Quantum Generative Models in HEP

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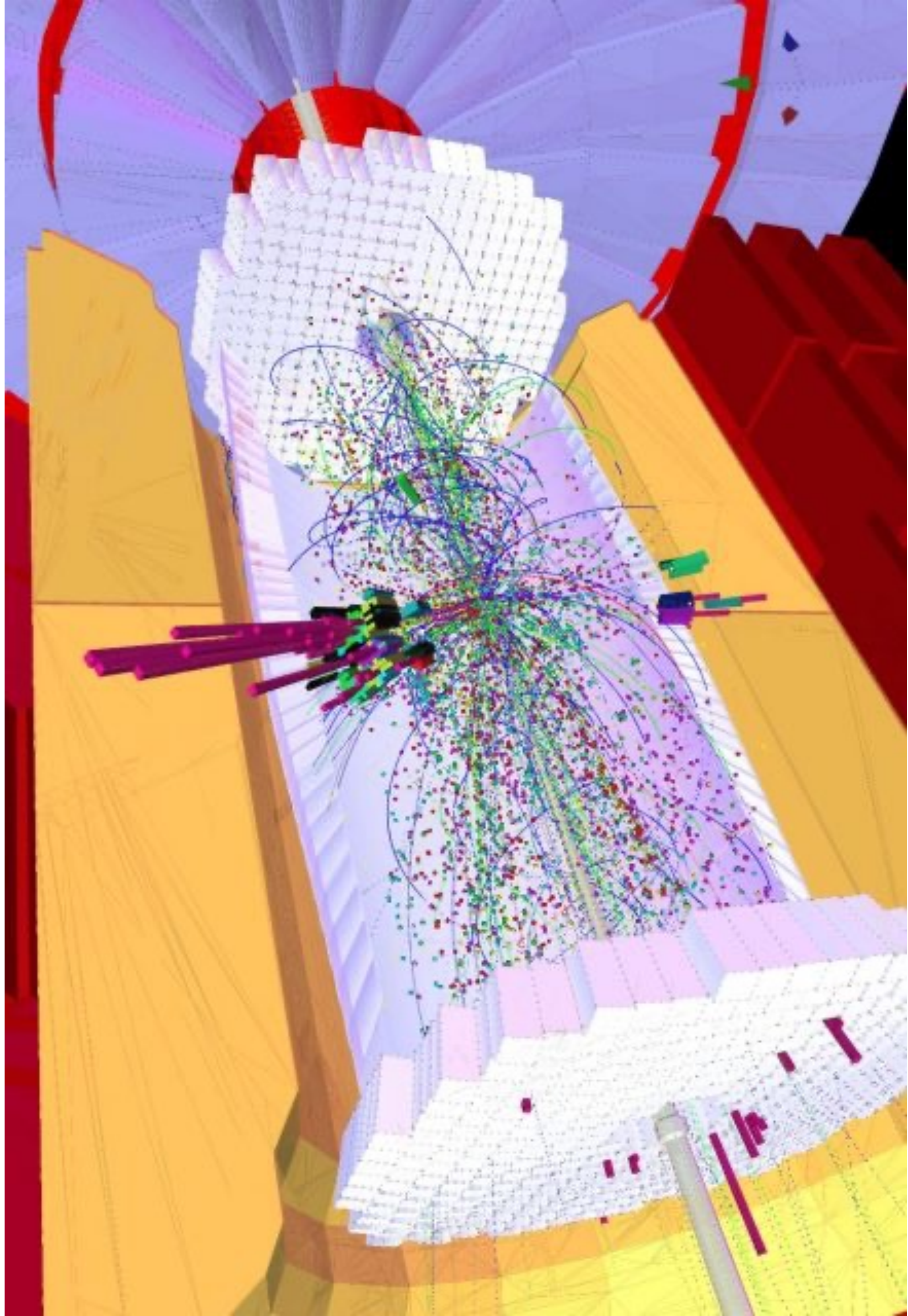
Outline

- Quantum Generative Models : An Overview
- Applications in data analysis in HEP
- Characterizing quantum generative models through model capacity and trainability.



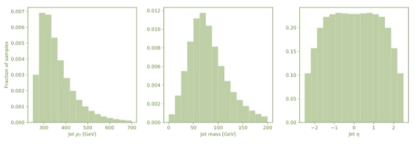
Quantum Generative Modeling

What?

- **Quantum Generative Models** are a powerful tool in QML to reproduce the statistics of a target distribution or quantum state ensemble, that can accordingly be used to generate new samples.

DATA SOURCE

Classical Data



Quantum Data

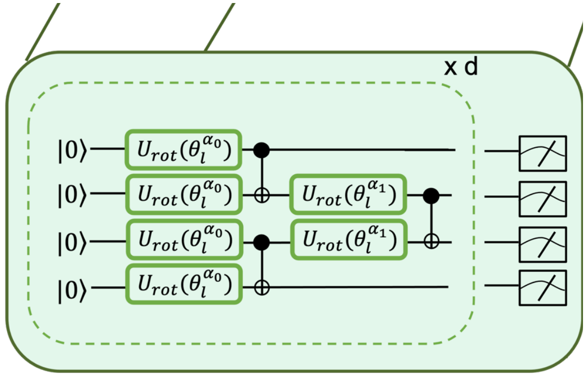
DATA LOAD

Probability distribution

Quantum Circuit

Quantum State

MODEL



Lloyd, Seth, and Christian Weedbrook. "Quantum Generative Adversarial Learning." *Physical Review Letters* 121, no. 4 (July 26, 2018): 040502. https://doi.org/10.1103/PhysRevLett.121.040502.

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Why?

- Motivated by the capacity of quantum processors to **learn, represent, and sample from high-dimensional probability distributions**.
- Relatively simple quantum systems can generate data whose statistics **cannot be generated efficiently by any classical system**.

QUANTUM PROCESSOR

Represent vectors in N-dimensional spaces using log(N) qubits

Perform manipulations of sparse and low-rank matrices in time O(poly(log(N)))

Lloyd, Seth, and Christian Weedbrook. “Quantum Generative Adversarial Learning.” *Physical Review Letters* 121, no. 4 (July 26, 2018): 040502. https://doi.org/10.1103/PhysRevLett.121.040502.

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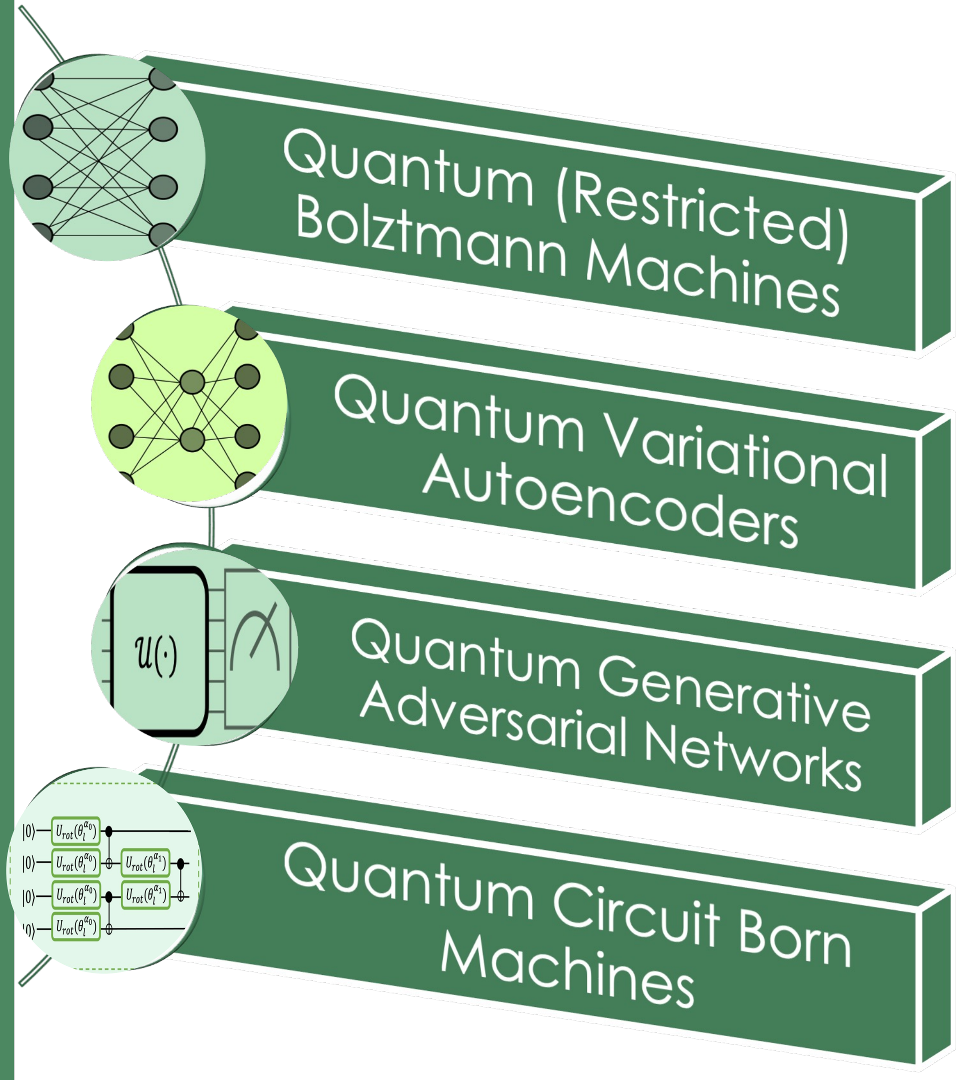
How?

- Several architectures explored, algorithms developed for quantum annealers, discrete and continuous variable.
- These models are **inspired by classical neural network models** and have been translated either as a standalone VQC or as a component in a hybrid network.

  Many quantum computing libraries have been developed that leverage existing classical ML libraries – TensorFlow Quantum, TorchQuantum, PennyLane.

Quantum Generative Models in HEP



- Inspired by applications in data augmentation, simulation, data compression tasks.
- HEP datasets provide a natural alternative to synthetic datasets to explore entanglement, expressiveness and scalability in QML models.
  - *If proven to be scalable can demonstrate to have an advantage in generating high-dimensional correlated events.*
- Also, can potentially have applications in large-scale quantum sensor networks, anomaly detection in quantum-enhanced probes for BSM physics, data embedding.
- Trained by minimizing the energy of a model (q-RBMs), the error when sampling from a target posterior (QCMBs), or through adversarial methods (q-GANs).

