Jet Discrimination with Quantum Complete Graph Neural Network

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[“Jet Discrimination with Quantum Complete Graph Neural Network” arXiv 2403.04990v3]

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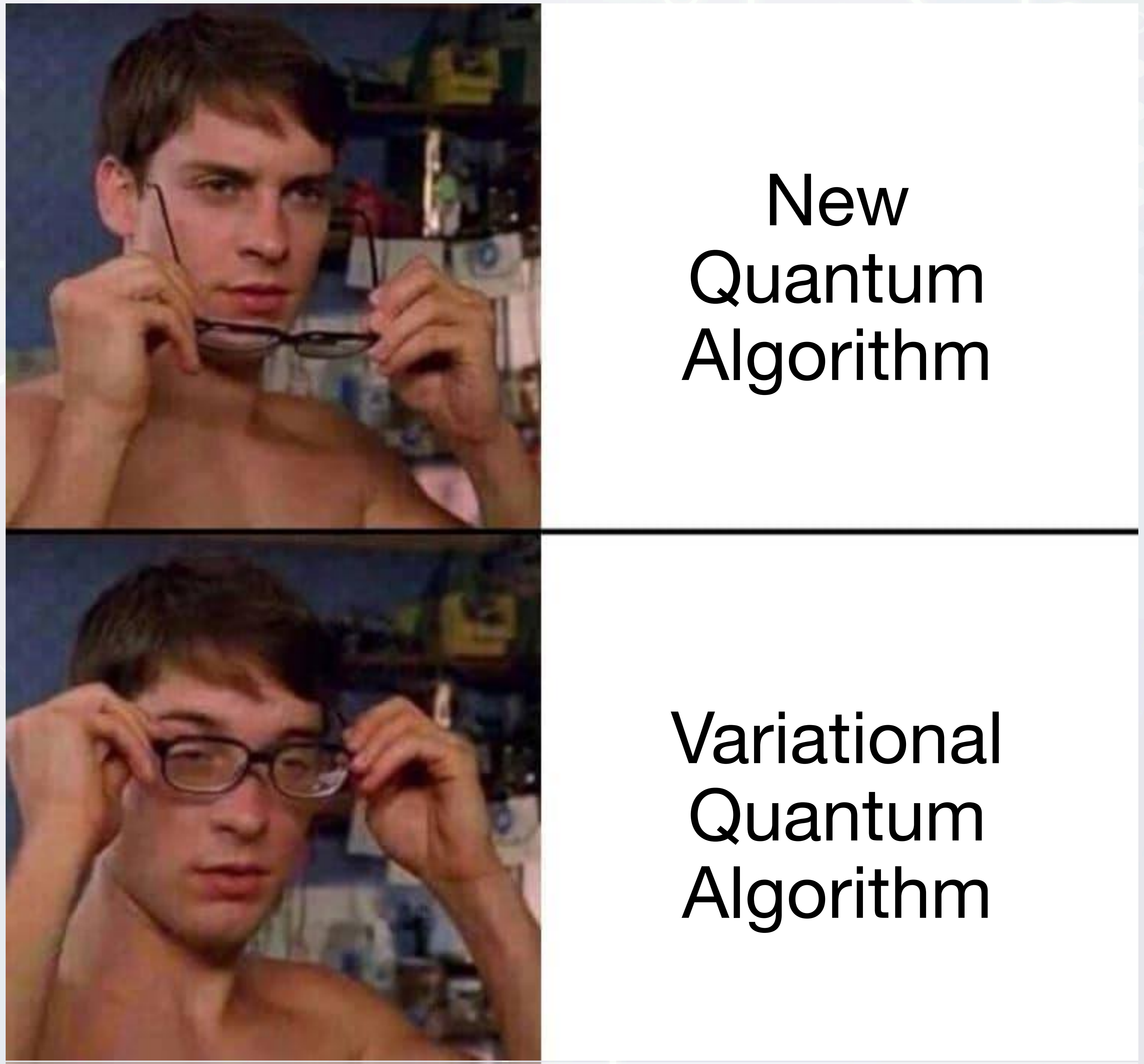
Outline

- **Classical Machine Learning**
  - Message-Passing Graph Neural Network
- **Quantum Machine Learning**
  - Variational Quantum Circuit
  - Quantum Complete Graph Neural Network
- **Dataset**
  - Public Monte Carlo Simulated Jet Data
- **Training X IBMQ X Summary**



Classical Machine Learning

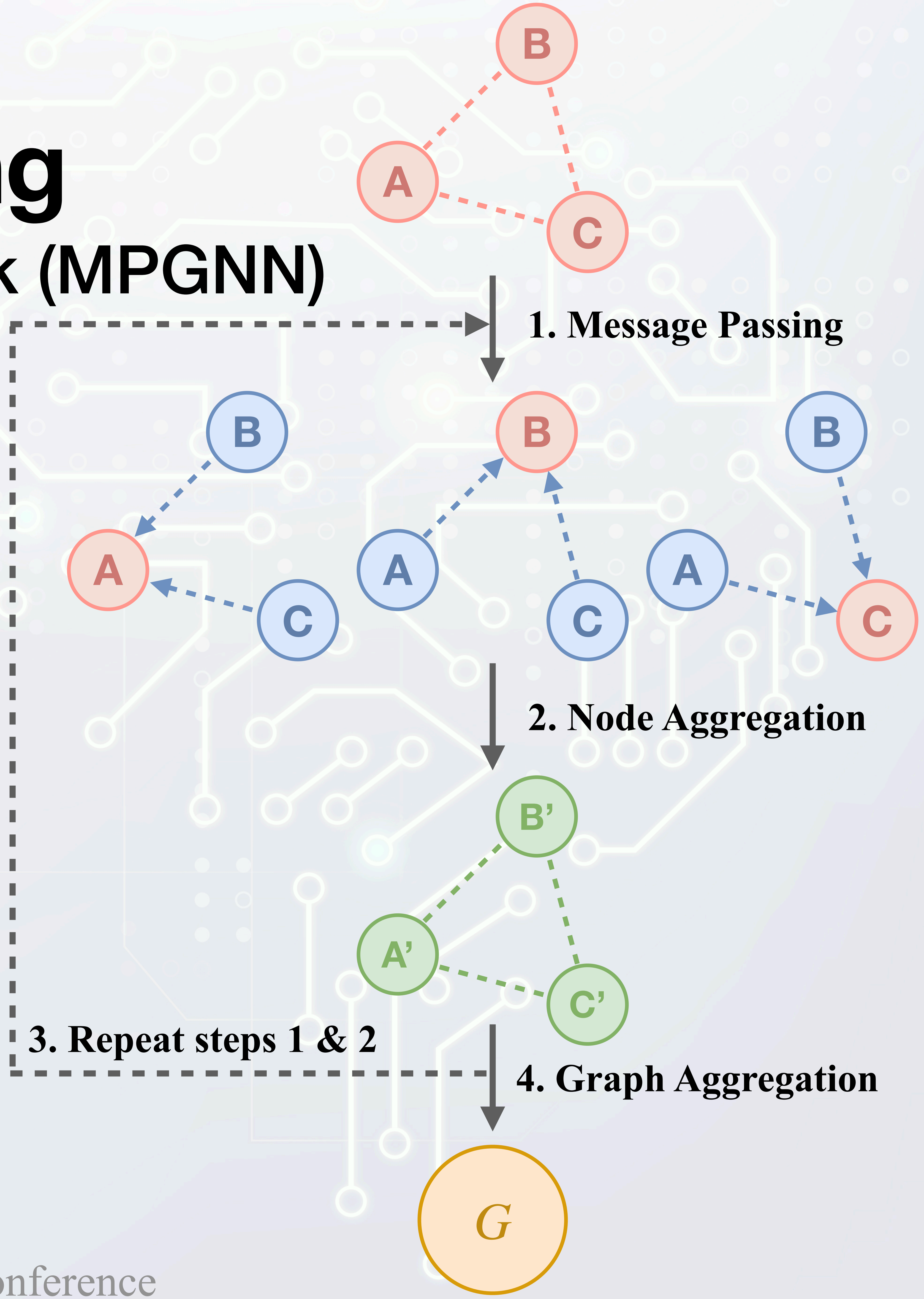
Message-Passing Graph Neural Network (MPGNN)

1. Message Passing: Compute the information for each particle pair through some parametrized transformation.

2. Node Aggregation: Aggregate the transformed information for each particle. Typically element-wise **summation** $\Longleftrightarrow$ **permutation-invariant**

3. Repeat step 1 & 2 for several times (optional).

4. Graph Aggregation: Aggregate the information of all particles.



Classical Machine Learning

Deep Sets Theorem and MPGNN

- Deep Sets Theorem (arXiv 1703.06114) : A function (model) f is permutation-invariant over a set X (particles) if and only if $f(X) = g\left(\sum_{\mathbf{x}_i \in X} h(\mathbf{x}_i)\right)$ for some suitable transformations g and h.

- The Message-Passing Graph Neural Network (MPGNN) obeys the Deep Sets Theorem, and is usually written as:

$$\mathbf{x}_i^{(k)} = \gamma^{(k)}\left(\mathbf{x}_i^{(k-1)}, \bigoplus_{j \in \mathcal{N}(i)} \phi^{(k)}\left(\mathbf{x}_i^{(k-1)}, \mathbf{x}_j^{(k-1)}, \mathbf{e}_{ij}\right)\right)$$

Aggregation function (MEAN, SUM, MAX, etc.)

