Full Quantum GAN Model for HEP Detector Simulations

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Florian Rehm [CERN, RWTH Aachen]

Sofia Vallecorsa [CERN], Michele Grossi [CERN], Kerstin Borras [DESY, RWTH Aachen], Dirk Krücker [DESY],
Simon Schnake [DESY, RWTH Aachen], Alexis-Harilaos Verney-Provatas [DESY, RWTH Aachen]

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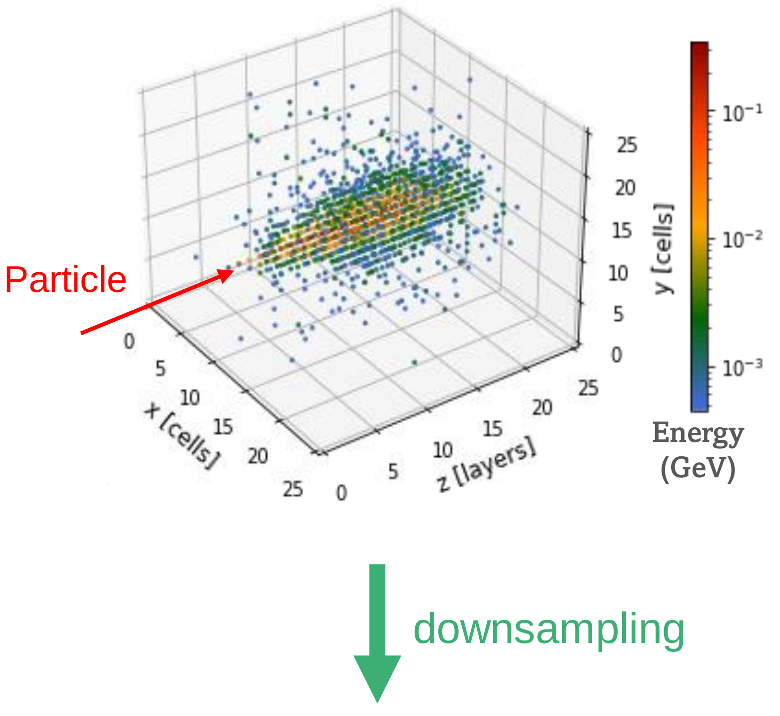
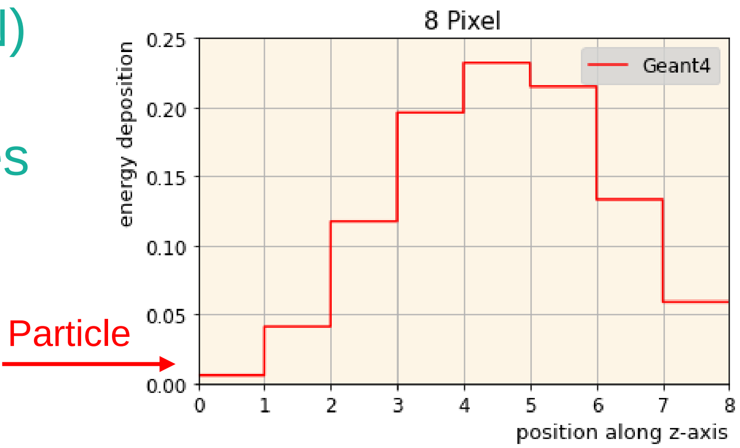
Introduction

- Explore present performance and potential of quantum computing
  - “Quantum Advantage” not yet reached
    → initial investigations with pioneering work



- Use case: calorimeter simulations
  - Machine learning: Generative Adversarial Network (GAN) models can represent the fullsize 3D shower image
  - Quantum Computing: Generate simplified shower images



- In this study: Investigate a full quantum GAN model

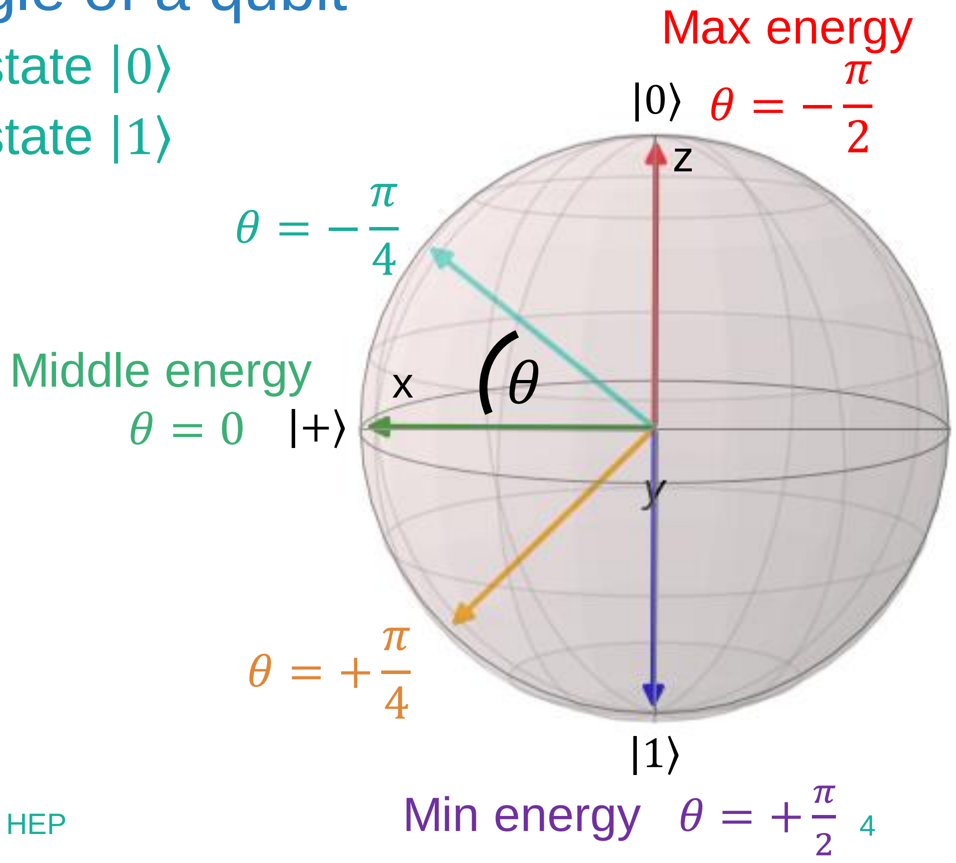
Angle Encoding - Decoding

Angle Encoding

- Encoding transfers classical images into a quantum state
- Encode the pixel energy into a rotational angle of a qubit
  - Max. energy corresponds to angle $\theta = -\pi/2$ → state $|0\rangle$
  - Min. energy corresponds to angle $\theta = +\pi/2$ → state $|1\rangle$