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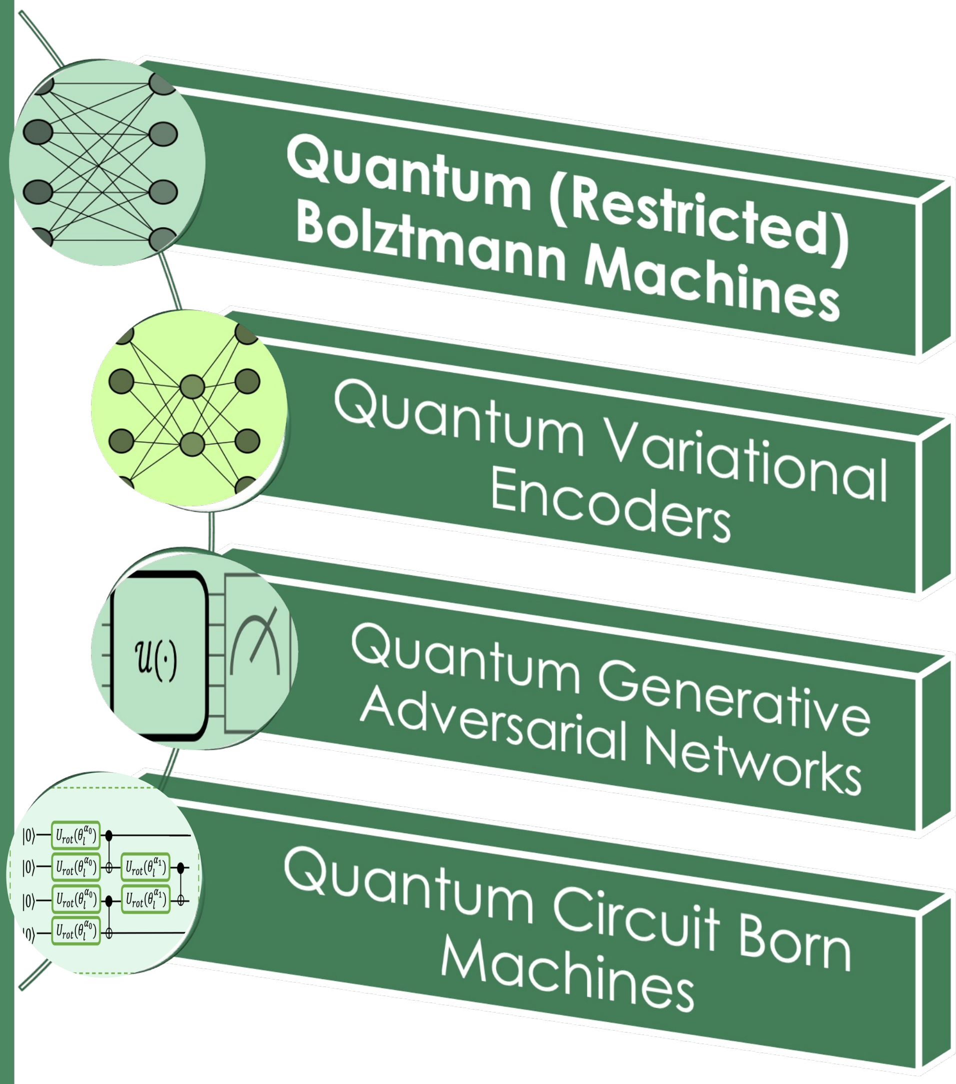
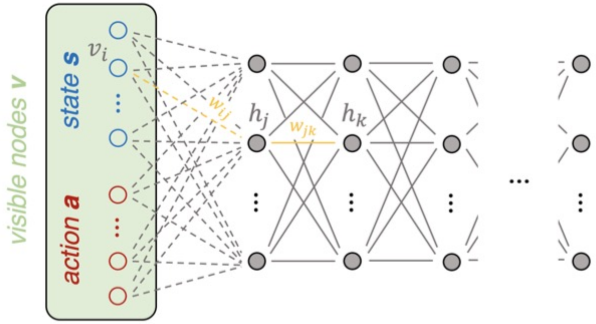
Quantum Generative Models in HEP



- **(Restricted) Boltzmann machines** are physically motivated NNs capable of generating new samples similar to the training data.
- Weights and biases are optimized by finding the ground state of a system's Hamiltonian – thus, *are perfectly suited for quantum annealers*.

Use free energy of QBM as an estimate of the Q-function in the training a reinforcement learning model to optimize a beam in a linear accelerator

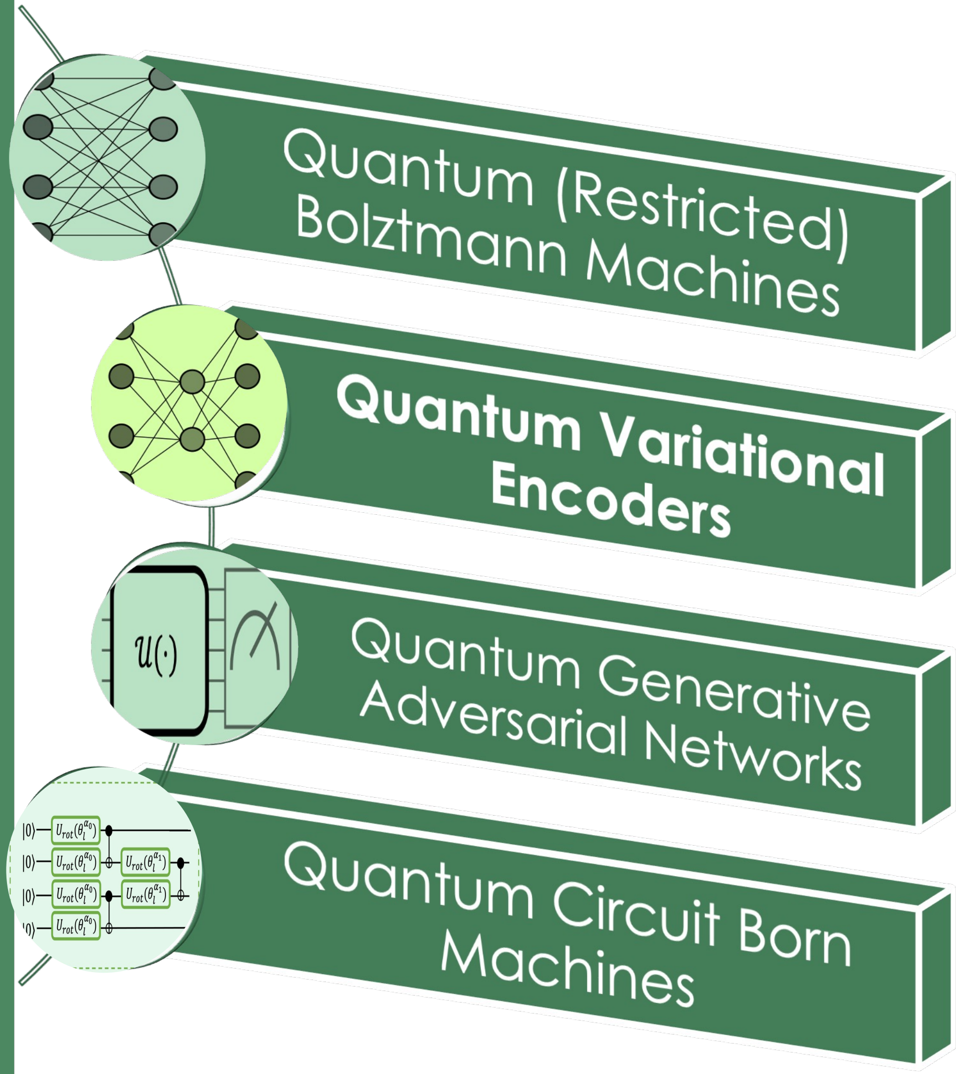


Schenk, Michael, Elías F. Combarro, Michele Grossi, et al "Hybrid Actor-Critic Algorithm for Quantum Reinforcement Learning at CERN Beam Lines." arXiv, September 22, 2022. https://doi.org/10.48550/arXiv.2209.11044.

QRBM for galaxy morphology classification with a quantum annealing

Caldeira, João, Joshua Job, et al. "Restricted Boltzmann Machines for Galaxy Morphology Classification with a Quantum Annealer." arXiv, February 13, 2020. http://arxiv.org/abs/1911.06259.

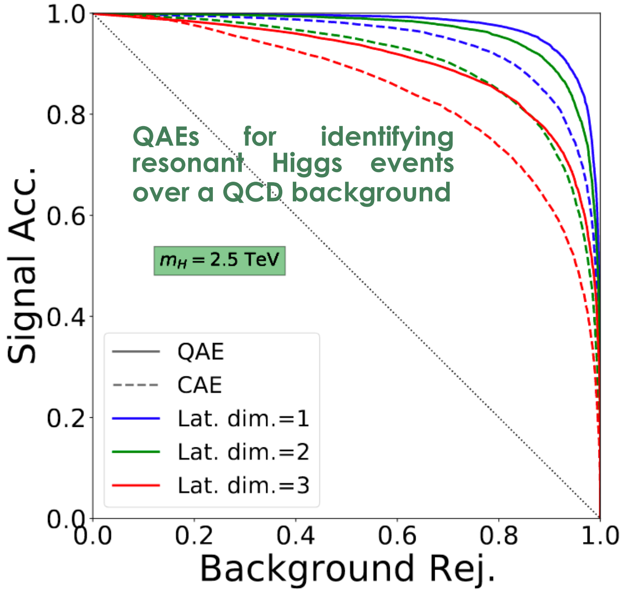
Quantum Generative Models in HEP



An **autoencoder** is a based on a two-component network:

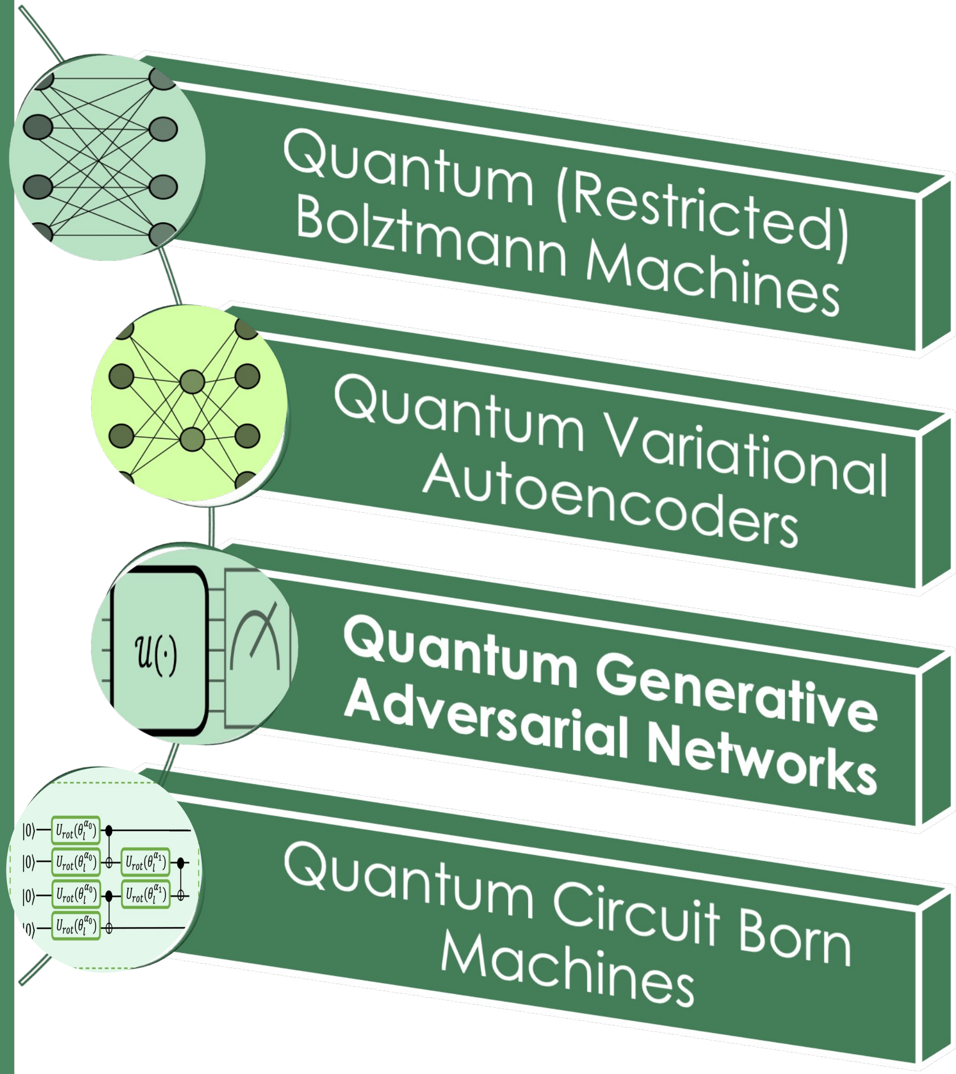
- A network maps an input vector x to a compressed "latent space".
- A second network maps back the latent vector into feature space.
- Network is trained to minimize the error of the reconstructed input state or vector.

