# Jet discrimination with a quantum complete graph neural network

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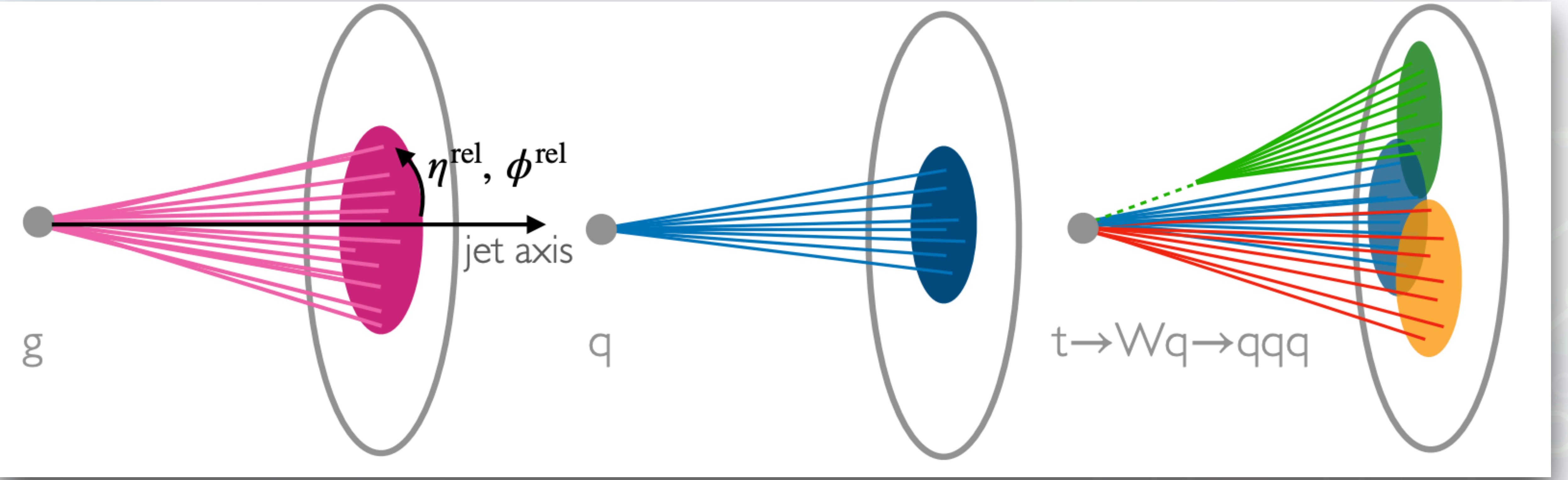
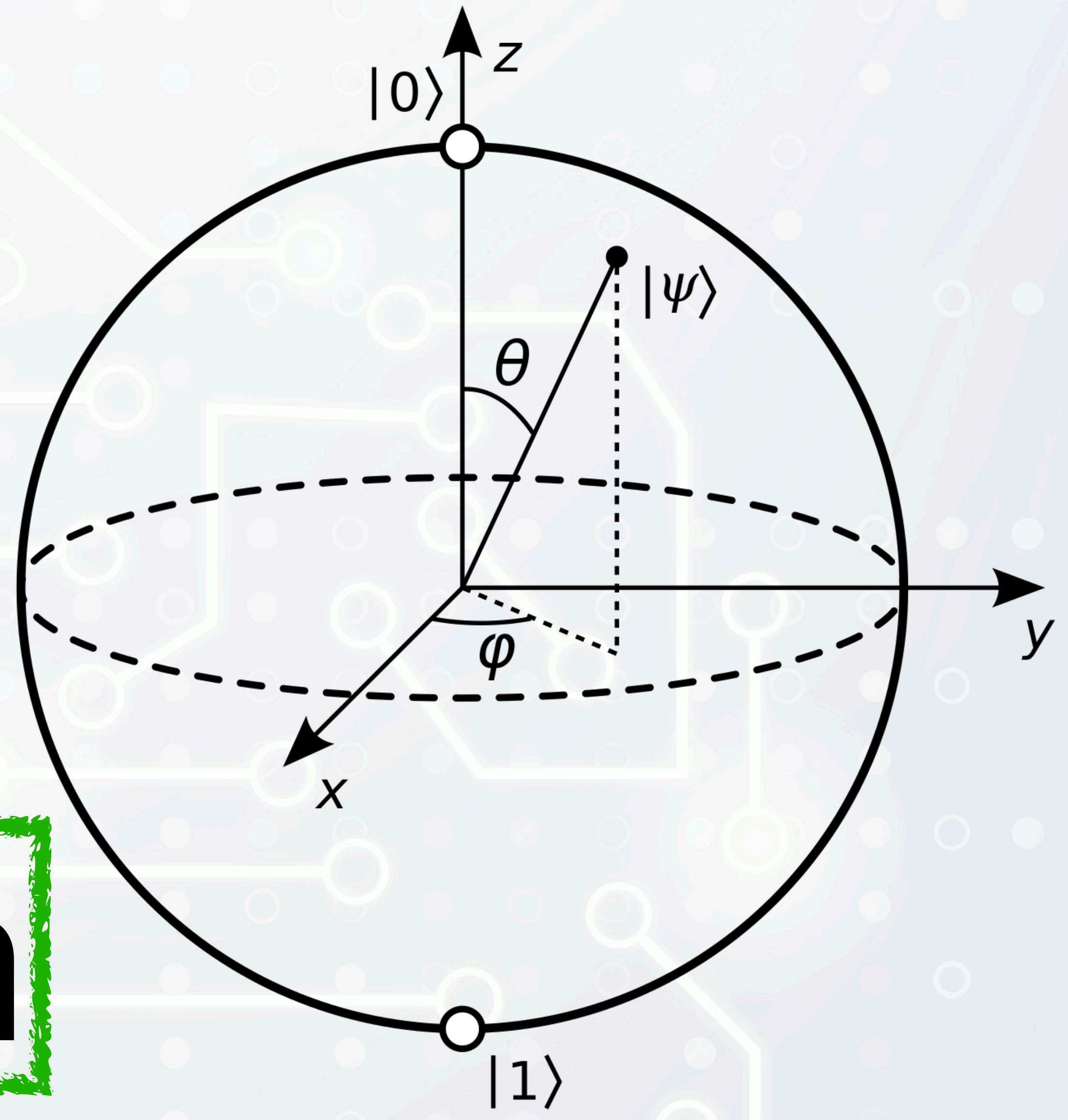
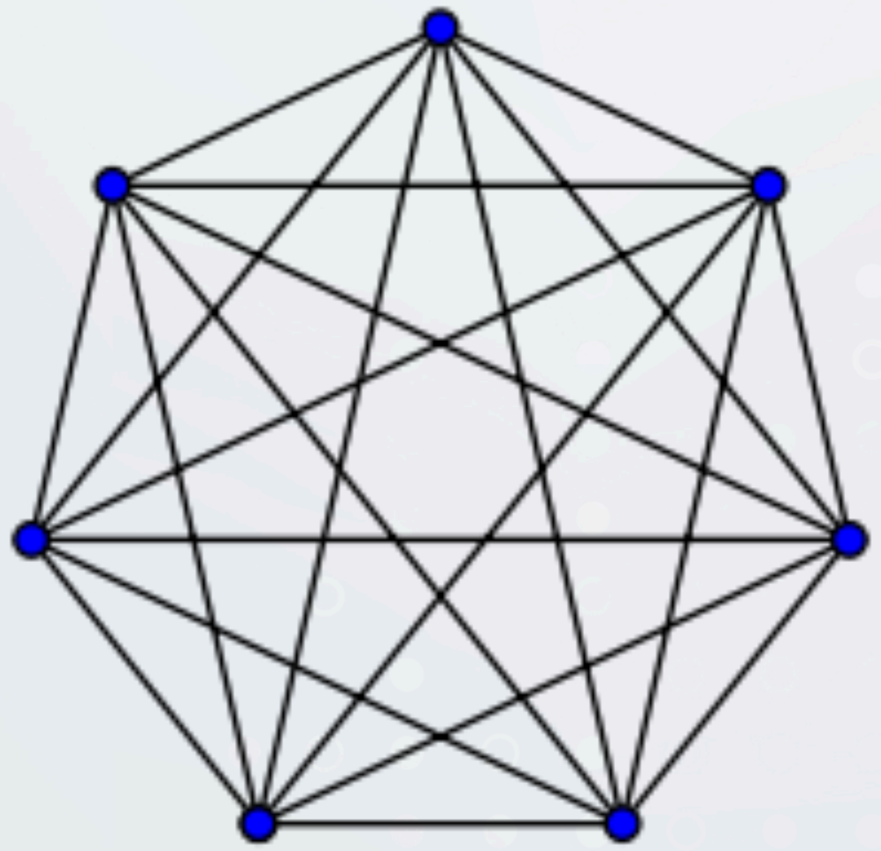



Jets, adapted from (arxiv 2106.11535)

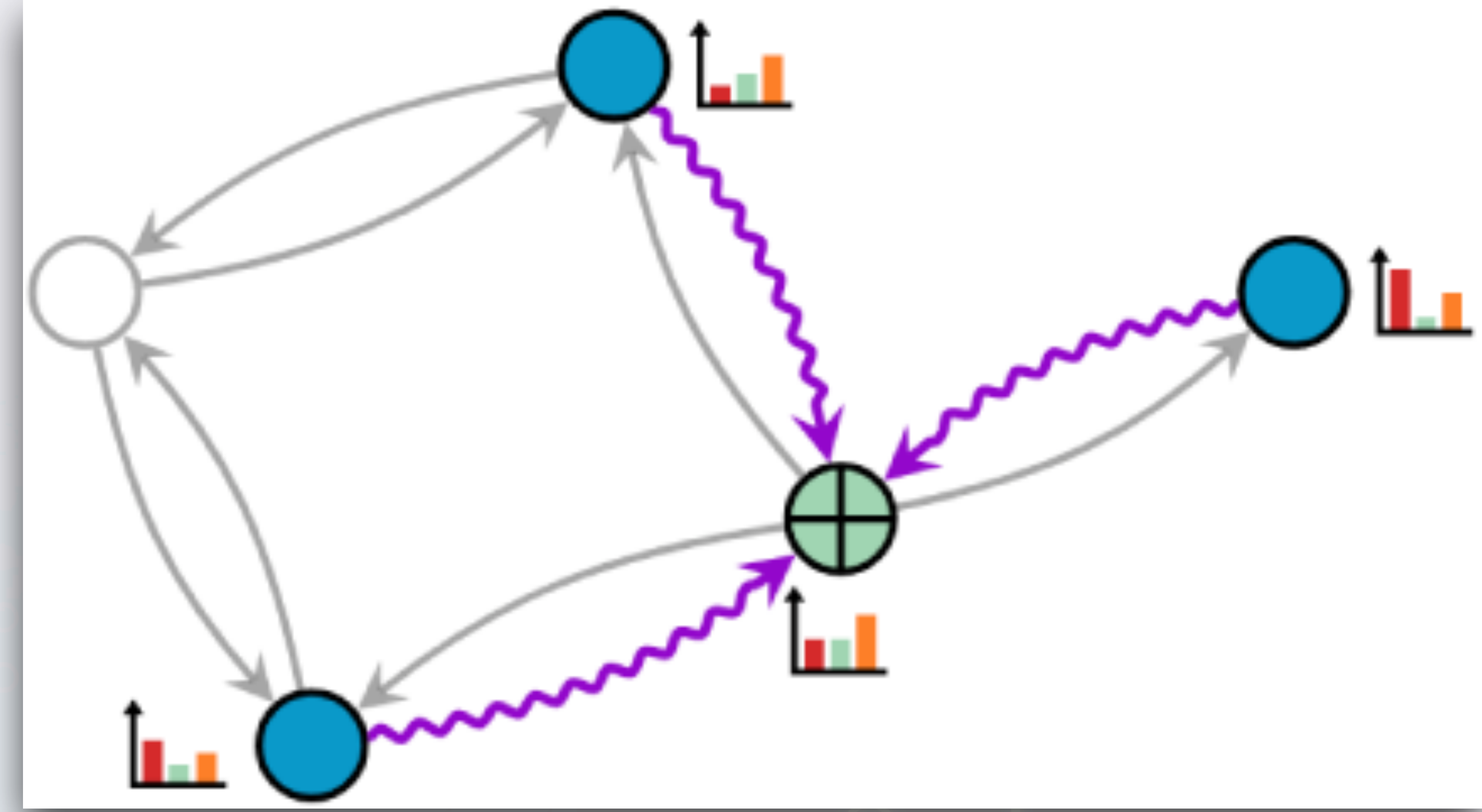



Bloch Sphere
(Adapted from Wikipedia)

# Jet discrimination with a quantum complete graph neural network



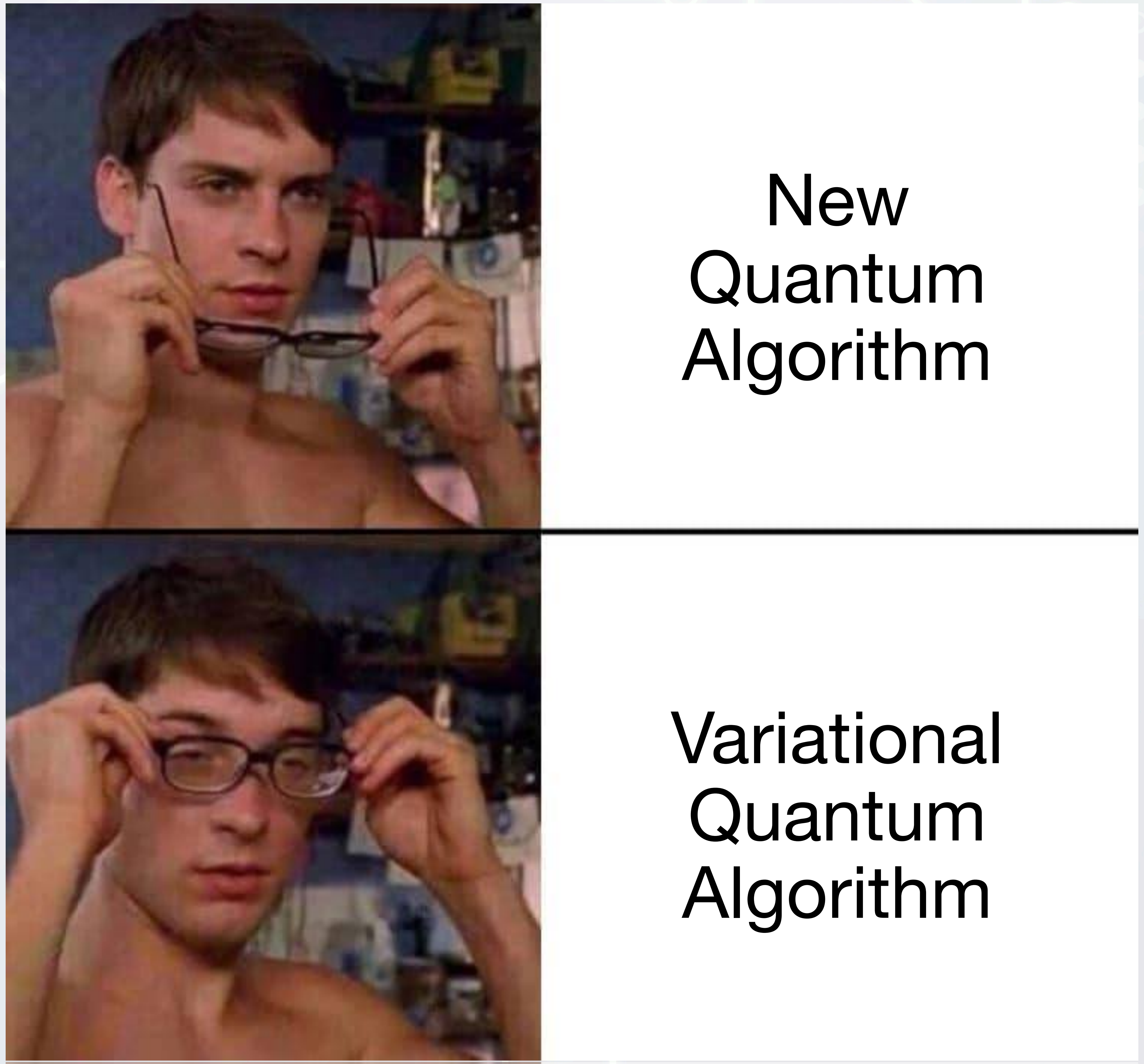
Complete Graph
(Adapted from Wikipedia)