- Visualization on Bloch sphere:
  - For all states: $y = 0\ (\varphi = 0)$

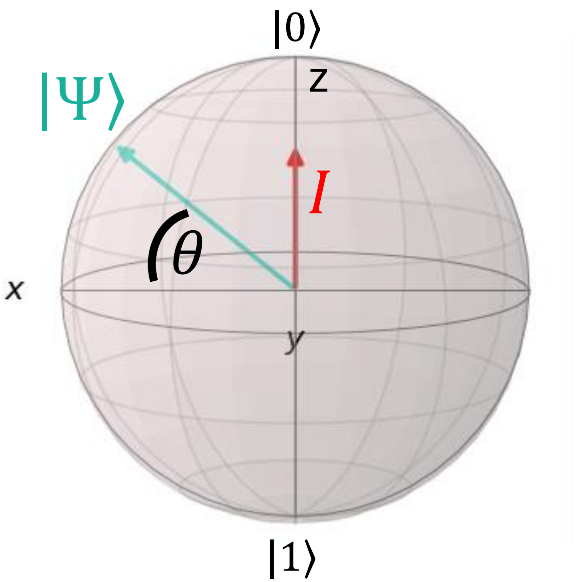
    → Moving only on the x-z-plane
- Implementation on hardware:
  - One H gate
  - One Ry gate



Angle Decoding

- Decoding transfers quantum state into an energy
- Measure the quantum state of each qubit multiple times (= nb_{shots})

- Bloch sphere example:



$$\frac{\#|0\rangle}{nb_{shots}} * 2 - 1 = \frac{954}{1024} * 2 - 1$$

Goal: Calculate angle θ of state $|\Psi\rangle$

→ Measurements M of 1024 shots: $M =$ {'0': 954, '1': 70}

→ Calculate z-axis intercept I (height): $I =$ 0.86

→ Calculate angle θ with trigonometry: $\theta =$ -0.76 $= \arcsin(I)$

$with\ a\ predefined\ equation\ this\ can\ be\ transferred\ into\ an\ energy$

Full Quantum GAN Model

The Full Quantum GAN Model

- GAN approach: two models are adversarial trained
  - Generator: generates fake images
  - Discriminator: classifies images as true or fake images

- Full quantum GAN: **quantum** generator + **quantum** discriminator
  - Previous hybrid GAN models are employing a classical discriminator *
  - Parameter optimization during training happens classical

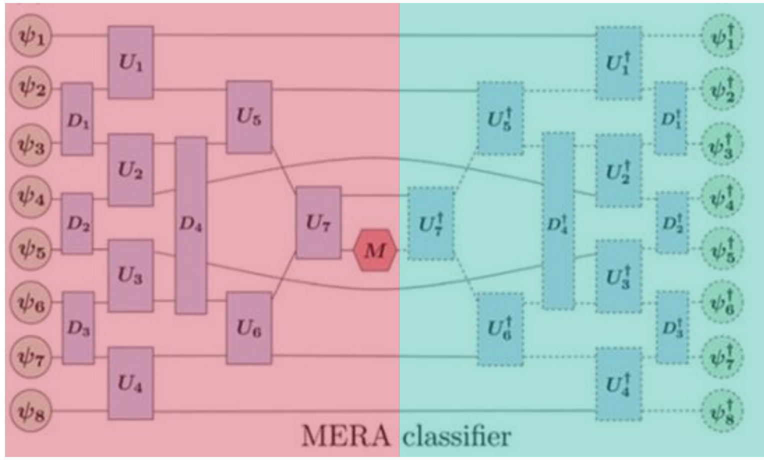
- For training and inference four distinct quantum circuits are required
  - Circuits provided on the following slides