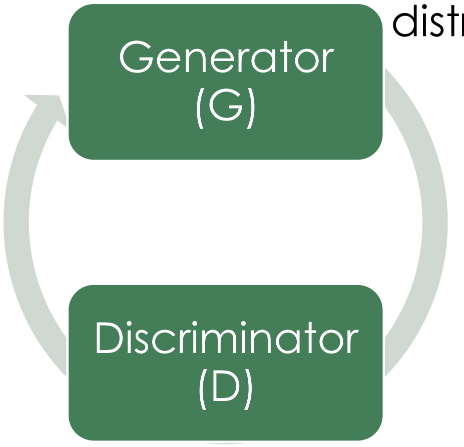
In the quantum setting, q-AEs can be used for generative modeling, data compression and anomaly detection.



Ngairangbam, V. S., et al, "Anomaly Detection in High-Energy Physics Using a Quantum Autoencoder." Accessed October 31, 2022. https://arxiv.org/abs/2112.04958.

Quantum Generative Models in HEP





G transforms samples from a prior to a target distribution

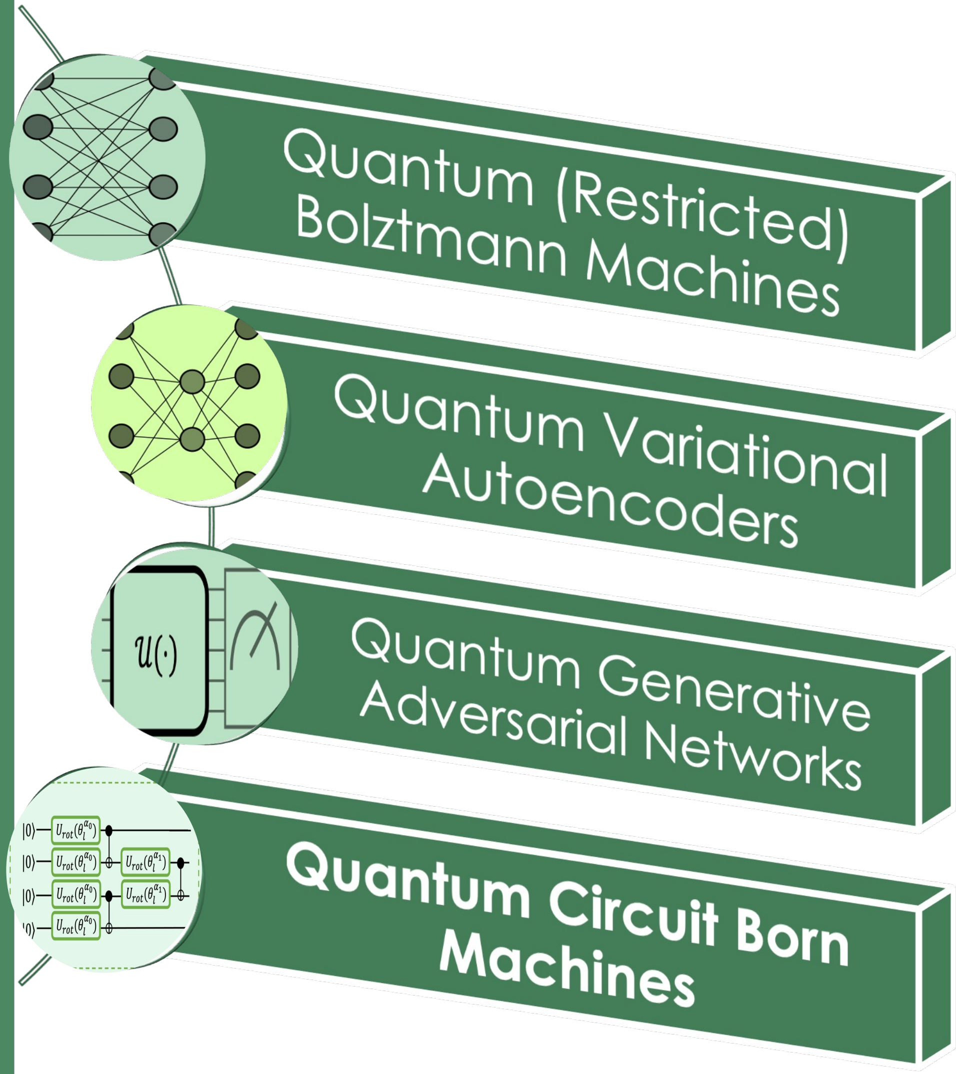
D takes generator and "real" samples and tries to distinguish between them.

Training corresponds to a minmax two player game

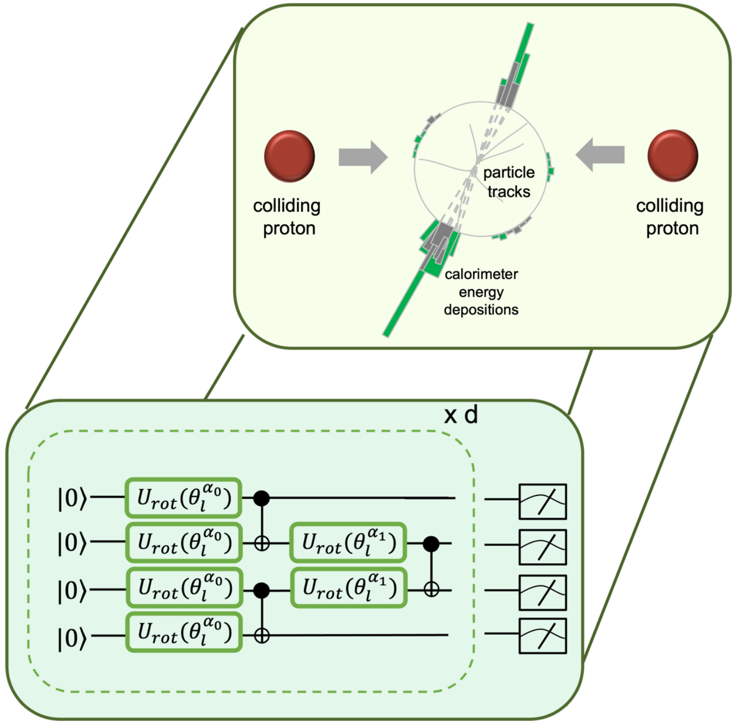
$$\min_{\phi_g} \mathcal{L}_G(\phi_g, \phi_d)\,, \quad \max_{\phi_d} \mathcal{L}_D(\phi_g, \phi_d)$$

- Adversarial training with quantum generator and classical or quantum discriminator.
- Applications:
    - Monte Carlo event generation: Carlos Bravo-Prieto, et al. Style-based quantum generative adversarial networks for monte carlo events. arXiv:2110.06933, 2021.
    - Detector simulation: Su Yeon Chang, et al. Dual- parameterized quantum circuit gan model in high energy physics. EPJ Web of Conferences, 251:03050, 2021.
    - Data loading for cross section integration: Gabriele Agliardi, et al,. "Quantum integration of elementary particle processes". arXiv preprint arXiv:2201.01547, 1 2022

Quantum Generative Models in HEP



- QCBMs are **parameterized quantum circuits** used with the objective of preparing a target distribution with high-fidelity.
- A QCBM rotates a fixed initial state to a final state, then samples from that final state.
- A commonly used ansatz for QCBMs is the **"hardware efficient ansatz":** constructed by alternating layers of rotation gates with layers of two-qubit entangling operations.

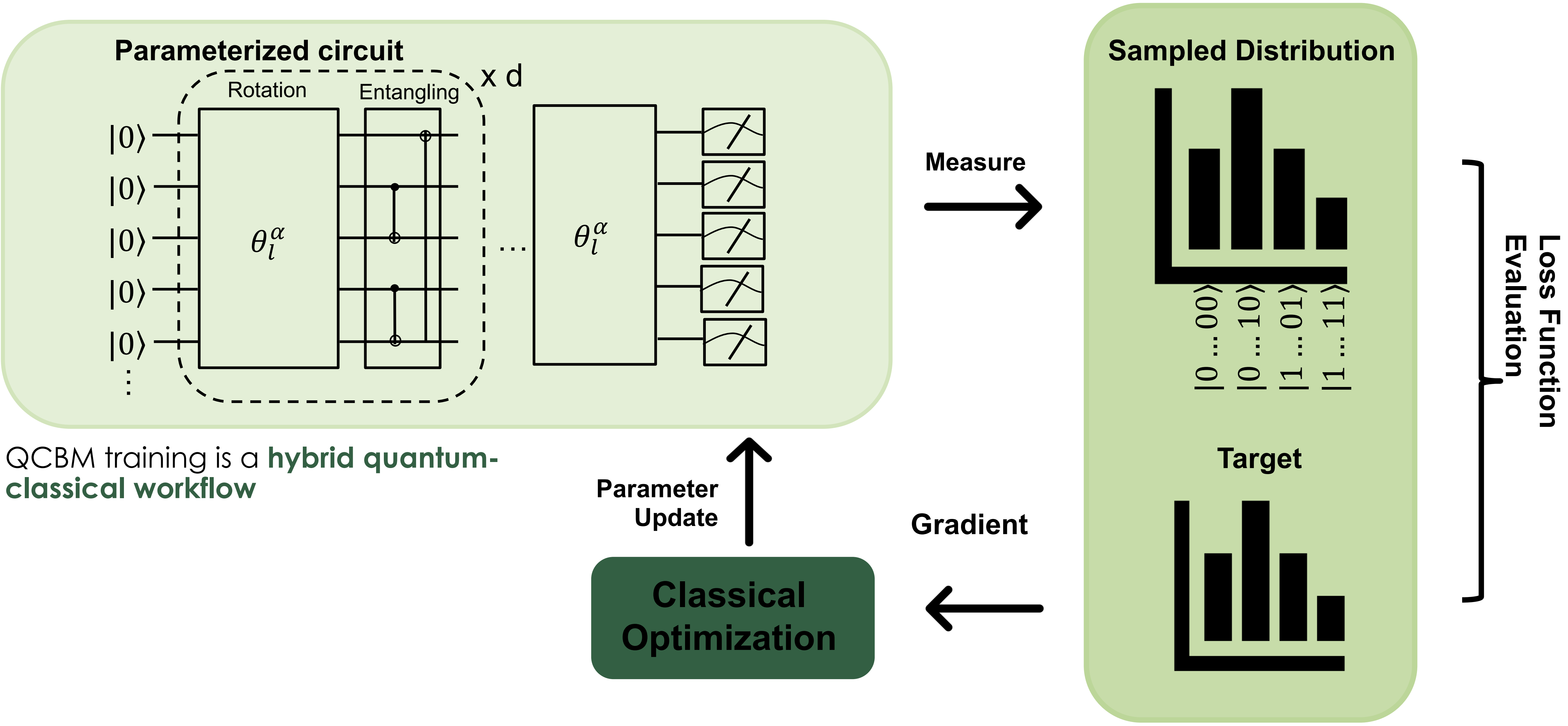


- The design space for QCBM models is large – there are many choices for initial state, ansatz, and measurement setting.
- Building **scalable QCBM models for HEP** must balance reproducing a target distribution with high fidelity with trainability and noise robustness.

