Intro to Quantum Computing ML for Neutrino Astronomy

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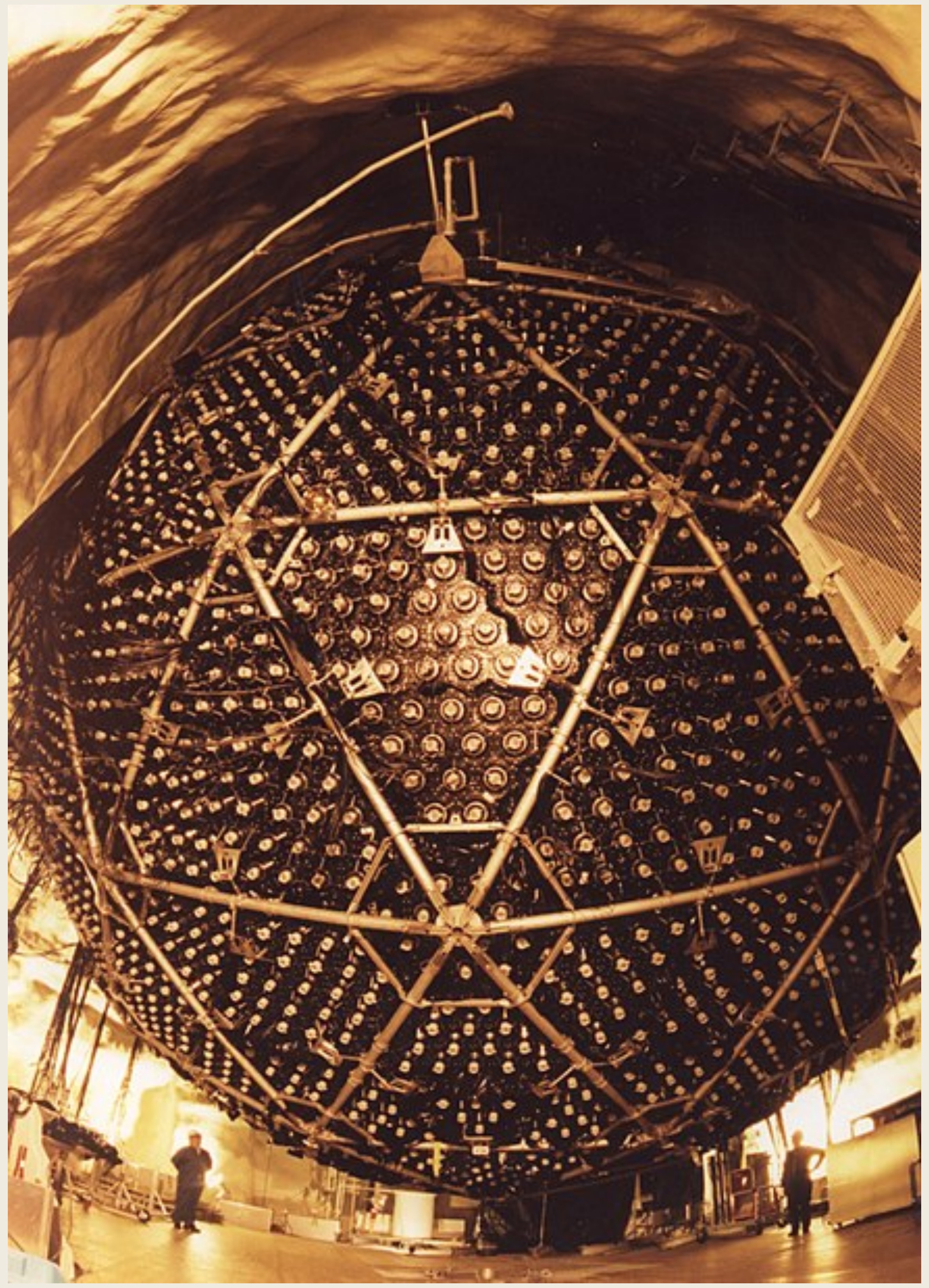
Machine Learning

- In the 1990s the initial exploration of ML in particle physics began: SNO experiment
- At the beginning, these neural networks did not outperform other statistical techniques but they did demonstrate capabilities
- However as expertise grew ML techniques began to surpass traditional reco
- Now ML has played a role in nearly every particle physics discovery and measurement since

Observation of high-energy neutrinos from the Galactic plane

ICECUBE COLLABORATION, R. ABBASI, M. ACKERMANN, J. ADAMS, J. A. AGUILAR, M. AHLERS, M. AHRENS, J. M. ALAMEDDINE, A. A. ALVES JR., [...], AND P. ZHELNIN

+380 authors Authors Info & Affiliations



https://en.wikipedia.org/wiki/Sudbury_Neutrino_Observatory

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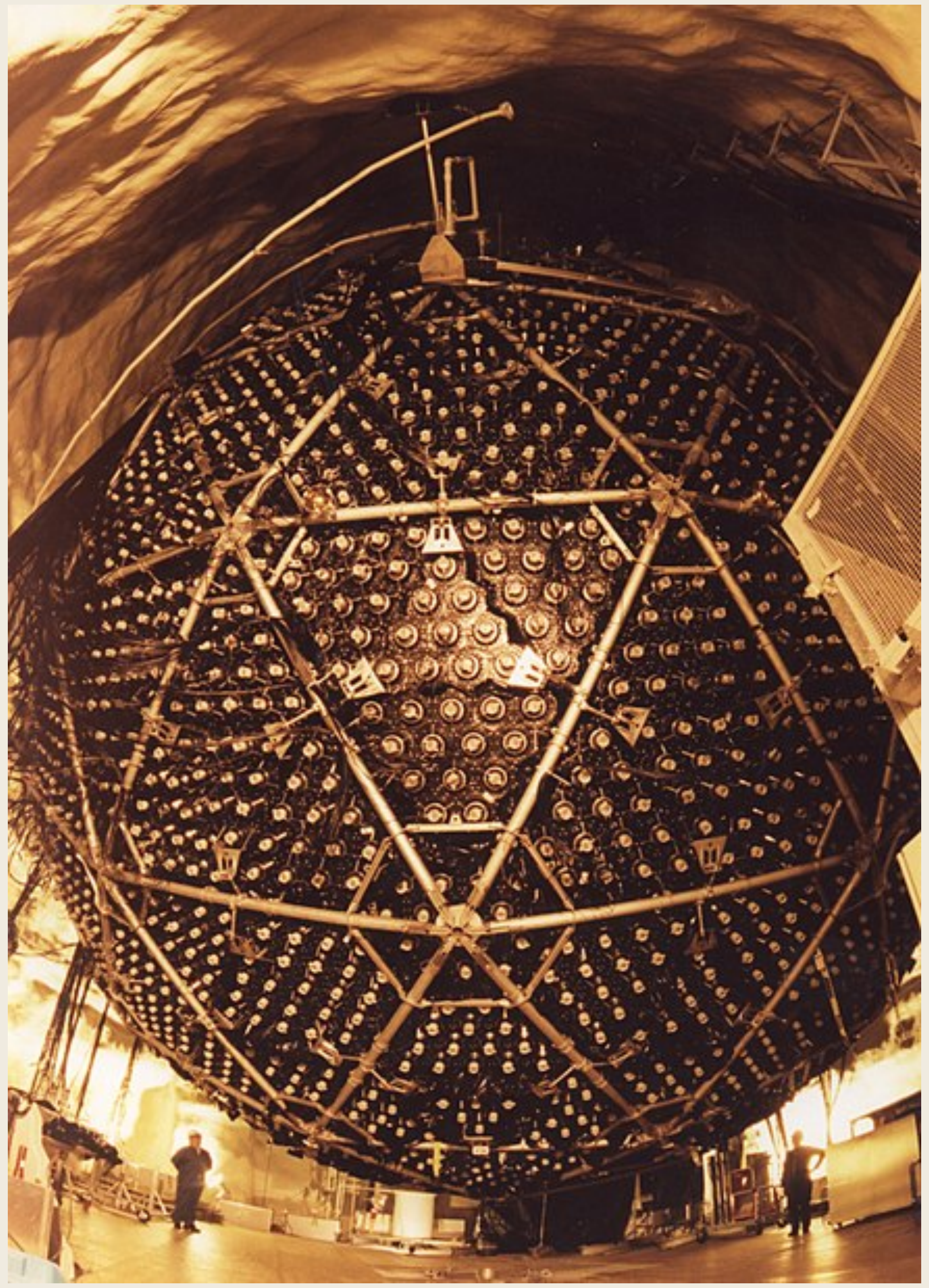
Measurement of the properties of Higgs boson production at $\sqrt{s} = 13$ TeV in the $H \rightarrow \gamma\gamma$ channel using 139 fb^{-1} of pp collision data with the ATLAS experiment