** Rehm, Florian, et al. "Quantum Machine Learning for HEP Detector Simulations." (2021).*

Circuit Architectures

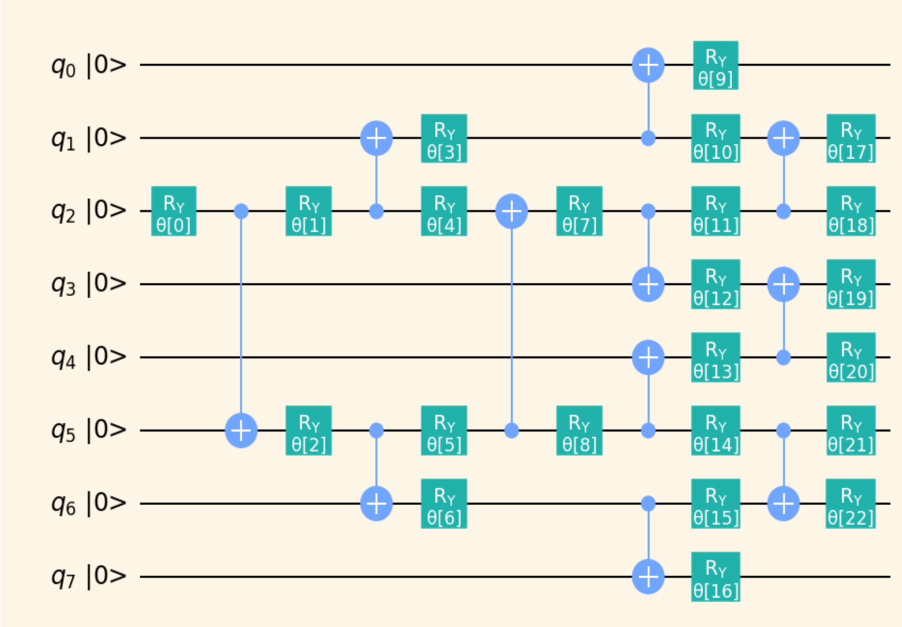
MERA-
downsampling

MERA-
upsampling

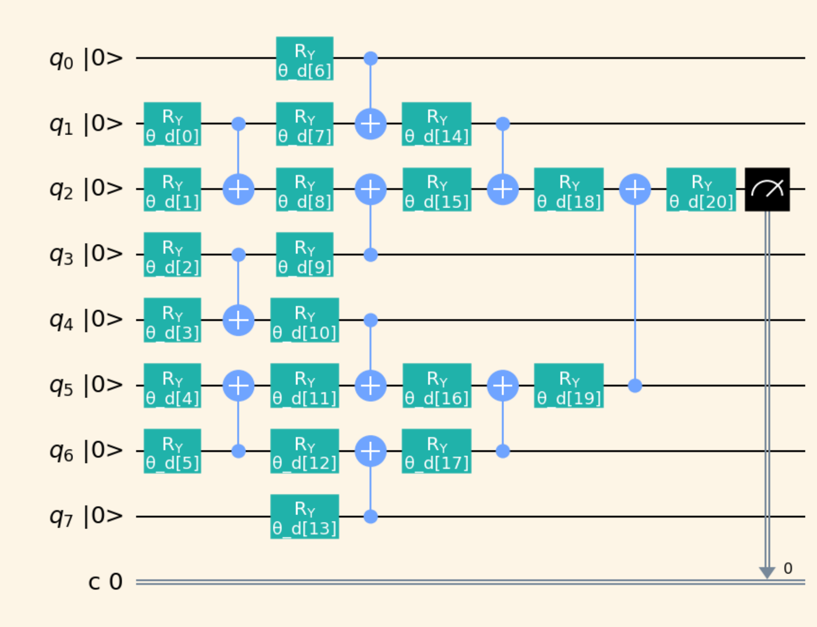


Grant, E., Benedetti, M., Cao, S. *et al.* **Hierarchical quantum classifiers**. *npj Quantum Inf* **4**, 65 (2018). https://doi.org/10.1038/s41534-018-0116-9

Generator: MERA-up



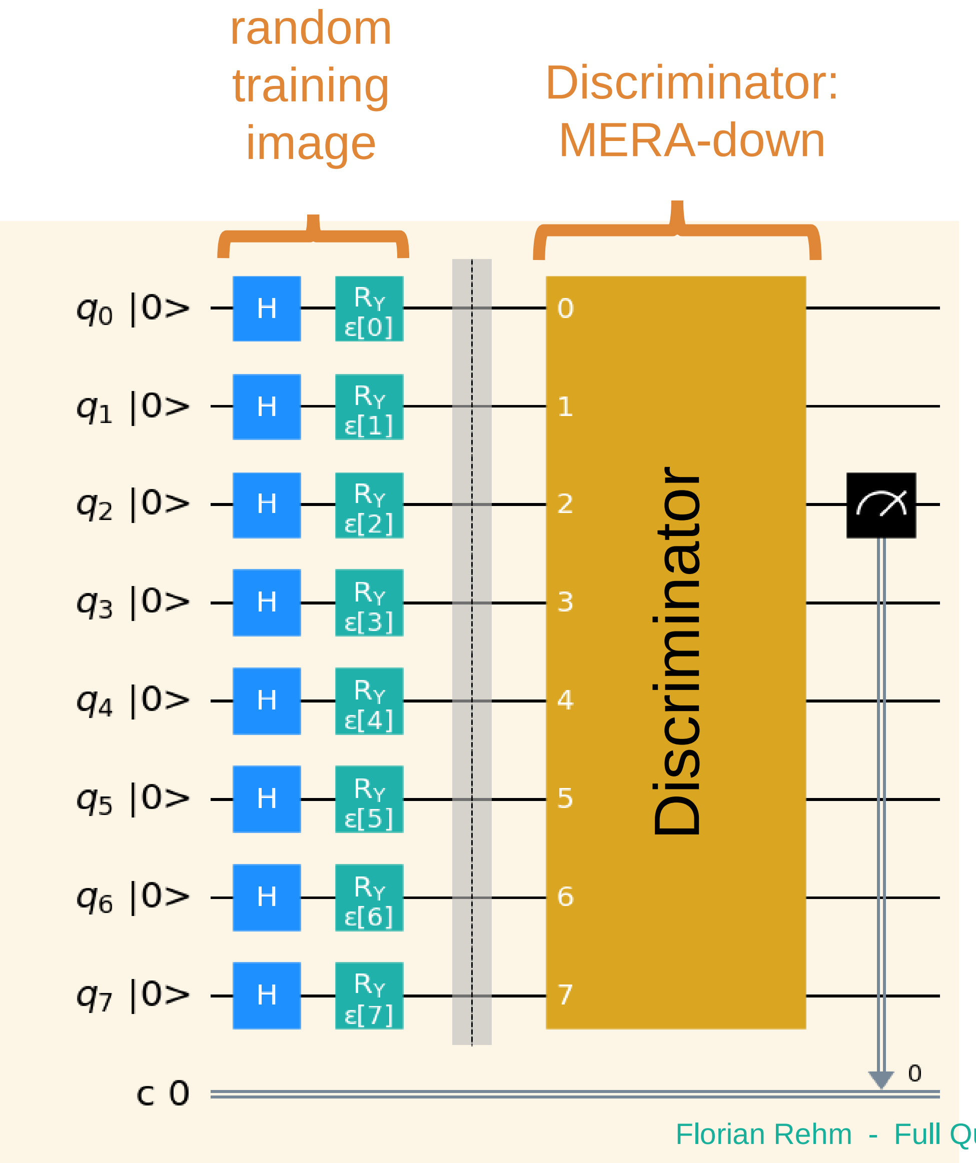
Discriminator: MERA-down



The unitary transformations consist of:

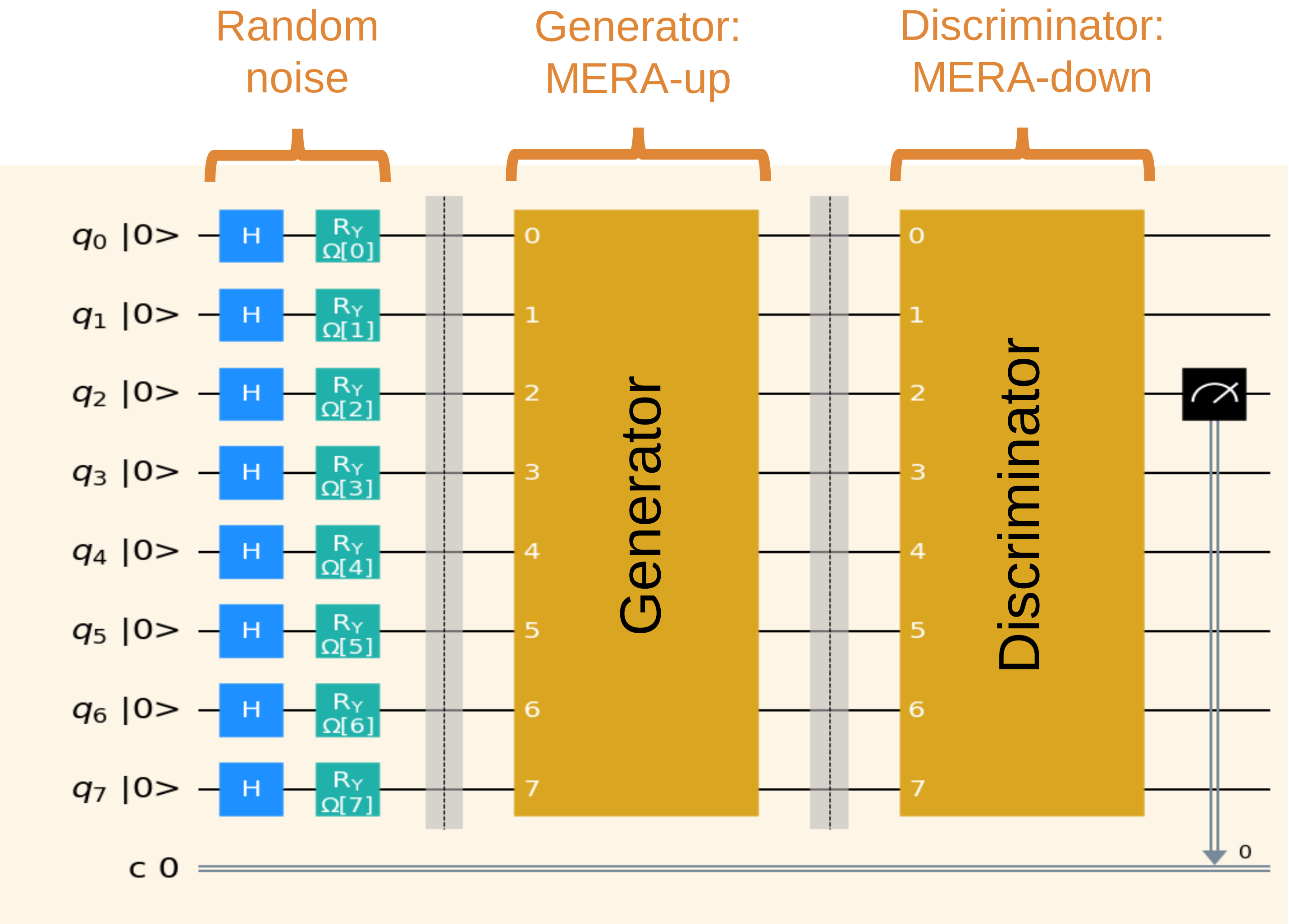
- Ry gates with trainable parameters
- Cx gates for enabeling entangling

1. Train True Discriminator



- Training image implemented via angle encoding
- True/Fake Probability: Measure the output of one qubit (q2)
  - Measure for multiple shots and count how often $|1\rangle$ is measured:
    - Probability close to 1 corresponds to True image
    - Probability close to 0 corresponds to Fake image

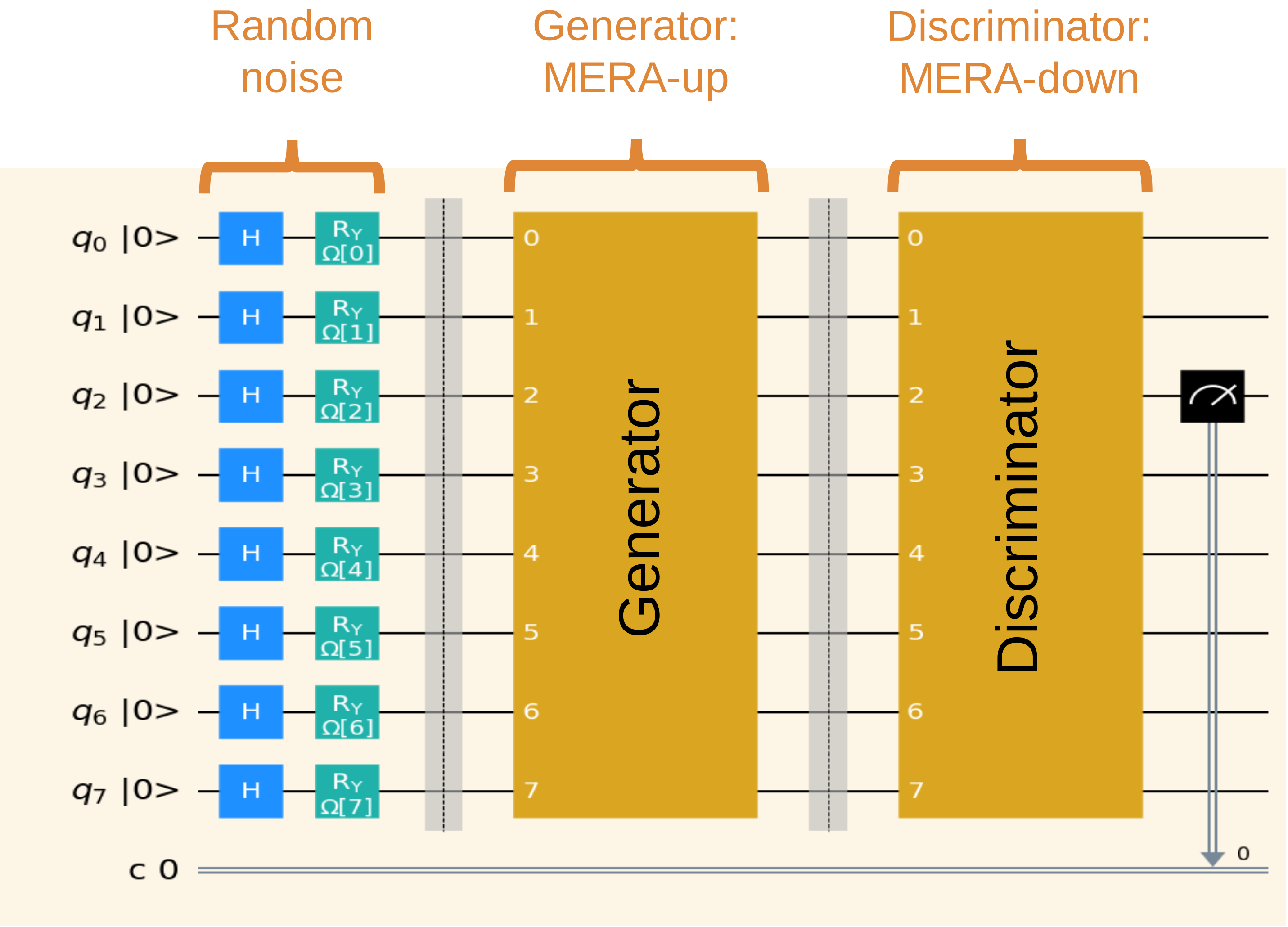
2. Train Fake Discriminator



- Random noise implementation
- Generator parameters frozen
- Dicsriminator parameters trainable