Delgado, Andrea, and Kathleen E. Hamilton. "Unsupervised Quantum Circuit Learning in High Energy Physics." arXiv, March 7, 2022. https://doi.org/10.48550/arXiv.2203.03578.

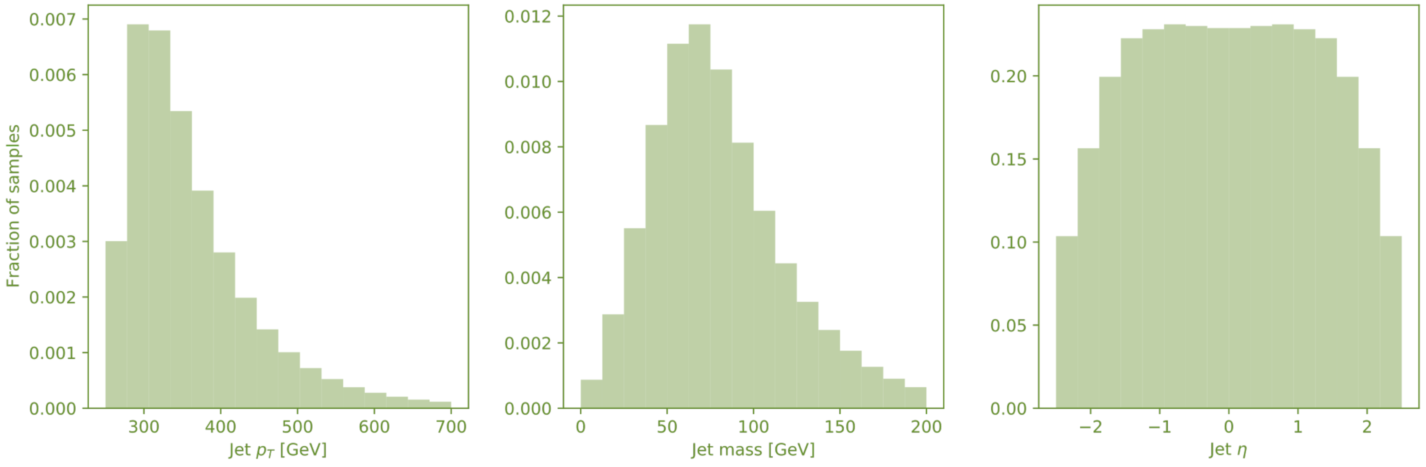
Kiss, Oriel, Michele Grossi, Enrique Kajomovitz, and Sofia Vallecorsa. "Conditional Born Machine for Monte Carlo Event Generation." *Physical Review A* 106, no. 2 (August 22, 2022): 022612. https://doi.org/10.1103/PhysRevA.106.022612.

Unsupervised Quantum Circuit Learning

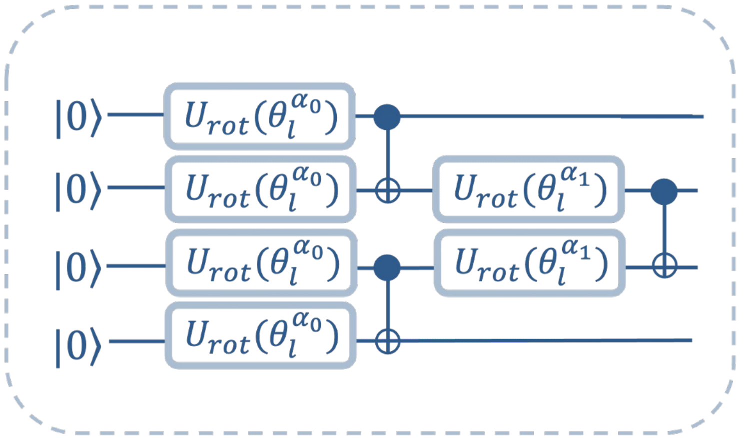


QCBM training is a **hybrid quantum-classical workflow**

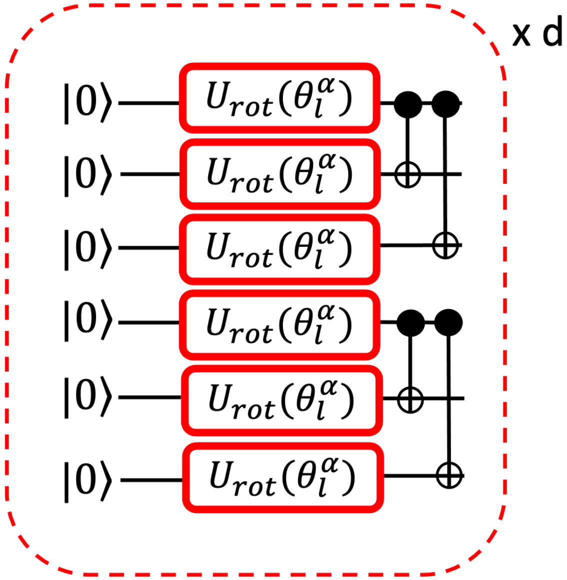
An Example: QCBMs for fitting 2 and 3-dimensional joint distributions



Ansatz 1



Ansatz 2



- Can we fit the marginal distributions?
- Are the correlations also preserved on the generated distribution?
- Ansatz choice: Trial and error

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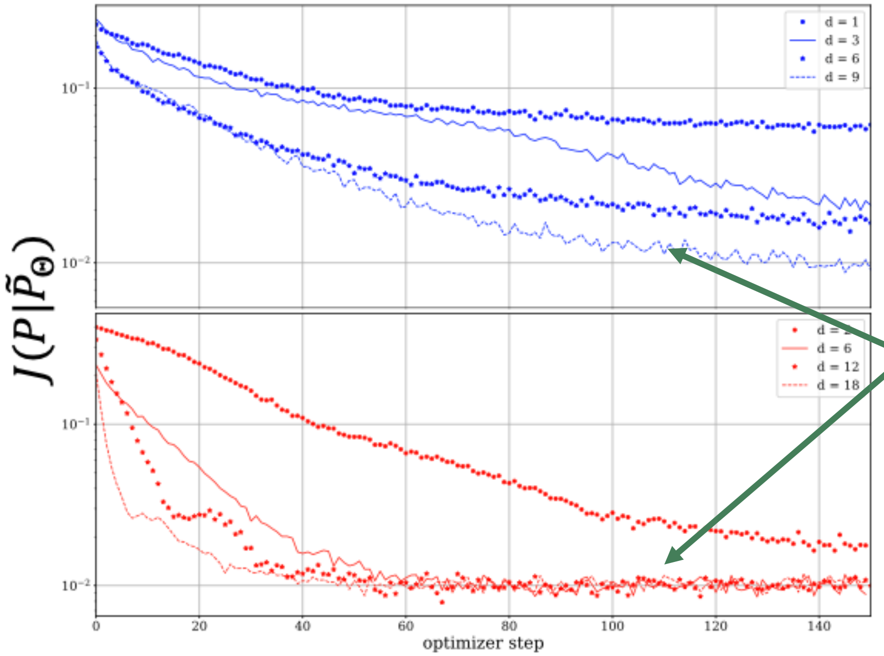
Hyperparameter Tuning

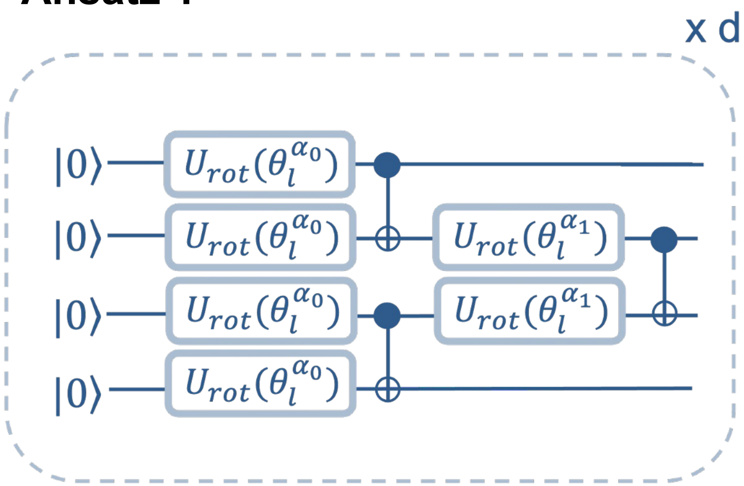


QCBM training simulated on CPU

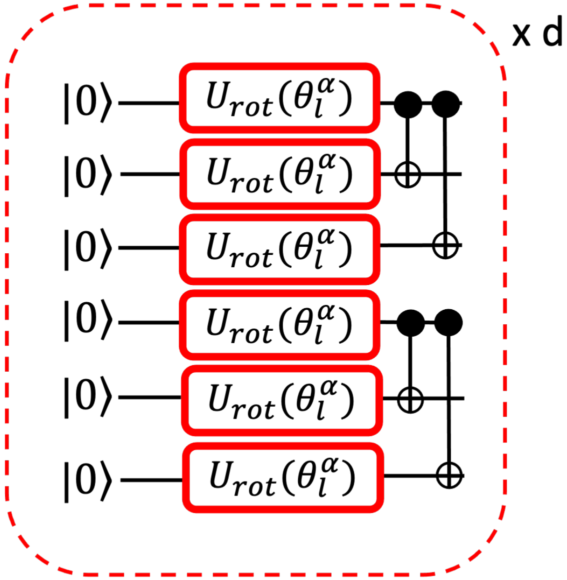
- *Using PennyLane library and Qulacs*
- *Adam optimizer*

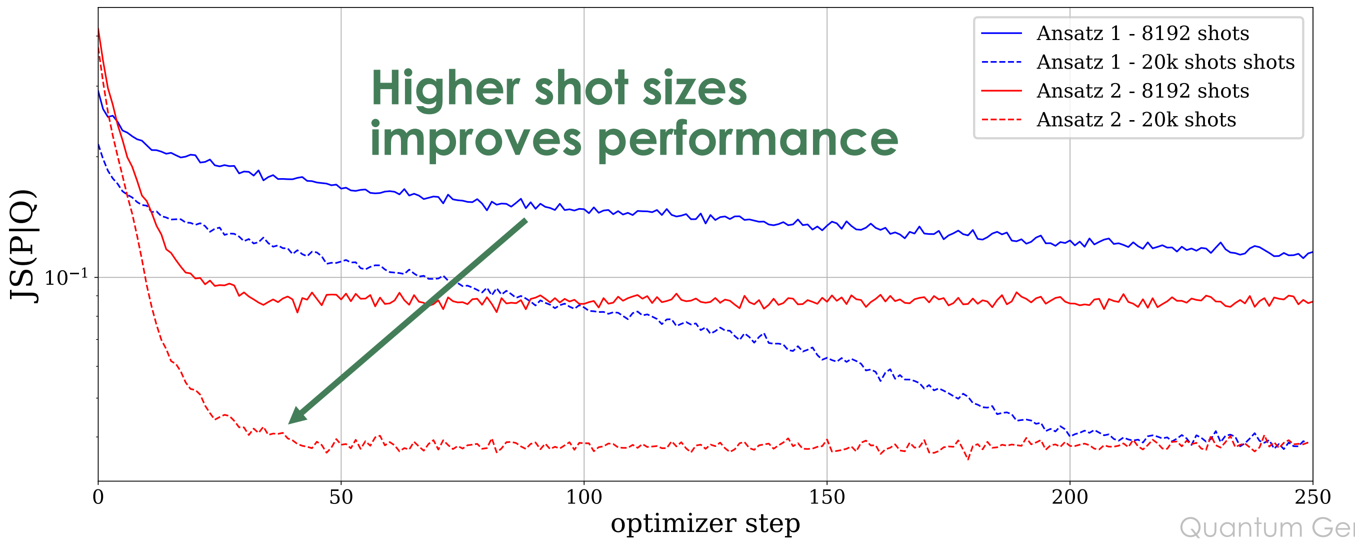
Larger circuits lead to faster convergence