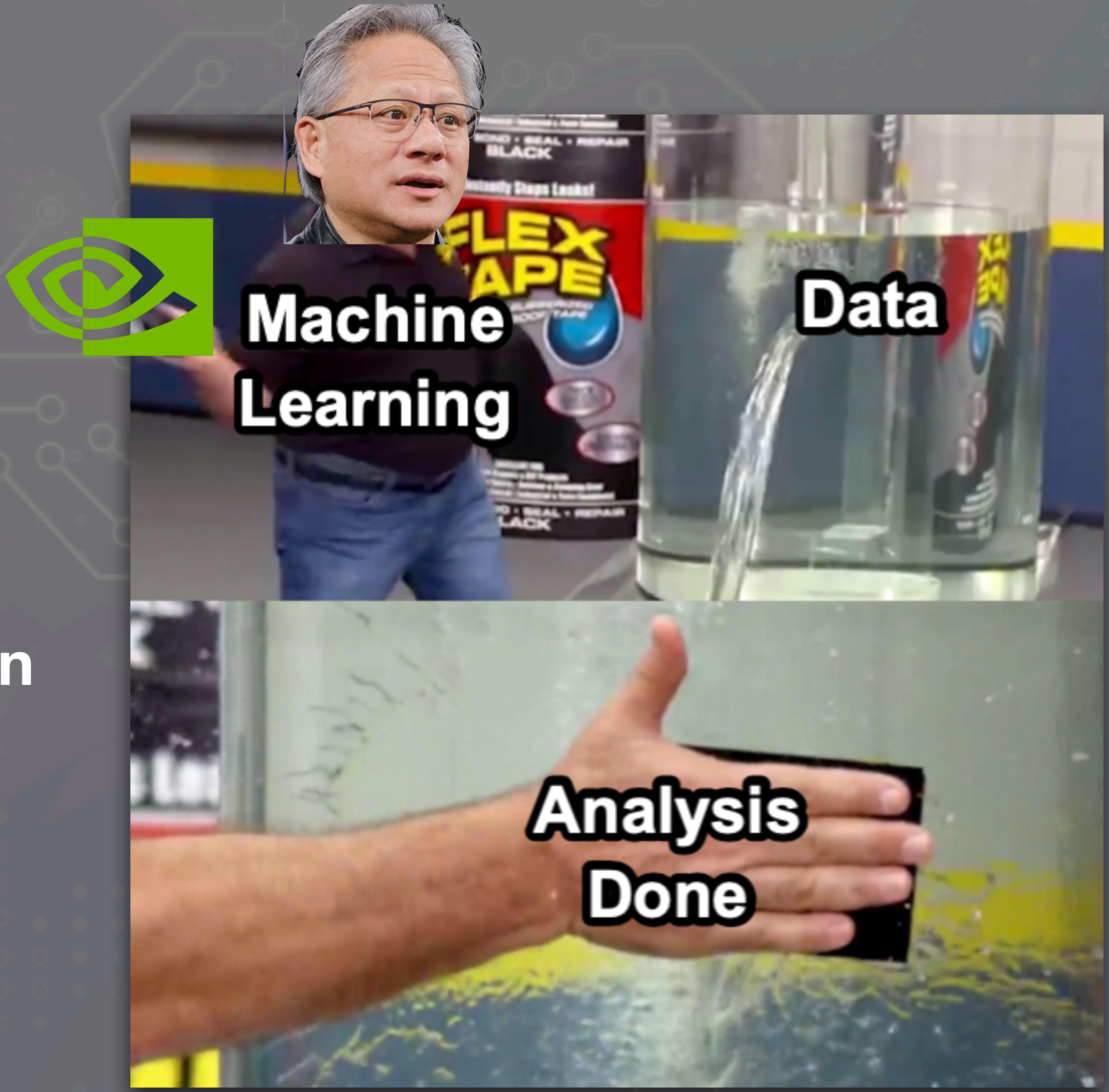
GNN (adapted from PyTorch-Geometric)

# Outline

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



# Classical
# Neural Networks
## Models for Jet Discrimination



# Jet Dataset

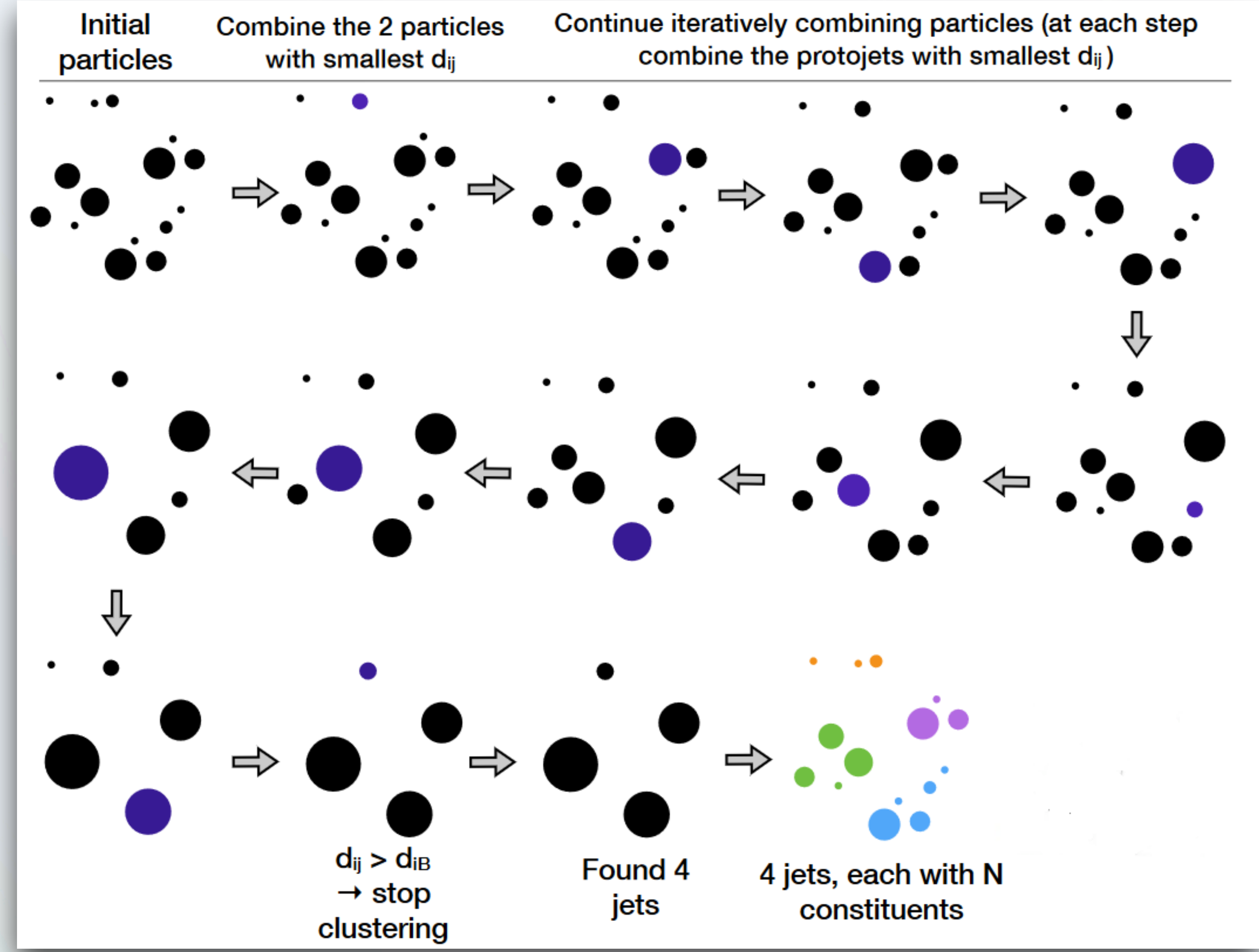
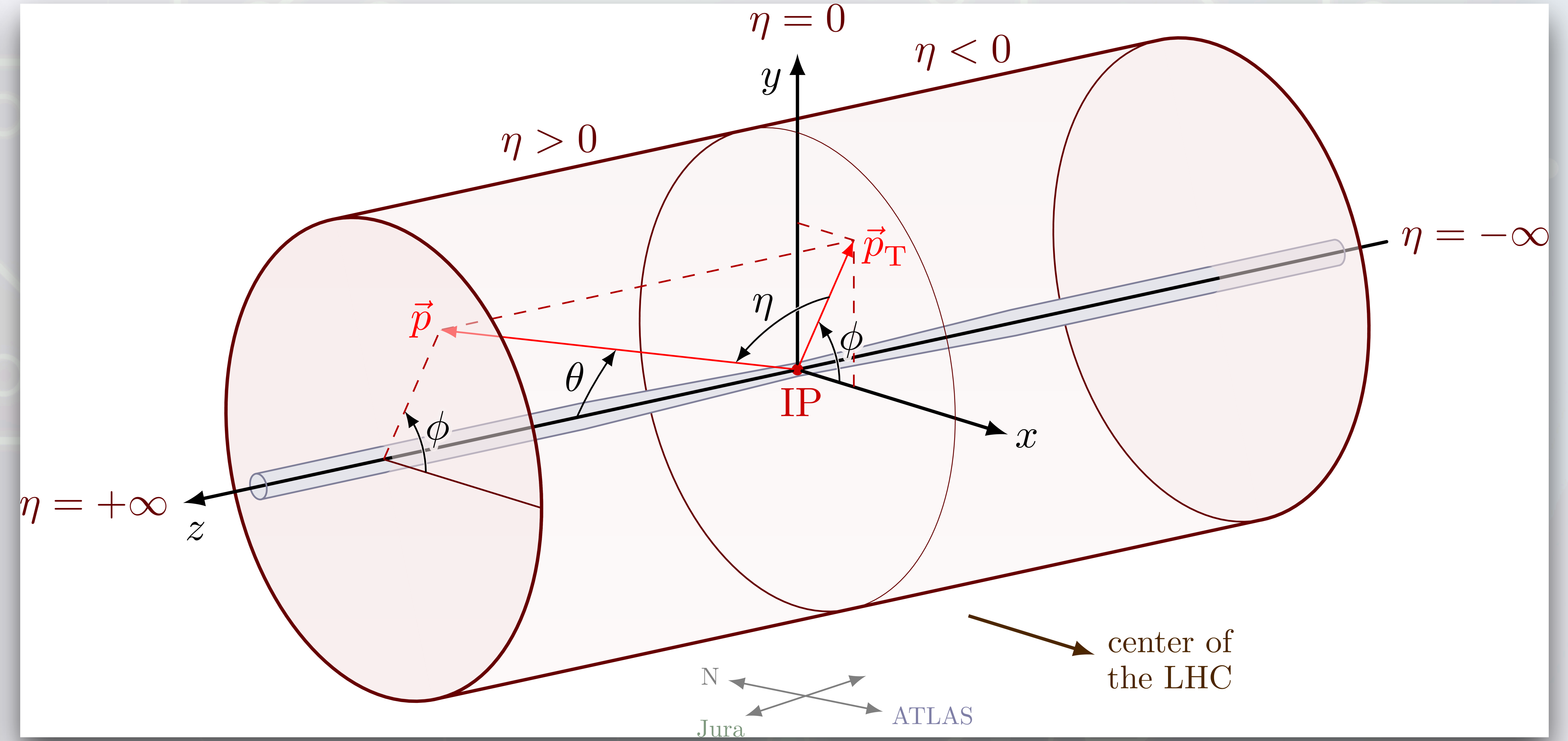