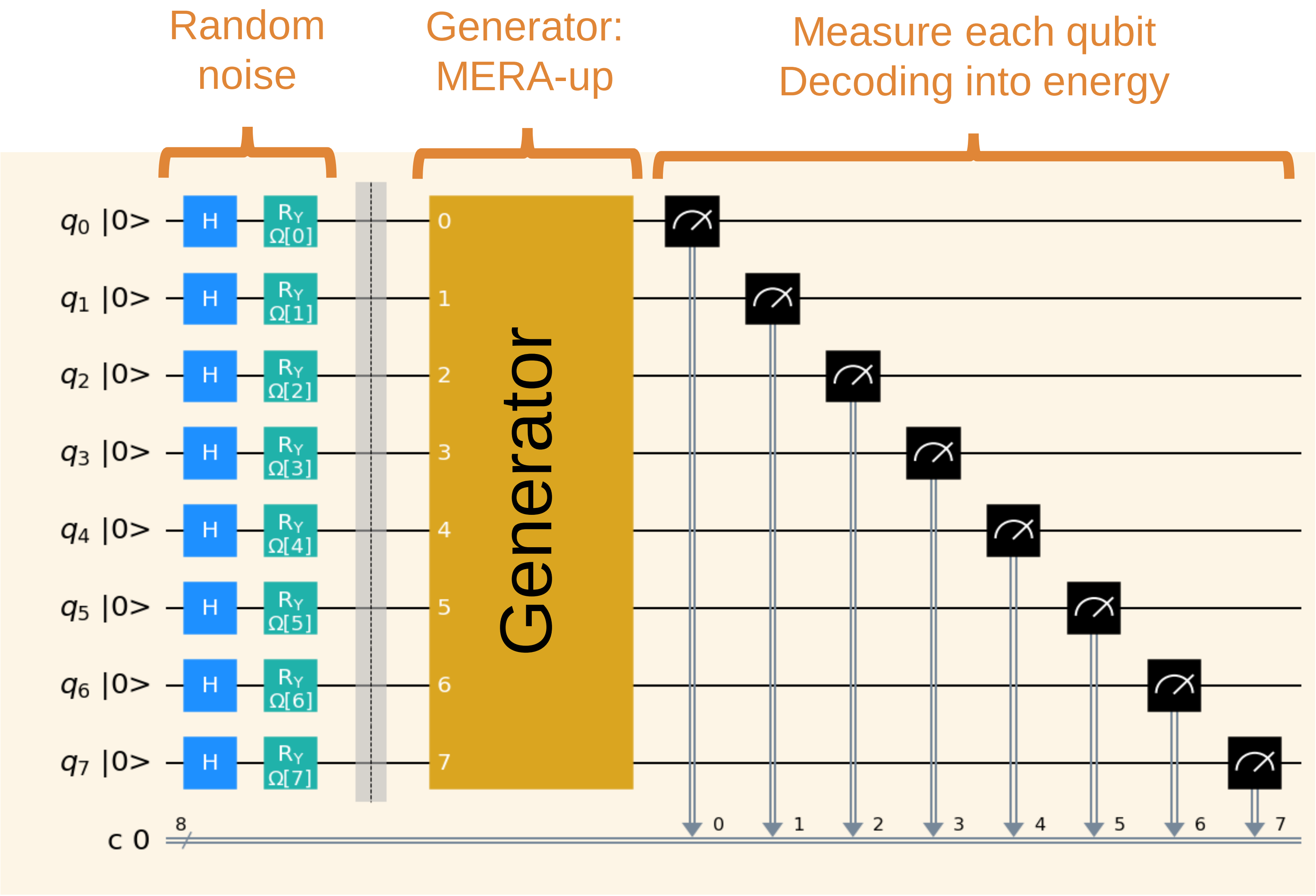
- **No conversion of the quantum image to classical required!**

3. Train Generator



- Similar as discriminator fake training except:
  - Generator trainable
  - Discriminator frozen

4. Generate Events

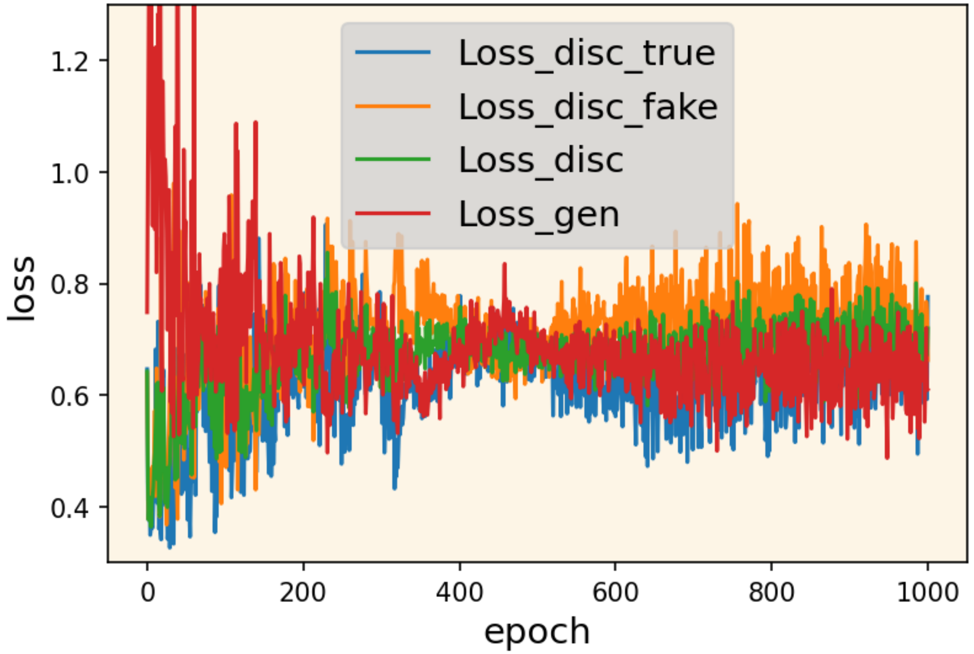


- Measure for multiple shots
- Angle decoding to convert measured angles into energies