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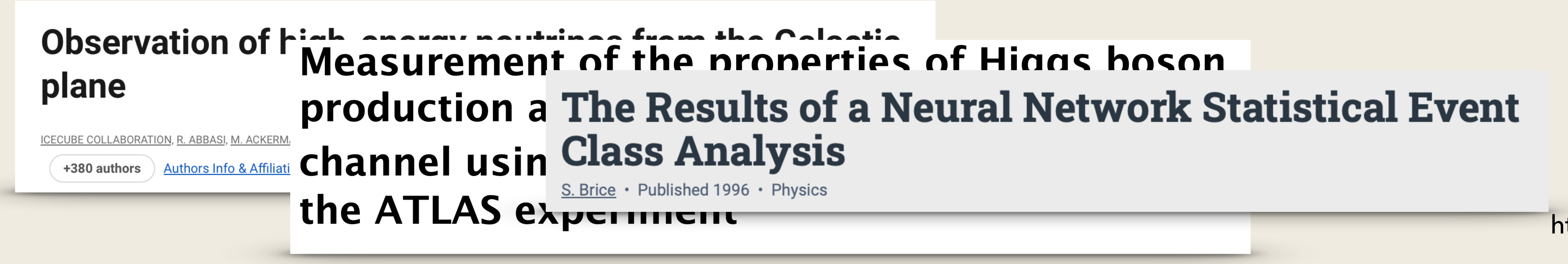
- In the 1990s the initial exploration of ML in particle physics began: SNO experiment
- At the beginning, these neural networks did not outperform other statistical techniques but they did demonstrate capabilities
- However as expertise grew ML techniques began to surpass traditional reco
- Now ML has played a role in nearly every particle physics discovery and measurement since
- What's the next iteration?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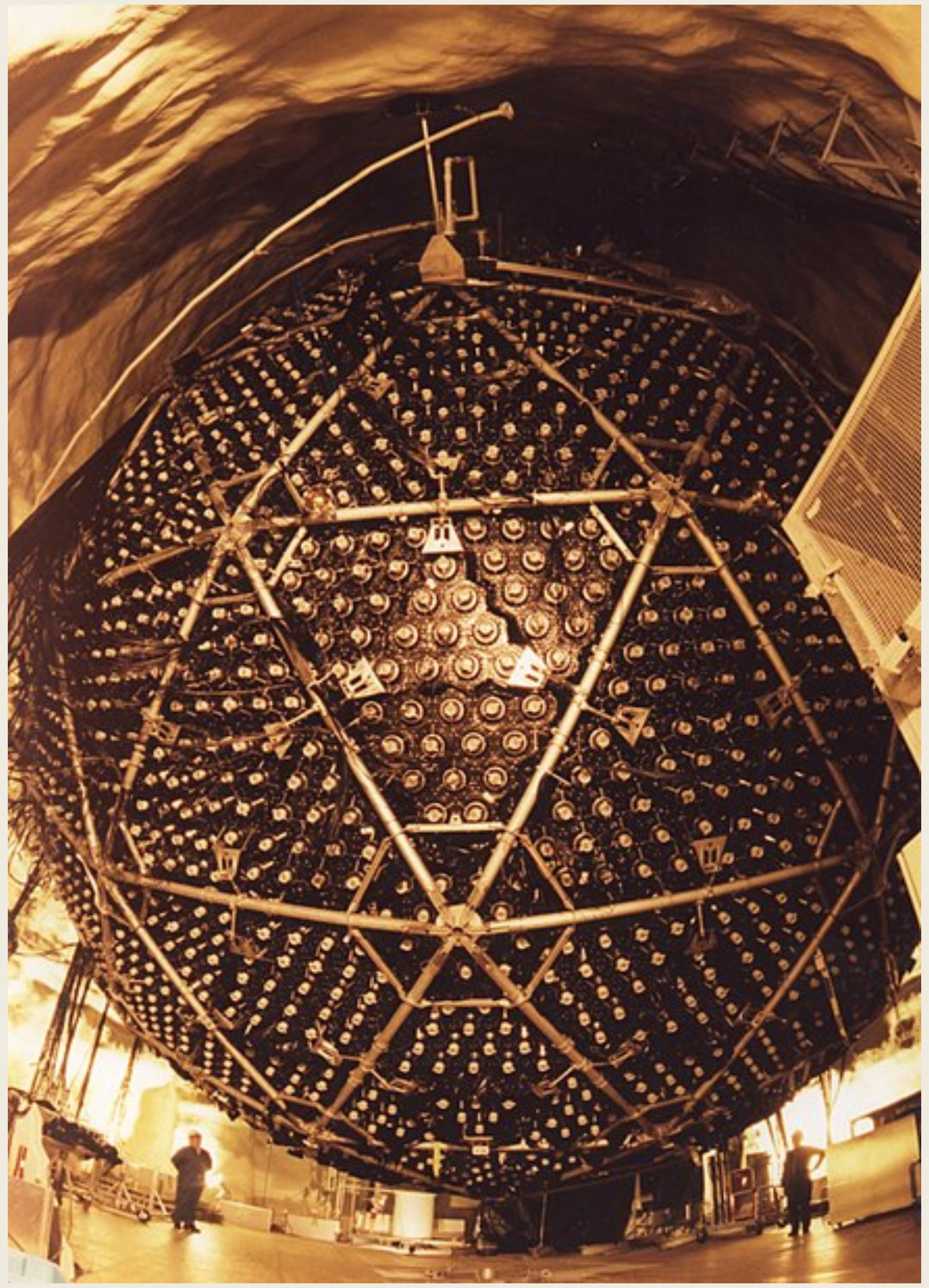
The Results of a Neural Network Statistical Event Class Analysis
S. Brice • Published 1996 • Physics



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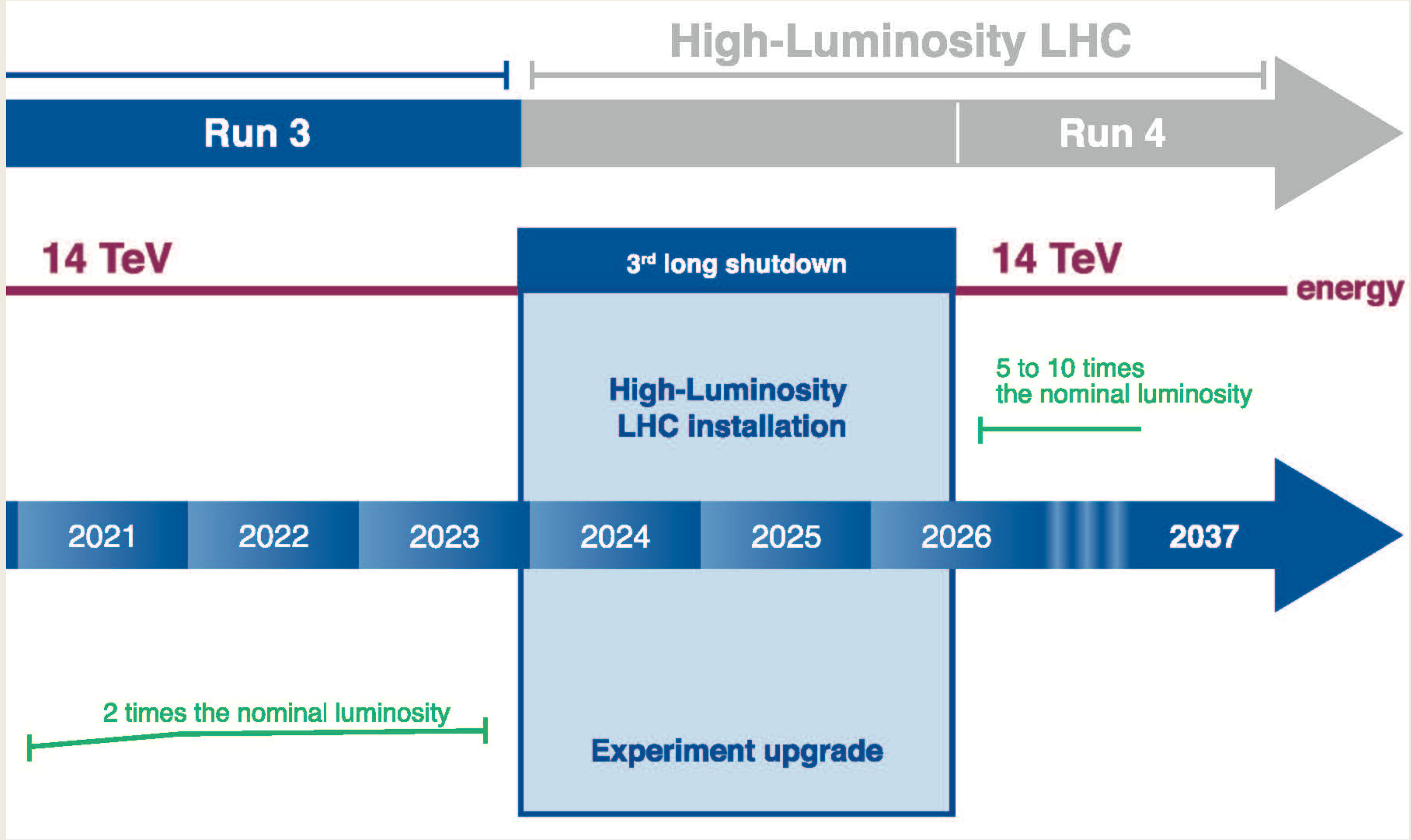
A Growing Data Challenge

- ML is essential in analyzing a commonality among experiments now: large data size
- In fact cuts are needed to manage modern experiments
- Even after cuts, datasets are huge
  - CERN produces > 300 TB of data per day
  - IceCube produces ~ 1 TB
- Templates based on our current understanding filters data
- Furthermore, next generation experiments will increase data output by an order of magnitude
- Could new physics be hiding in cut data?

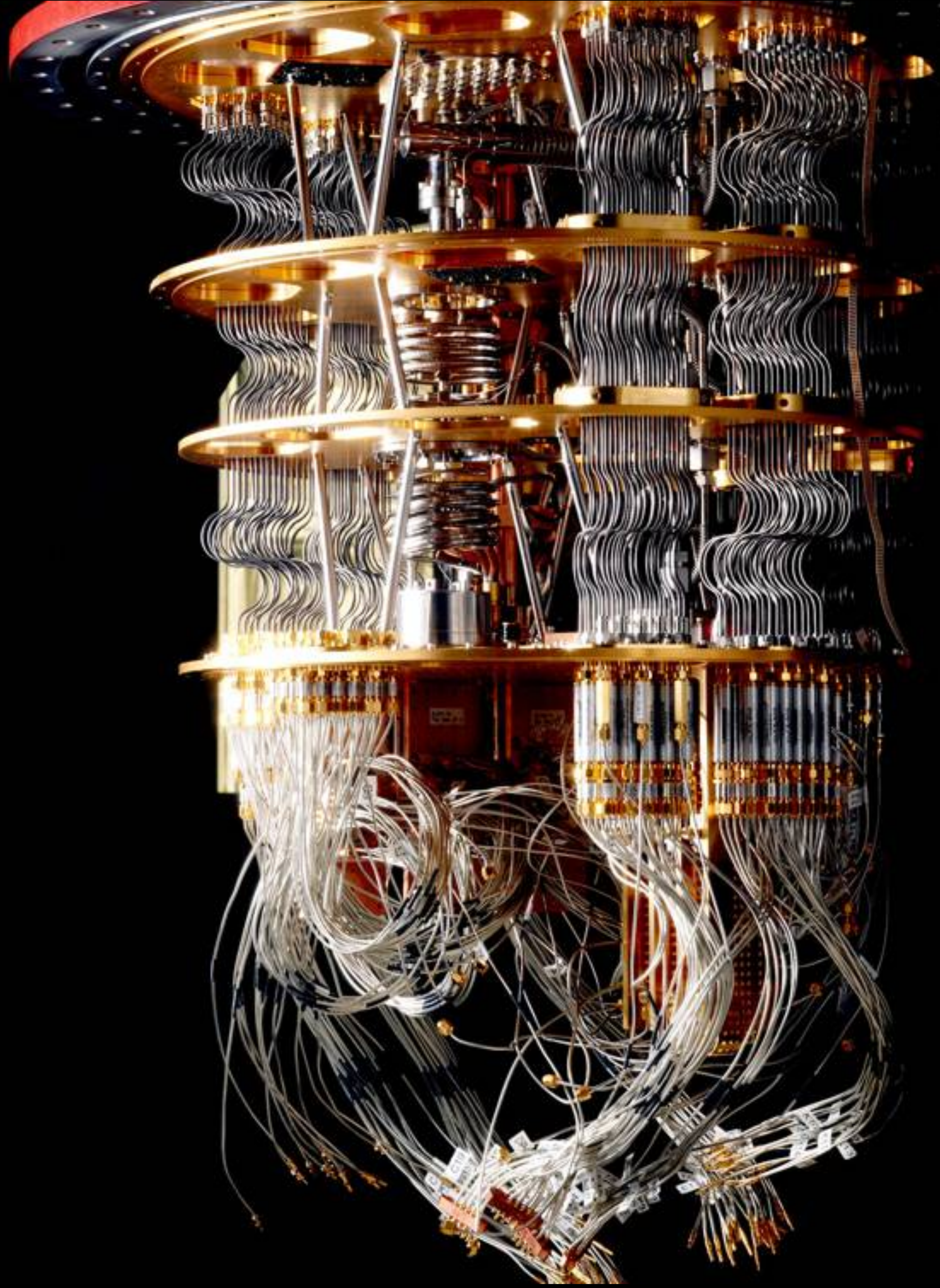


A Growing Challenge cont.