Figure adapted from 2021 CMS Open Data Workshop

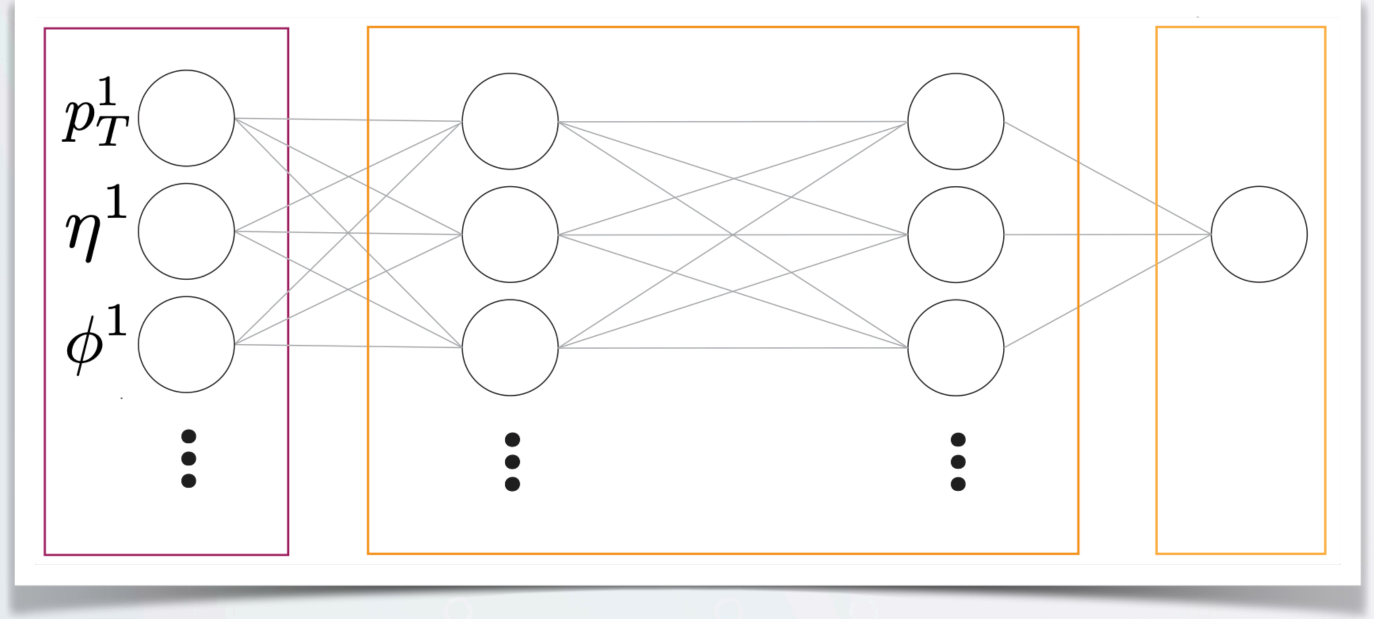



CMS Coordinate System by Izaak Neutelings

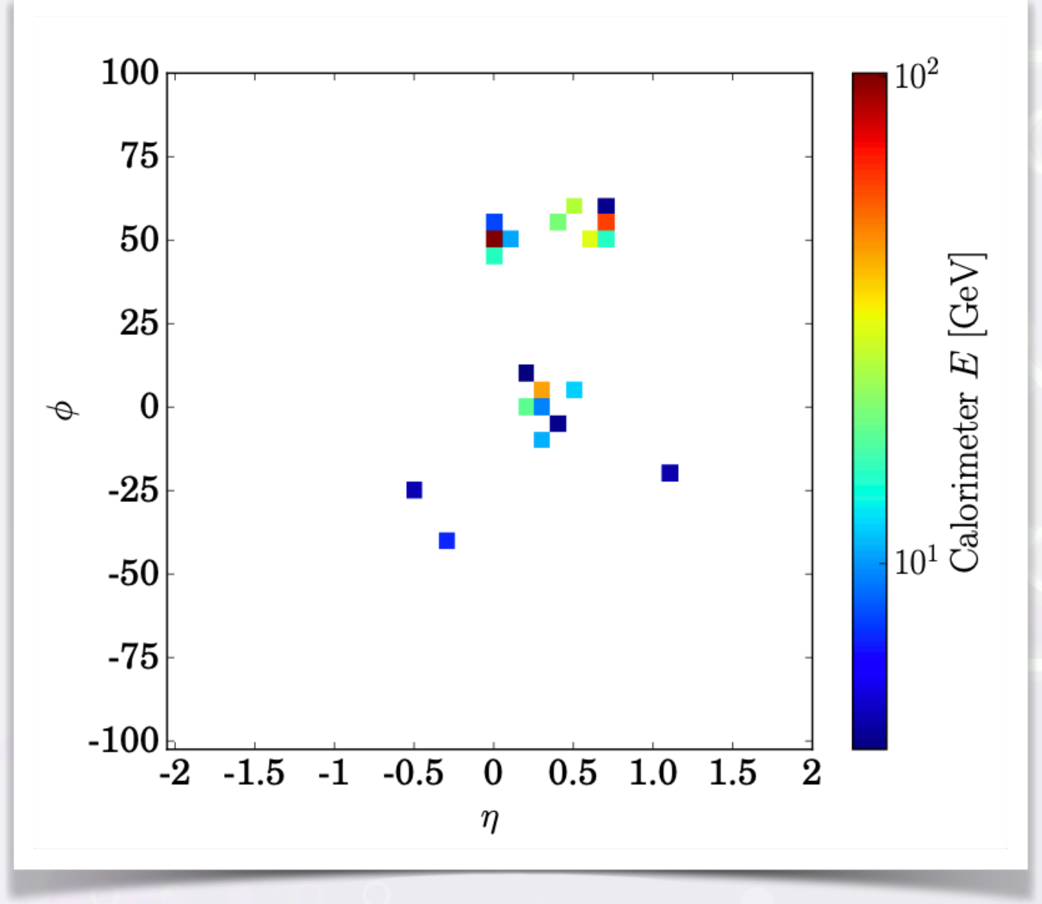
$$\overrightarrow{x} = (p_T, \Delta\eta, \Delta\phi)$$

# Classical ML for Jets

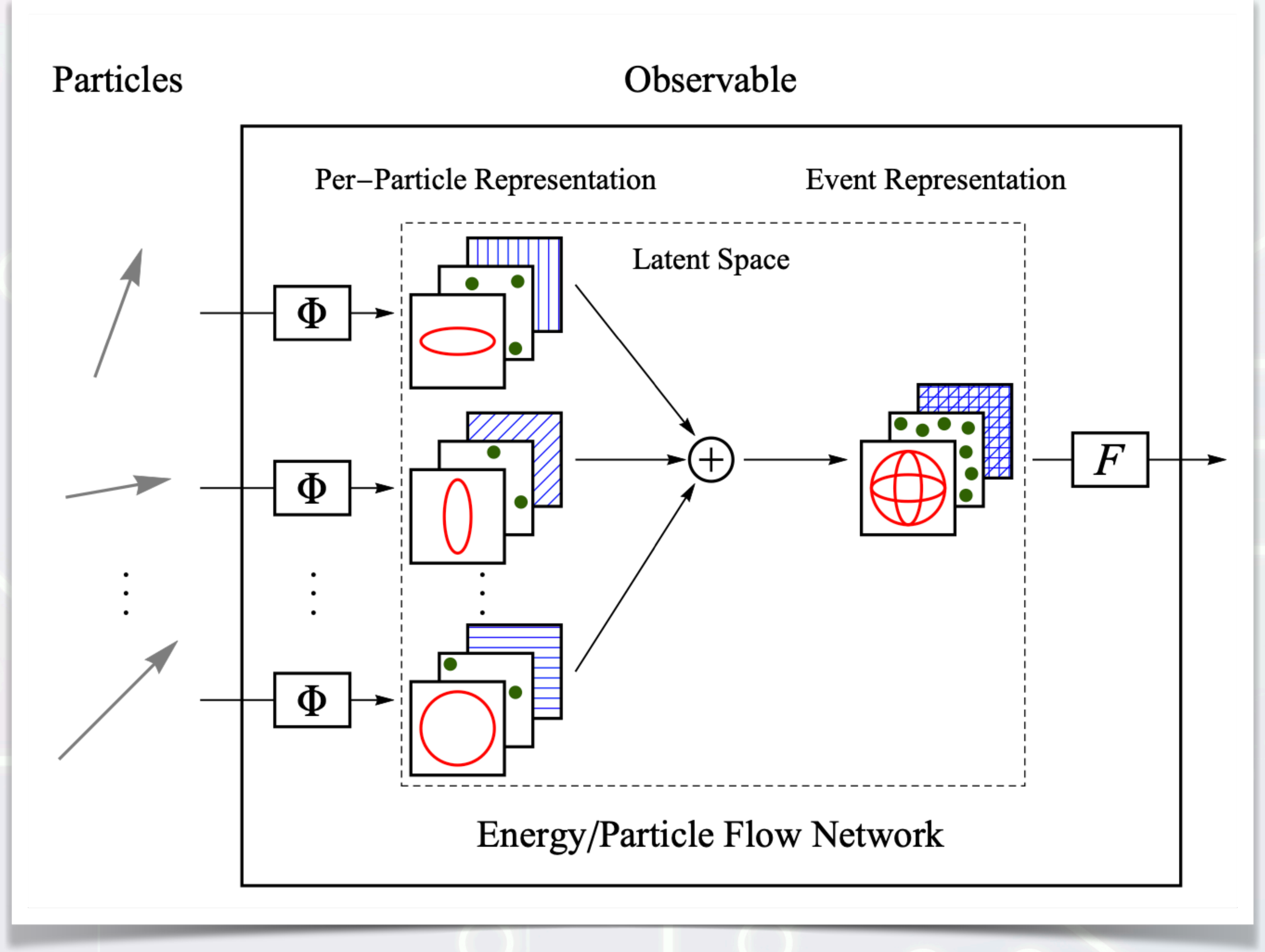
## Overview



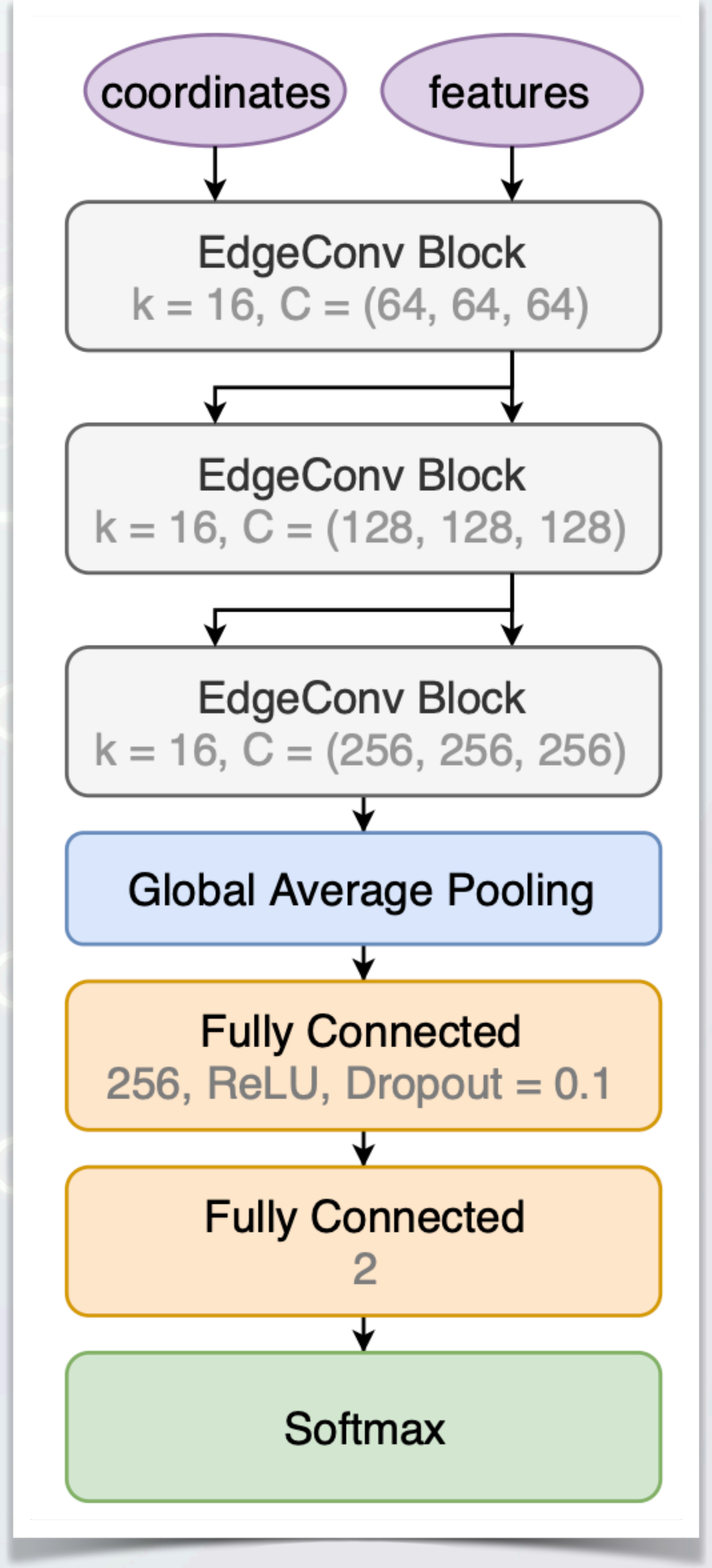

DNN (arXiv 1704.02124)



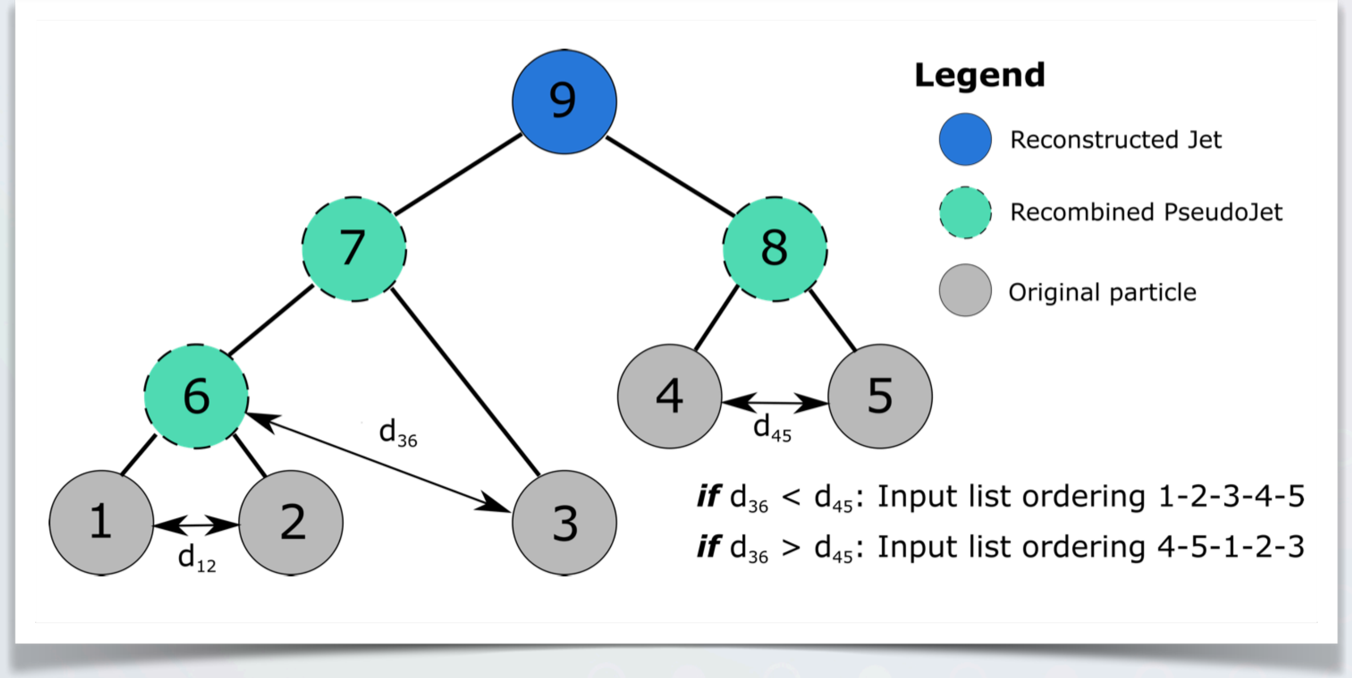

CNN (arXiv 1707.08966)



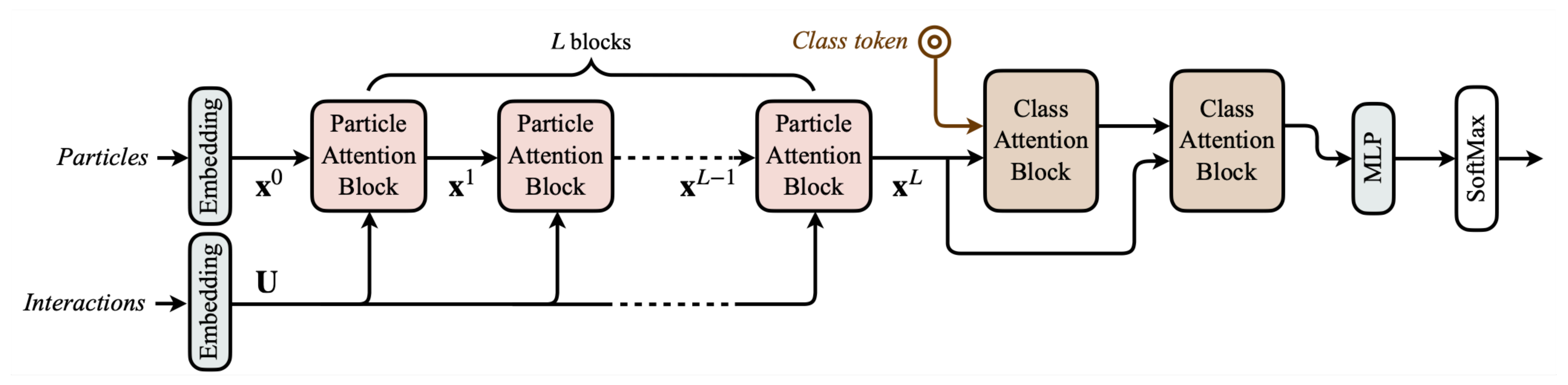

Deep Sets: EFN/PFN
(arXiv 1810.05165)




Particle Net
(arXiv 1902.08570)




LSTM (arXiv 1711.09059)




Particle Transformer (arXiv 2202.03772)