Quantum Machine Learning

Variational Quantum Circuit

QCGNN

Quantum Complete Graph Neural Network

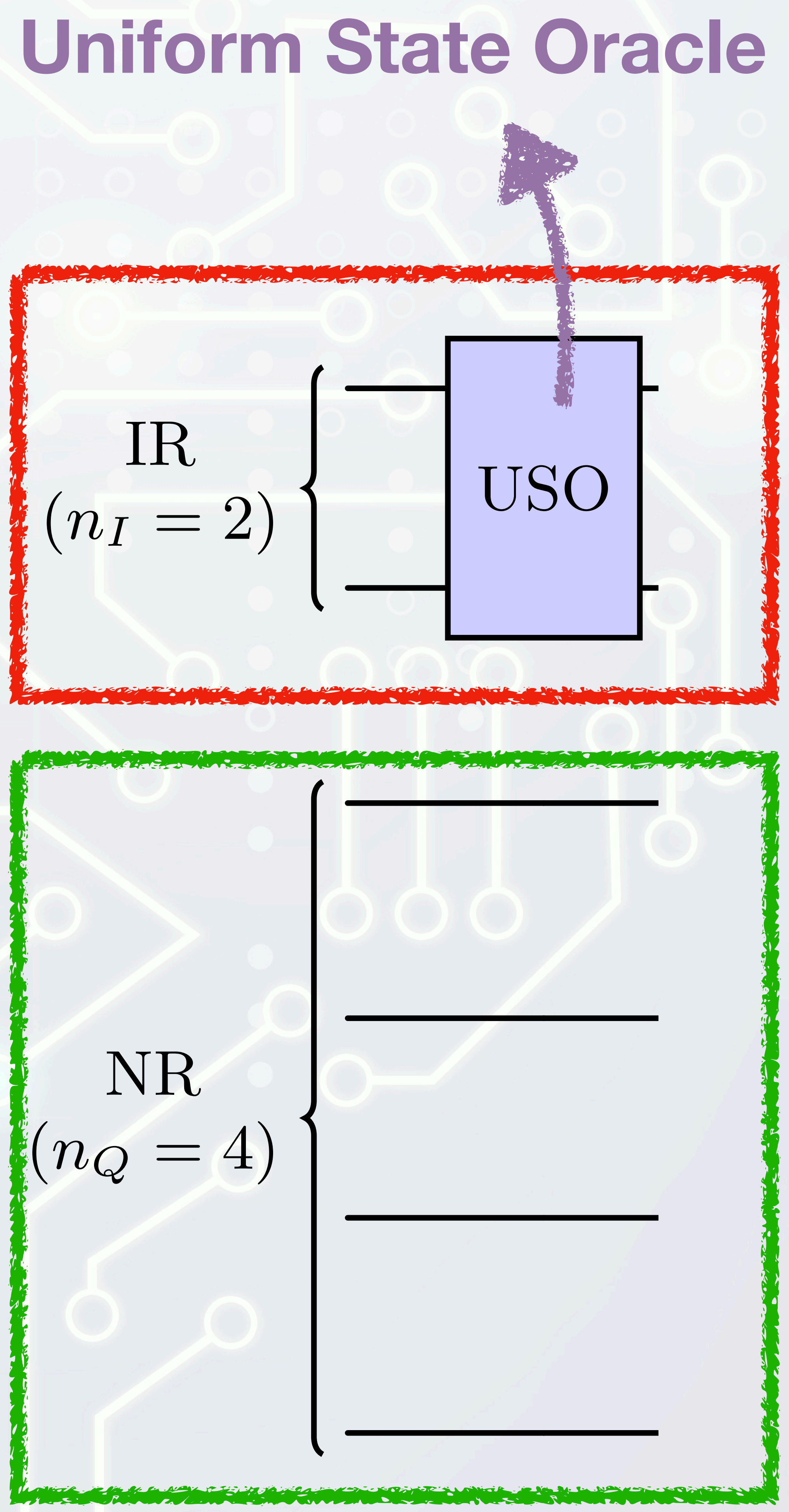
Suppose we have N particles with features $\{\mathbf{x}_i \mid 0 \le i \le N-1\}$. We prepare a quantum circuit with $n_I + n_Q$ qubits where

- $n_I = \lceil \log_2 N \rceil$ is the number of qubits in the **index register (*IR*)**
- n_Q is the number of qubits in the **network register (*NR*)**

The initial quantum state is initialized as

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle |0\rangle^{\otimes n_Q}$$

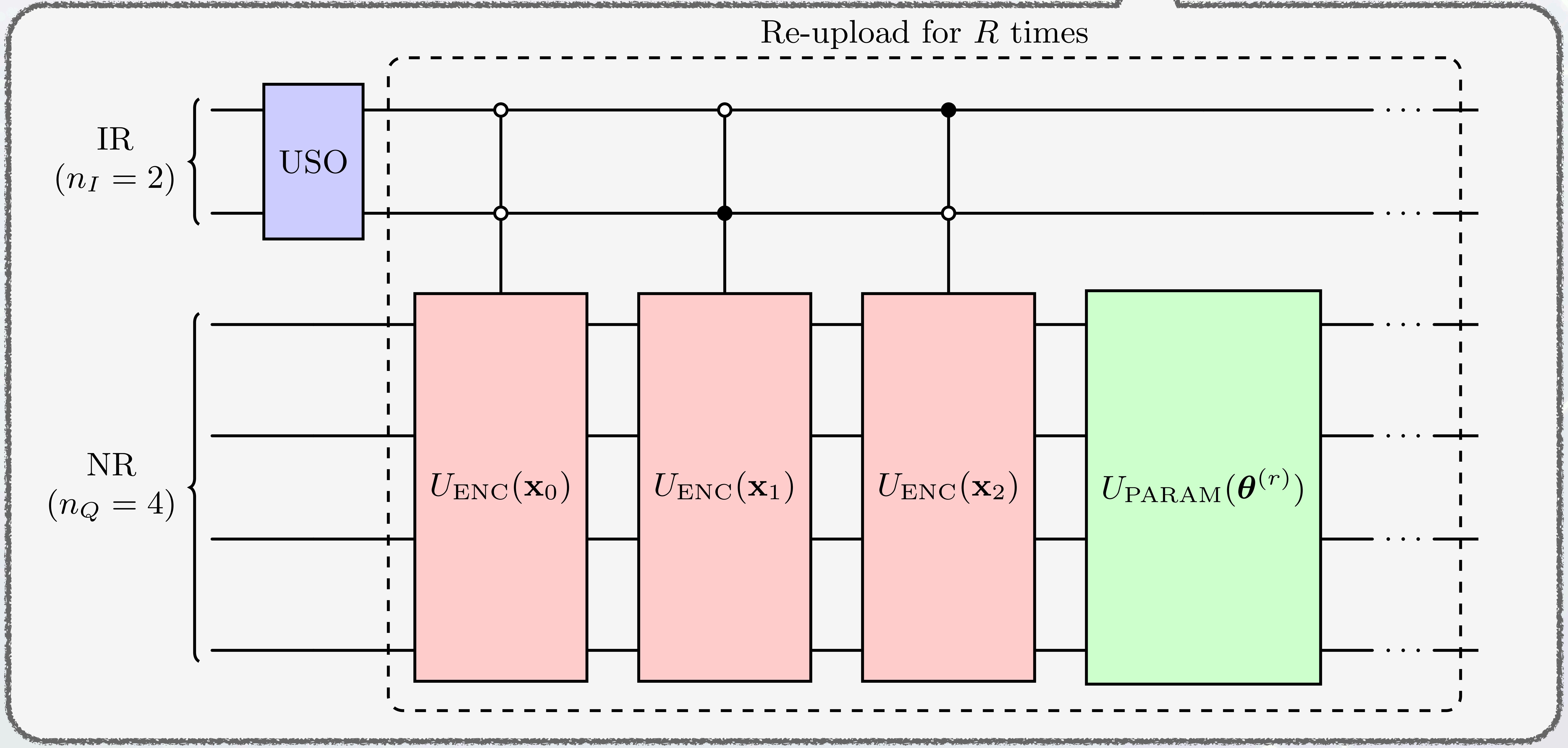
If $N = 2^{n_I}$, then we can simply use Hadamard gates. Otherwise, one should use some *Uniform State Oracle* (USO) to prepare the state.