- We could be missing new physics due to un-modeled interactions **(streetlight effect)**
- Allowing additional data may be necessary for new physics
- For this, a paradigmatic shift is needed in data management to process trigger-level data

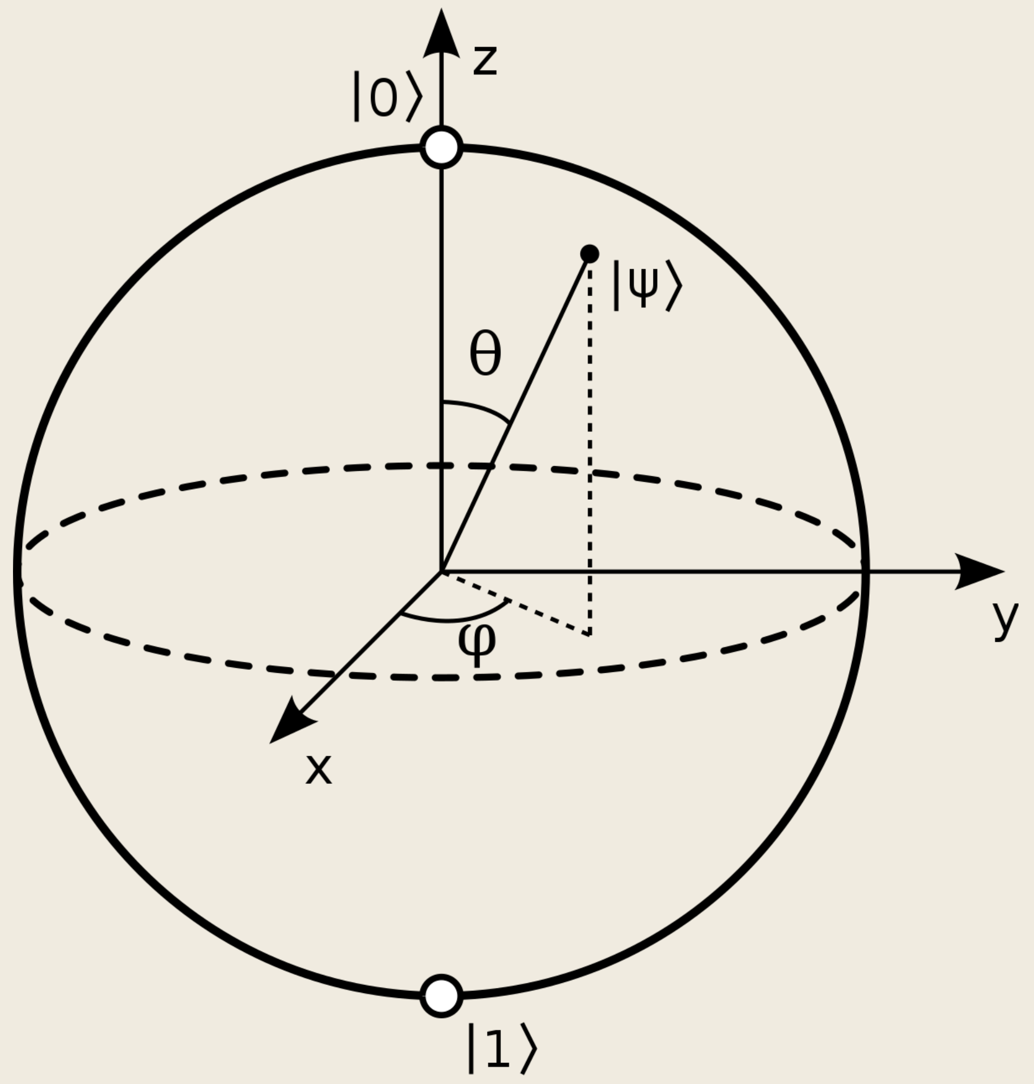
Quantum Computing

- A computer whose computations can only be described with the laws of quantum theory
  - **Exponentially large Hilbert space**
  - Entanglement
  - Superposition
  - Interference
- 2^N advantage over classical computers
- E.g. 8 classical bits → 3 "qubits", 64 bits → 6 "qubits", can store all of Google Drive cloud storage in ~60 qubits



Basics of Quantum Computing

- **Qubits** = basic unit of information in a QC (akin to a bit)
- Often represented by a Bloch sphere



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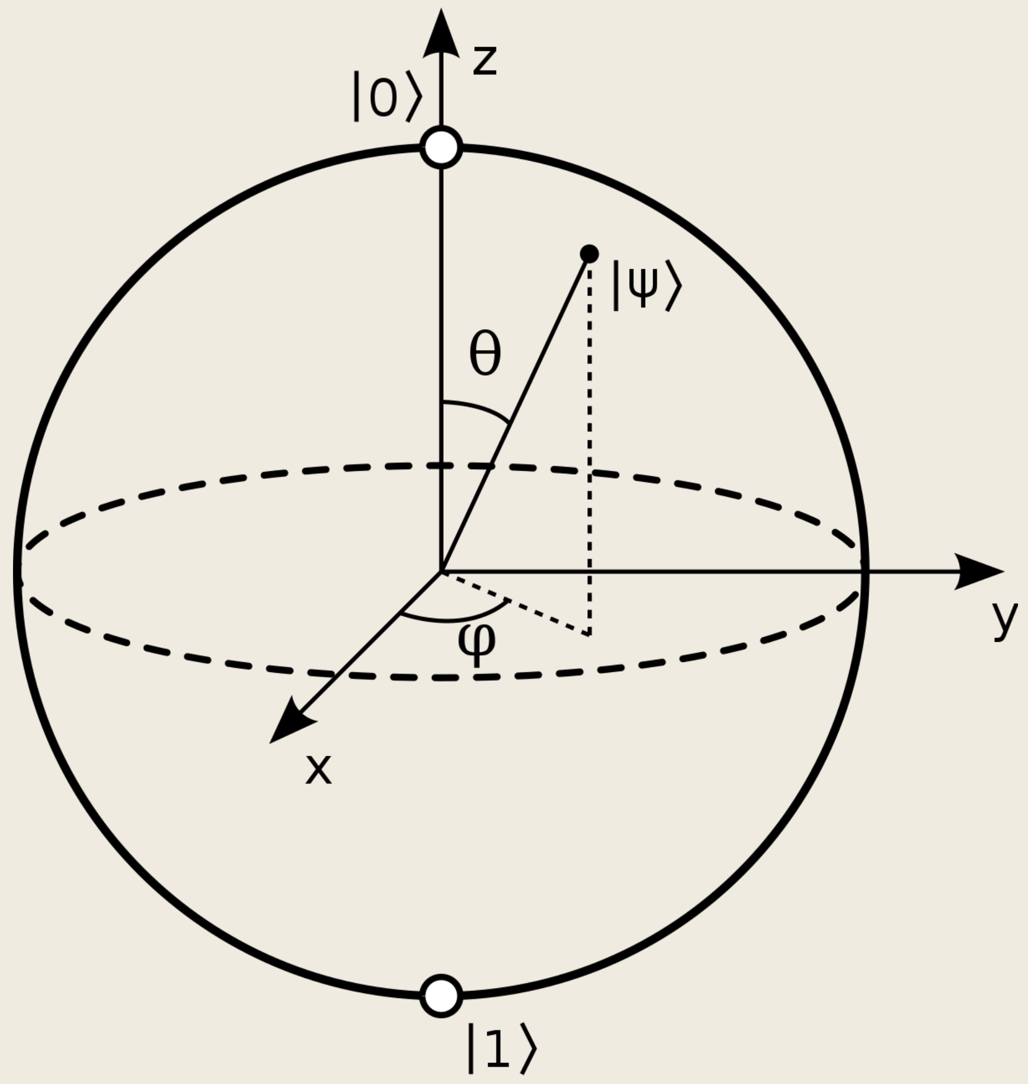
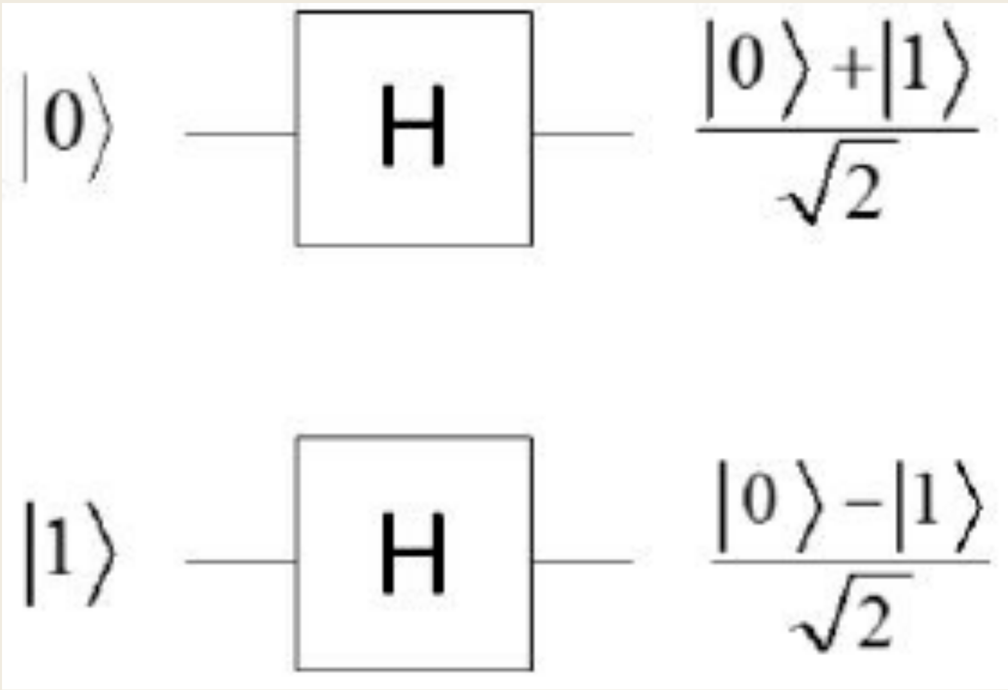
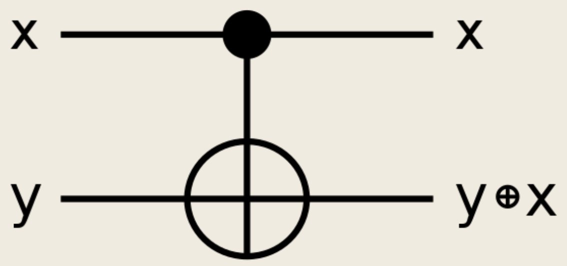
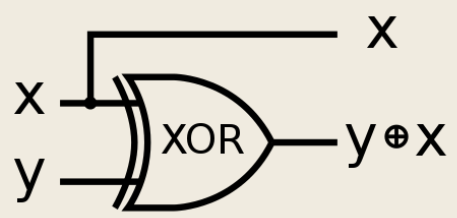