# Classical Machine Learning

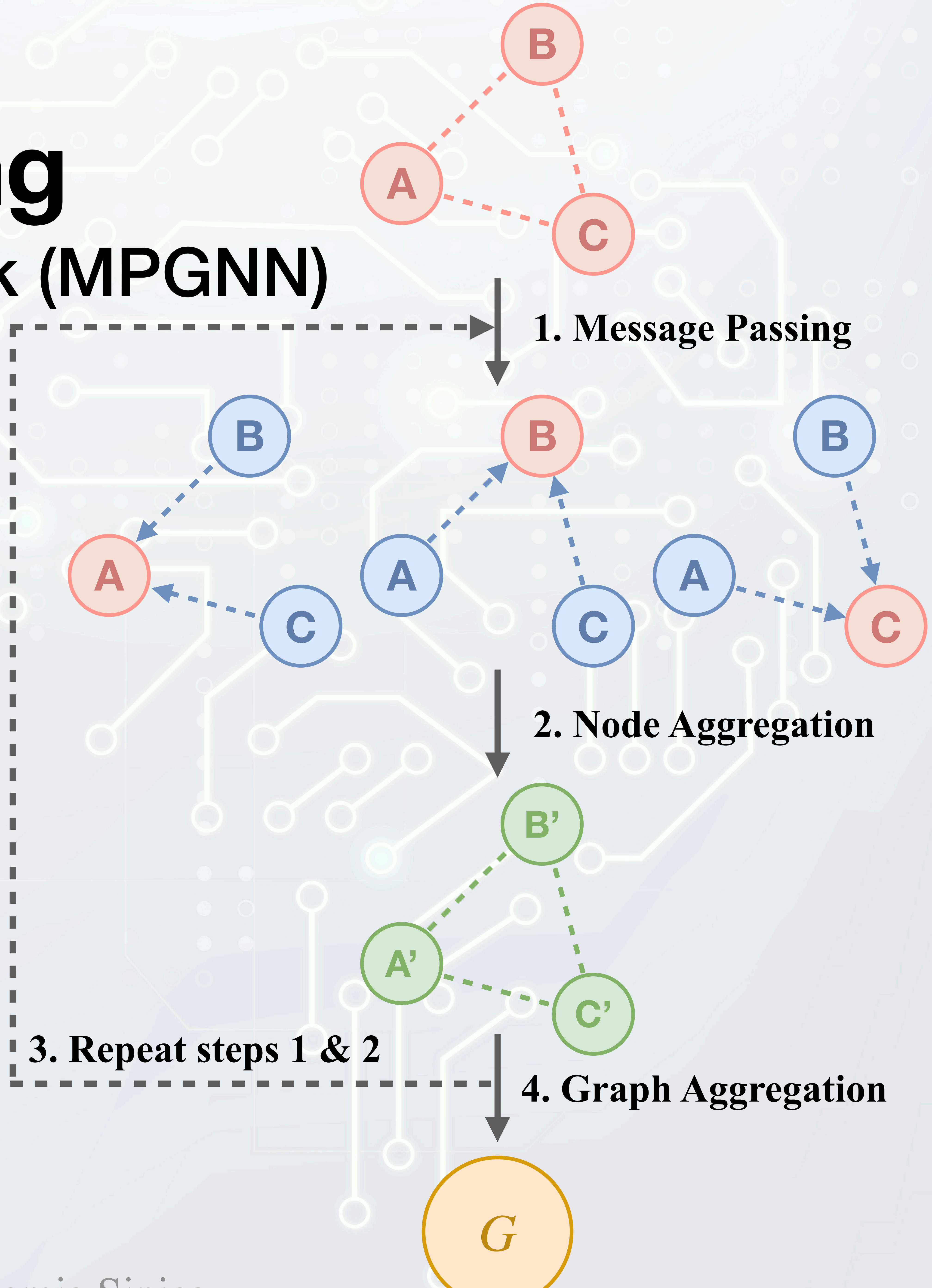
## Message-Passing Graph Neural Network (MPGNN)

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 $f(X) = g\left(\sum_{\mathbf{x}_i \in X} \boxed{h(\mathbf{x}_i)}\right)$ for some suitable transformations $g$ and $h$.

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

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

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

# QCGNN

## Quantum Complete Graph Neural Network

# Quantum Machine Learning

## Variational Quantum Circuit

# QCGNN

## Quantum Complete Graph Neural Network

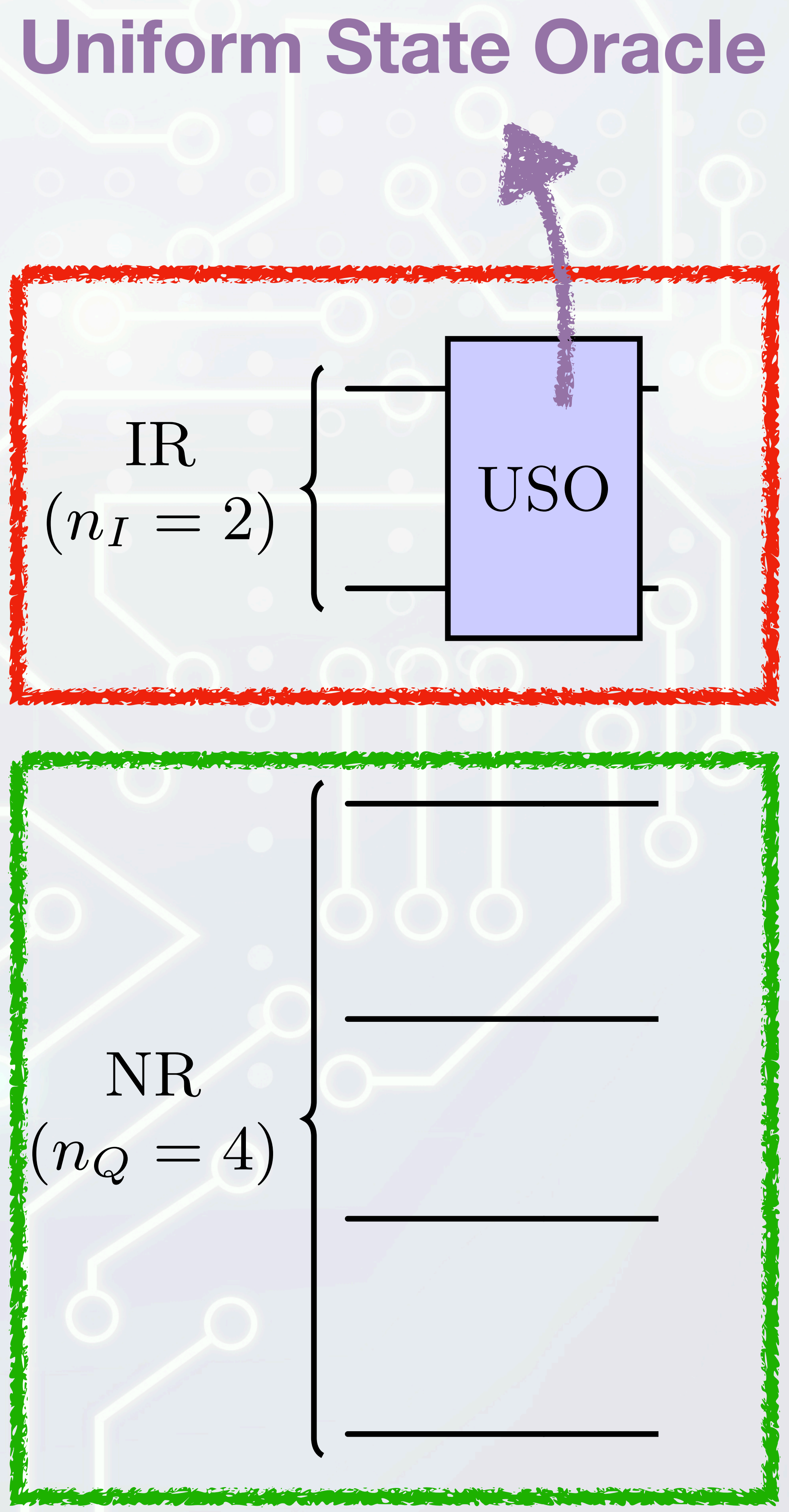
Suppose we have $N$ particles with features $\{\mathbf{x}_i \mid 0 \leq i \leq N-1\}$. We prepare a quantum circuit with $n_I + n_Q$ qubits where

- $n_I = \lceil \log_2 N \rceil$ 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**

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

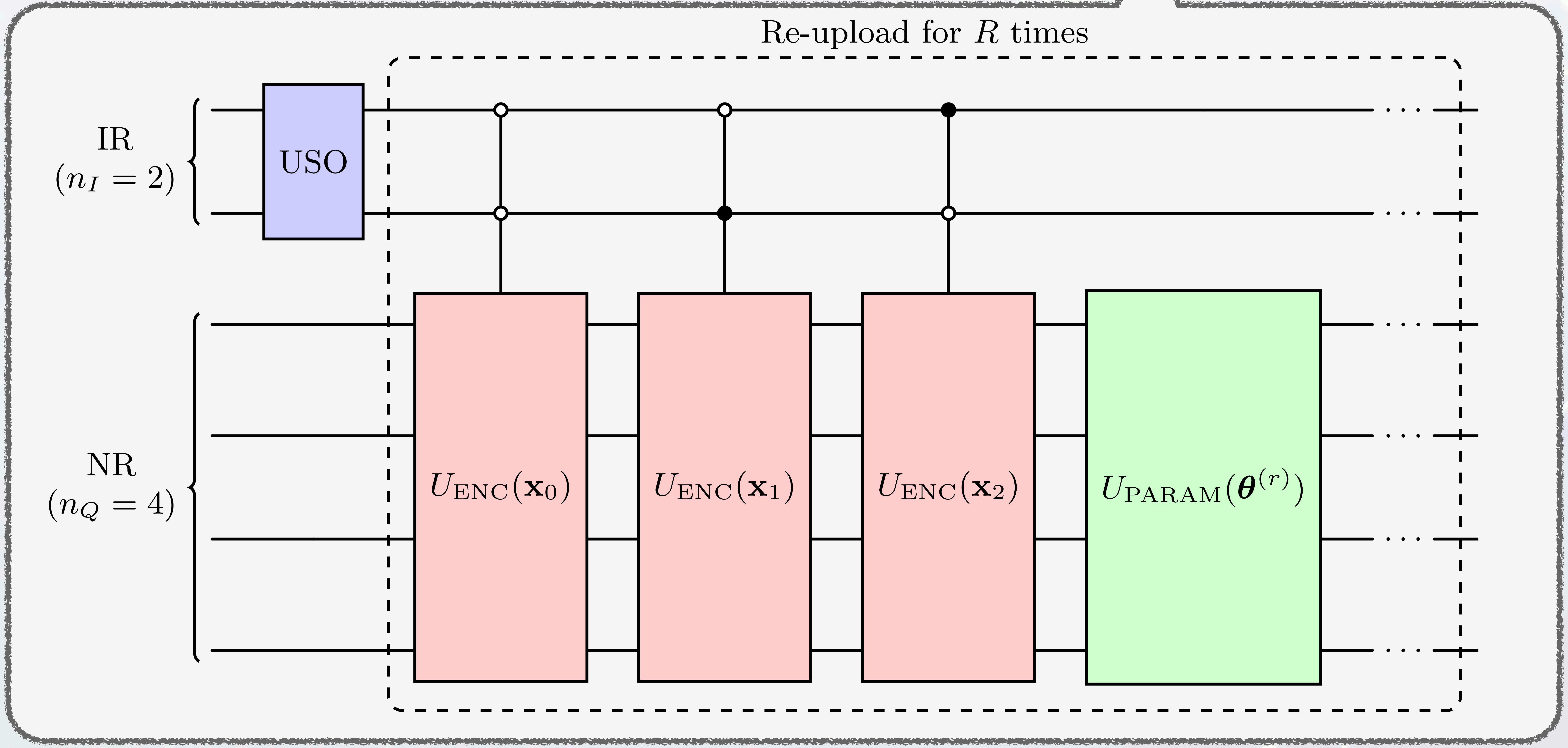
If $N = 2^{n_I}$, then we can simply use Hadamard gates. Otherwise, one should use some *Uniform State Oracle* (USO) to prepare the state.