QCGNN

Quantum Circuit

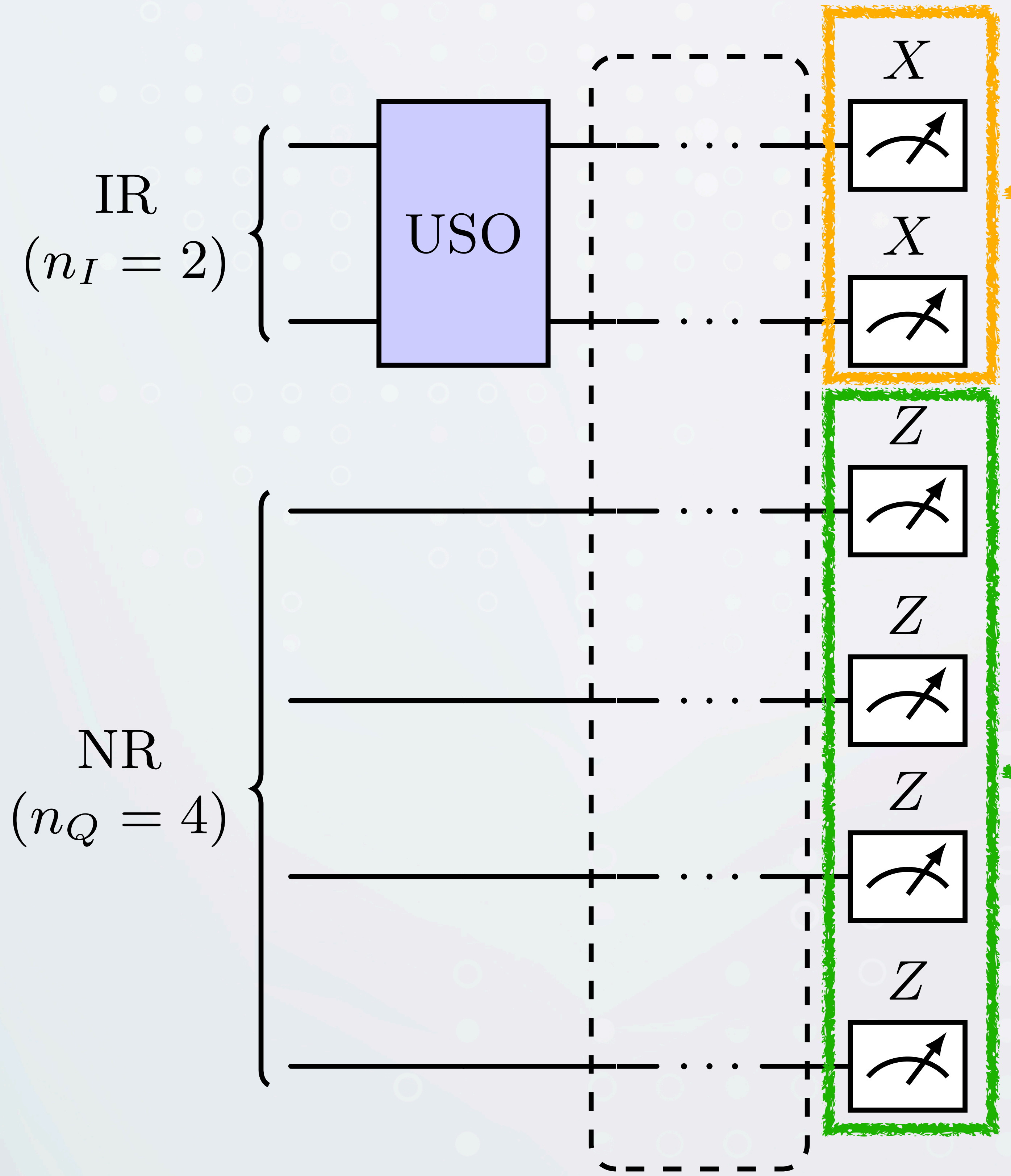
$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |\mathbf{x}_i, \theta\rangle$$



The QCGNN quantum circuit of a 3-particle jet, with $n_I = 2$ and $n_Q = 4$.

QCGNN

Measurement



The quantum state before measurement is $|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |\mathbf{x}_i, \theta\rangle$

Consider a Hermitian matrix J with dimension $2^{n_I} \times 2^{n_I}$ full of ones, i.e.,

$$J = \begin{bmatrix} 1 & \dots & 1 \\ \vdots & & \vdots \\ 1 & \dots & 1 \end{bmatrix} = (I + X)^{\otimes n_I}.$$

Denote the observables on NR as P, then

$$\langle \psi | J \otimes P | \psi \rangle = \frac{1}{N} \sum_{i<N} \sum_{j<N} \langle \mathbf{x}_i; \theta | P | \mathbf{x}_j; \theta \rangle$$

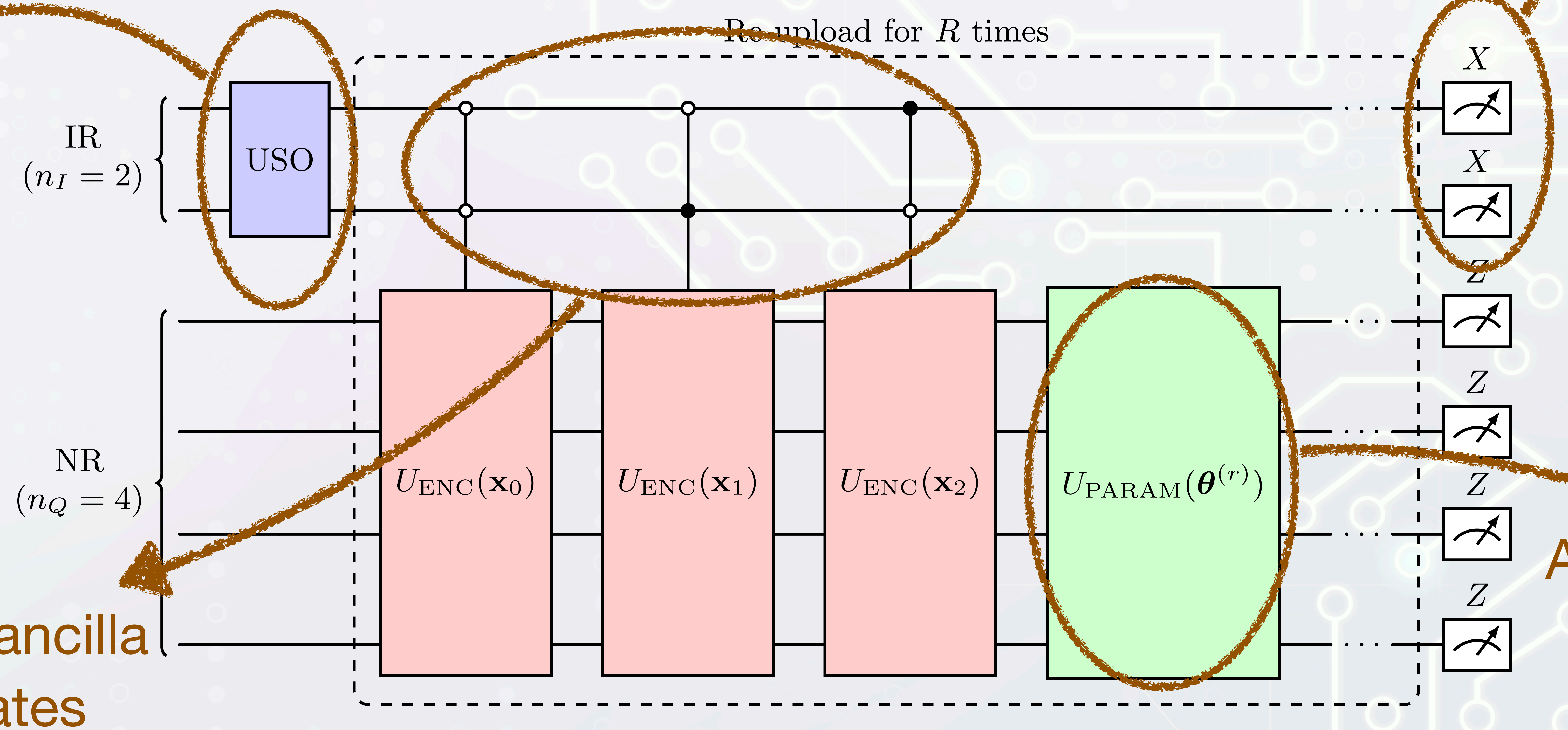
Similar to MPGNN, with automatic aggregation.

QCGNN

Gate and Computational Complexity

$O(\log_2 N)$ gates and circuit depth

$O(N)$ Pauli-string observables



Assuming Deep VQC

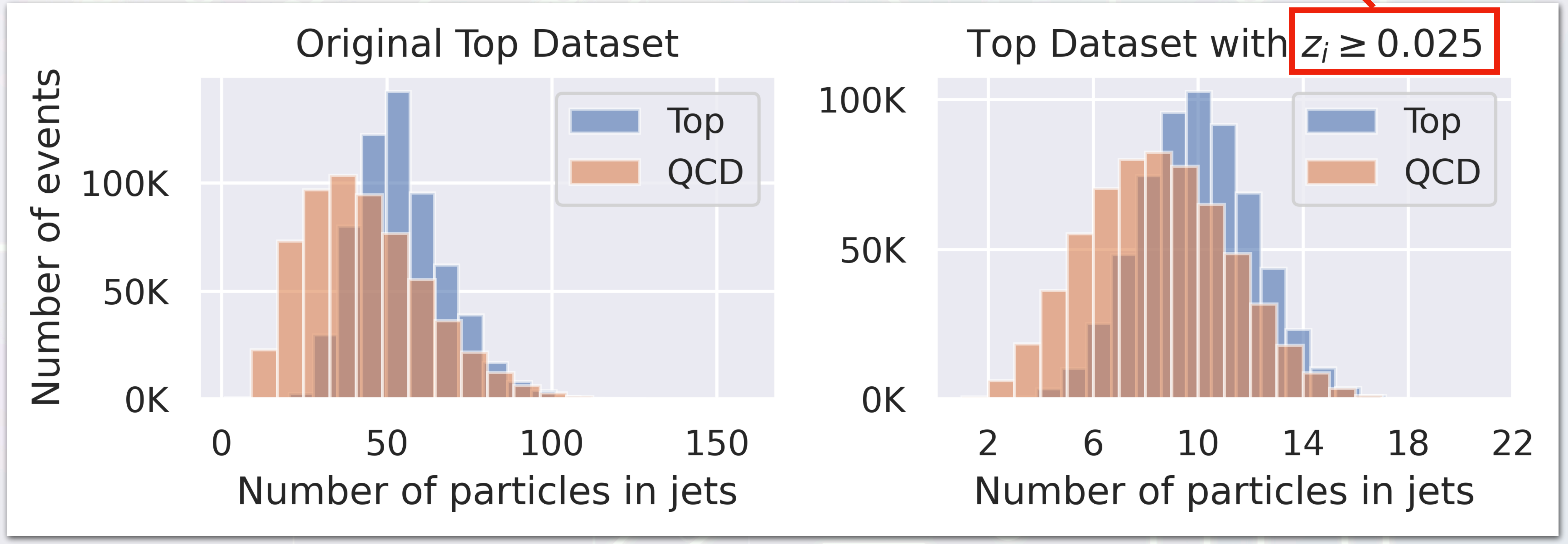
Additional $O(\log_2 N)$ ancilla qubits and Toffoli gates