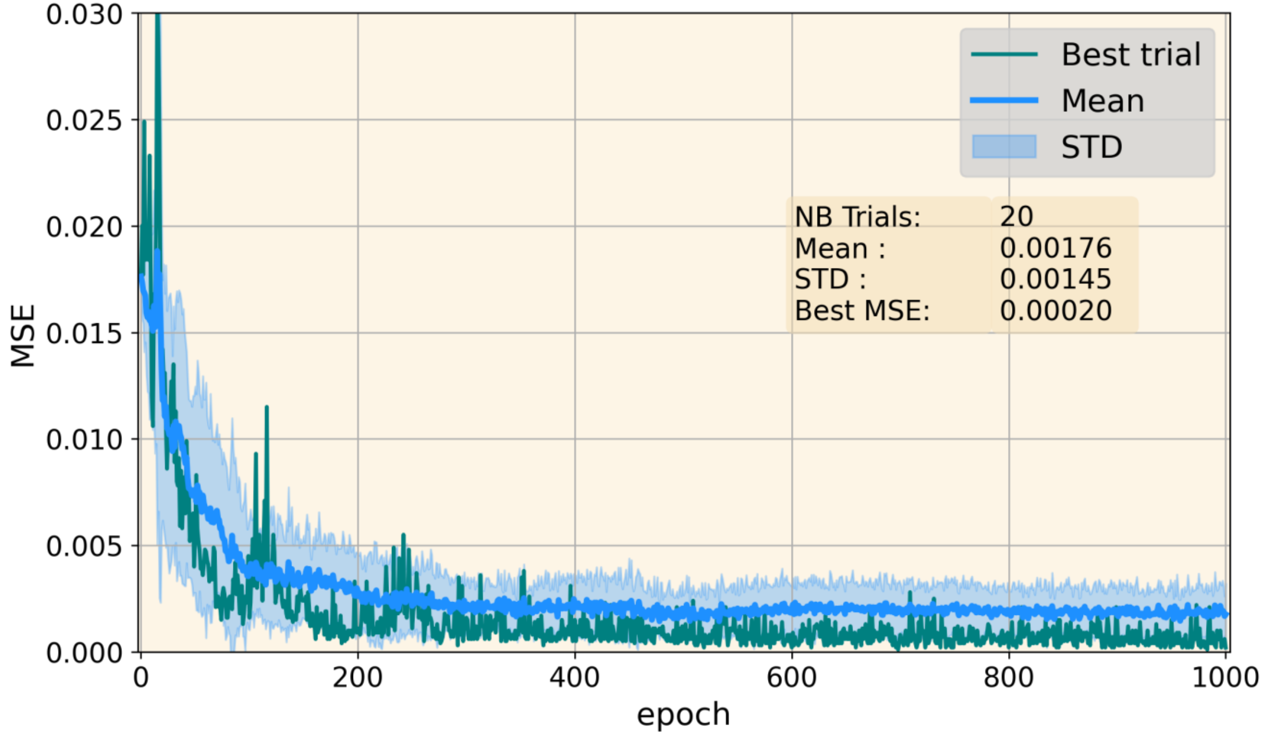
Training Evaluation

Training Results

Training Losses



Statistics Evaluation



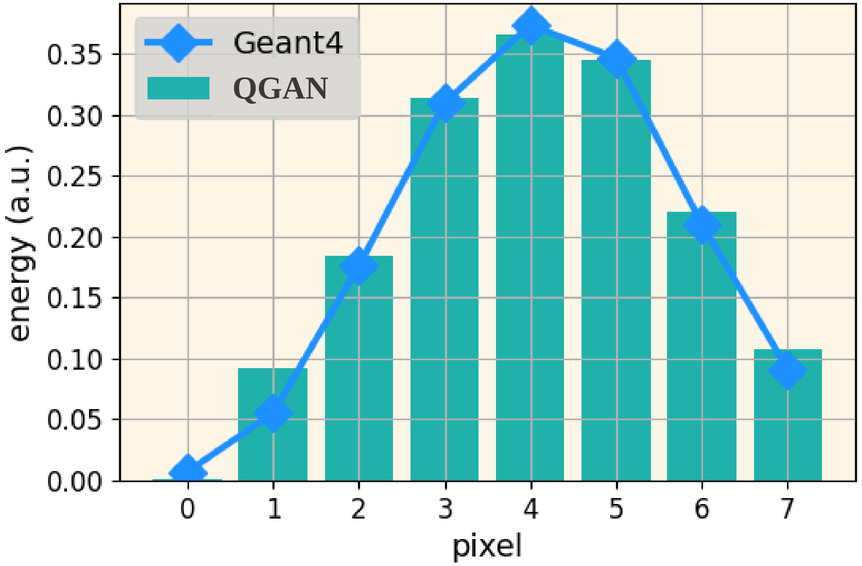
- Losses of best trial oscillate a lot
- At the end, generator and discriminator loss convergence to equal values

- MSE as accuracy metrics: pixelwise computed between average true and fake data
- MSE‘s of all trials converge
  → stable training (due to extensive hyperparameter optimization)

