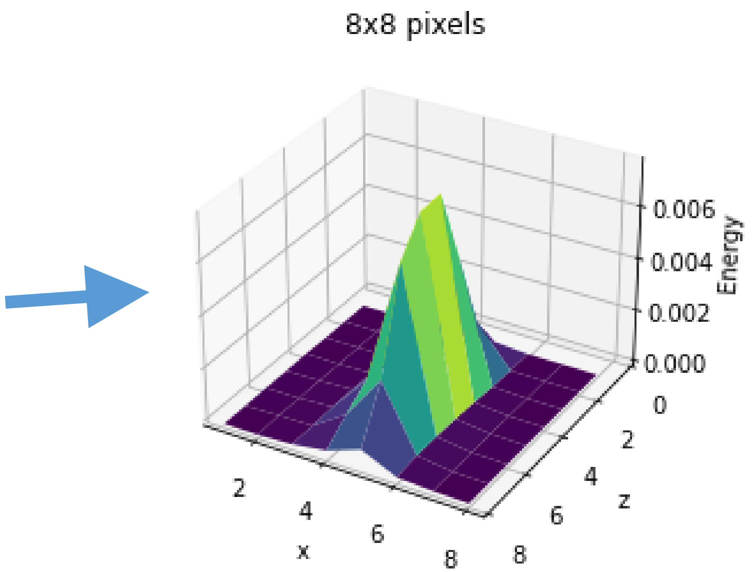
2D qGAN

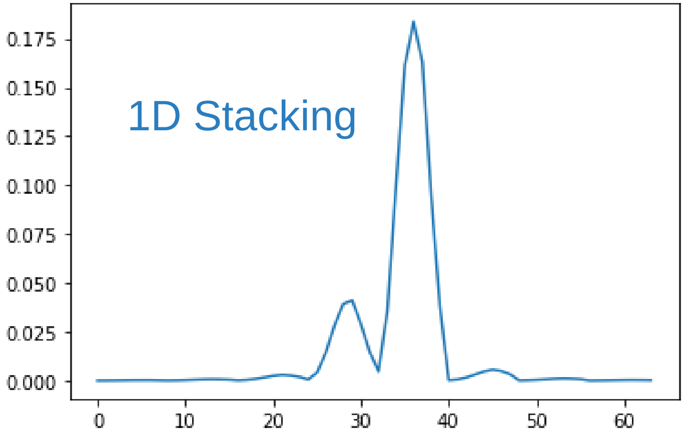
2D Data Representation

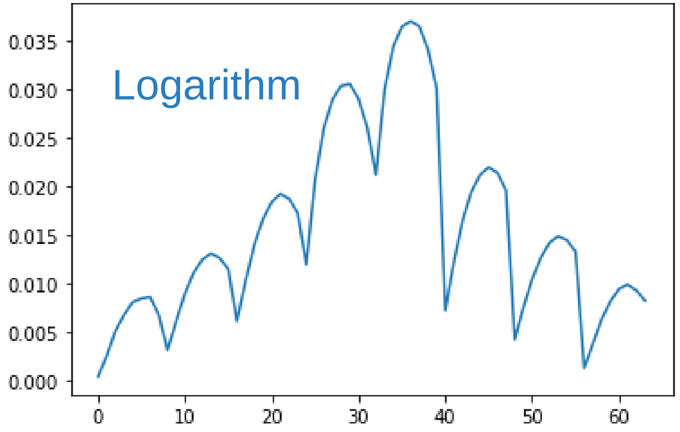
2D: 8x8 = 64 pixels = 2^6 → **6 qubits**