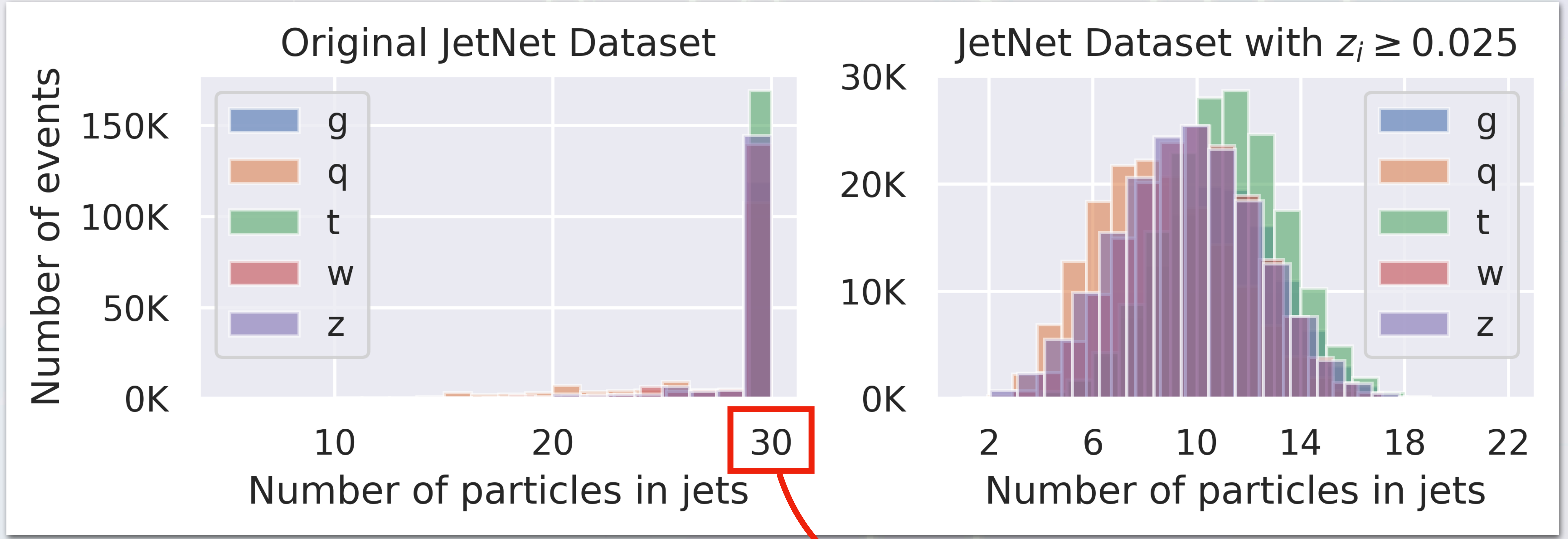
When N is large and the parametrized gates are deep comparing to encoding gates, **QCGNN only needs $O(N)$ computations**, while classical MPGNN requires $O(N^2)$ computations!

Jet Dataset

- **Top-Taggers (arXiv 1902.09914)**
  - Top v.s. Gluon / Light Quarks
  - Jet $p_T \in [550{,}650]GeV$
  - Pythia / Delphes (ATLAS)
  - FastJet with $R = 0.8$
- **JetNet (arXiv 2106.11535)**
  - Multi-class $\{g, q, t, W, Z\}$
  - Jet $p_T \sim 1TeV$
  - MadGraph / Pythia
  - FastJet with $R = 0.8$

$$z_i \equiv \frac{p_{T_i}}{p_{T_{jet}}}$$





Only the 30 highest p_T particles are provided

Training Results

AUC and Accuracy

- Each training process was conducted with 5 different random seeds and 30 epochs.
- Each class has 25K training samples, 2.5K validation samples, and 2.5K testing samples.
- The number of particles of jets lies between 4~16 $\Longrightarrow$ At most $n_I = 4$ qubits for IR is needed.
- The performance of the state-of-the-art classical models is also presented.

State-of-the-art classical models

Classical models for benchmarking

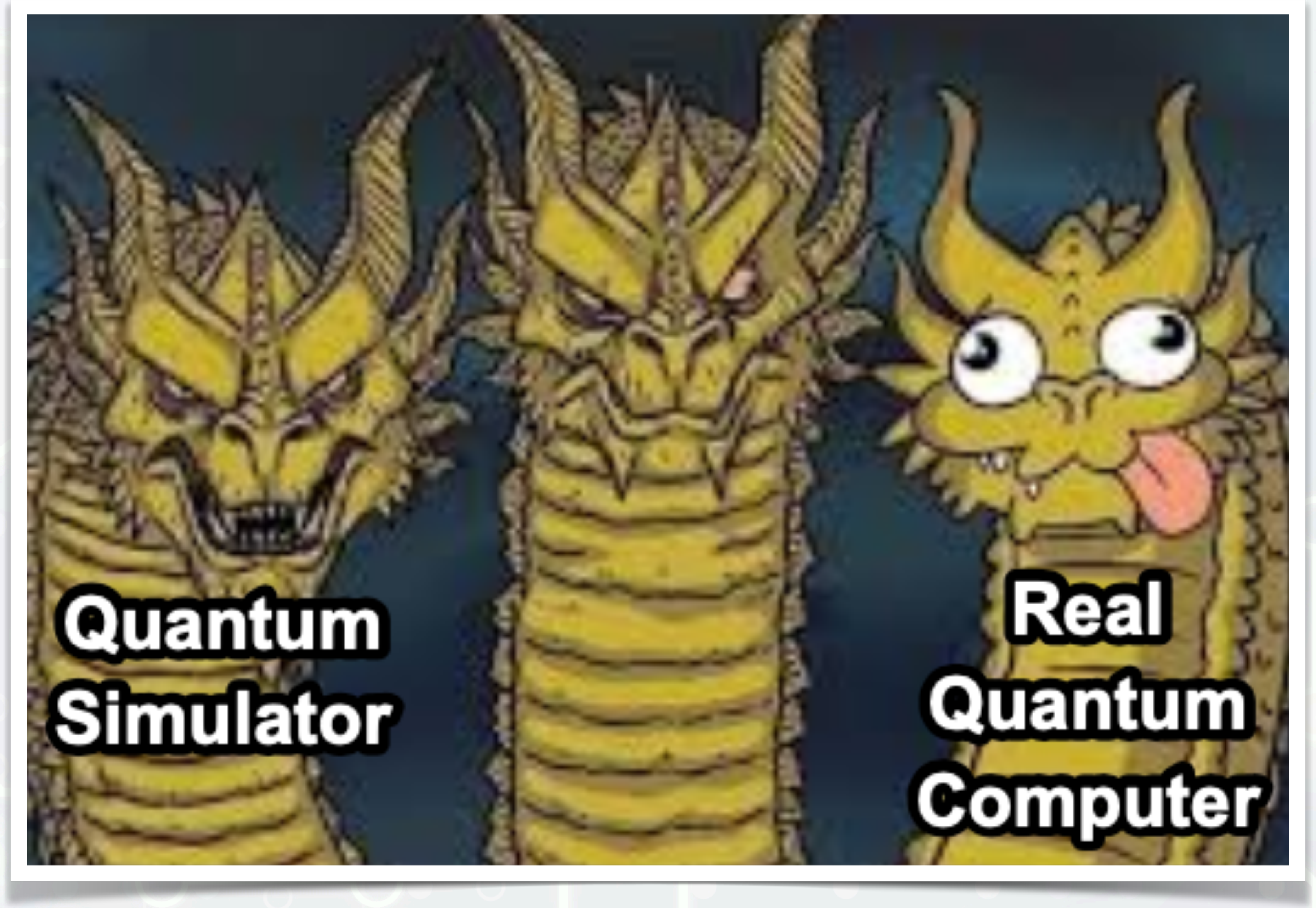
QCGNN with $n_Q = 3$ and $n_Q = 6$ (On simulators)

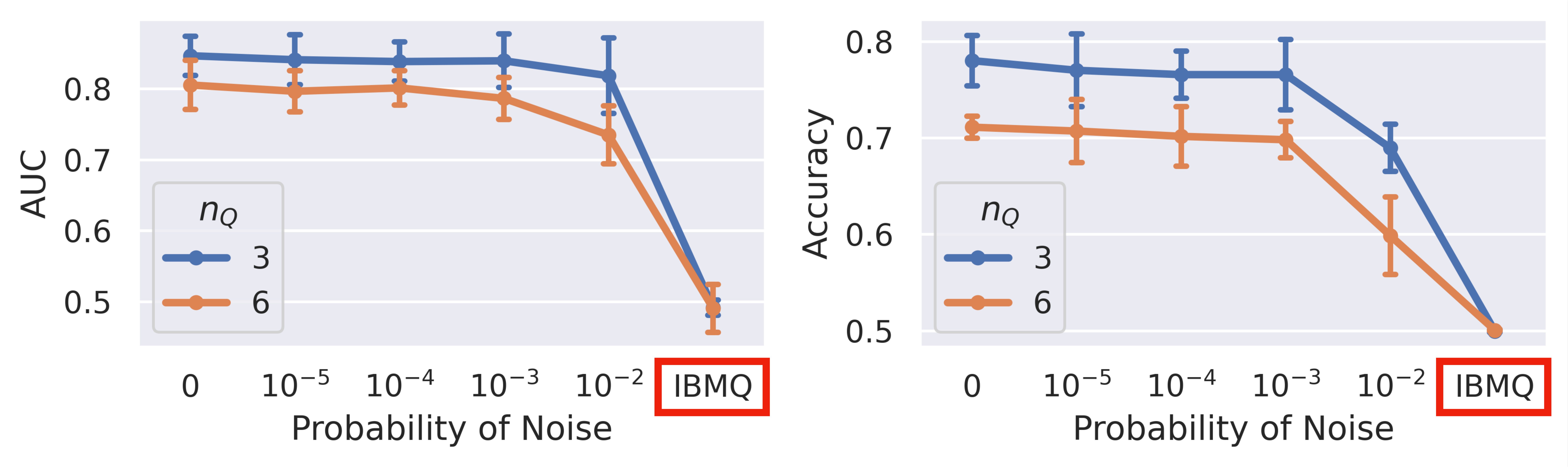
Model	Top Dataset (2 classes)			JetNet Dataset (5 classes)		
	# params	AUC	Accuracy	# params	AUC	Accuracy
Particle Transformer	2.2M	0.946±0.005	0.868±0.009	2.2M	0.889±0.002	0.656±0.006
Particle Net	177K	0.953±0.003	0.885±0.006	178K	0.896±0.003	0.669±0.004
Particle Flow Network	72.3K	0.954±0.004	0.885±0.005	72.7K	0.900±0.003	0.675±0.005
MPGNN - $n_M = 64$	13K	0.961±0.003	0.896±0.003	13.3K	0.903±0.002	0.683±0.007
MPGNN - $n_M = 6$	255	0.924±0.006	0.866±0.006	323	0.865±0.004	0.615±0.010
MPGNN - $n_M = 3$	126	0.922±0.005	0.864±0.006	194	0.757±0.110	0.475±0.141
QCGNN - $n_Q = 6$	201	0.932±0.004	0.868±0.005	269	0.822±0.003	0.543±0.006
QCGNN - $n_Q = 3$	99	0.919±0.006	0.864±0.005	167	0.796±0.009	0.505±0.014