- **Quantum gates** = most basic operation that can performed on a qubit (or set of qubits)
- Two basic quantum gates: Hadamard/CNOT
- Hadamard creates superpositions
- CNOT entangles
- Combination makes a Bell State





input		output	
x	y	x	y+x
|0⟩	|0⟩	|0⟩	|0⟩
|0⟩	|1⟩	|0⟩	|1⟩
|1⟩	|0⟩	|1⟩	|1⟩
|1⟩	|1⟩	|1⟩	|0⟩



input		output	
x	y	x	y+x
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

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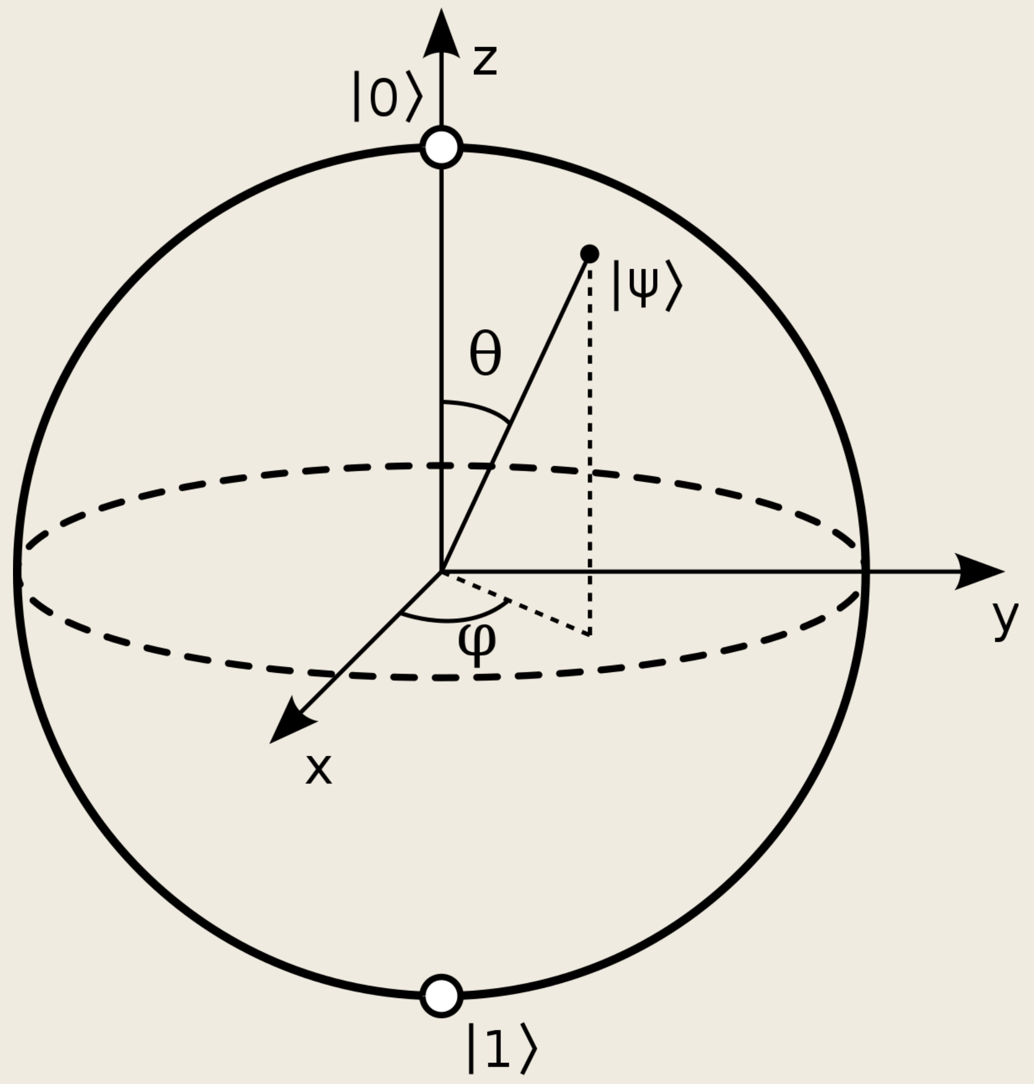

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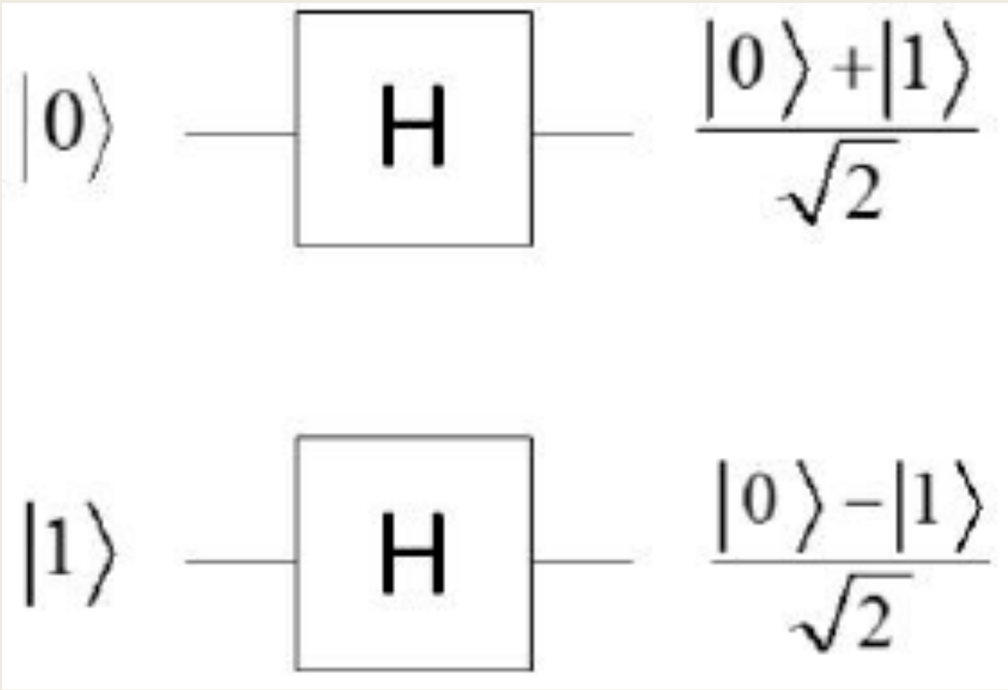

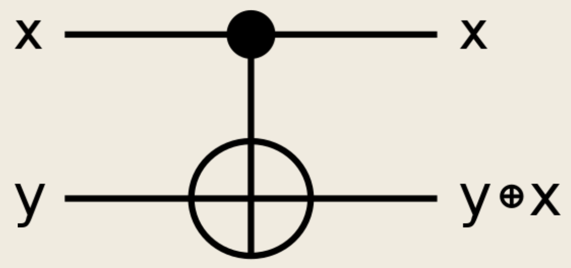

input		output	
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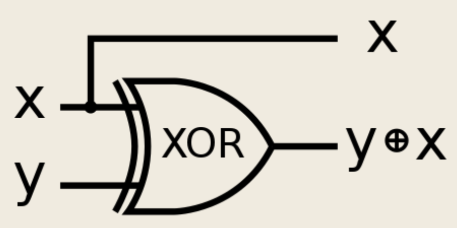
|0⟩	|0⟩	|0⟩	|0⟩
|0⟩	|1⟩	|0⟩	|1⟩
|1⟩	|0⟩	|1⟩	|1⟩
|1⟩	|1⟩	|1⟩	|0⟩



input		output	
x	y	x	y+x
0	0	0	0
0	1	0	1
1	0	1	1
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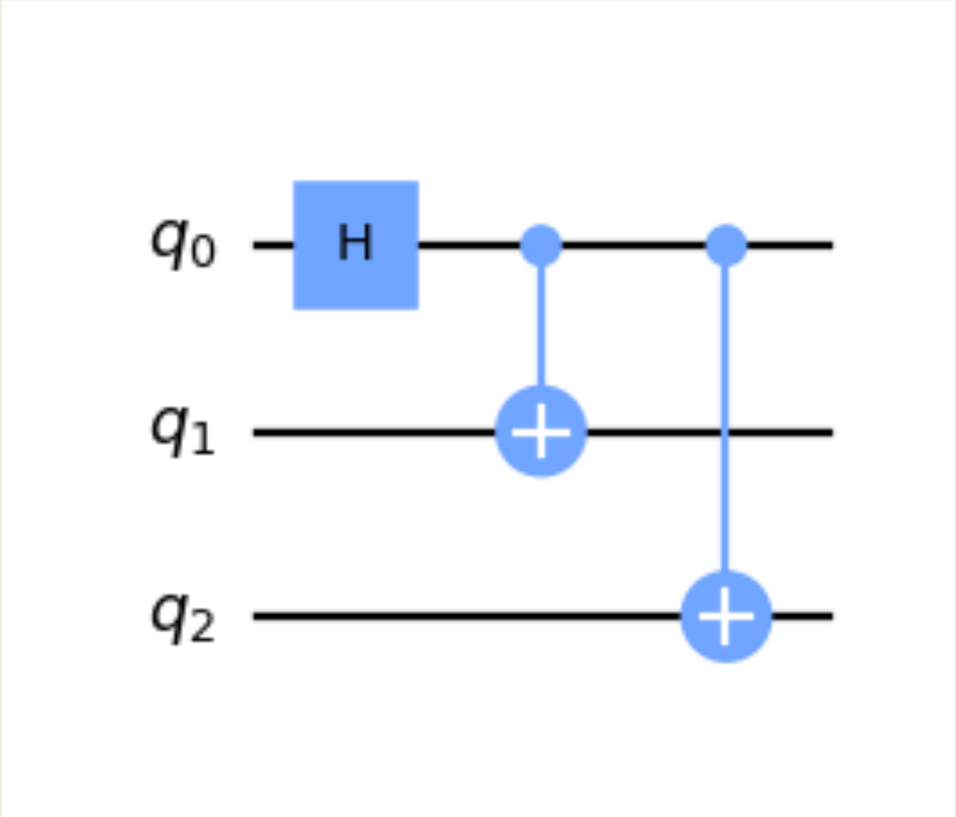
- **Quantum circuit** = a model for quantum computation in which a sequence of quantum gates are applied to a set of n qubits