Inference Evaluation

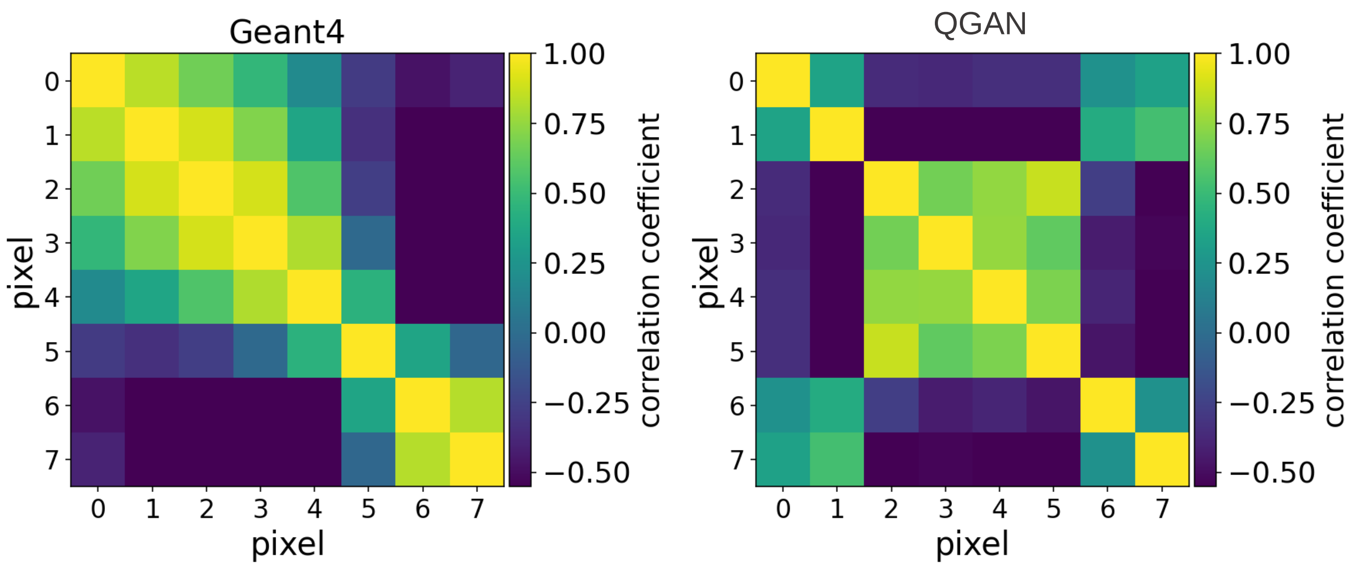
Inference Results

Average Shower Image



- Good agreement between classical and quantum image

Pixelwise correlation



- Pixelwise correlation pattern cannot be represented by the full quantum GAN
  → topic for future studies

Summary

- Successful implementation of a full quantum GAN.
- Good accuracy accomplished for the average shower shape.
- Future work: investigate why the pixelwise correlations are not learned and try to improve.

Thank you for Listening!

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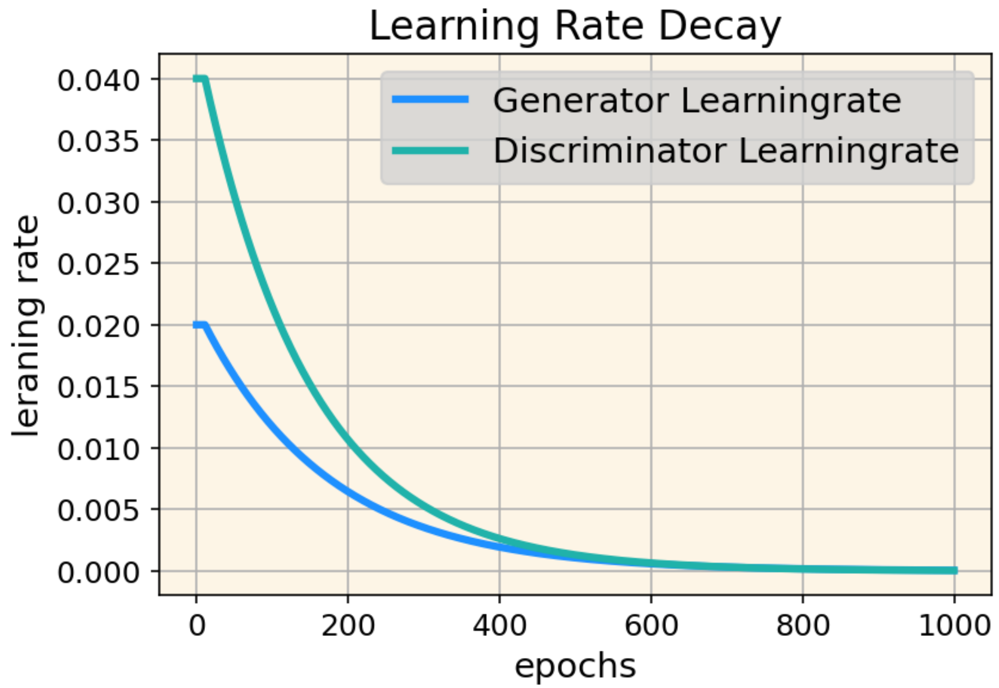
Training Hyperparameters

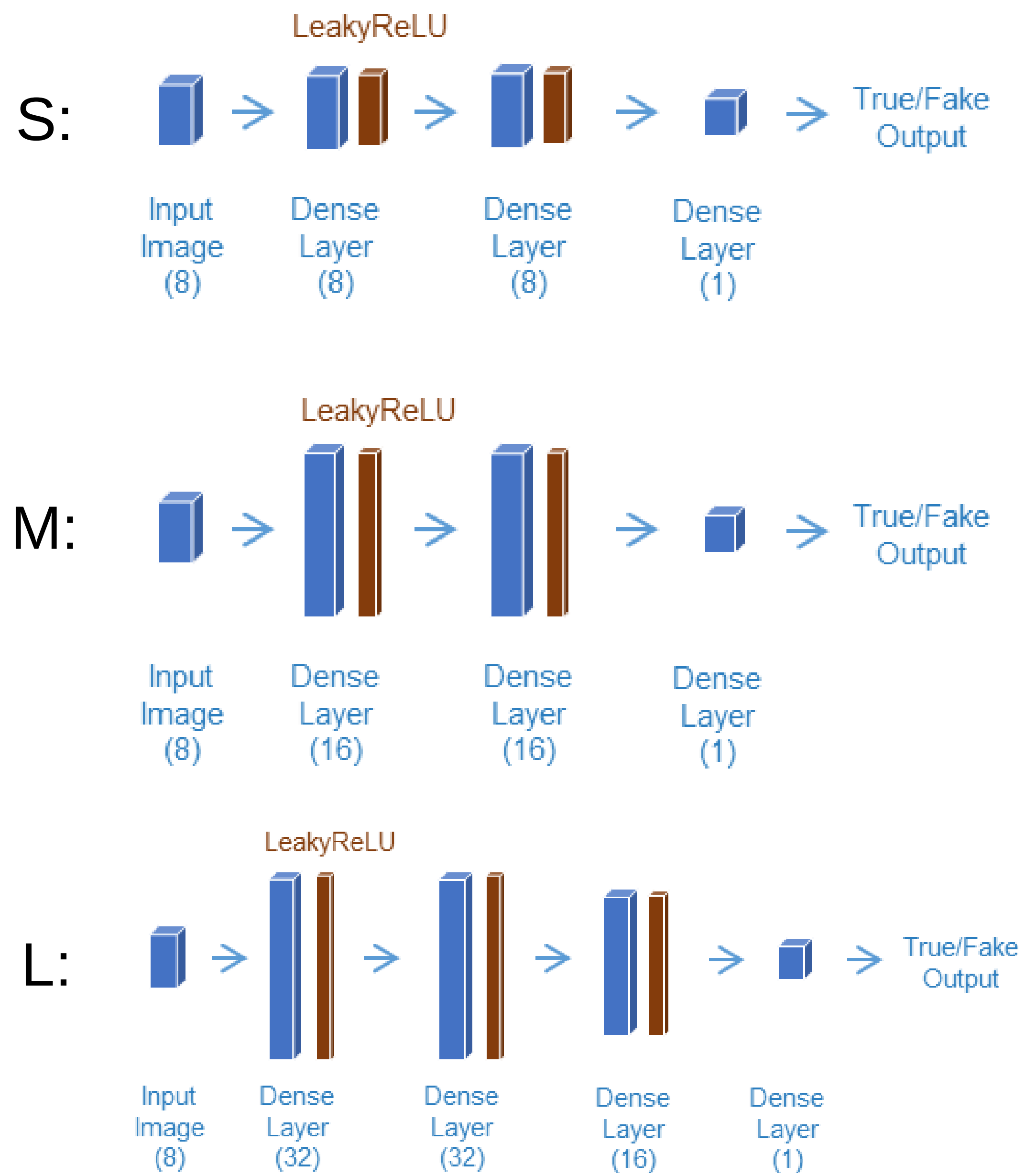
- Training for 1000 epochs
- Separate generator and discriminator learning rate
- Exponential learning rate decay
- Train the discriminator circuit 5 times more frequently than the generator
- Generator and discriminator parameters are zero-initialized
- Training with SPSA optimizer