IBMQ Results

Noise Extrapolation

- The training of QCGNN is done with simulators.
- The pre-trained QCGNN is tested on ***ibm_brussels***.





Summary

- In the task of jet discrimination, a set, or equivalently a complete graph serves as a natural representation. MPGNN provides a natural way to design permutation-invariant model.

- **Motivated by the MPGNN, we propose a VQC based model QCGNN. If the parametrized gates are deep enough, the cost of QCGNN only scales as $O(N)$, while classical MPGNN requires $O(N^2)$.**

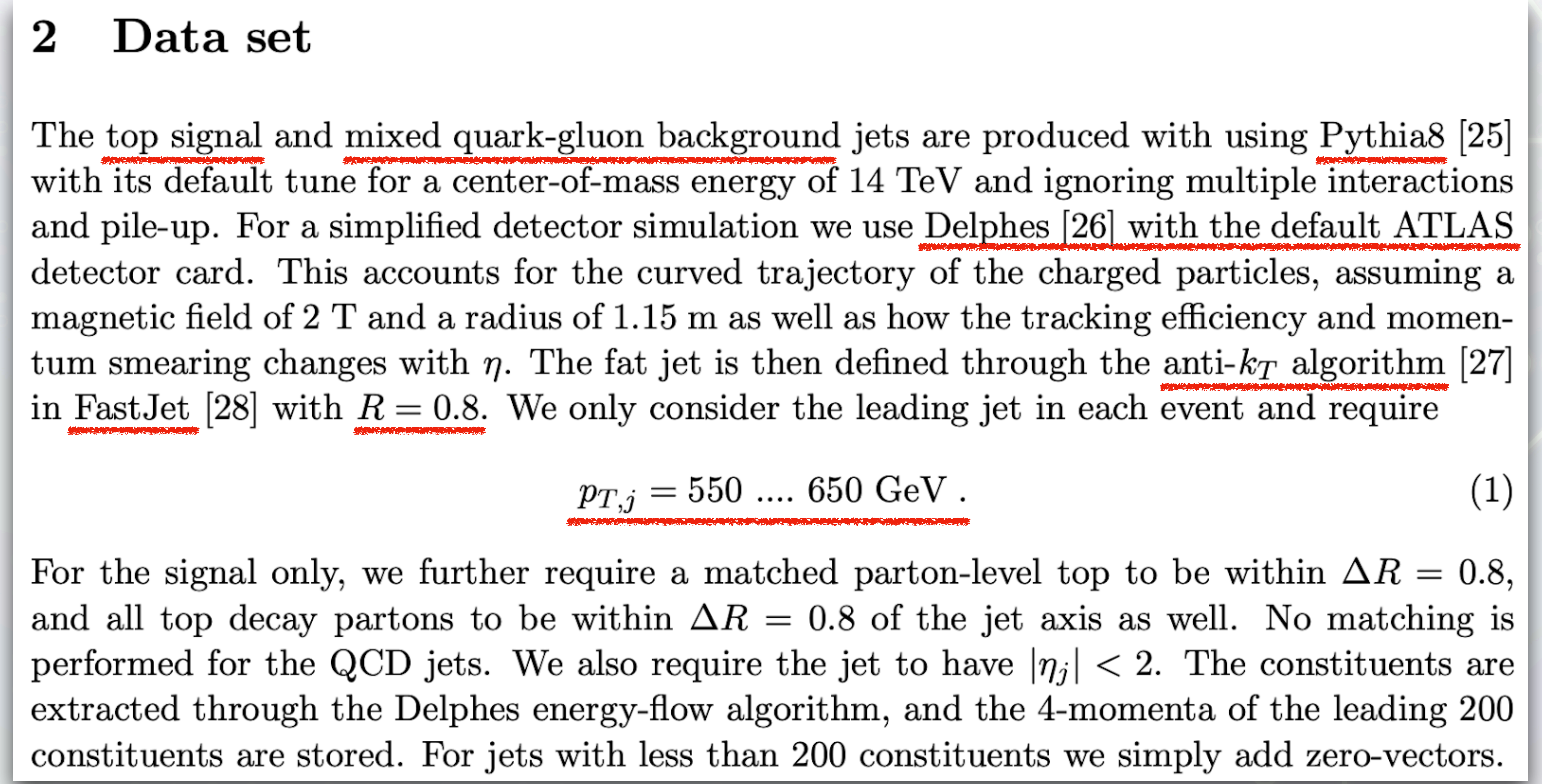
- QCGNN has also been tested on IBMQ real quantum devices. However, due to noise in the quantum circuits, information transmission was unsuccessful.

- As the quantum computers becoming more robust in the future, the potential for quantum advantage of the QCGNN can be studied.

Backup Slides

Dataset

Top Tagging (arXiv 1902.09914)


2 Data set

The top signal and mixed quark-gluon background jets are produced with using Pythia8 [25] with its default tune for a center-of-mass energy of 14 TeV and ignoring multiple interactions and pile-up. For a simplified detector simulation we use Delphes [26] with the default ATLAS detector card. This accounts for the curved trajectory of the charged particles, assuming a magnetic field of 2 T and a radius of 1.15 m as well as how the tracking efficiency and momentum smearing changes with η. The fat jet is then defined through the anti-k_T algorithm [27] in FastJet [28] with $R = 0.8$. We only consider the leading jet in each event and require

$$p_{T,j} = 550 \; .... \; 650 \text{ GeV} \; . \qquad (1)$$

For the signal only, we further require a matched parton-level top to be within $\Delta R = 0.8$, and all top decay partons to be within $\Delta R = 0.8$ of the jet axis as well. No matching is performed for the QCD jets. We also require the jet to have $|\eta_j| < 2$. The constituents are extracted through the Delphes energy-flow algorithm, and the 4-momenta of the leading 200 constituents are stored. For jets with less than 200 constituents we simply add zero-vectors.

Dataset

JetNet (arXiv 2106.11535)

B JetNet Generation

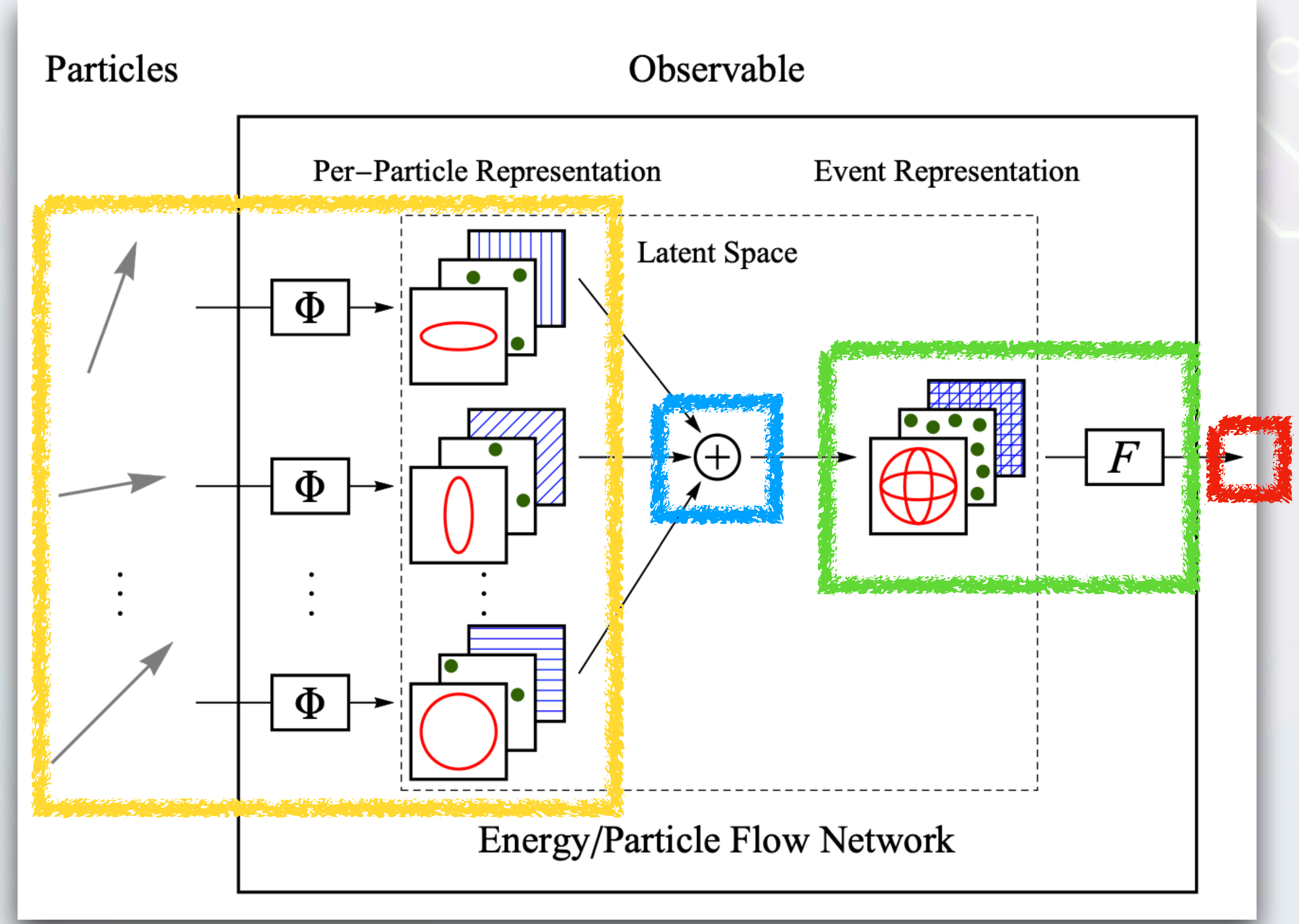
The so-called parton-level events are first produced at leading-order using MADGRAPH5_aMCATNLO 2.3.1 [51] with the NNPDF 2.3LO1 parton distribution functions [52]. To focus on a relatively narrow kinematic range, the transverse momenta of the partons and undecayed gauge bosons are generated in a window with energy spread given by $\Delta p_{\mathrm{T}}/p_{\mathrm{T}} = 0.01$, centered at 1 TeV. These parton-level events are then decayed and showered in PYTHIA 8.212 [5] with the Monash 2013 tune [53], including the contribution from the underlying event. For each original particle type, 200,000 events are generated. Jets are clustered using the anti-k_{T} algorithm [54], with a distance parameter of $R = 0.8$ using the FASTJET 3.1.3 and FASTJET CONTRIB 1.027 packages [55, 56]. Even though the parton-level p_{T} distribution is narrow, the jet p_{T} spectrum is significantly broadened by kinematic recoil from the parton shower and energy migration in and out of the jet cone. We apply a restriction on the measured jet p_{T} to remove extreme events outside of a window of $0.8\,\mathrm{TeV} < p_{\mathrm{T}} < 1.6\,\mathrm{TeV}$ for the $p_{\mathrm{T}} = 1\,\mathrm{TeV}$ bin. This generation is a significantly simplified version of the official simulation and reconstruction steps used for real detectors at the LHC, so as to remain experiment-independent and allow public access to the dataset.