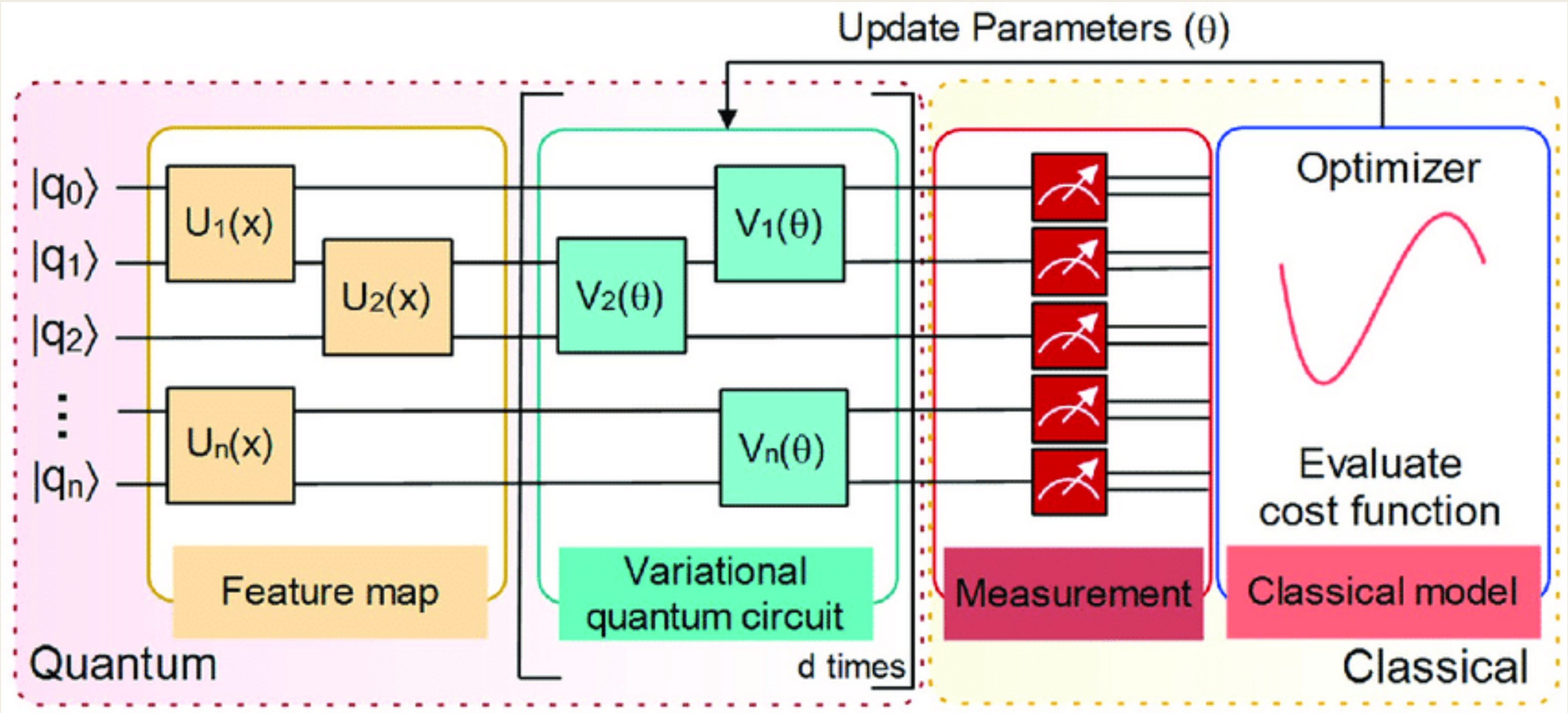


A Data Processing Pipeline Using QC

- We don't want to just store data on a QC, we want to process it as well
- Its runtime is costly to do: classical → quantum or quantum → classical transfers of data
- We want a fully "quantum pipeline", no classical preprocessing

E.g. …

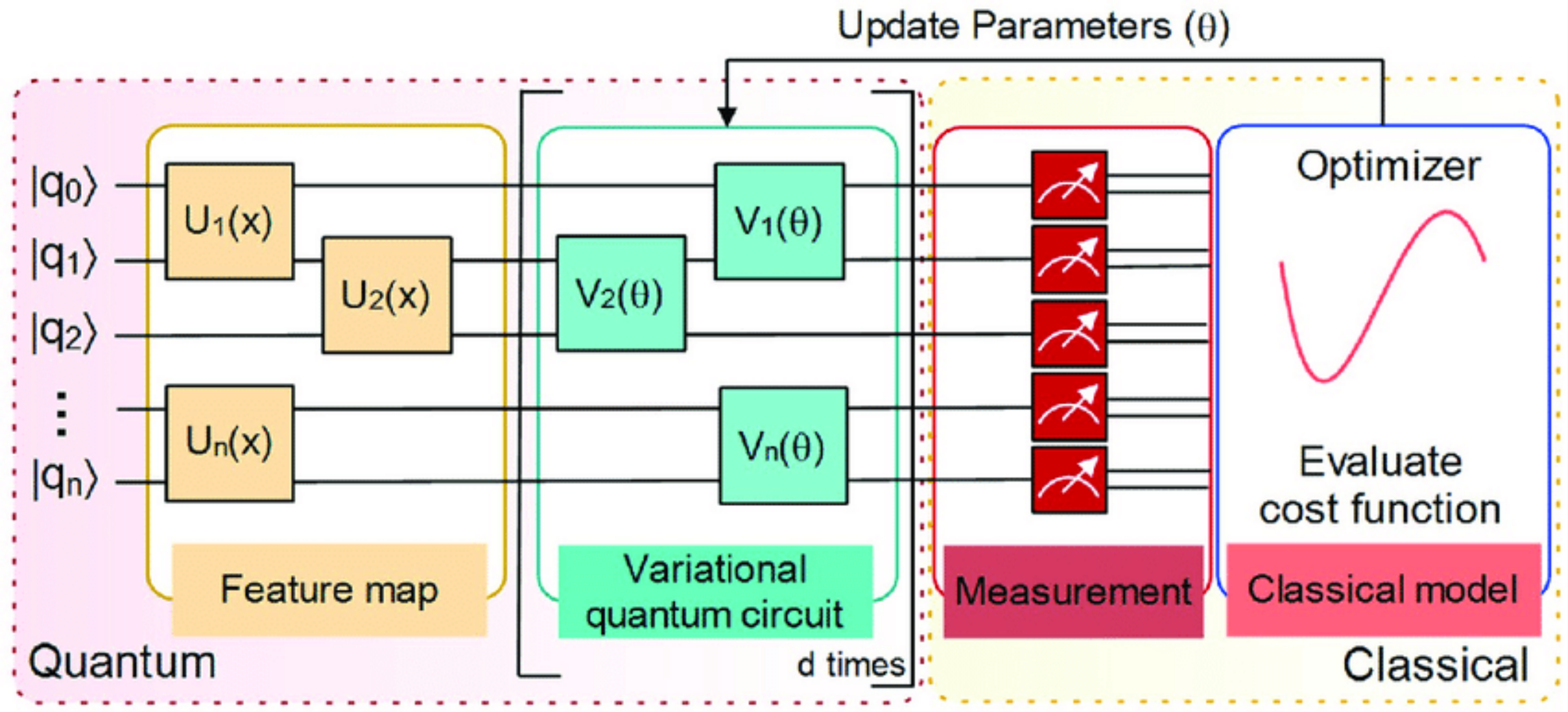
Classical Data →



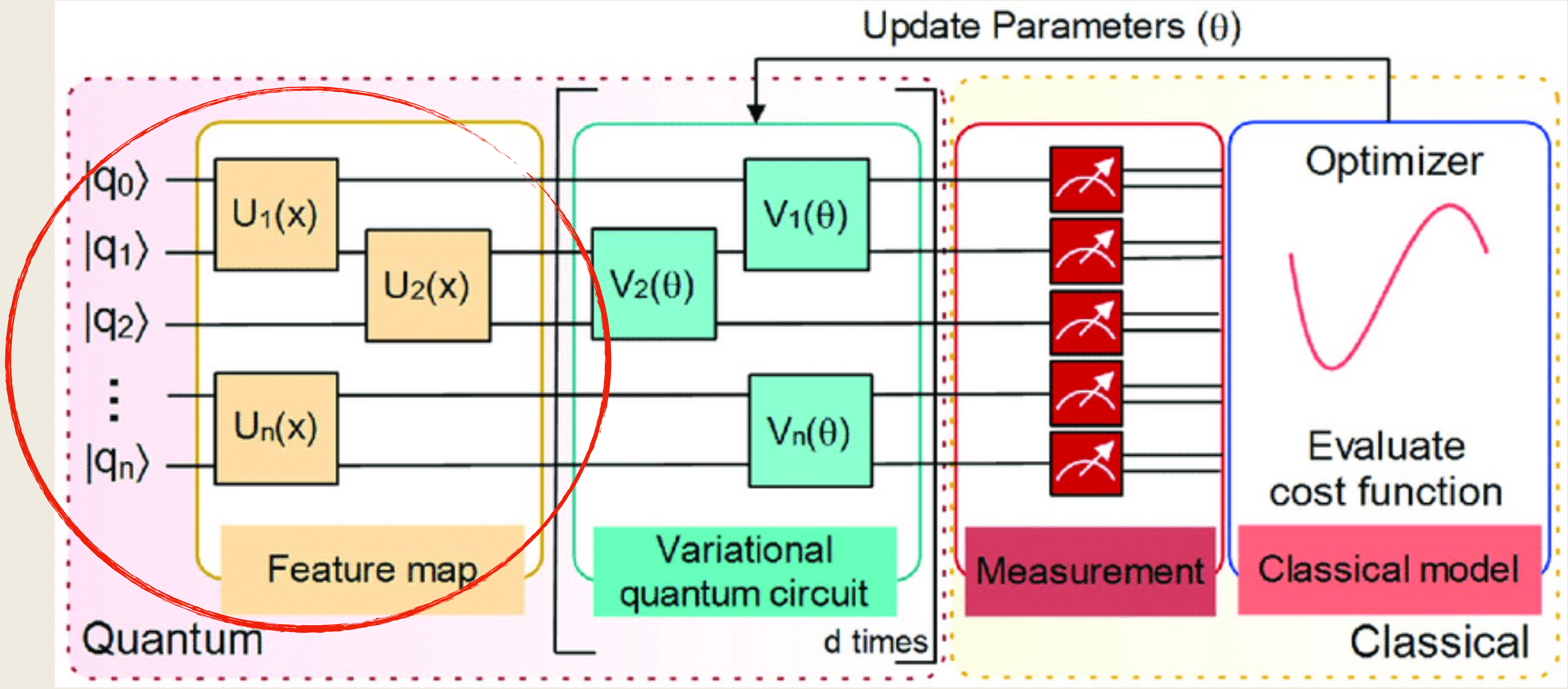
→ Classification

Rest of the talk: QML with a Variational Quantum Circuit

A VQC is a low depth, low width choice suitable for ML applications on current quantum computers.