Ansatz 1



Ansatz 2





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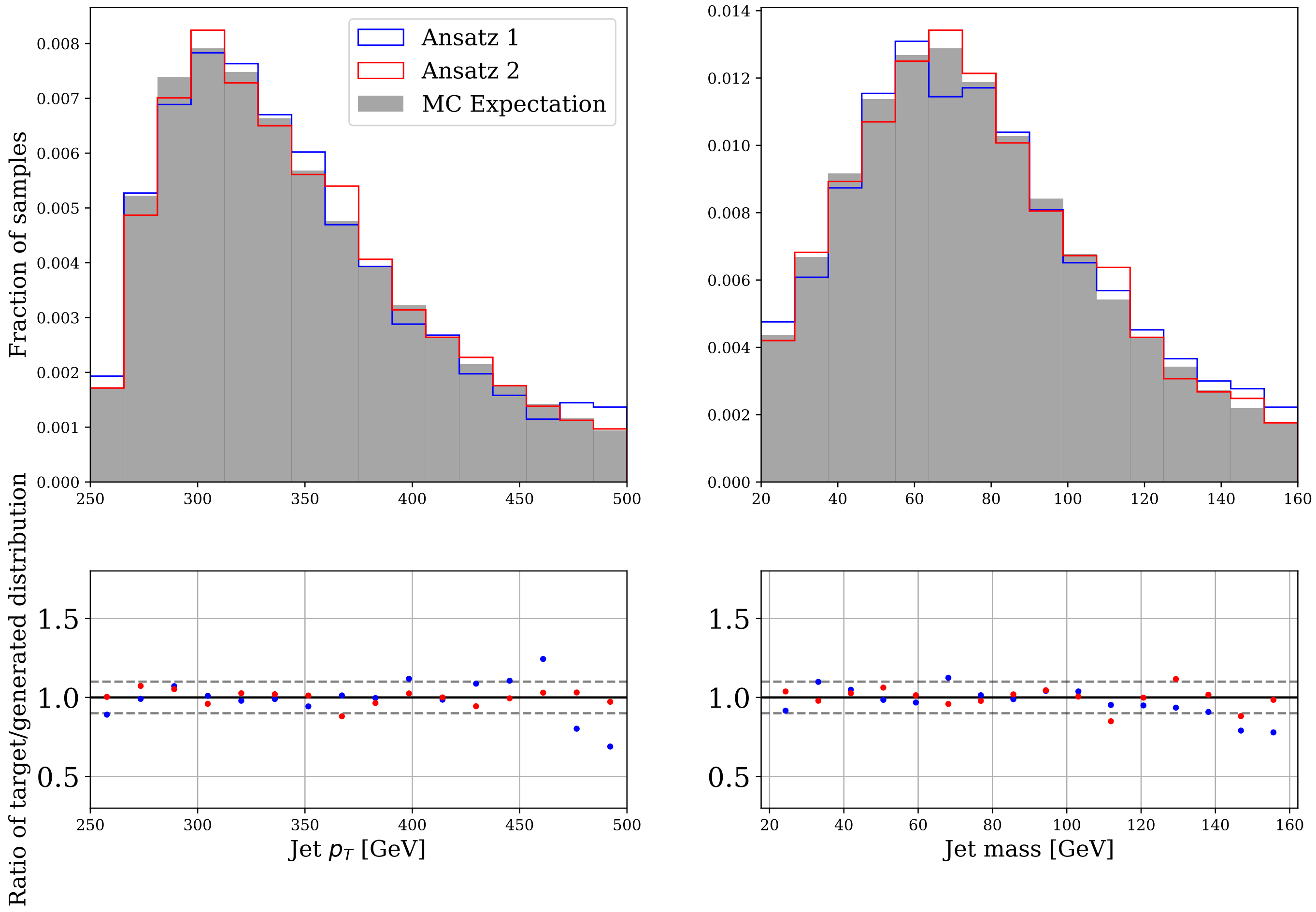
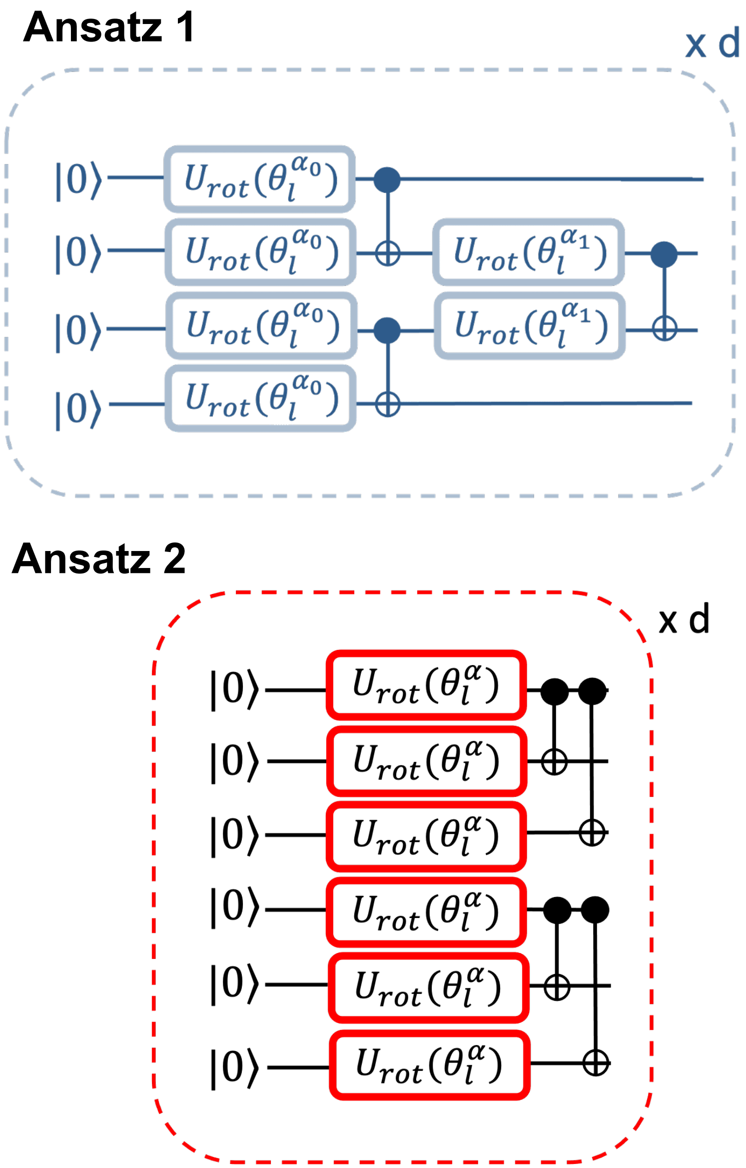
Marginal Fitting: 2D Joint Distributions (8 qubits)





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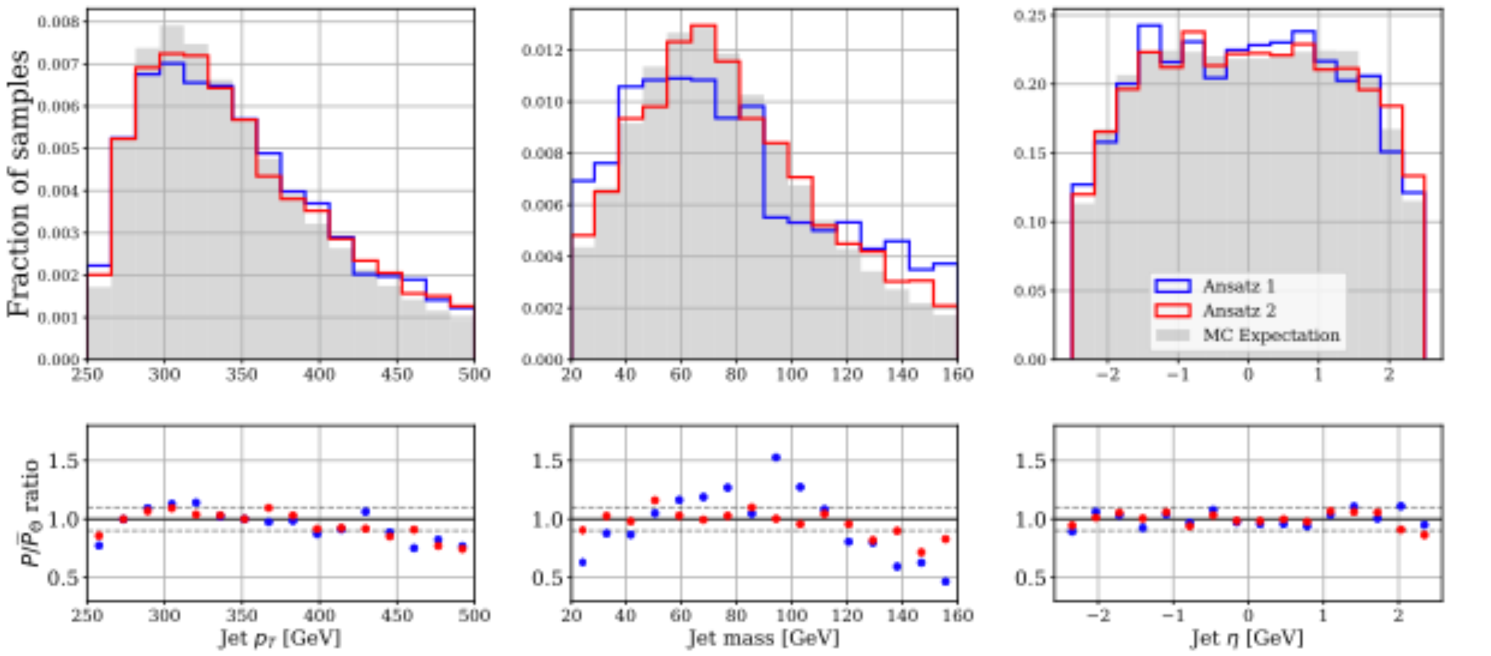
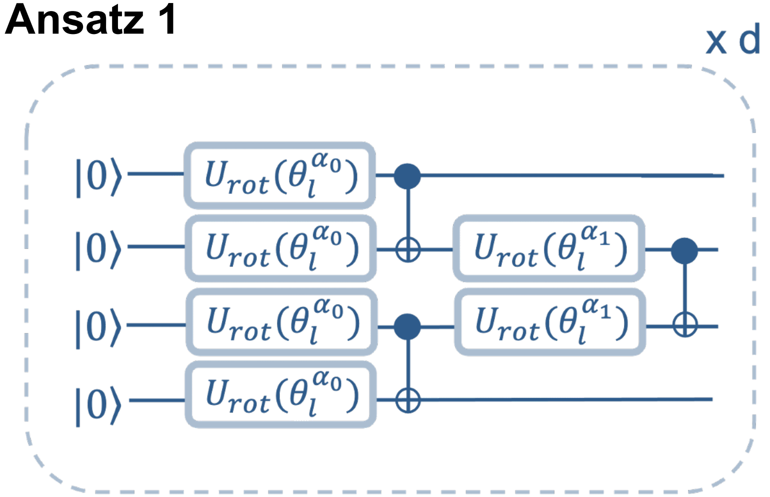
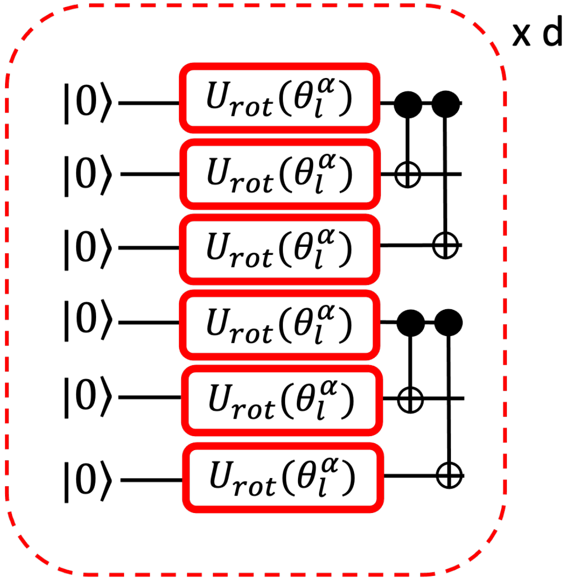
Marginal Fitting: 3D Joint Distributions (12 qubits)