1. Down sample
2. 1D stacking
3. Apply logarithm



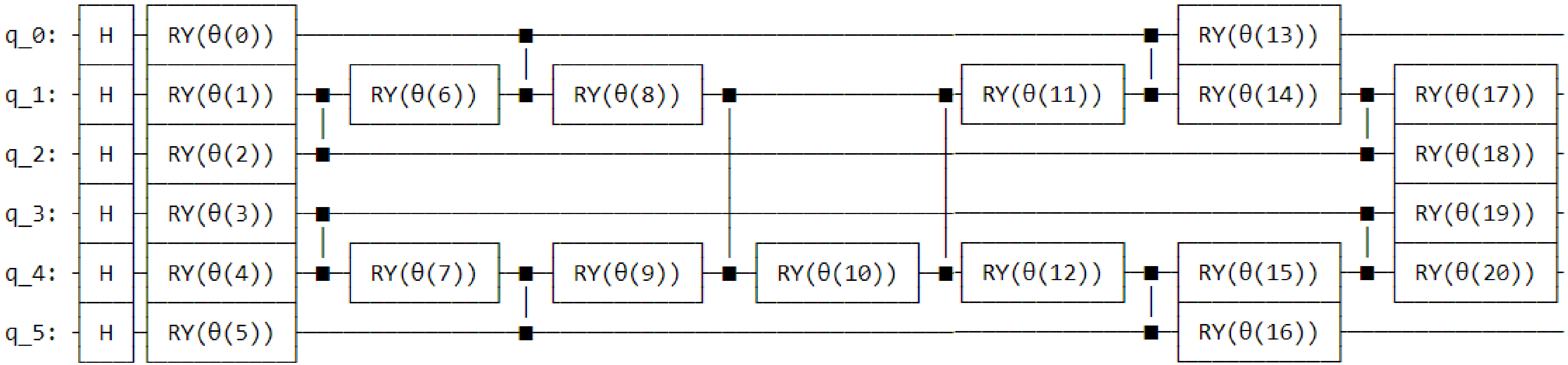


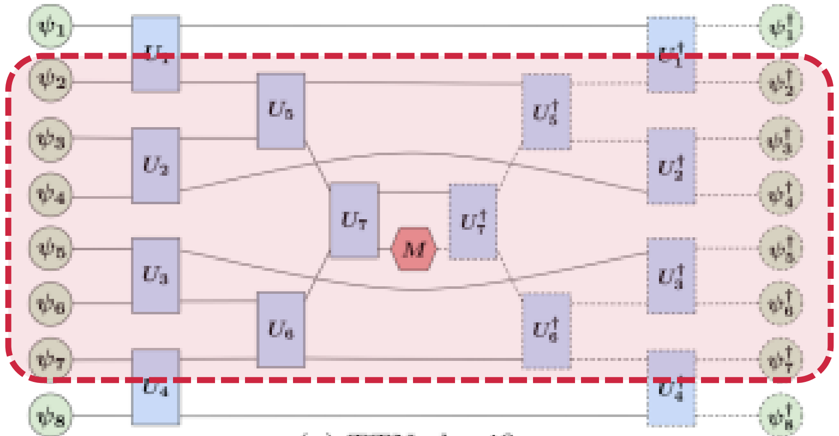




2D Quantum Generator Circuit

Tree Tensor Network Architecture





(a) TTN classifier

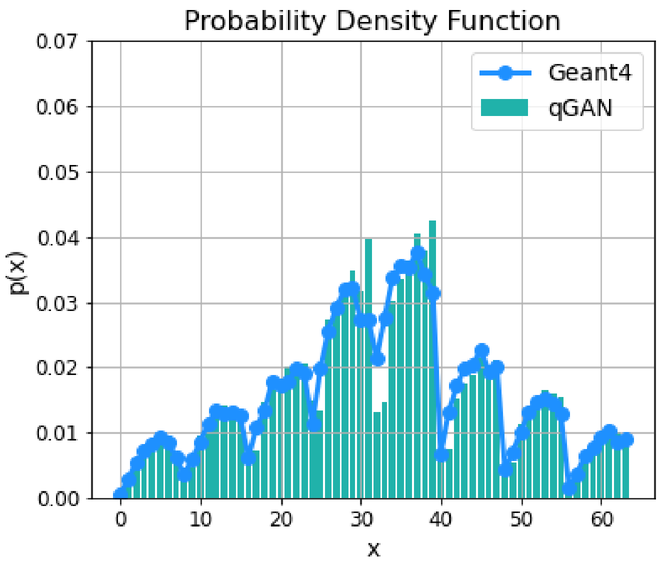
Only 6 qubits

Grant, E., Benedetti, M., Cao, S. *et al.* Hierarchical quantum classifiers. *npj Quantum Inf* **4,** 65 (2018). https://doi.org/10.1038/s41534-018-0116-9

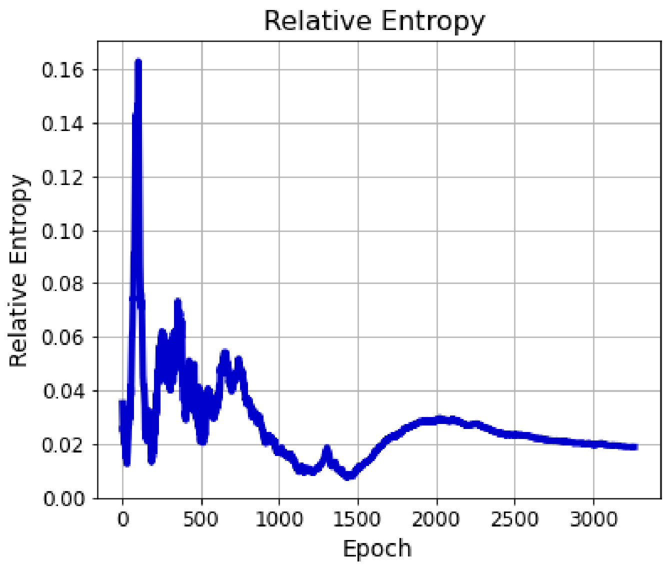
2D qGAN

Best Results

- Run on quantum simulator without noise



Trained Model



qGAN Future Work

- 2D qGAN:
  - Improve training convergence
    - Rare that training converges
  - Decrease training time: recently ~5 days
    - Hyperparameter optimization

- 1D qGAN:
  - More tests with the full noise model
    - Test error mitigation techniques
  - Conditional qGAN

QUESTIONS?

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