Rest of the talk: QML



Data Encoding

- "Data encoding is often the most crucial step in QML with classical data: it influences potential quantum advantage, learning performance and runtime."
- Most other QML encoding schemes involve some classical preprocessing then using either amplitude/basis encoding (arXiv:2012.11560, arXiv.1907.00397, arXiv.2010.07335)
- We want to avoid classical preprocessing while still working within the constraints of Near-Intermediate Scale Quantum (NISQ) computers

Shuld et al. Machine Learning with Quantum Computers

Background: Data Encoding

- **Amplitude encoding** can store information with 2^N efficiency
  - Susceptible to decoherence

$$\mathbf{x} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}$$

$$|\psi_{\mathbf{x}}\rangle = \sum_{i=0}^{N-1} x_i |i\rangle.$$

$$|\mathbf{x}\rangle = \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle - \frac{1}{2}|10\rangle - \frac{1}{2}|11\rangle$$

Background: Data Encoding

- **Amplitude encoding** can store information with 2^N efficiency
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- **Basis encoding** is the simplest encoding
  - No quantum advantage, a 1 to 1 mapping

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$$x = 1011 \rightarrow |1011\rangle$$

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$$x = 1011 \rightarrow |1011\rangle$$

- **Angle encoding**
  - Rotations around principle axes of Bloch sphere
  - Principle encoding scheme by others in QML HEP

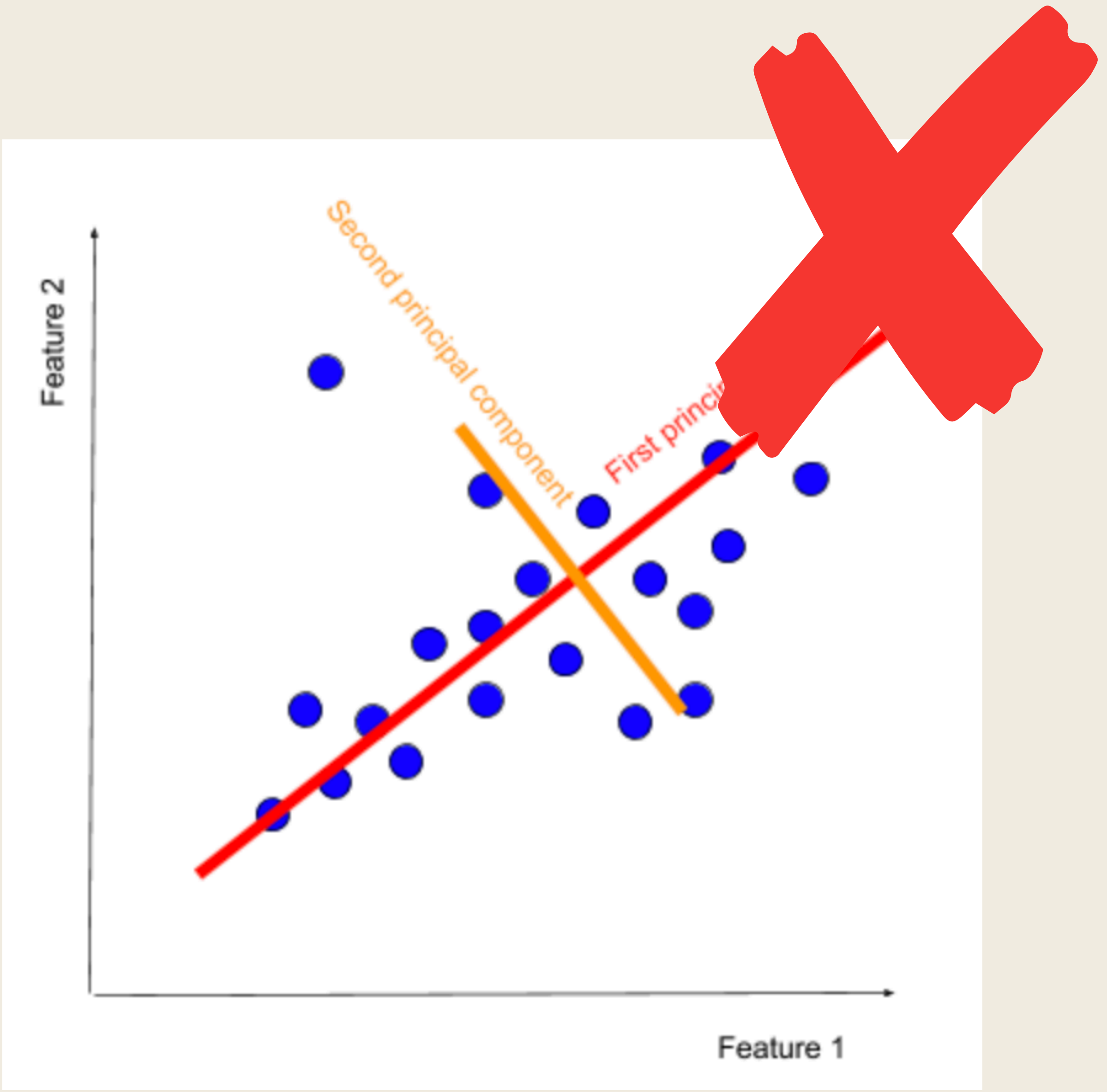
$$|\mathbf{x}\rangle = \bigotimes_{i}^{n} R(\mathbf{x}_i)\,|0^n\rangle$$

Rotation by pi around y axis on Bloch sphere

$$\mathbf{x} = \begin{bmatrix} \pi \\ \pi \\ \pi \end{bmatrix} \rightarrow |111\rangle$$

Recap so far

- We want to use quantum computers because they can handle computational challenges of increase data loads of upcoming experiments
- This way we can investigate more data
- We don’t want to reduce the complexity of our data (no PCA, no classical dimension reduction)
- Traditional quantum encoding schemes either don’t use quantum advantage or are overly susceptible to decoherence
- So we want a near lossless quantum encoding scheme with quantum advantage

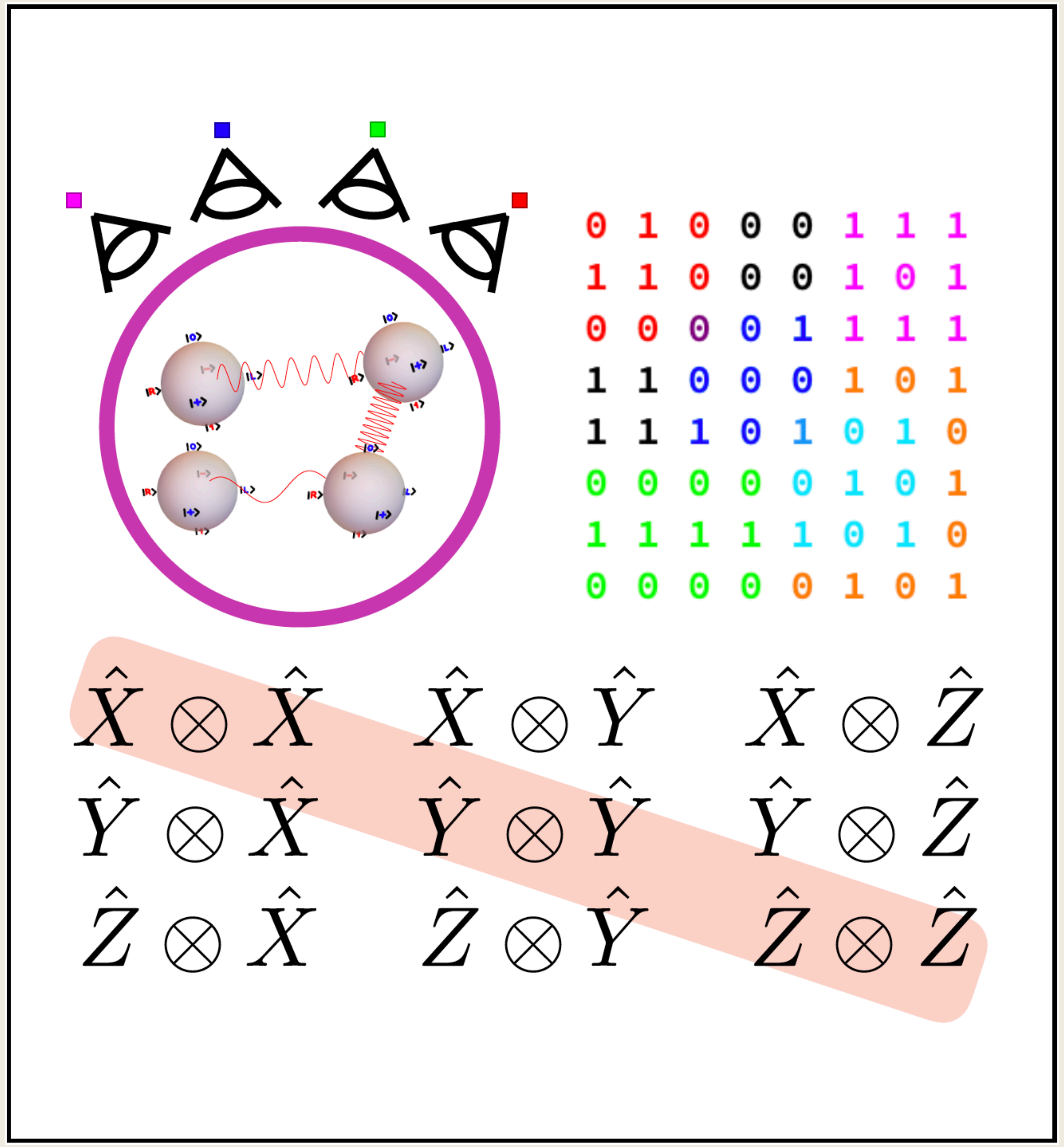


Quantum Random Access Codes (QRAC)

- We want a resilient data encoding scheme that still occupies some advantage over classical systems
- Encodes digital information in correlations between qubits
- ~a 1.5^N advantage over classical systems
- It's resilient: for N $\geq$ 18 nearly lossless (0.999) recovery rate
- For N $\geq$ 14 QRAC has greater success than classical counterparts

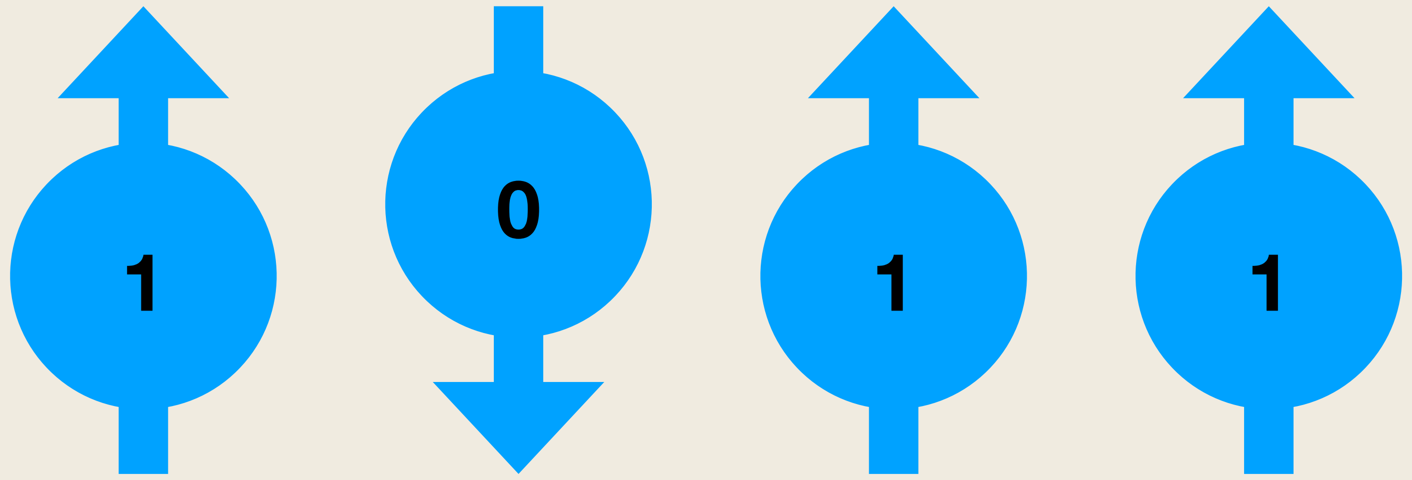
Random access codes via quantum contextual redundancy