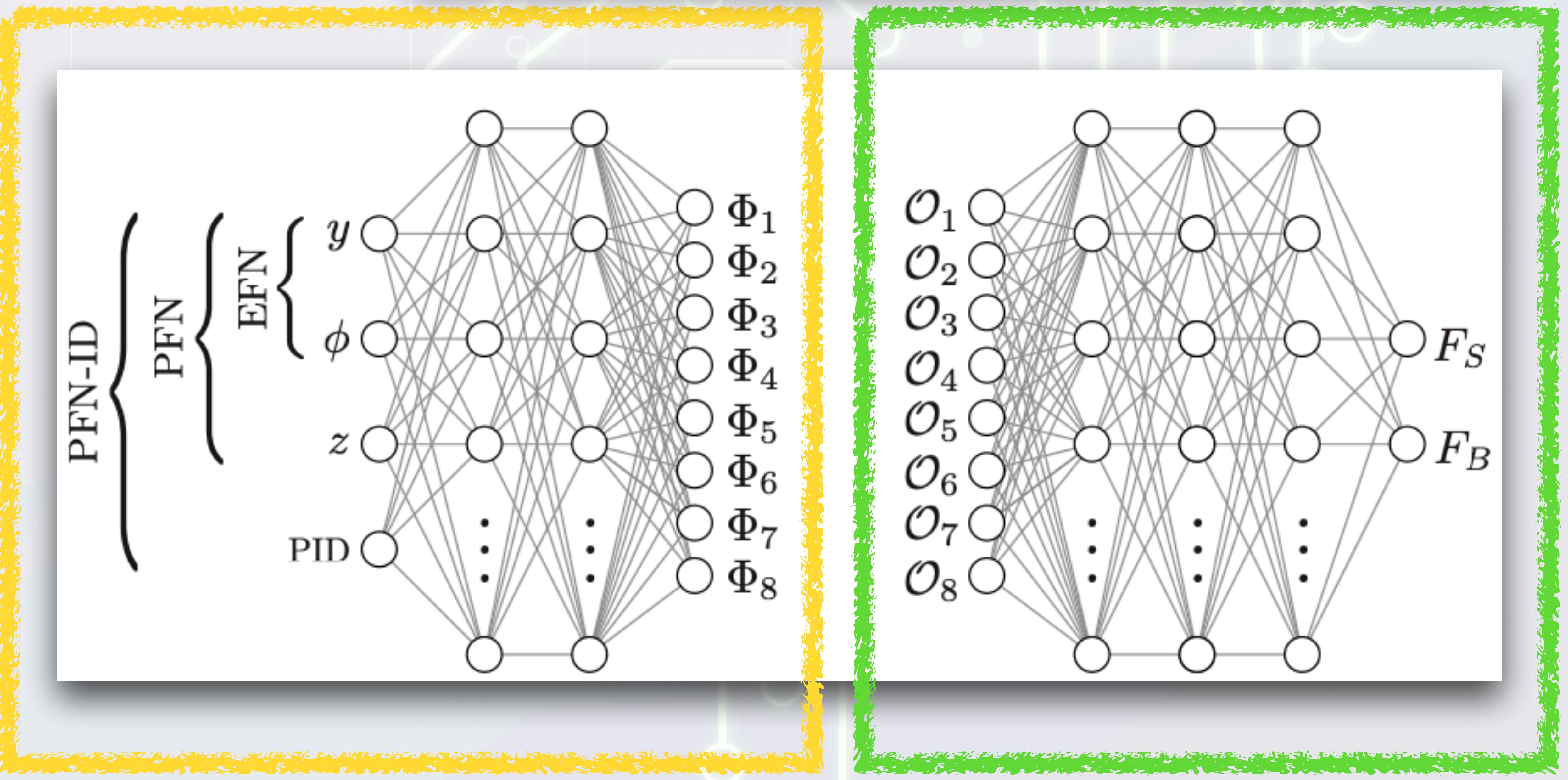
Particle Flow Network

arXiv 1810.05165

Motivated by the *Deep Set Theorem*

$$\mathcal{O}(\{p_1,\ldots,p_M\}) = F\left(\sum_{i=1}^{M}\Phi(p_i)\right)$$





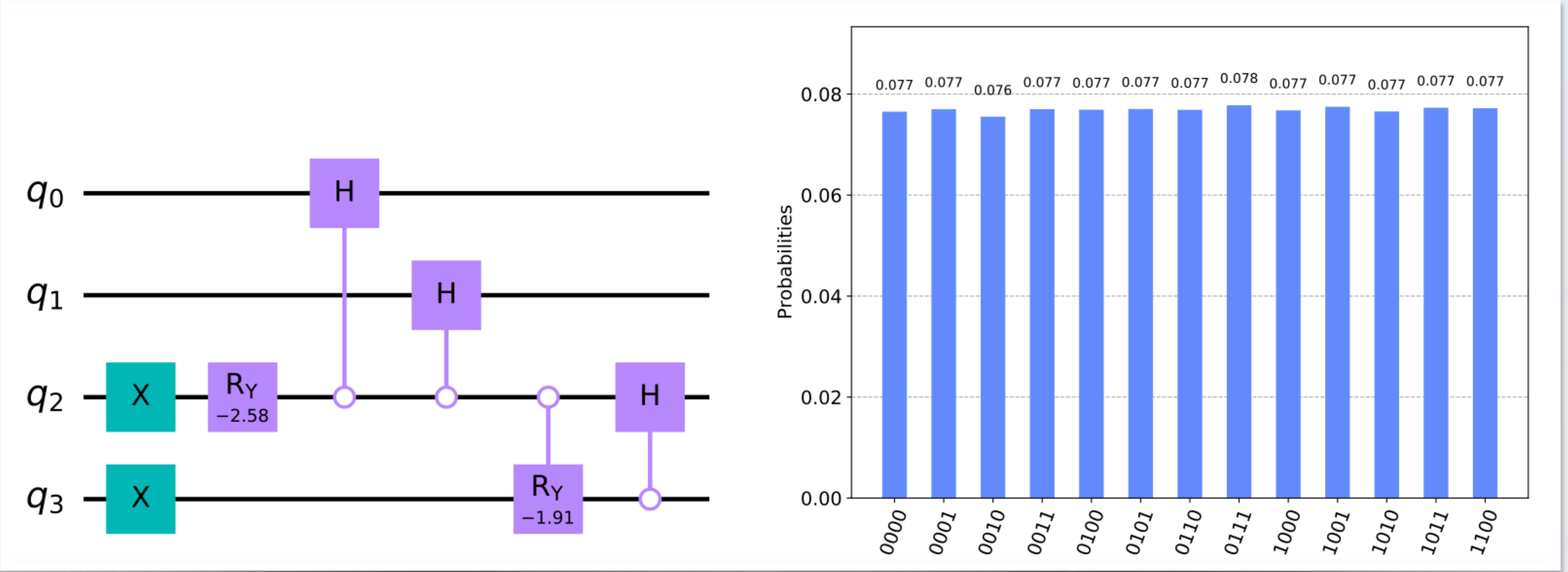
Uniform State Oracle

arXiv 2306.11747

In this paper, we propose an efficient approach for quantum state preparation of uniform superposition state $|\Psi\rangle = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} |j\rangle$ that offers a significant (exponential) reduction in gate complexity and circuit depth without the use of ancillary qubits. We show that using only $n = \lceil \log_2 M \rceil$ qubits, the uniform superposition state $|\Psi\rangle$ can be prepared for arbitrary M with a gate complexity and circuit depth of $O(\log_2 M)$.