Ansatz 1



Ansatz 2



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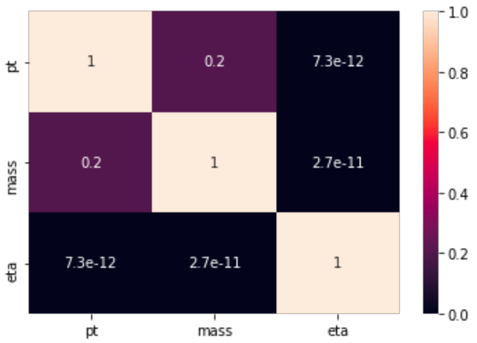
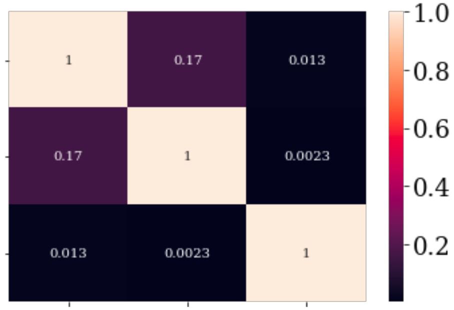
Correlation Fitting

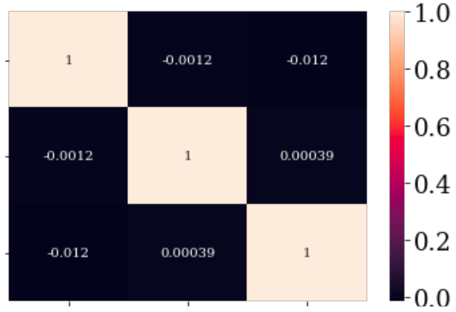
MC (Truth)



Ansatz 1



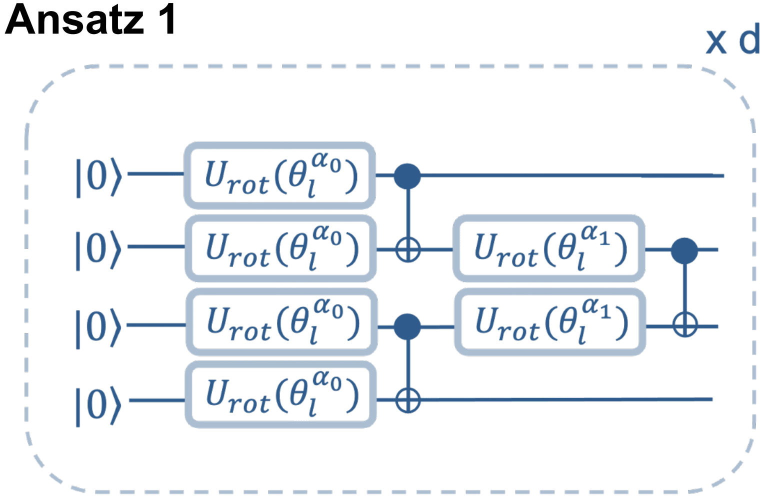
Ansatz 2



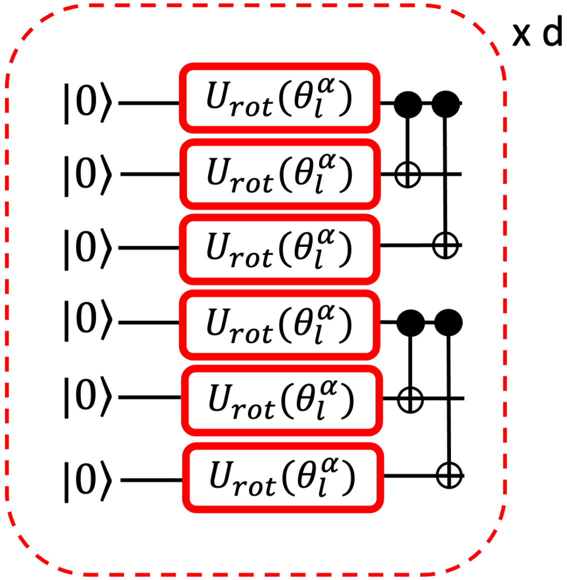
With d=1 layer all n-qubits can be entangled together

With d=1 layer n-qubits are prepared as separated sub-systems of m-qubits

Ansatz 1



Ansatz 2



The road to quantum advantage…

Harder

*Train circuits that are **harder** to simulate in classical devices (classically intractable regime of QML)?*

Better

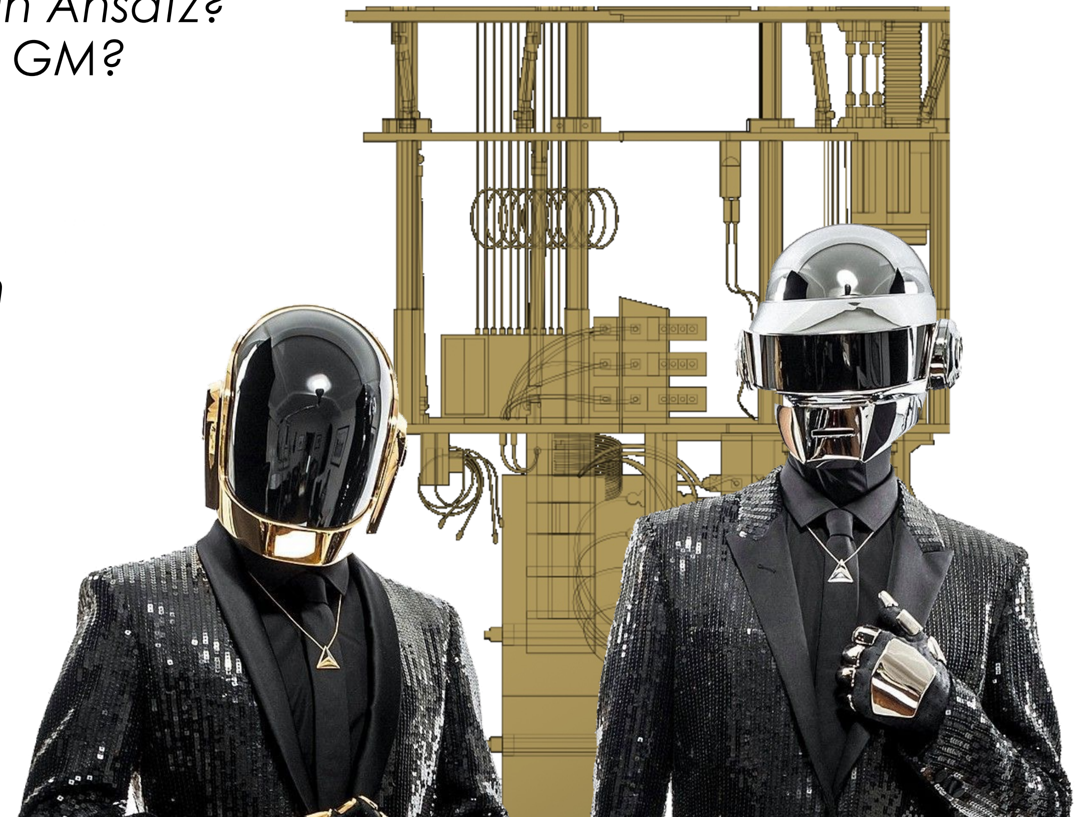
*Can we do **better** than trial and error when selecting an Ansatz? Produce a systematic method to characterize PQCs in GM?*

Faster

*Can we train circuits **faster**? By optimizing circuit design and reduce the number of executions on hardware.*

Stronger

*Develop **stronger**, scalable error mitigation/correction techniques.*



The road to quantum advantage…

Harder

Train circuits that are ***harder*** *to simulate in classical devices (classically intractable regime of QML)?*

Actively working on it… trained QCBMs up to 15 qubits

Better

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Preliminary results on some ideas to tackle these