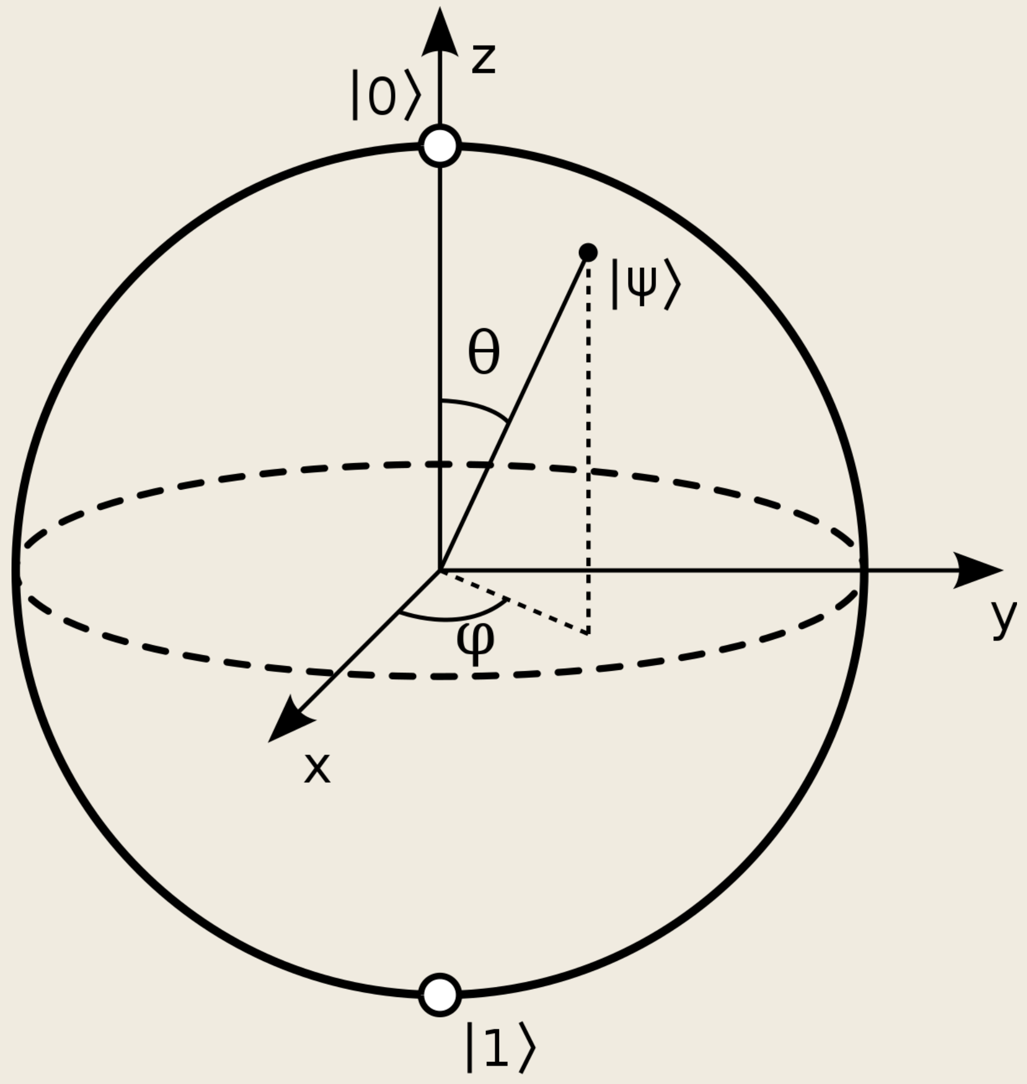
Giancarlo Gatti,[1,2,*] Daniel Huerga,[1,†] Enrique Solano,[1,3,4,5,‡] and Mikel Sanz[1,4,5,§]



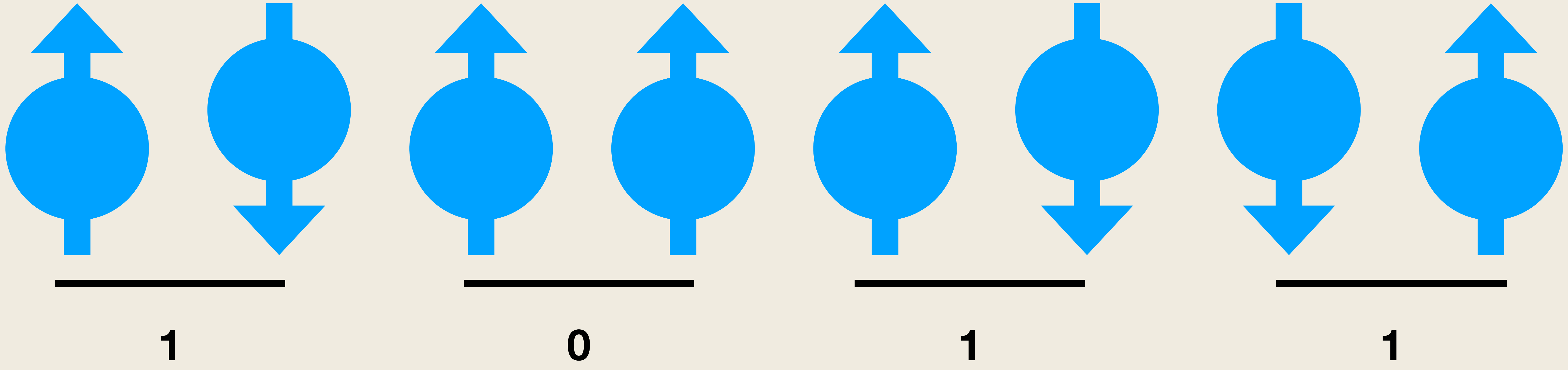
Digital Quantum Encoding

- For example, I want to encode the bit string '1011'
- Option 0: One-to-one mapping to z-spin





- Option 1: Two-to-one mapping to z-spins (have two options to encode)



Correlation-based digital encoding

- The set $\{X, Y, Z\}^{\otimes N}$ are parity observables (POs) where N is number of qubits
- Measuring using POs always yield a ± 1
- Instead of assigning a bit to each PO, assign a bit to each pair of POs, $0 \leftrightarrow =$ and $1 \leftrightarrow \neq$
- We create eigenstates of sets of commuting POs, these are our compressed states that when measured later recover our input data

b^{target}	1		0		1		1		
PO relationship	$\neq$		$=$		$\neq$		$\neq$		ZZ
POs	XX	XY	XZ	YX	YY	YZ	ZX	ZY	NA
Option 1	$+1$	-1	$+1$	$+1$	$+1$	-1	$+1$	-1	NA
Option 2	-1	$+1$	-1	-1	-1	$+1$	-1	$+1$	NA

Example for encoding '1011' in two qubits

0 Let us use n-qubit systems
(and draw figures for n=4)

1 Alice has m bits of data

1	1	0	0	1	0	0	1
0	0	0	0	1	1	1	1
1	1	0	1	1	0	1	0
1	0	1	0	0	0	1	0
0	0	1	0	0	0	0	1

that she wants Bob to randomly access

$m = (3^n - 1)/2$

2 Alice maps her data to outcomes of n-body Pauli observables

1 $\begin{cases} X_1X_2X_3X_4 & \text{yields +1 (more than -1)} \\ X_1X_2X_3Y_4 & \text{yields -1 (more than +1)} \end{cases}$

1 $\begin{cases} X_1X_2X_3Z_4 & \text{yields -1 (more than +1)} \\ X_1X_2Y_3X_4 & \text{yields +1 (more than -1)} \end{cases}$

0 $\begin{cases} X_1X_2Y_3Y_4 & \text{yields -1 (more than +1)} \\ X_1X_2Y_3Z_4 & \text{yields -1 (more than +1)} \end{cases}$

⋮ 3^n observables

3a Alice prepares a group of n-qubit states which collectively have those outcome preferences

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$$
$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0001\rangle + i\,|1110\rangle)$$
$$|\psi_3\rangle = \frac{1}{\sqrt{2}}(|000+\rangle - |111-\rangle)$$

⋮ $O(n(3/2)^n)$ states

She sends a few copies of each state to Bob (k/n states in total)

3b E.g., the state $|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$ yields

+1 in $X_1X_2X_3X_4$, -1 in $X_1X_2Y_3Y_4$,
-1 in $X_1Y_2X_3Y_4$, -1 in $X_1Y_2Y_3X_4$,
-1 in $Y_1X_2X_3Y_4$, -1 in $Y_1X_2Y_3X_4$,
-1 in $Y_1Y_2X_3X_4$, +1 in $Y_1Y_2Y_3Y_4$
and +1 in $Z_1Z_2Z_3Z_4$, with probability 1

4 Bob measures the states with some of the observables

$|\psi_1\rangle$ $\mathcal{O}$ $|\psi_2\rangle$ $\mathcal{O}$ $|\psi_3\rangle$ $\mathcal{O}$

He finds their preferred outcomes

5 Bob reconstructs a fragment of Alice's original data

1	1	0

$m \rightarrow k$ QRAC

Optimizations

- Which set of preferred parities to chose from out of 2^N choices where N are number of couples of POs
  - First compute all compatible well-defined outcomes for all possible eigenstates
  - Compare eigenvalues from this optimization to compatible preferred parities
- Which eigenstates best represents that chosen preferred parity order
  - We want a low sampling requirement
  - Least number of states