# QCGNN

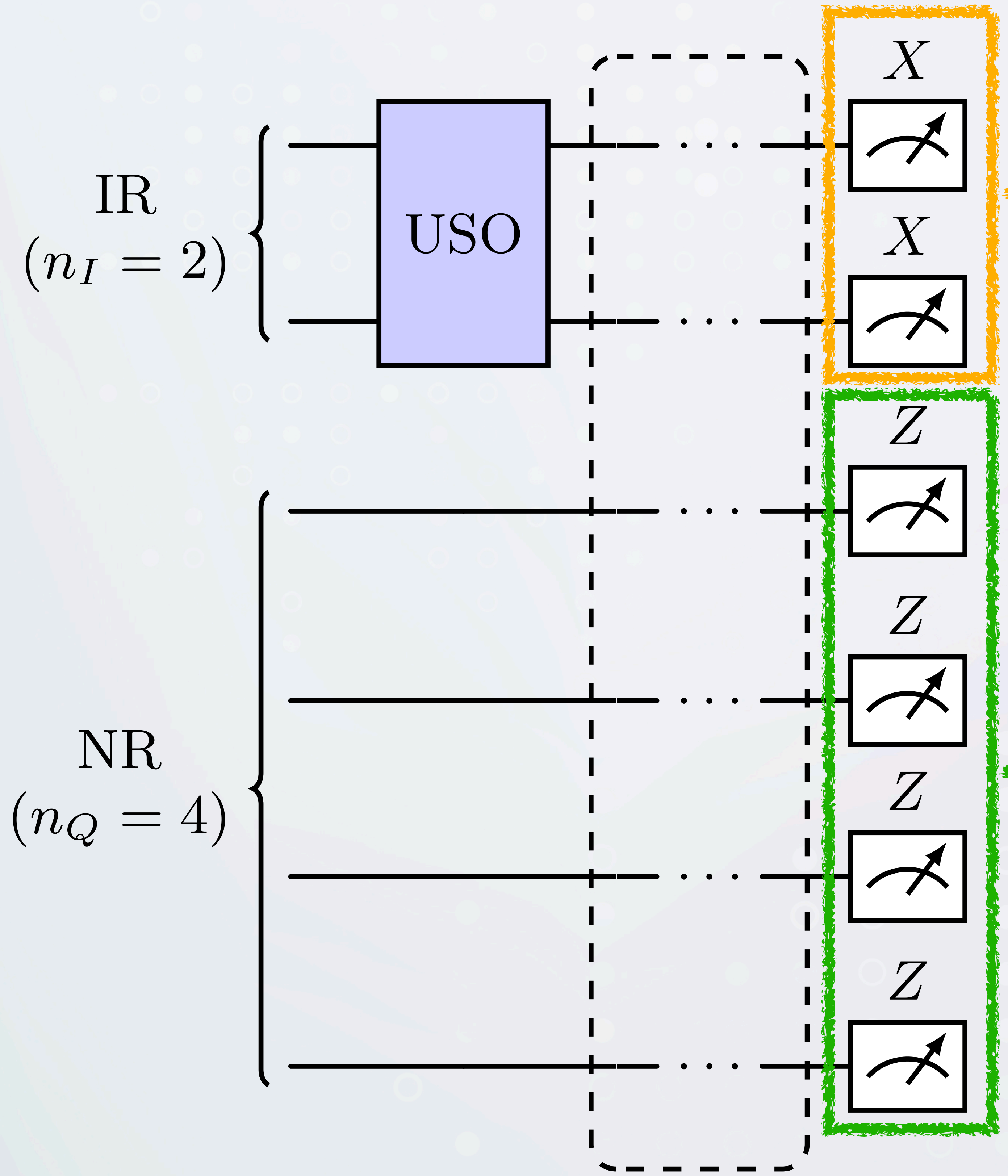
## Quantum Circuit

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




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

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

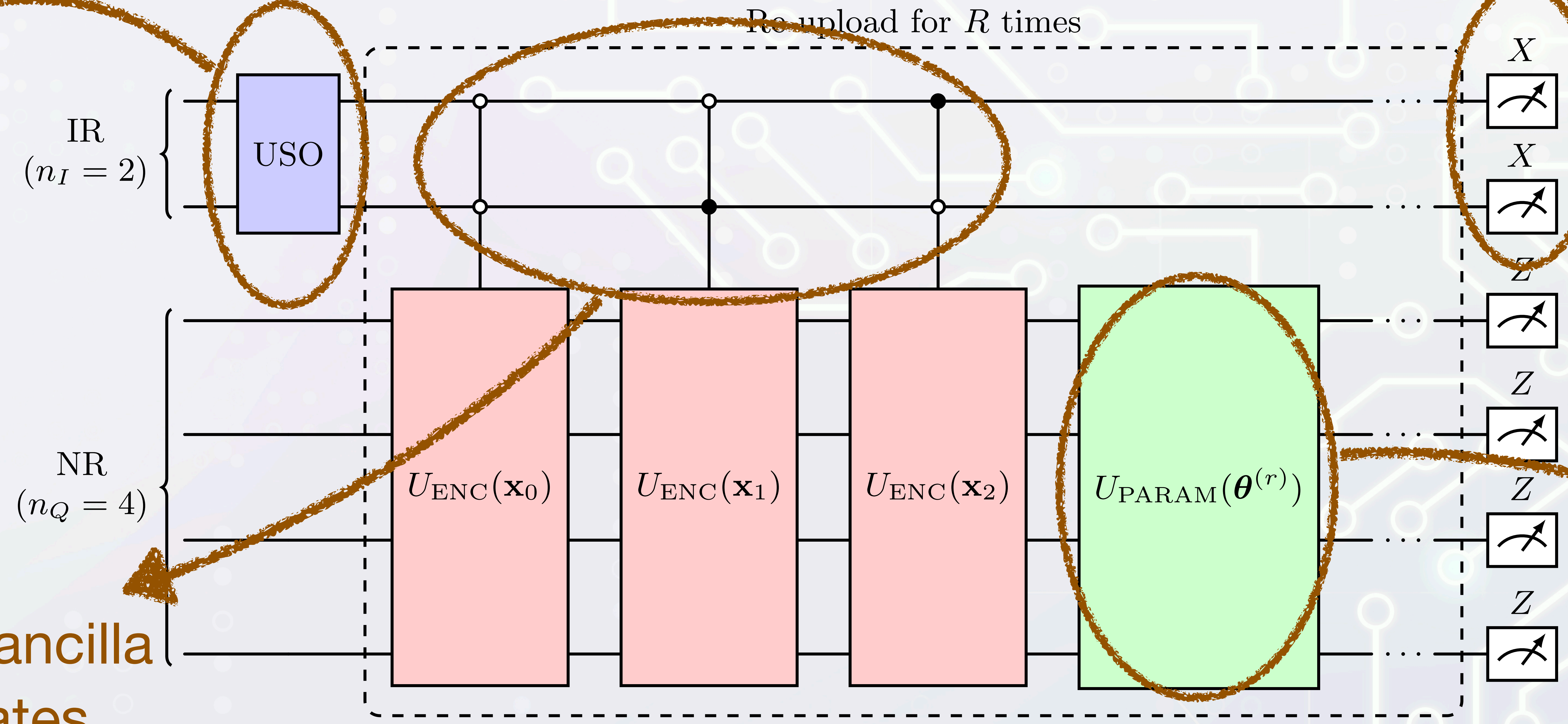
**Similar to MPGNN, with automatic aggregation.**

# QCGNN

## Gate and Computational Complexity

$O(N)$ Pauli-string observables

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




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!

# Experiments Results

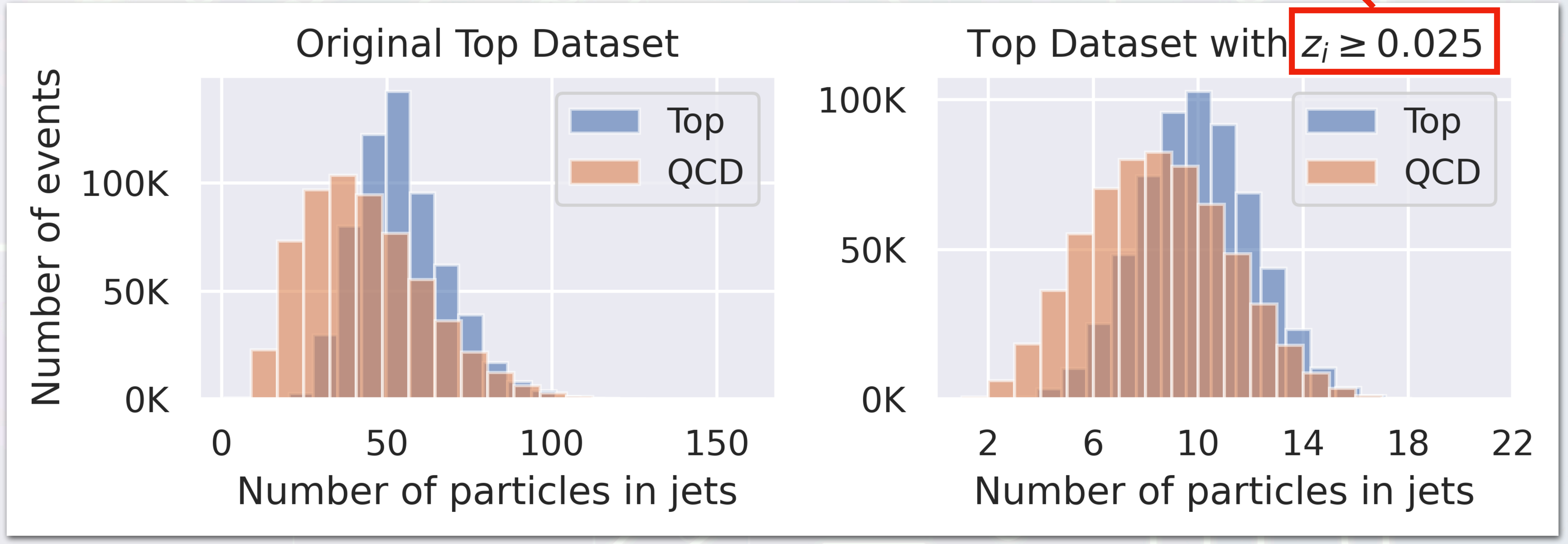
## Quantum Simulators & IBMQ


Jet Substructure (CMS 2022 Open Data Workshop)

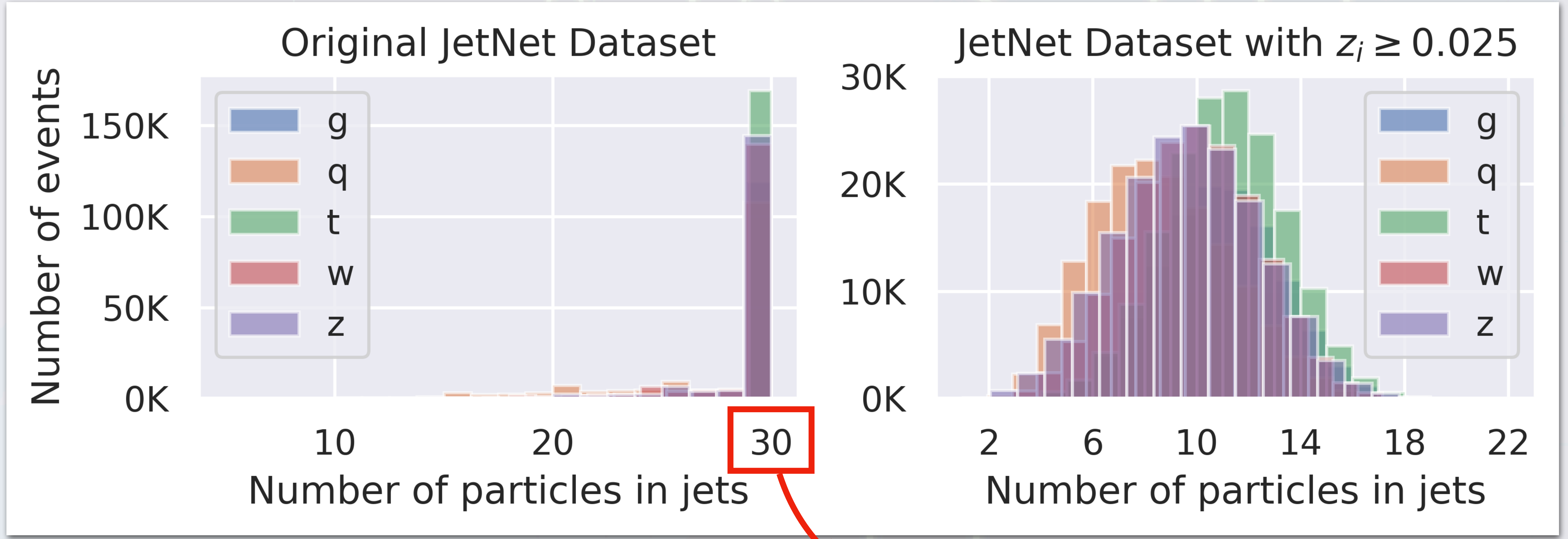
# Jet Dataset

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

- **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 $R = 0.8$




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

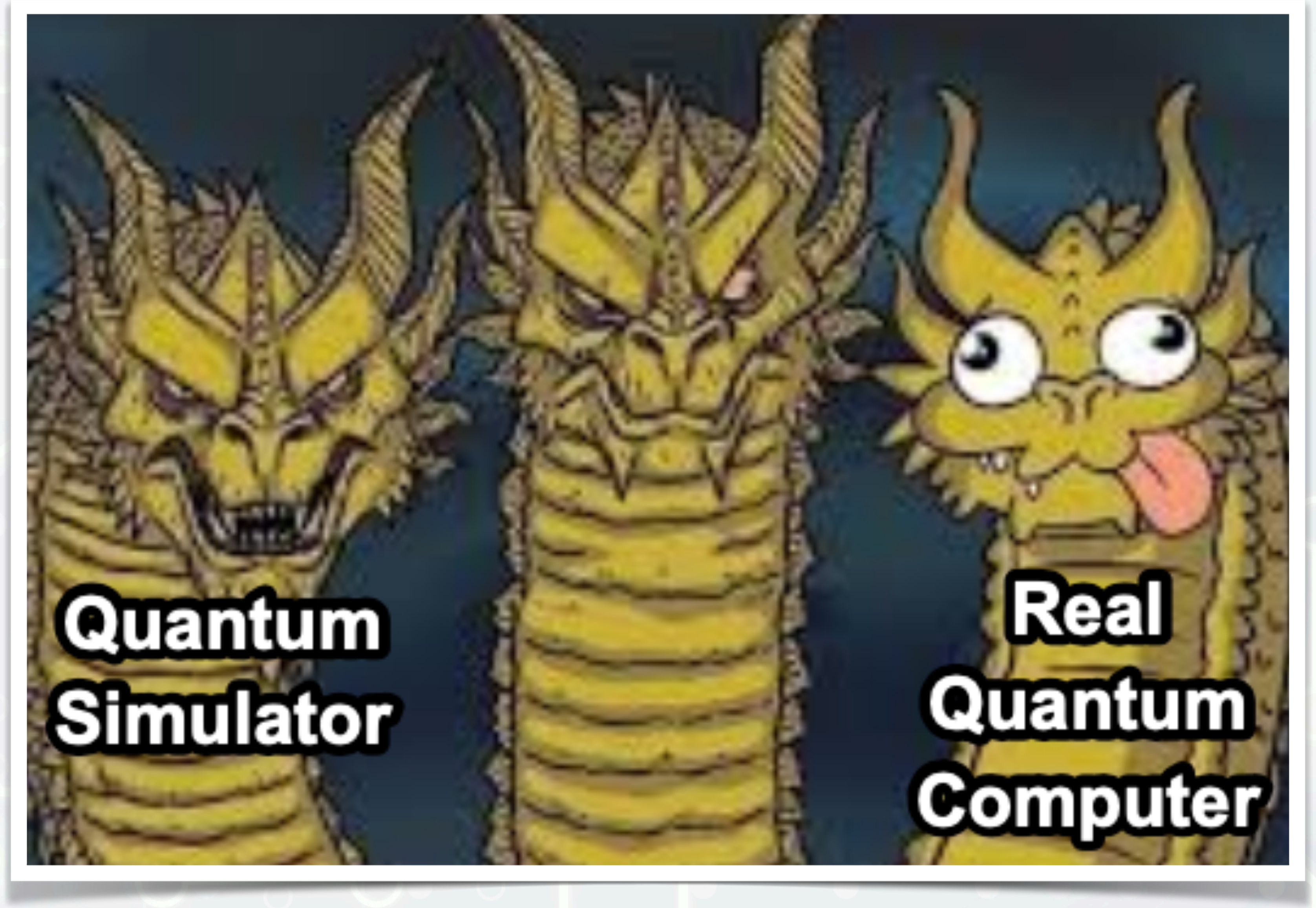
QCGNN with $n_Q = 3$ and $n_Q = 6$ (On simulators)

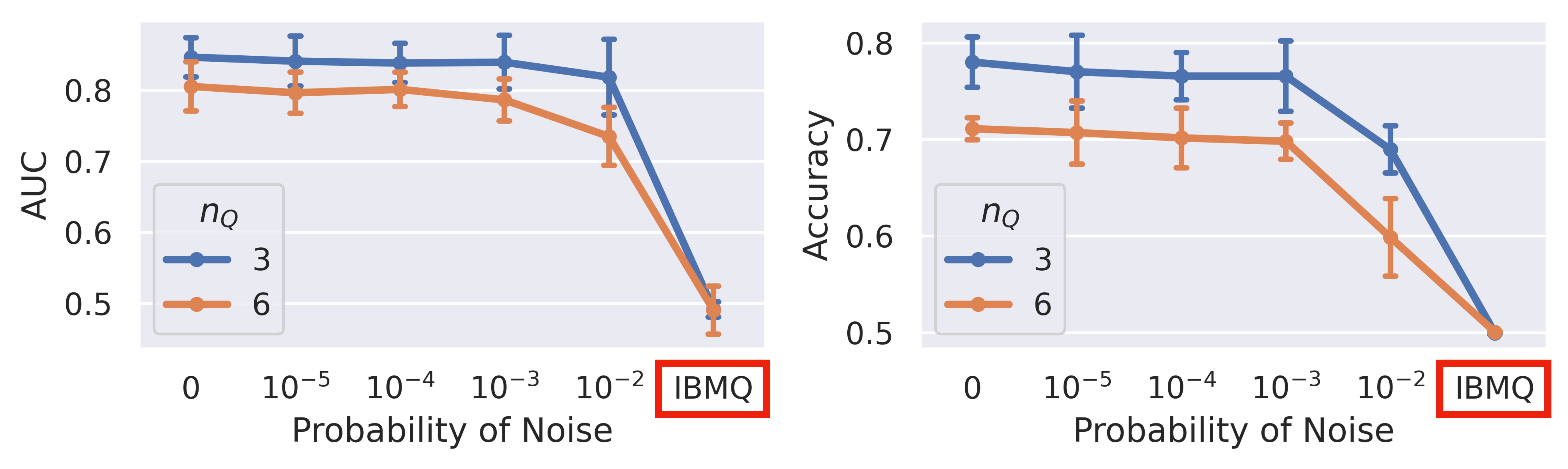
| Model | Top Dataset (2 classes) | | | JetNet Dataset (5 classes) | | |
|---|---|---|---|---|---|---|
| | # params | AUC | Accuracy | # params | AUC | Accuracy |
| Particle Transformer | 2.2M | 0.946±0.005 | 0.868±0.009 | 2.2M | 0.889±0.002 | 0.656±0.006 |
| Particle Net | 177K | 0.953±0.003 | 0.885±0.006 | 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***.