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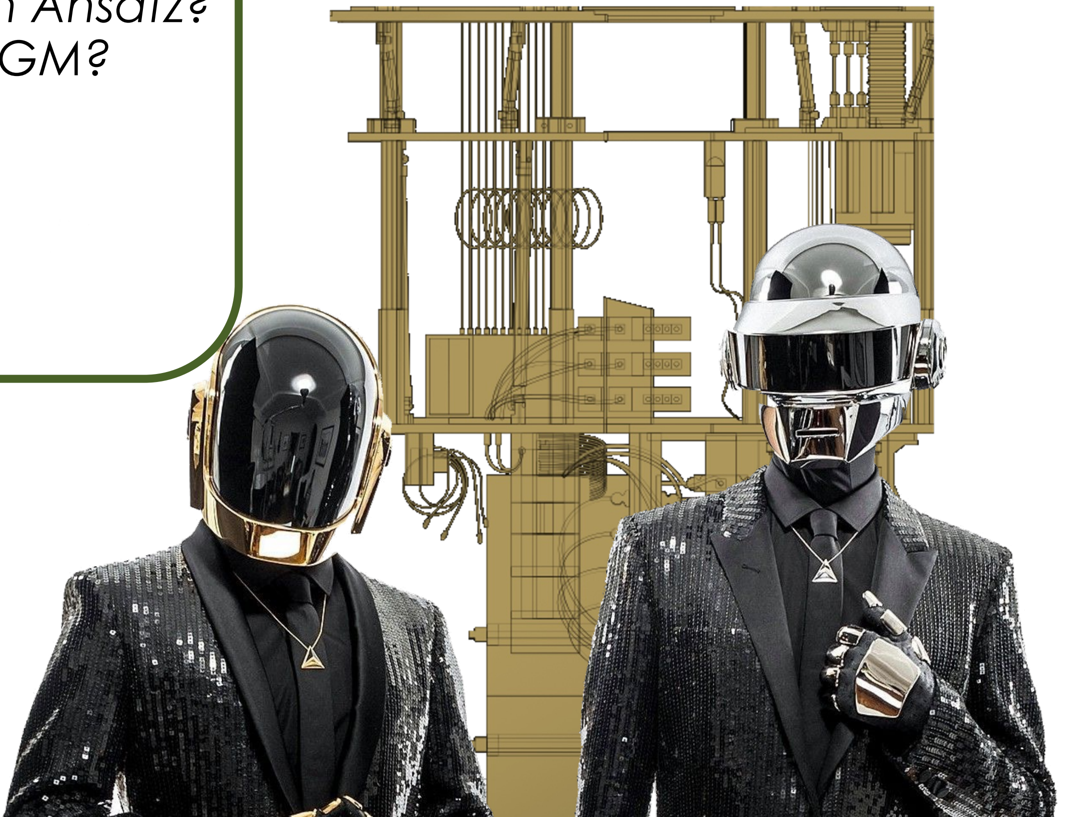
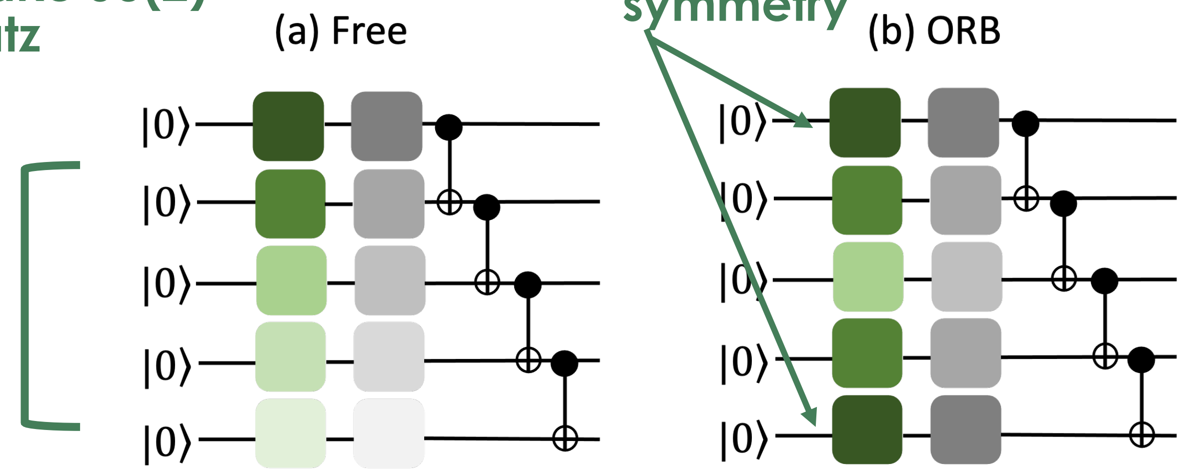


Building Symmetries into Quantum Circuit Learning

- How can we reduce the number of parameters in our circuit?
- Is there any symmetry we can exploit for QML applications?
- Inspired by ORB-type circuits.
  - Parameters are grouped into “orbits” with shared parameters.

(1) Take SU(2) Ansatz

(2) Group rotational gates on qubits that can be swapped without affecting symmetry



(3) Operations on the same orbit share parameters, reducing the number of trainable parameters

Sauvage, Frederic, Martin Larocca, Patrick J. Coles, and M. Cerezo. “Building Spatial Symmetries into Parameterized Quantum Circuits for Faster Training.” arXiv, July 28, 2022. https://doi.org/10.48550/arXiv.2207.14413.

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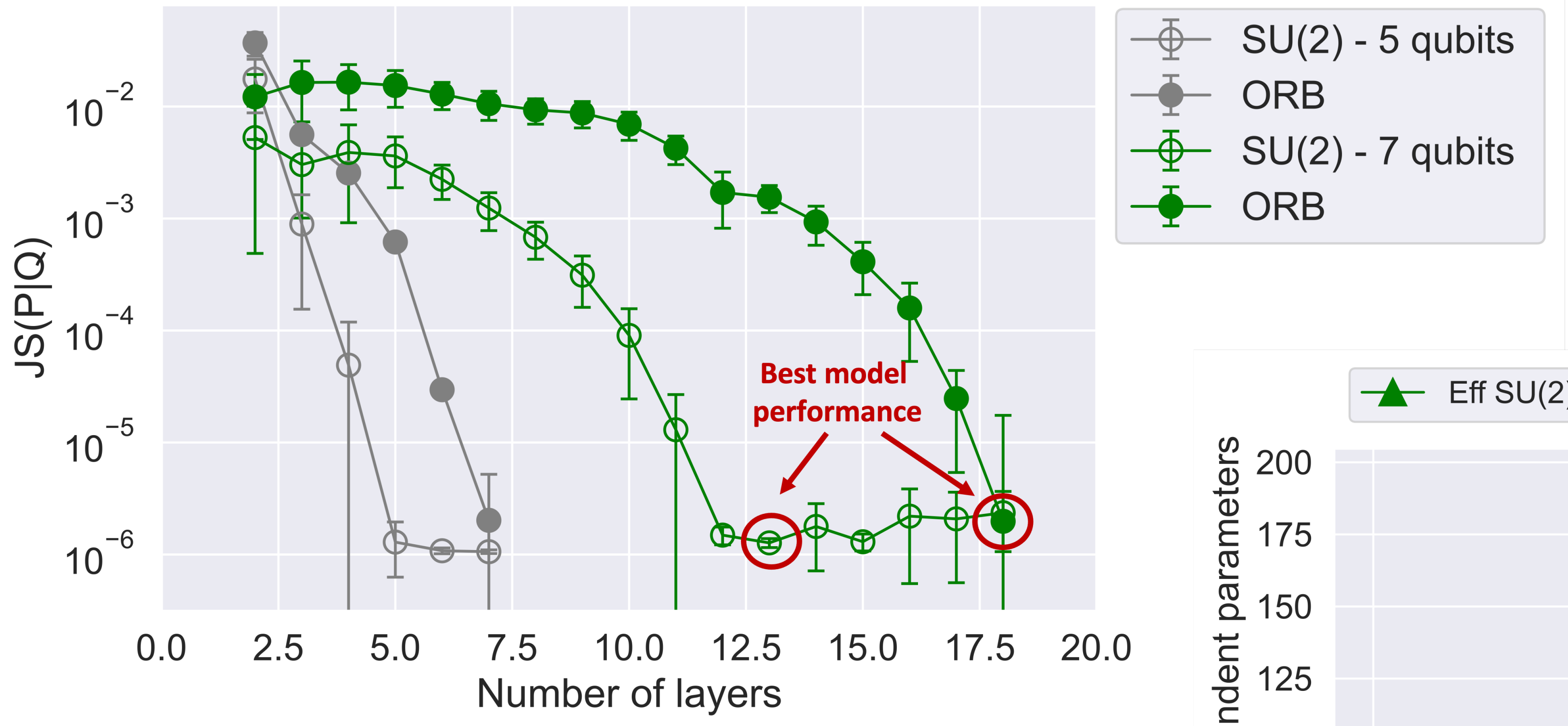
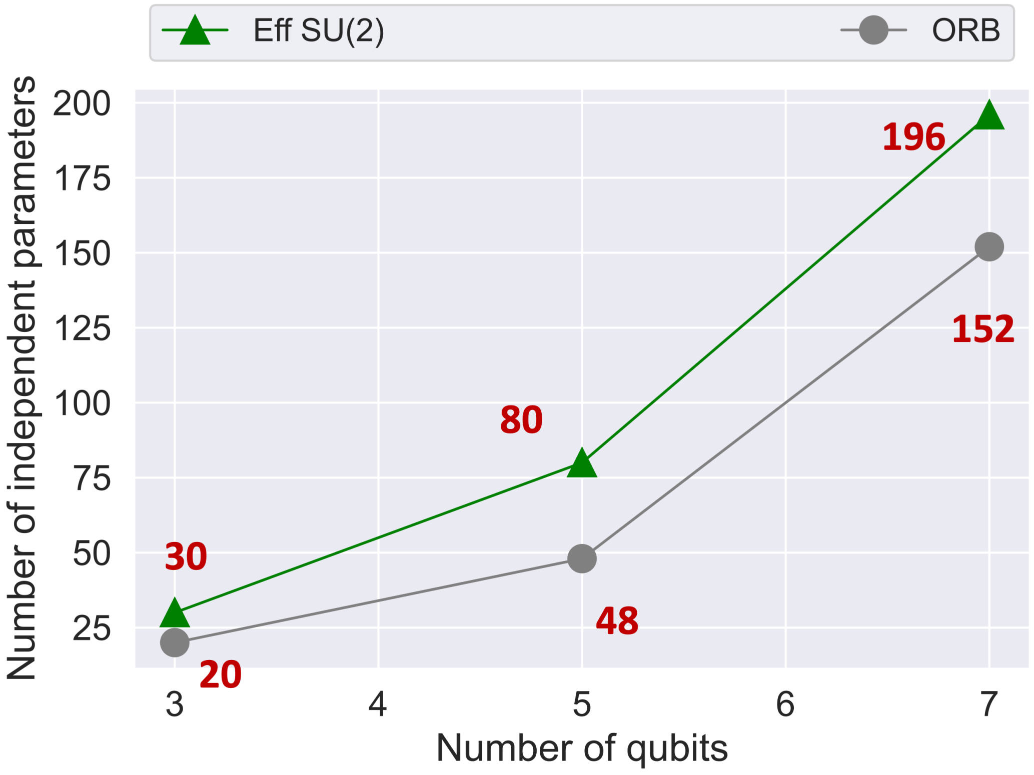
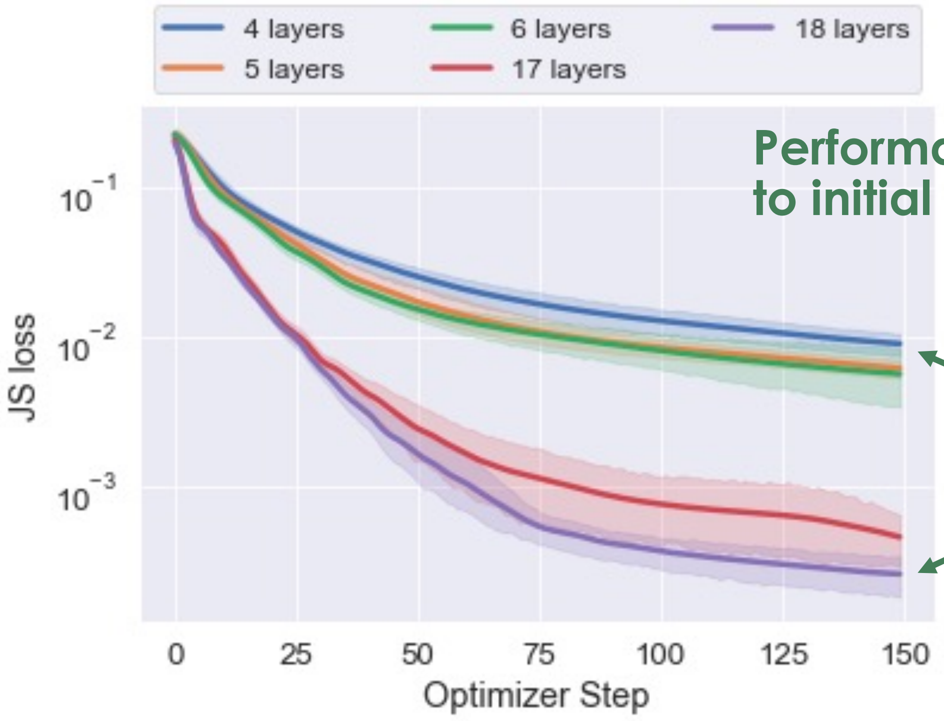




More layers needed in Orb-type circuits to achieve similar performance than fully-parameterized circuits.