Hybrid Quantum GAN

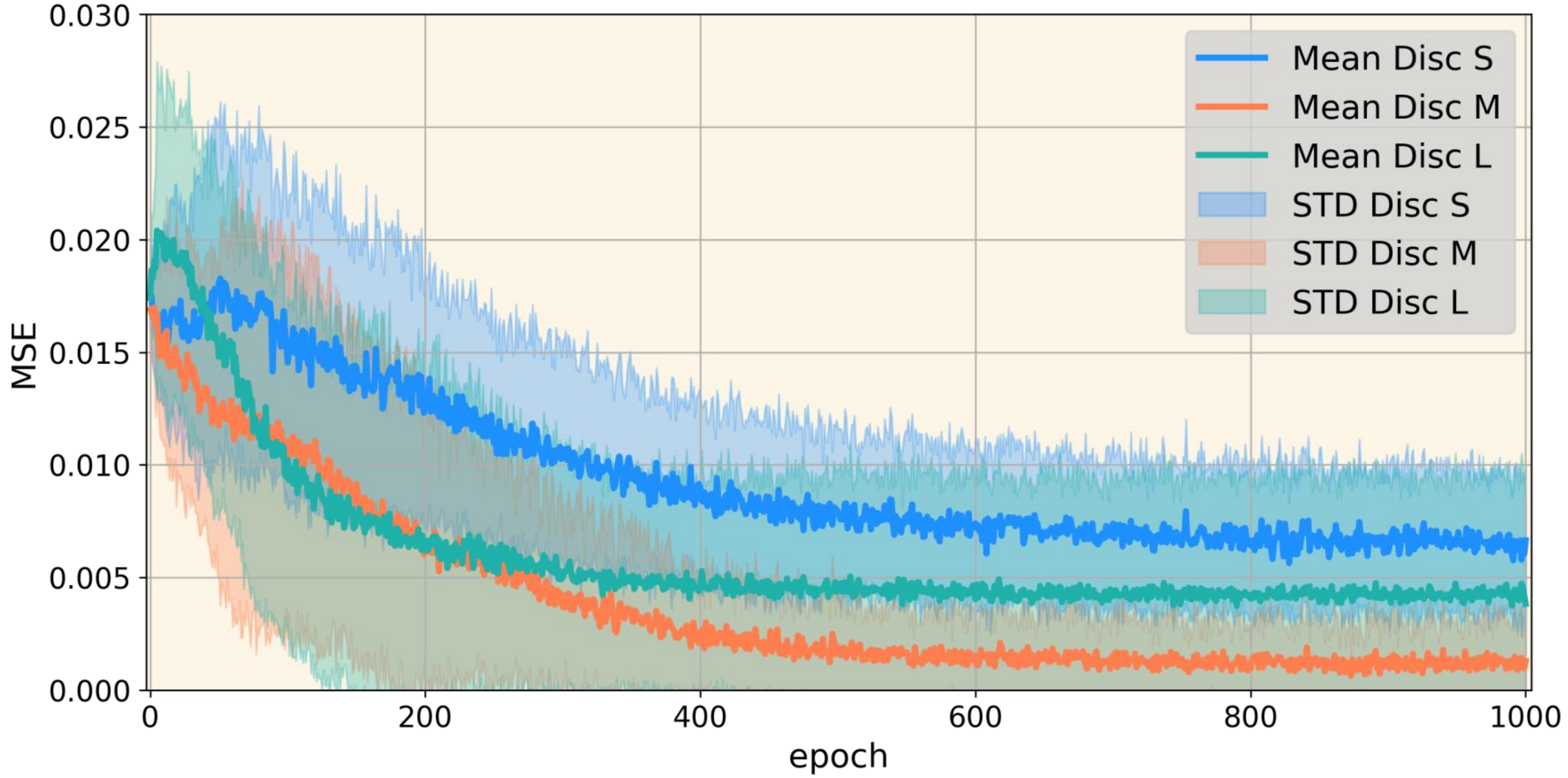
Hybrid GAN

- Hybrid quantum-classical GAN
  - **Quantum** generator circuit
    - MERA-up architecture
  - Classical discriminator neural network
    - Consists of dense (fully connected) layers
    - Three discriminator sizes evaluated
      - S: 153 trainable parameters
      - M: 433 trainable parameters
      - L: 1889 trainable parameters



- Hybrid GAN for comparison

Results Training



Model	MSE $(* 10^{-3})$
Full Quantum GAN	1.76 ± 1.45
Hybrid S	6.64 ± 3.28
Hybrid M	1.28 ± 2.22
Hybrid L	3.83 ± 4.42
QAG*	0.67 ± 0.56

* QAG: Quantum Angle Generator

- New enhanced quantum generative model
- Discriminator replaced by objective function
- Even able to correctly represent the pixelwise correlation

- Only the hybrid M model outperforms the full quantum GAN
  - Hybrid L model: not balanced, discriminator too powerful