# 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 | $T_{\text{ENC}}$ | $T_{\text{PARAM}}$ |
|---|---|---|---|
| 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 $O(1)$

# Summary

- In the task of jet discrimination, graph is one of the natural representation. To design permutation-invariant models, graph neural networks have become a popular architecture.
- **We introduce a new quantum model, the Quantum Complete Graph Neural Network. 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.


Thanks for your attention!
Hypergeometric functions
functions
Special functions
contour
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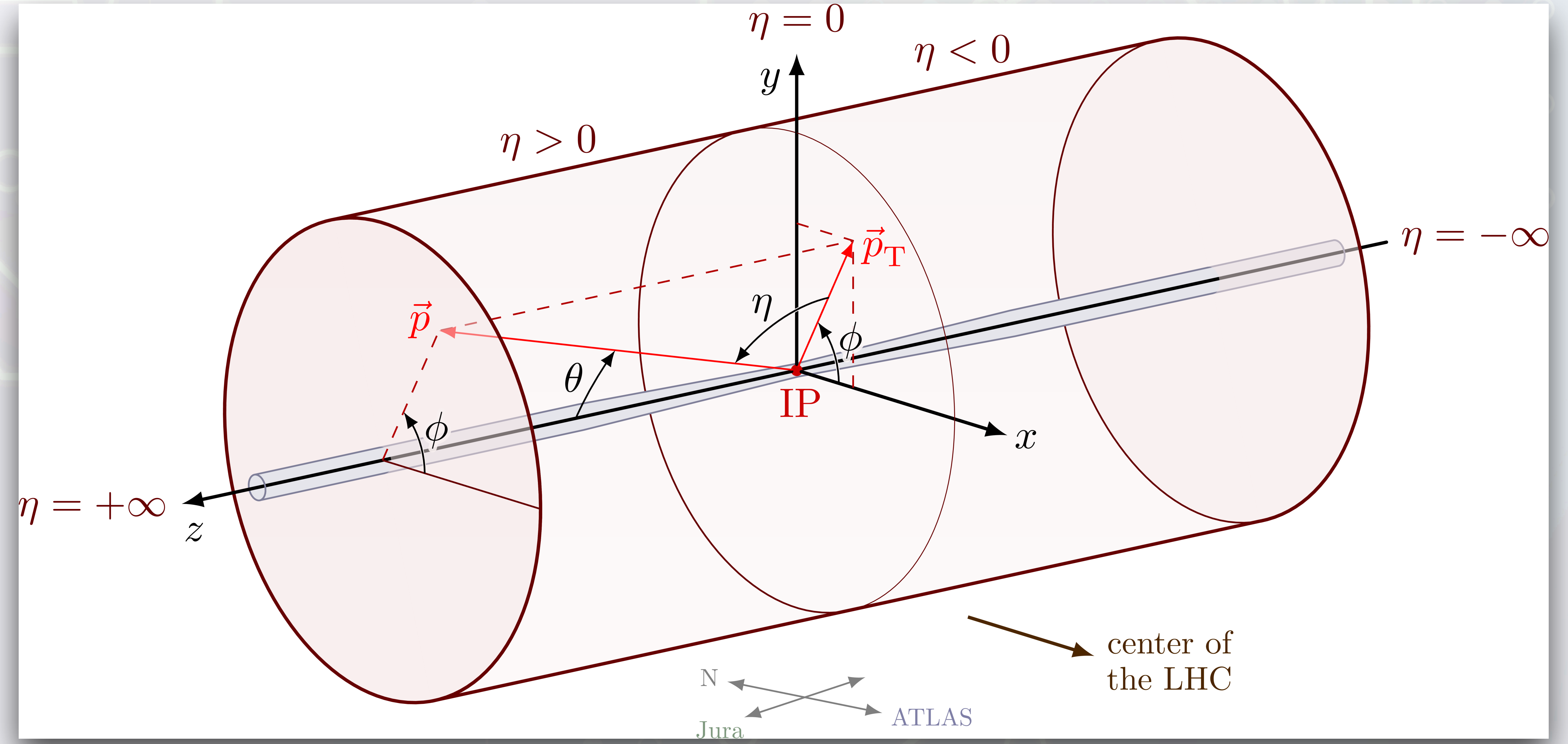
# Backup Slides

# CMS Coordinate System

The particle flow is defined as

- The transverse momentum $p_T = \sqrt{p_x^2 + p_y^2}$
- The azimuthal angle $\phi = \tan^{-1}(\frac{p_y}{p_x})$
- The pseudo-rapidity $\eta = -\ln\left[\tan(\frac{\theta}{2})\right]$

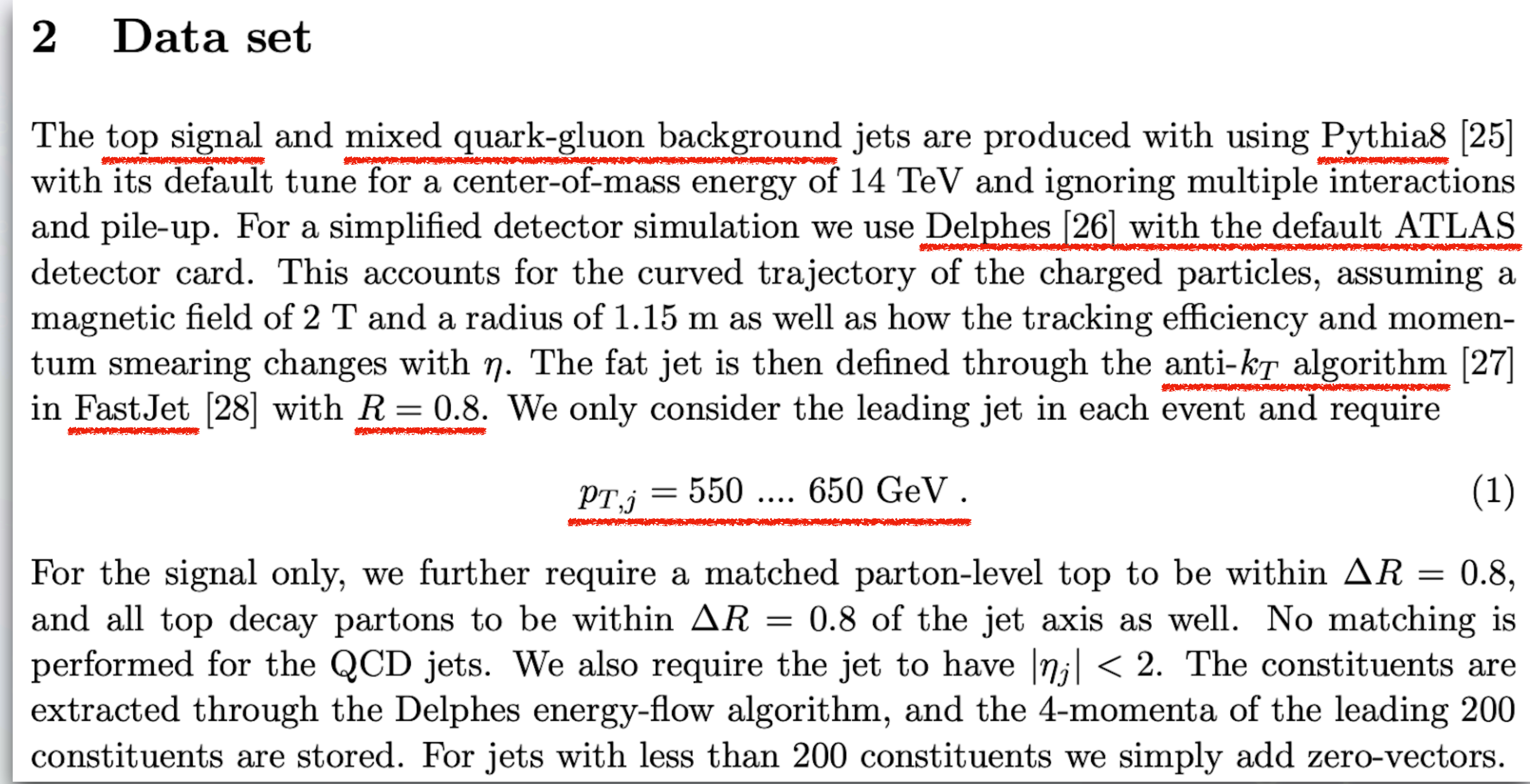


CMS Coordinate System by Izaak Neutelings

In jet analysis, the differences $\Delta\phi$ and $\Delta\eta$ relative to the jets is adopted, since they are Lorentz invariant under boosts in $z$-direction.

# 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 $\eta$. 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

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

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-$k_{\mathrm{T}}$ 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 $p_{\mathrm{T}}$ distribution is narrow, the jet $p_{\mathrm{T}}$ 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 $p_{\mathrm{T}}$ 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.

# Classical ML for Jets

## Message Passing GNN

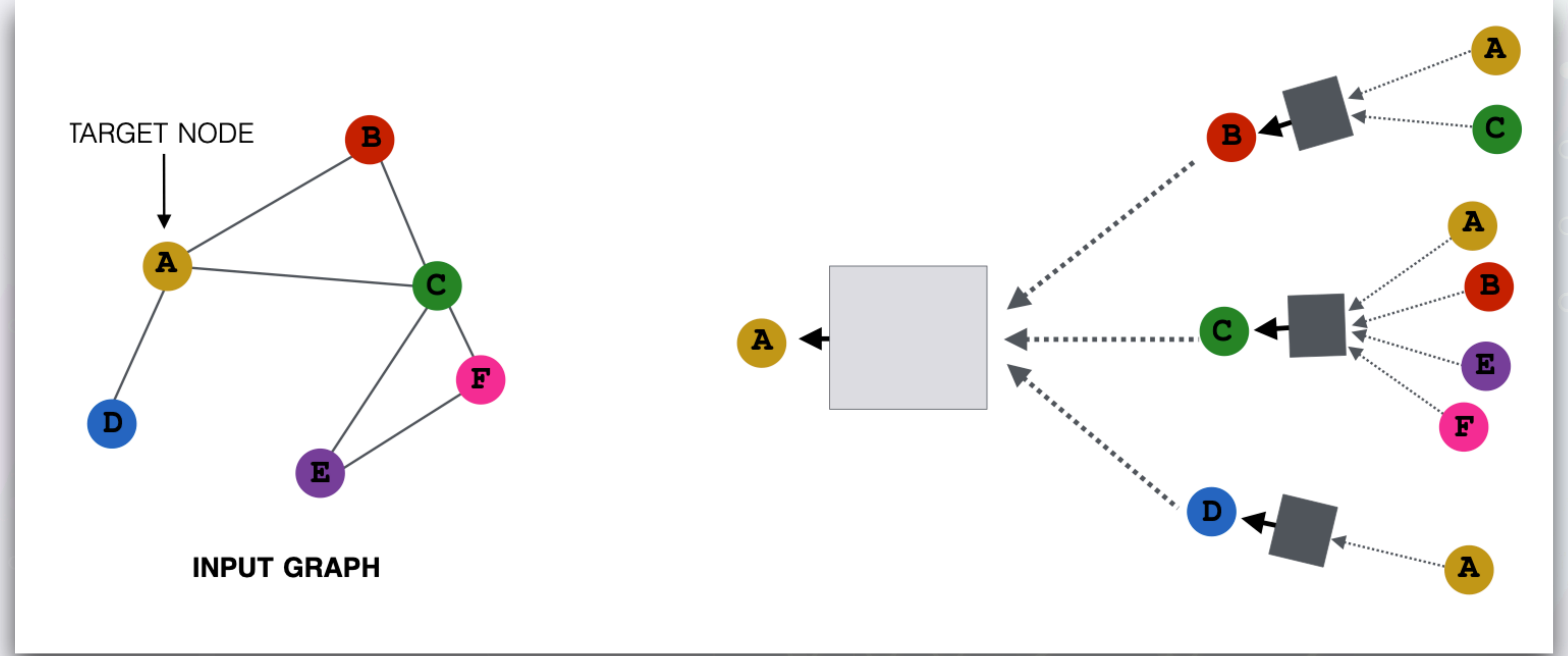



Figure adapted from "Stanford CS224W: Machine Learning with Graphs" by J.Leskovec.

$$f(X) = g\left(\sum_{\vec{x}_i \in X} \boxed{h(\vec{x}_i)}\right)$$

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

$k$-th update

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

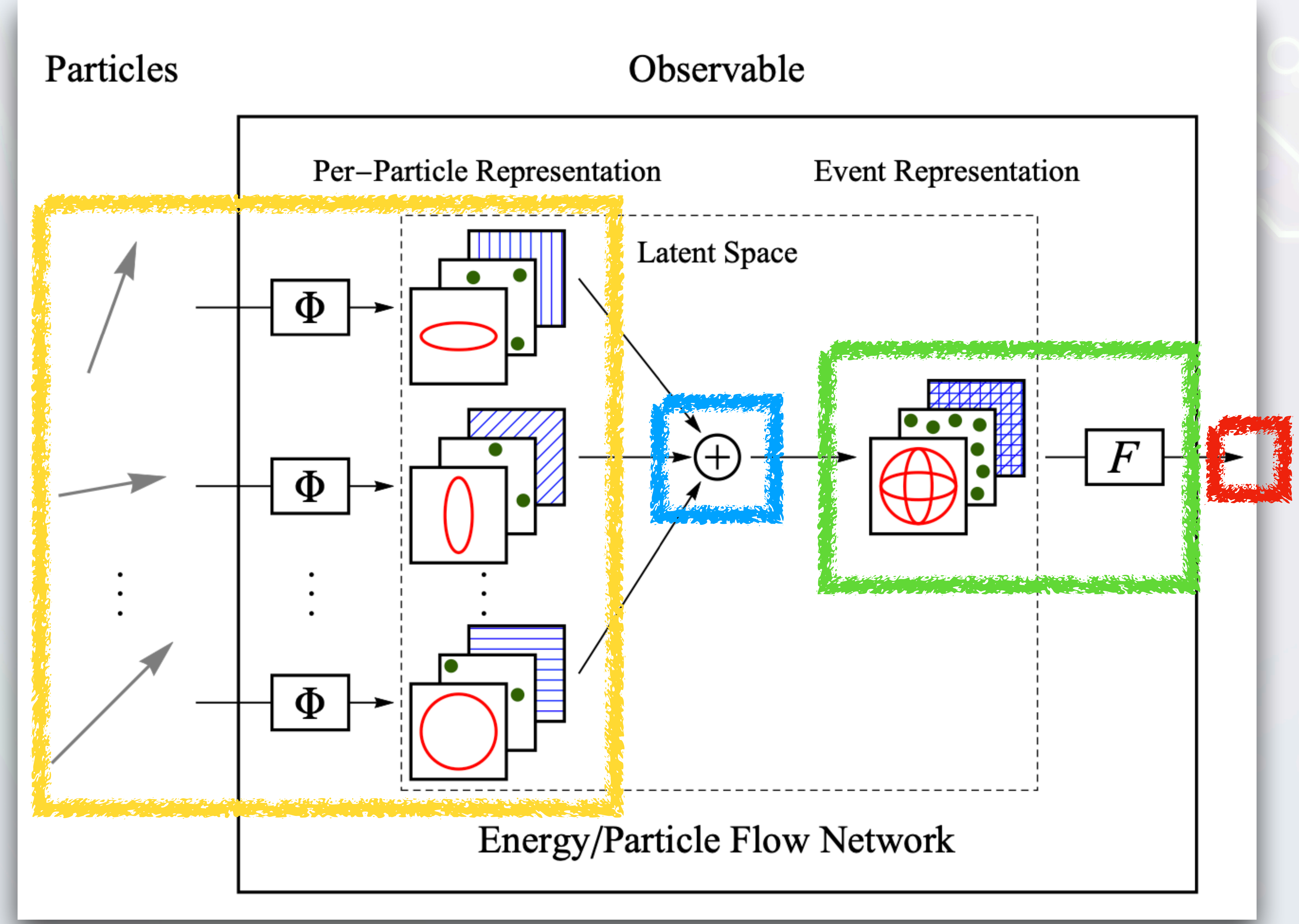
- GCN (arXiv 1609.02907)
- GraphSAGE (arXiv 1706.02216)
- GAT (arXiv 1710.10903)
- EdgeConv (arXiv 1801.07829)