But effective number of trainable parameters is reduced.

Capacity and Trainability of Quantum Generative Models

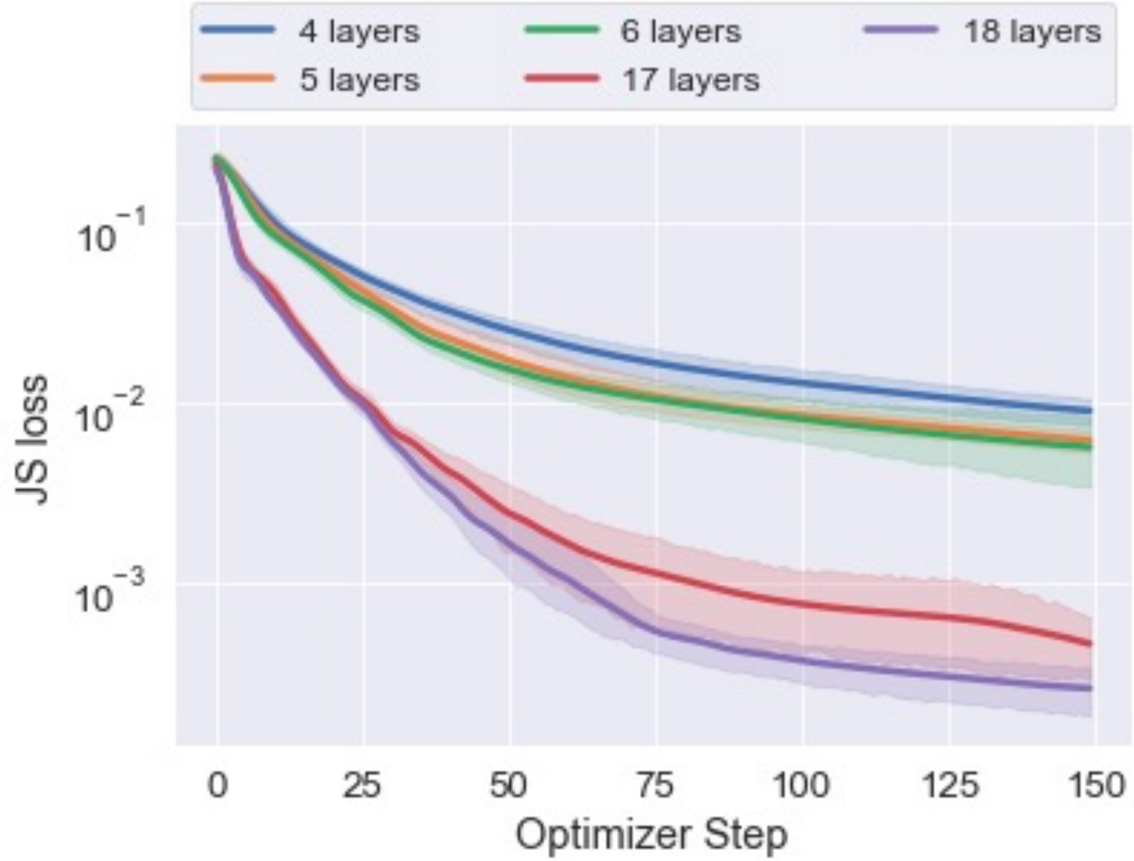


Performance also related to initial parameters

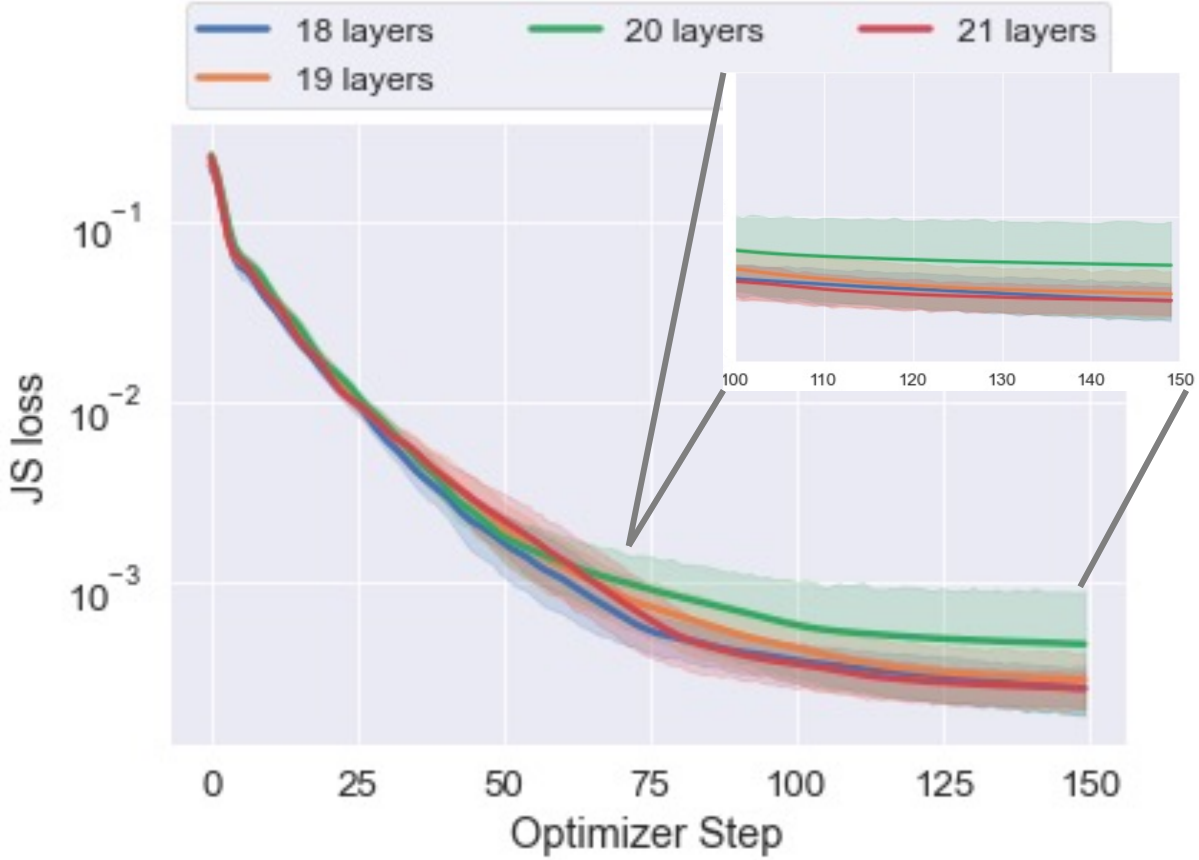
As we add more layers, we get to lower JS values

Capacity and Trainability of Quantum Generative Models

But… there is a limit to the model capacity



… after a critical number of layers, performance can't get any better



Coinciding with the saturation in the QFI matrix rank!

→ **But how does it relate to the circuit entangling structure?**

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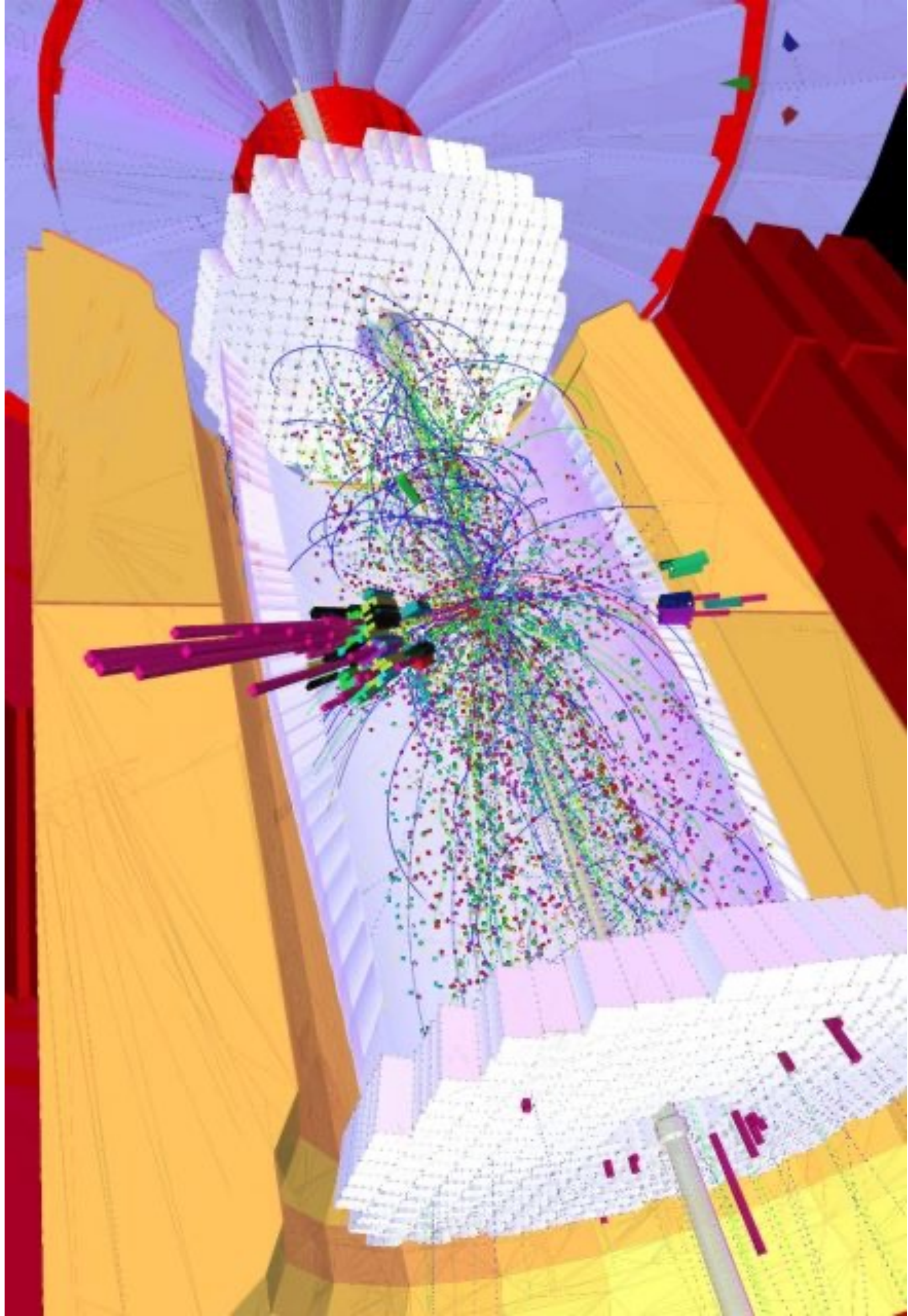
Summary

- Quantum generative models are currently a promising candidate for quantum advantage in QML, with current performance comparable to classical methods. Still a lot of open questions:
  - Scalability?
  - Model capacity and how it is affected by entanglement in circuit.
  - Transitions in trainability.
  - Scalable error correction.
- Promising applications in HEP.
  - Finding complex correlations in data.
  - As a data augmentation tool.
  - As input models for other quantum algorithms.
  - To complement quantum-enhanced searches for BSM physics – i.e. quantum sensor networks.

An exciting time to work on QML!



Thank you!

Collaborators: ***Dr. Kathleen Hamilton*** *(ORNL).*

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