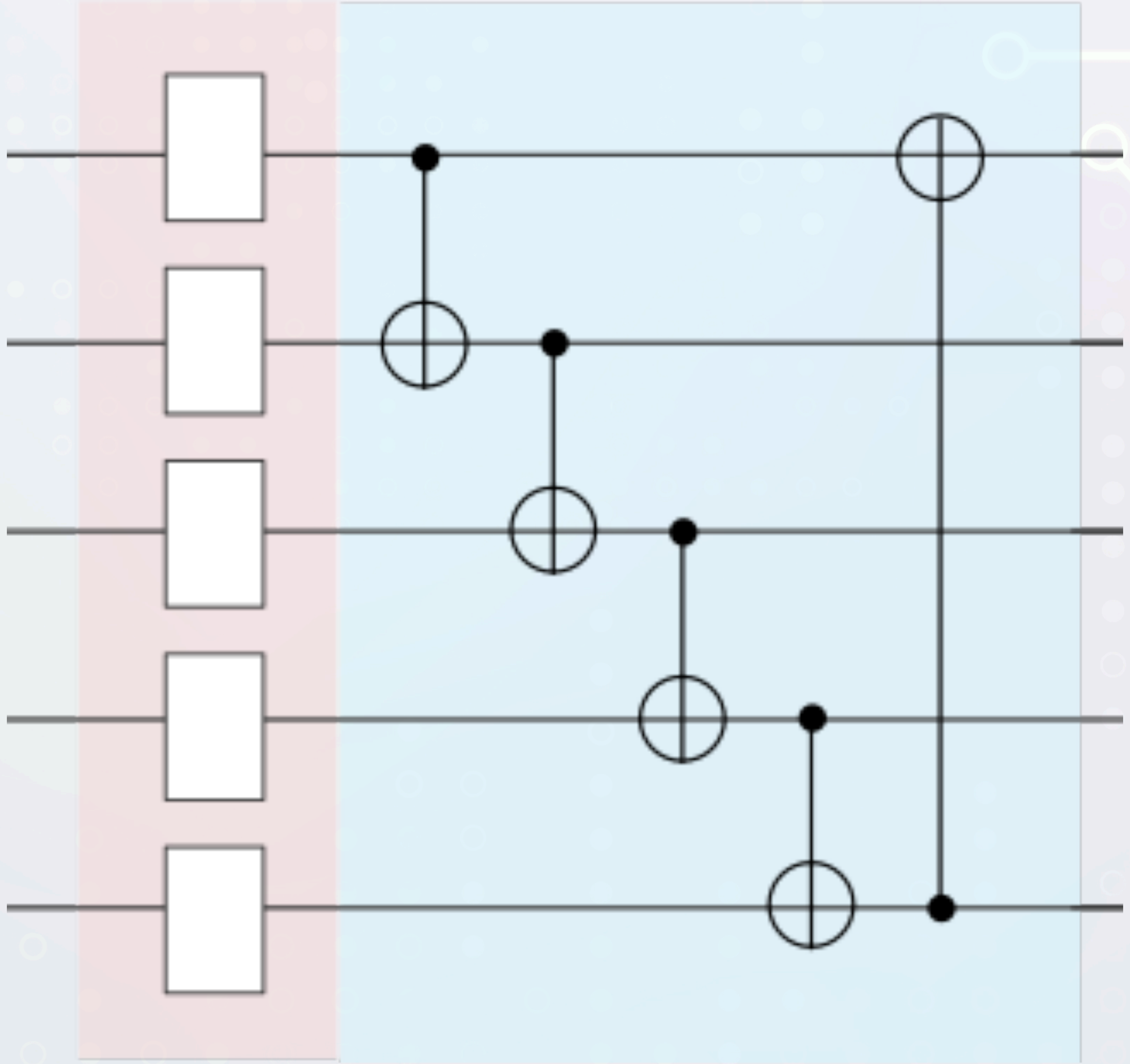
Quantum circuit for generating a 13-basis uniform state:

$$|\psi\rangle = \frac{1}{\sqrt{13}} \sum_{i=0}^{12} |i\rangle$$

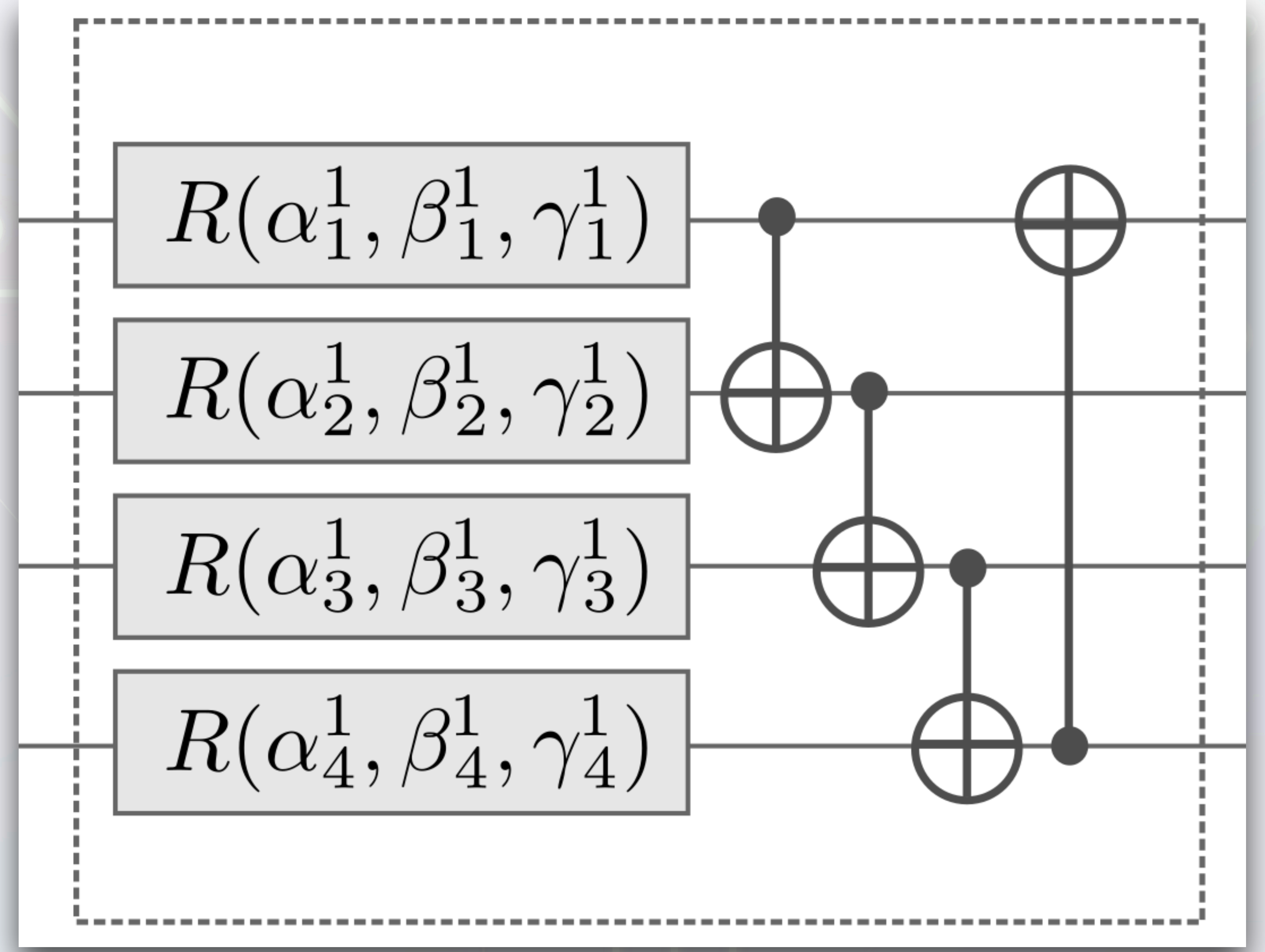


VQC Ansatz

PennyLane

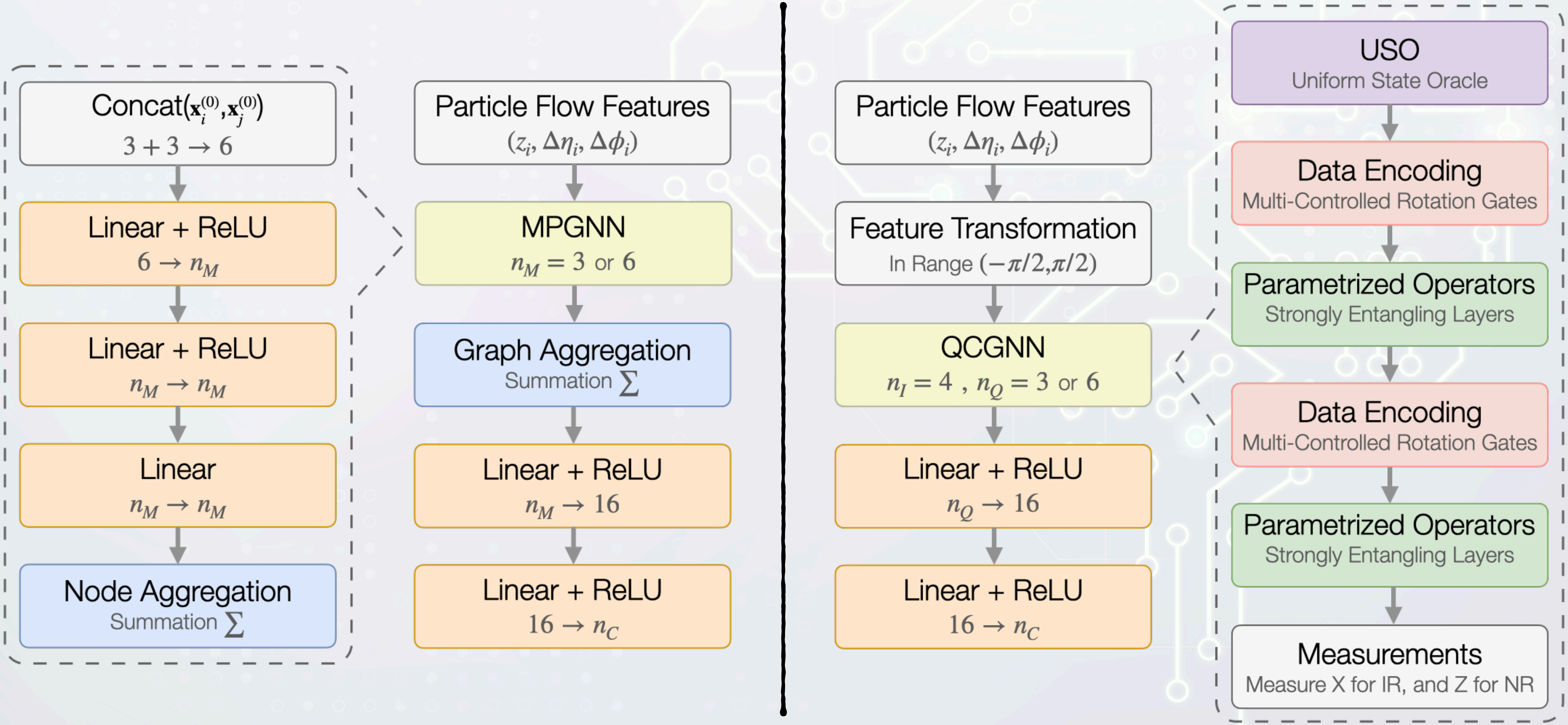


qml.BasicEntanglerLayers



qml.StronglyEntanglingLayers

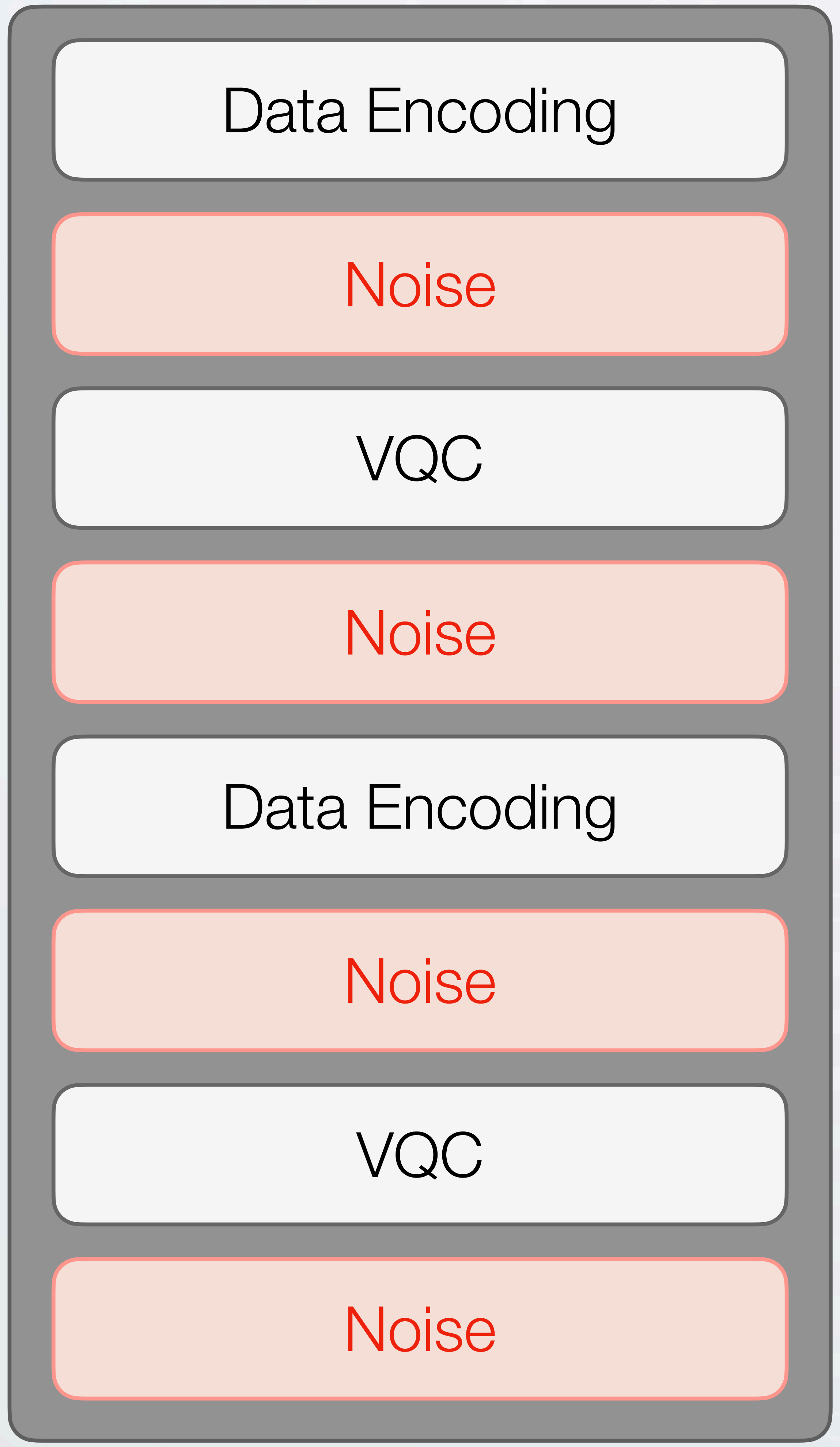
Model Setup



Concat($\mathbf{x}_i^{(0)}$,$\mathbf{x}_j^{(0)}$)
$3+3 \to 6$
Linear + ReLU
$6 \to n_M$
Linear + ReLU
$n_M \to n_M$
Linear
$n_M \to n_M$
Node Aggregation
Summation $\sum$
Particle Flow Features
$(z_i, \Delta\eta_i, \Delta\phi_i)$
MPGNN
$n_M = 3$ or 6
Graph Aggregation
Summation $\sum$
Linear + ReLU
$n_M \to 16$
Linear + ReLU
$16 \to n_C$
Particle Flow Features
$(z_i, \Delta\eta_i, \Delta\phi_i)$
Feature Transformation
In Range $(-\pi/2, \pi/2)$
QCGNN
$n_I = 4$, $n_Q = 3$ or 6
Linear + ReLU
$n_Q \to 16$
Linear + ReLU
$16 \to n_C$
USO
Uniform State Oracle
Data Encoding
Multi-Controlled Rotation Gates
Parametrized Operators
Strongly Entangling Layers
Data Encoding
Multi-Controlled Rotation Gates
Parametrized Operators
Strongly Entangling Layers
Measurements
Measure X for IR, and Z for NR

Noise

Simulated with PennyLane



qml.DepolarizingChannel

$$K_0 = \sqrt{1-p}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

$$K_1 = \sqrt{p/3}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$$

$$K_2 = \sqrt{p/3}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$$

$$K_3 = \sqrt{p/3}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

qml.GeneralizedAmplitudeDamping

$$K_0 = \sqrt{p}\begin{bmatrix}1 & 0\\ 0 & \sqrt{1-\gamma}\end{bmatrix}$$

$$K_1 = \sqrt{p}\begin{bmatrix}0 & \sqrt{\gamma}\\ 0 & 0\end{bmatrix}$$

$$K_2 = \sqrt{1-p}\begin{bmatrix}\sqrt{1-\gamma} & 0\\ 0 & 1\end{bmatrix}$$

$$K_3 = \sqrt{1-p}\begin{bmatrix}0 & 0\\ \sqrt{\gamma} & 0\end{bmatrix}$$

IBMQ Results

Runtime of Quantum Gates

- The gate runtime experiment is conducted with two different IBMQ backends for 10 times.
- T_{ENC} and T_{PARAM} are the time for encoding and parametrized gates respectively.

IBMQ Backend	N	T_{ENC}	T_{PARAM}
ibm_nazca	2	2.567	0.209
	4	5.352	0.197
	8	10.551	0.219
ibm_strasbourg	2	2.595	0.217
	4	5.416	0.197
	8	11.085	0.211

Scales as $O(N)$

Constant time $O(1)$

Parameter Shift Rule

arXiv 1905.13311

Gradients of parameterized quantum gates using the parameter-shift rule and gate decomposition

Gavin E. Crooks*
California Institute of Technology, Pasadena, CA 91125, USA and
Berkeley Institute for Theoretical Sciences, Berkeley, CA 94706, USA

- Consider a VQC output $f(\theta) = \langle\psi|\, U_G^\dagger(\theta) A U_G(\theta)\, |\psi\rangle$, where A is some Hermitian operator of observable and $U_G(\theta) = e^{-ia\theta G}$ with some Hermitian operator G.

- If G has two unique eigenvalues e_0 and e_1, the gradient can be calculated by

$$\frac{d}{dx} f(x) = r\left[f(\theta + \frac{\pi}{4r}) - f(\theta - \frac{\pi}{4r})\right] \qquad \text{with} \qquad r = \frac{a}{2}(e_1 - e_0)$$

Barren Plateau

arXiv 2309.09342

$$\mathrm{Var}_{\boldsymbol{\theta}}[\ell_{\boldsymbol{\theta}}(\rho, O)] = \frac{\mathcal{P}_{\mathfrak{g}}(\rho)\mathcal{P}_{\mathfrak{g}}(O)}{\dim(\mathfrak{g})}$$