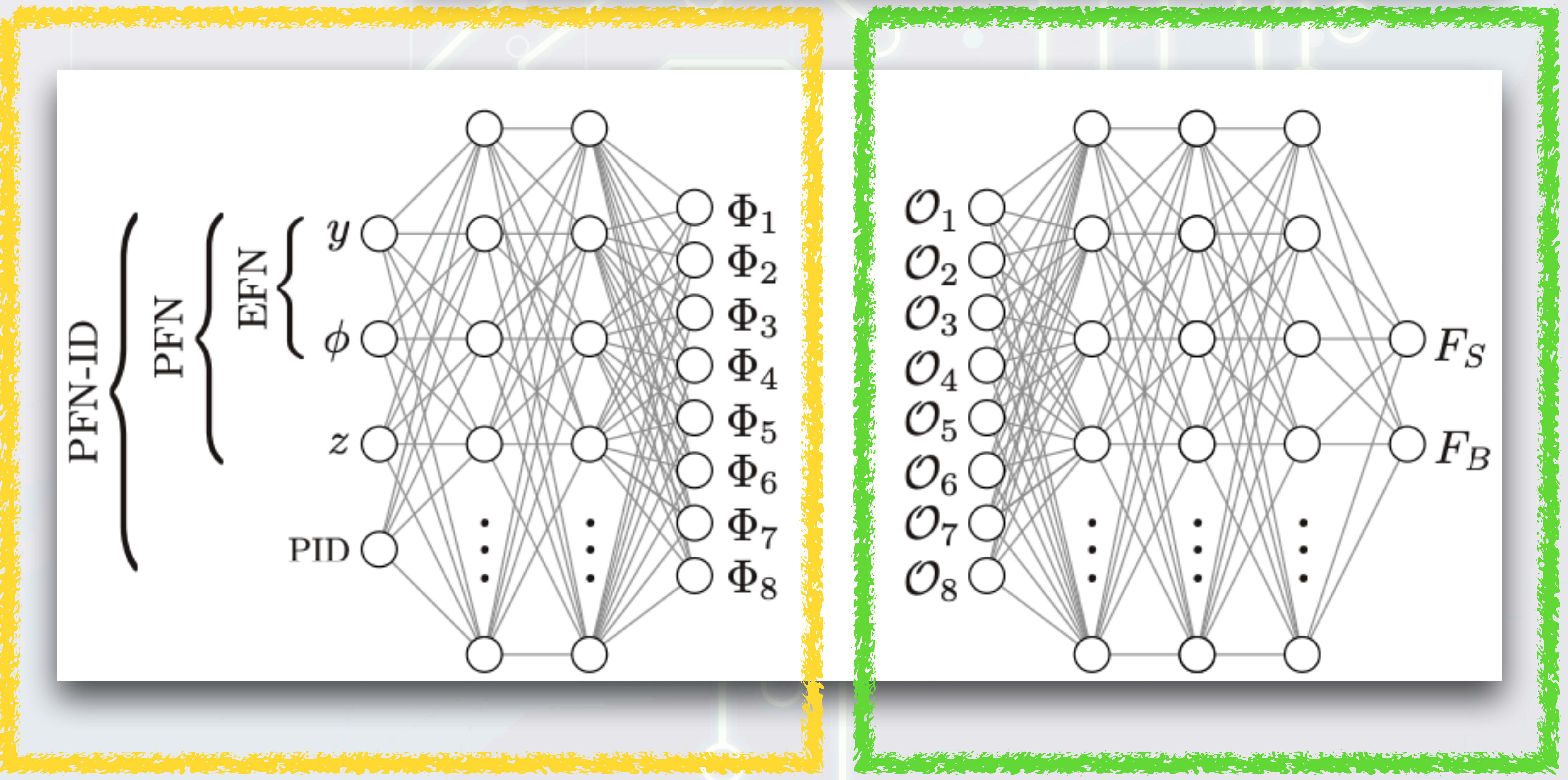
# Particle Flow Network

## arXiv 1810.05165

Motivated by the *Deep Set Theorem*

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



# Single Qubit Gates

## Rotation Gates

*Theorem 4.1*: (**$Z$-$Y$ decomposition for a single qubit**) Suppose $U$ is a unitary operation on a single qubit. Then there exist real numbers $\alpha, \beta, \gamma$ and $\delta$ such that

$$U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta). \tag{4.11}$$

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{4.4}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{4.5}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}. \tag{4.6}$$

# Multi-Qubit Gates

## Decomposition of Multi-Controlled Gates

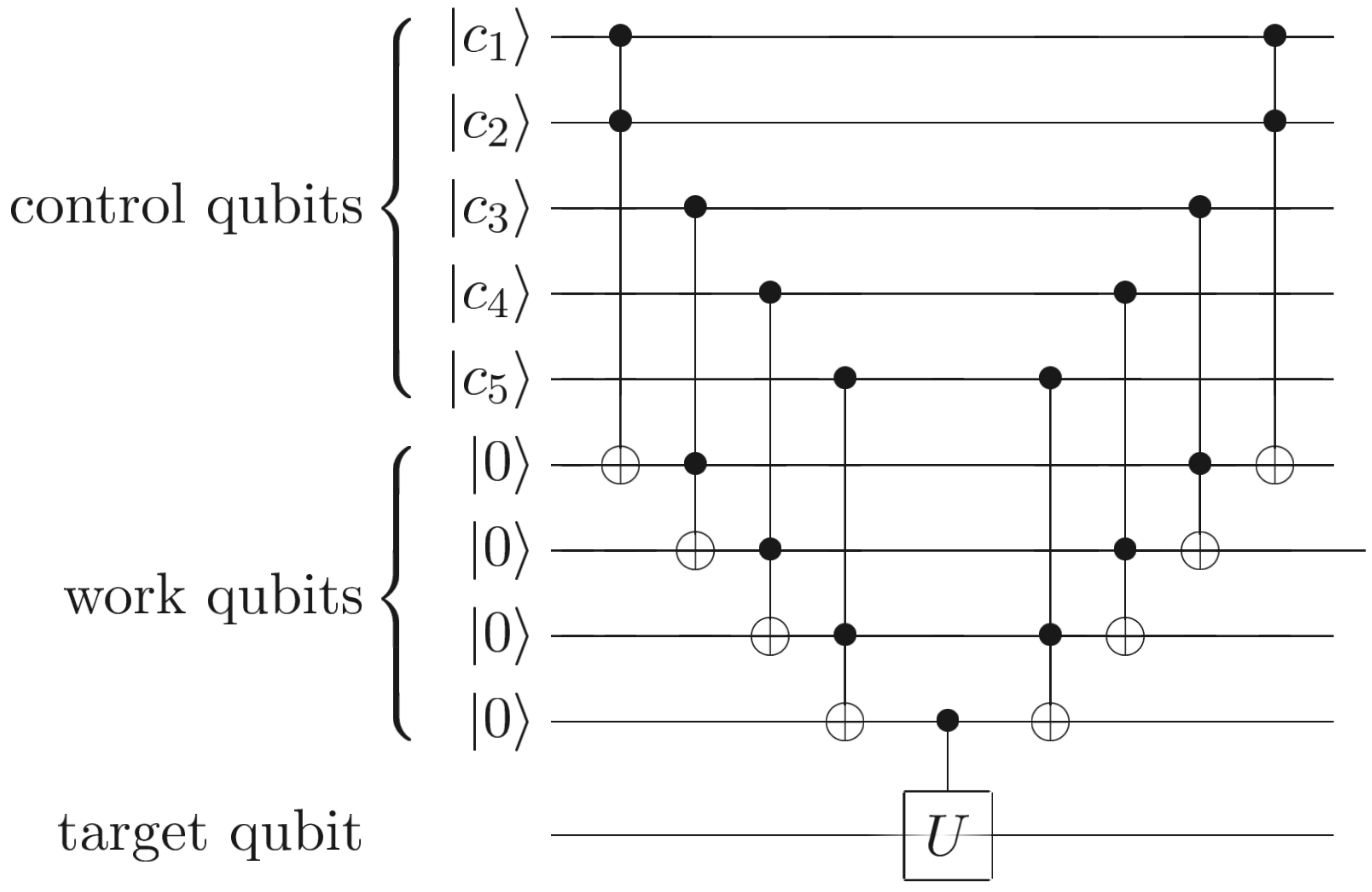



Figure 4.10. Network implementing the $C^n(U)$ operation, for the case $n = 5$.

Adopted from "Quantum Computation and Quantum Information" by N & C.

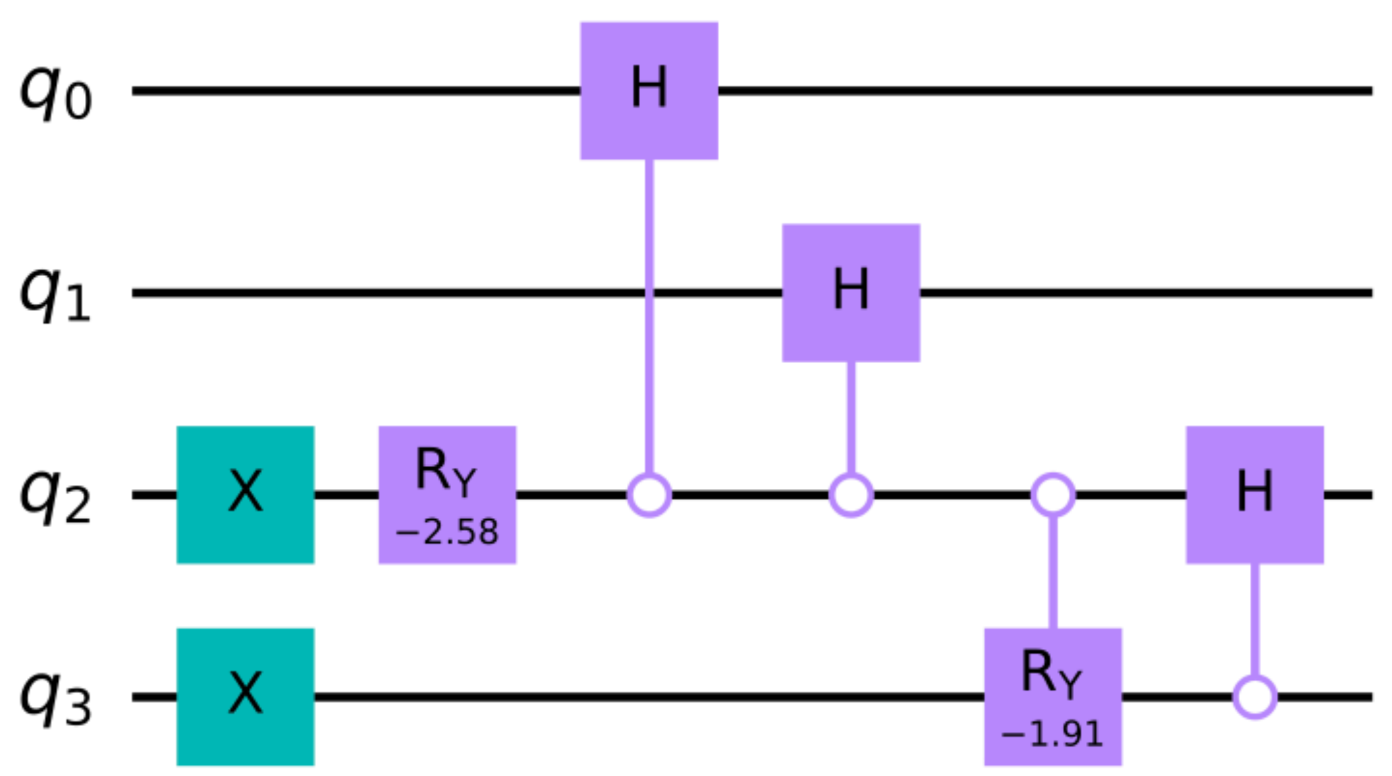
# Uniform State Oracle

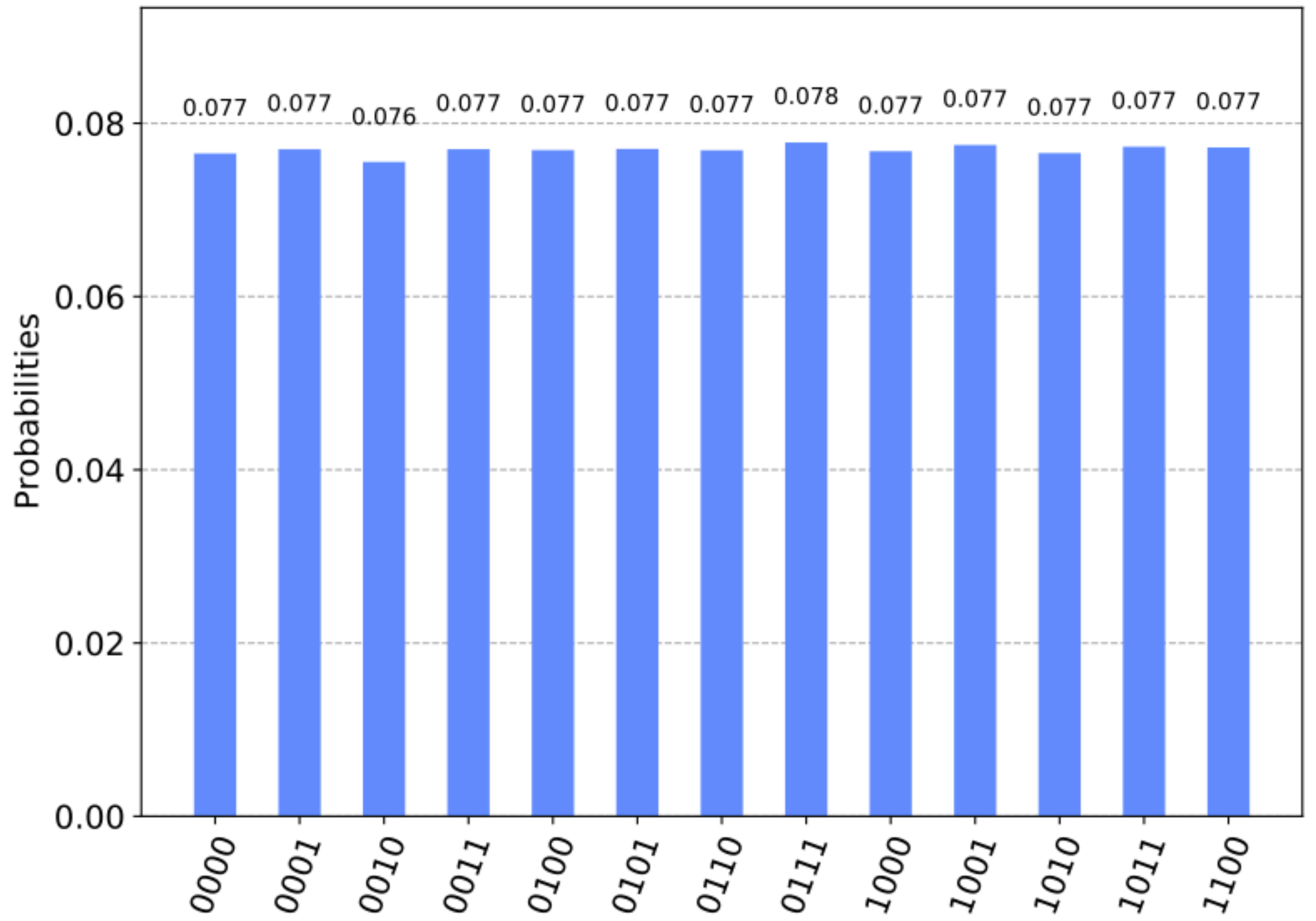
## arXiv 2306.11747

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:

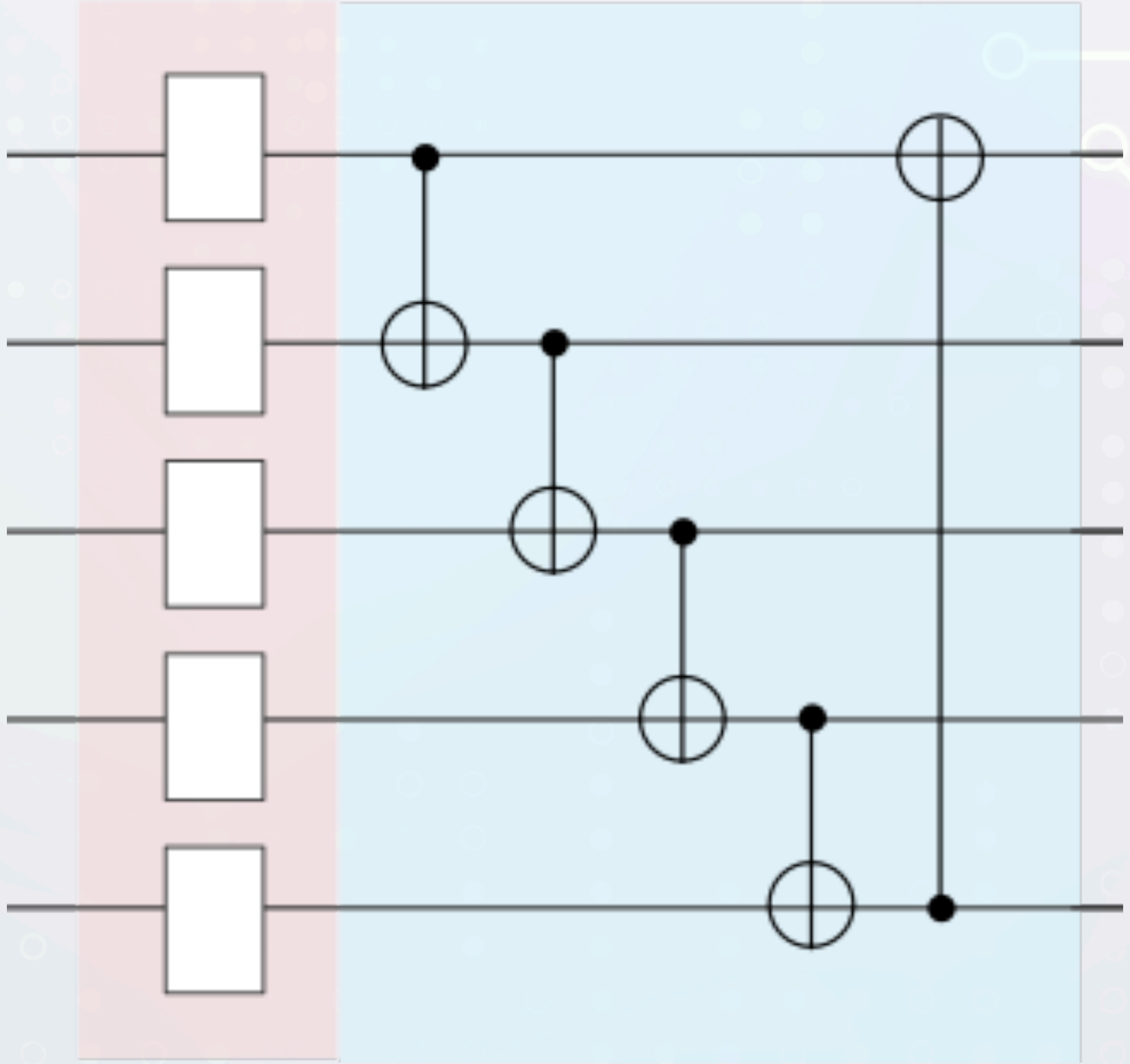
$$|\psi\rangle = \frac{1}{\sqrt{13}} \sum_{i=0}^{12} |i\rangle$$



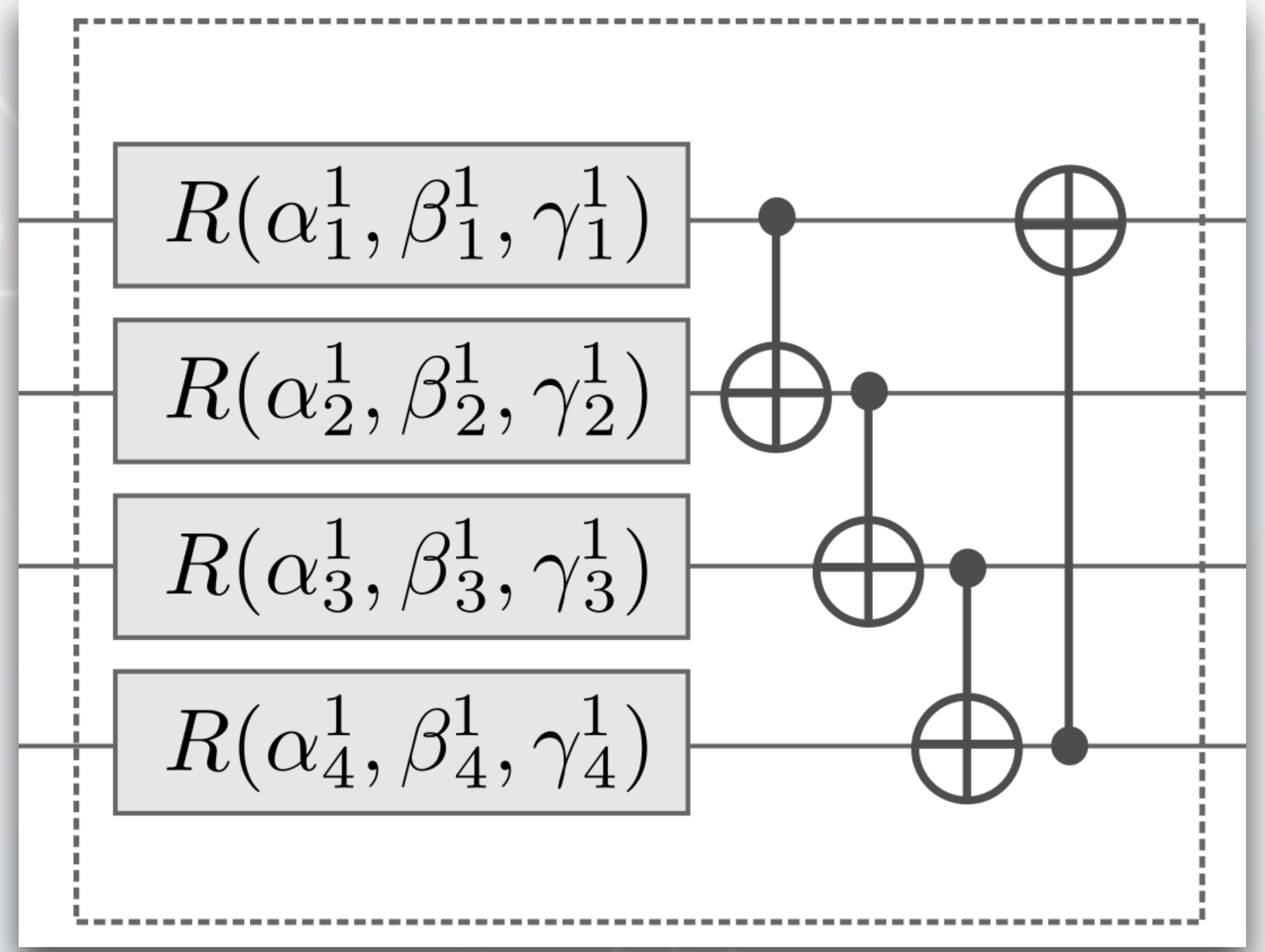



# VQC Ansatz

## PennyLane

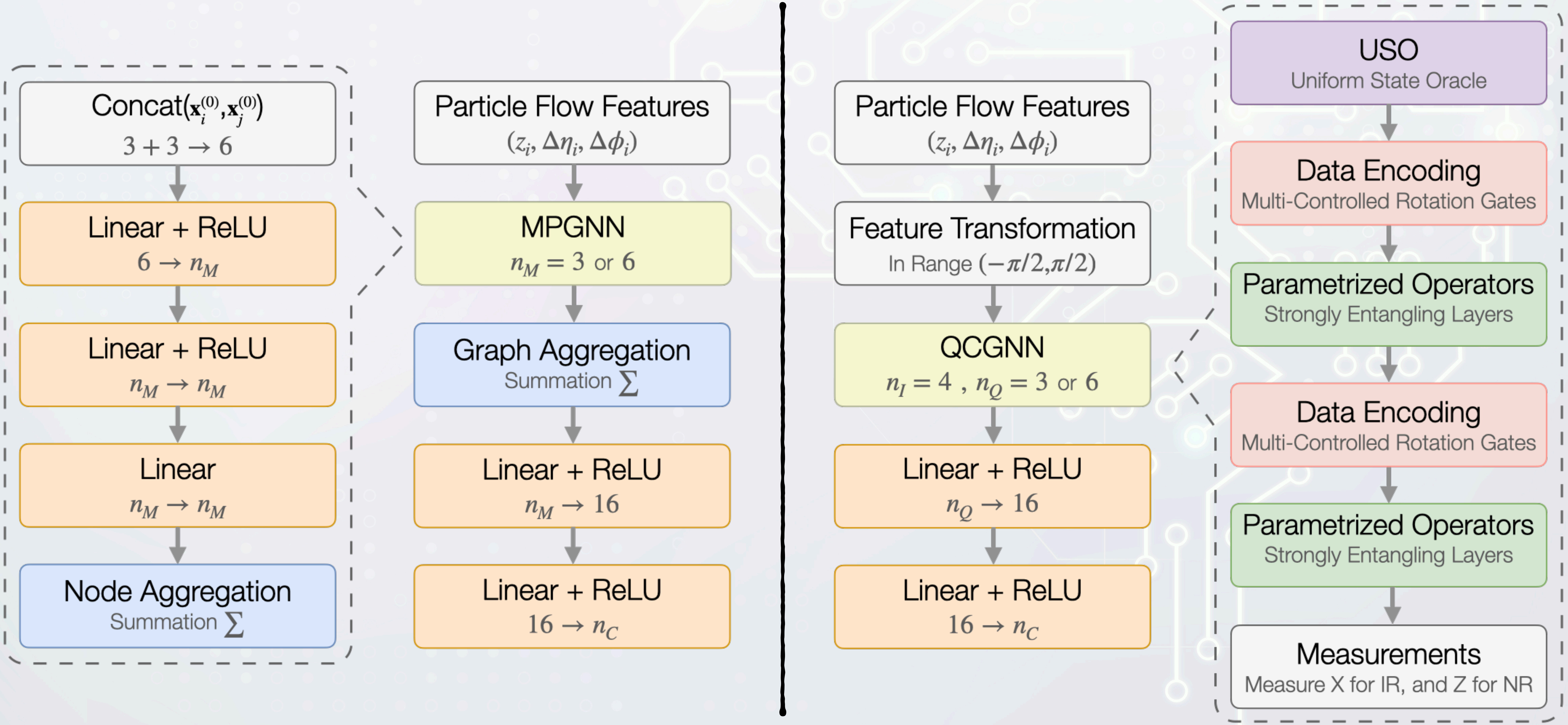


qml.BasicEntanglerLayers



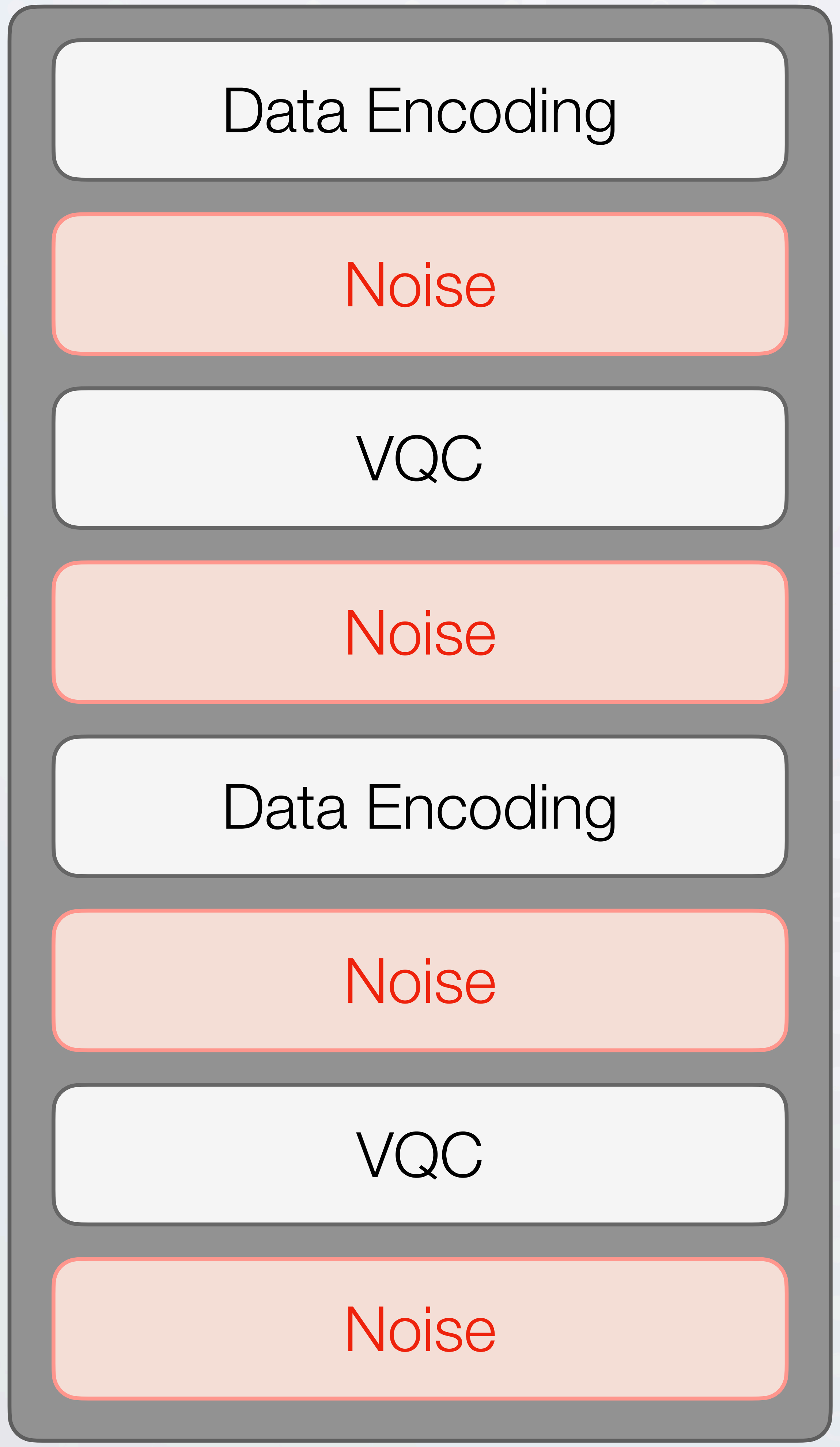

qml.StronglyEntanglingLayers

# 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**

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

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

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

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

# Parameter Shift Rule

## arXiv 1905.13311

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

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- 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

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