Neutrino Astronomy: IceCube Events

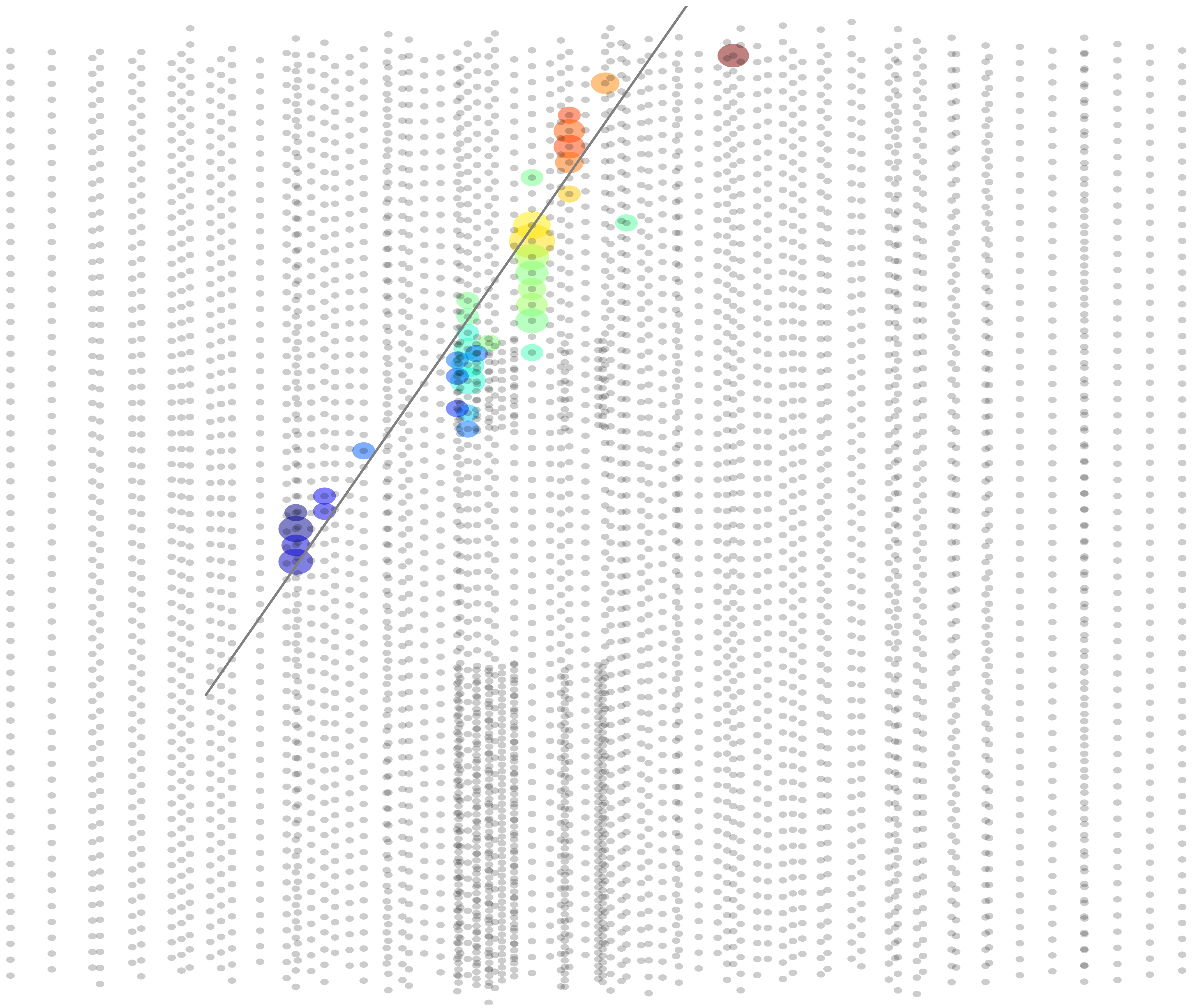
x	95.3 m	01000010101111101001100110011010
y	75.8 m	11000010100101111001100110011010
z	484.6 m	01000011111100100100110011001101
Q_{tot}	2.84 PE	01000000001101011100001010001111
$\bar{t}$	26.2 ns	01000001110100011001100110011010

0100001010111110100110011001101011000010100
1011110011001100110100100001111110010010011
0011001101010000000011010111000010100011110
1000001110100011001100110011010

Digitization Scheme: takes Optical Module (OM) position, light and time information and converts to binary. Each circle in image is a OM, size of circle indicates amount of light, color indicates time (red → purple)

This is our input to our QRAC

Event example:



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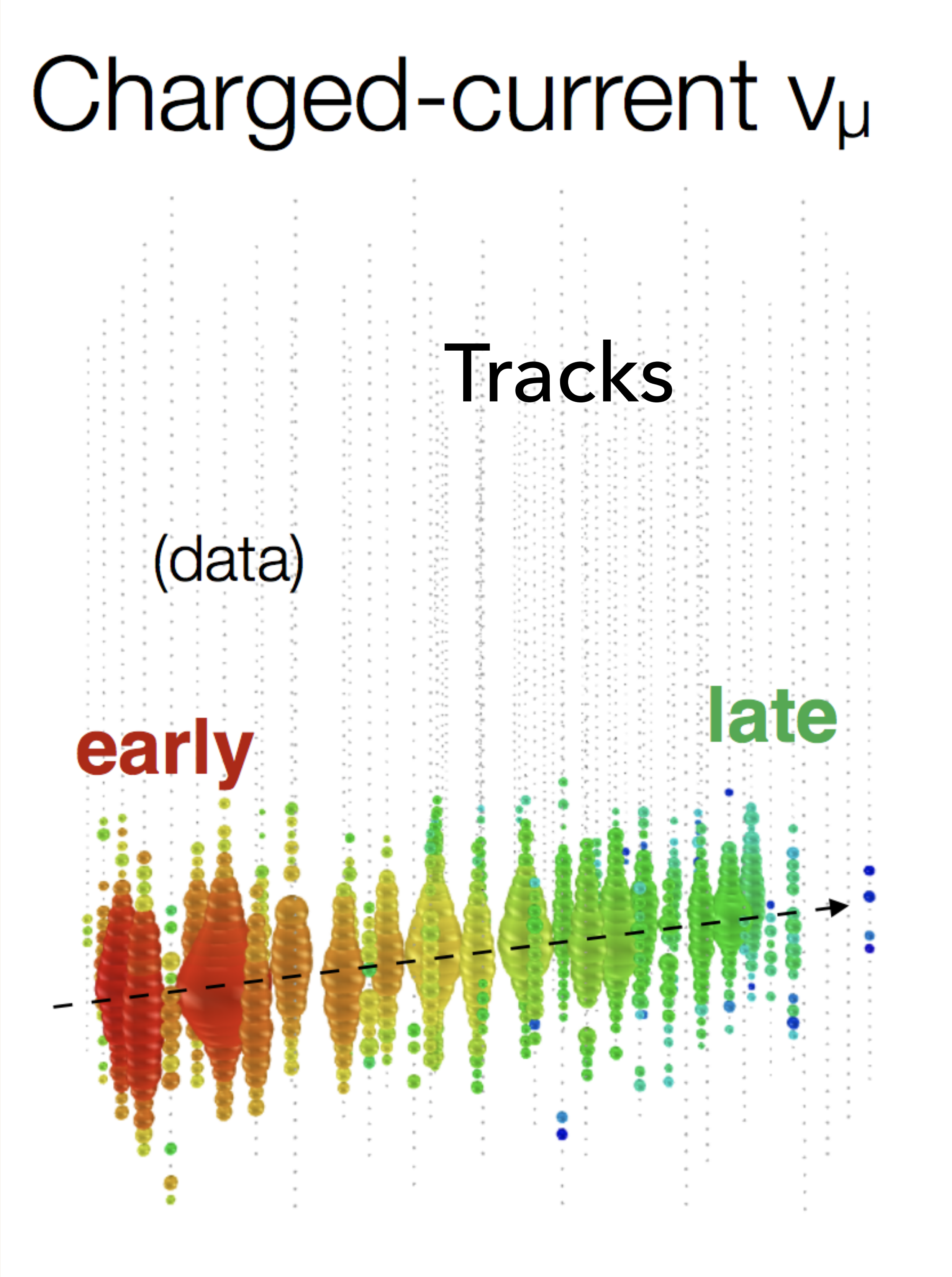
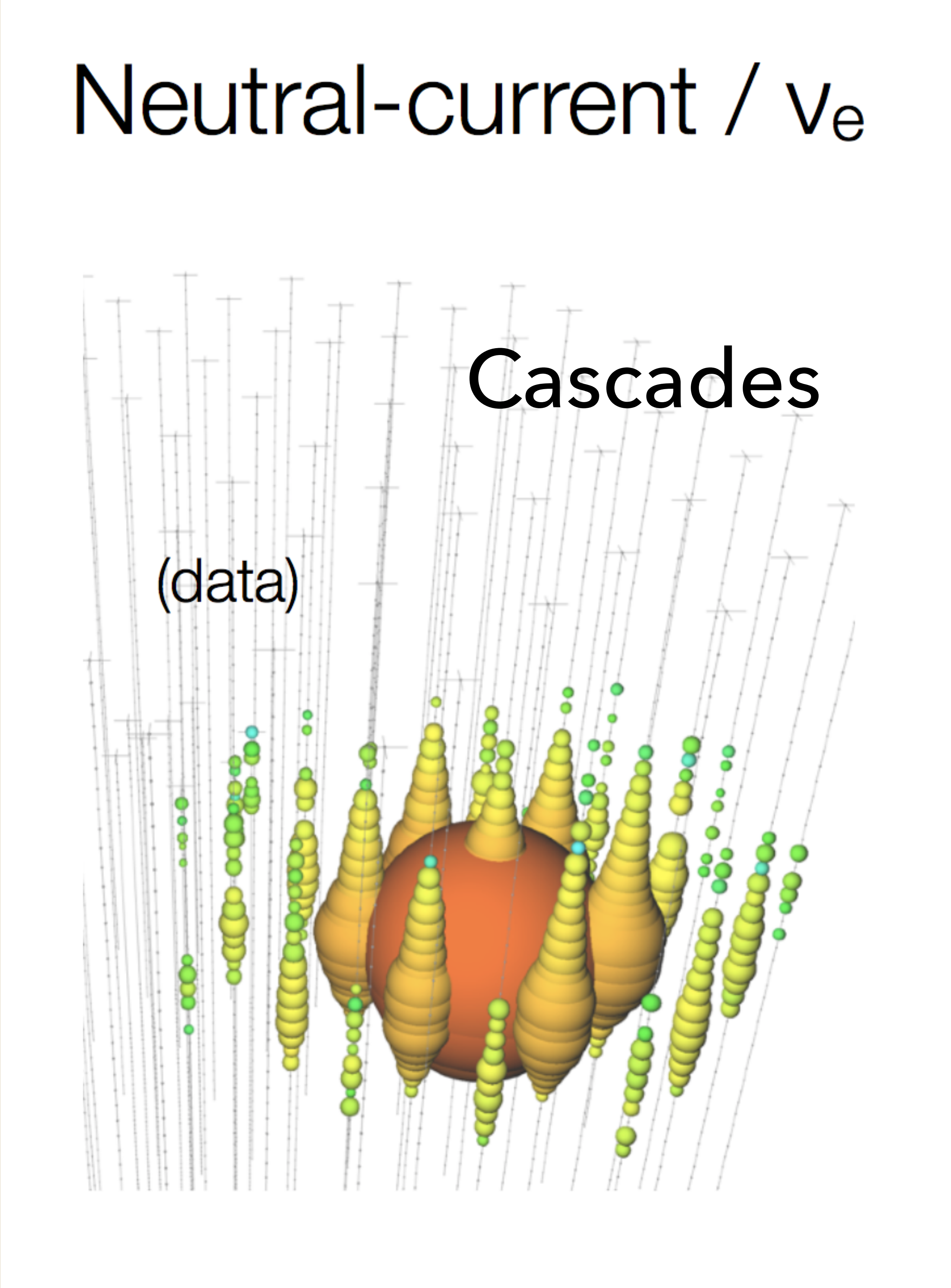
QRAC: What has been done so far

- Have achieved compression with 8 qubits
- Almost demonstrated storage/retrieval of IceCube simulation data with 14 qubits

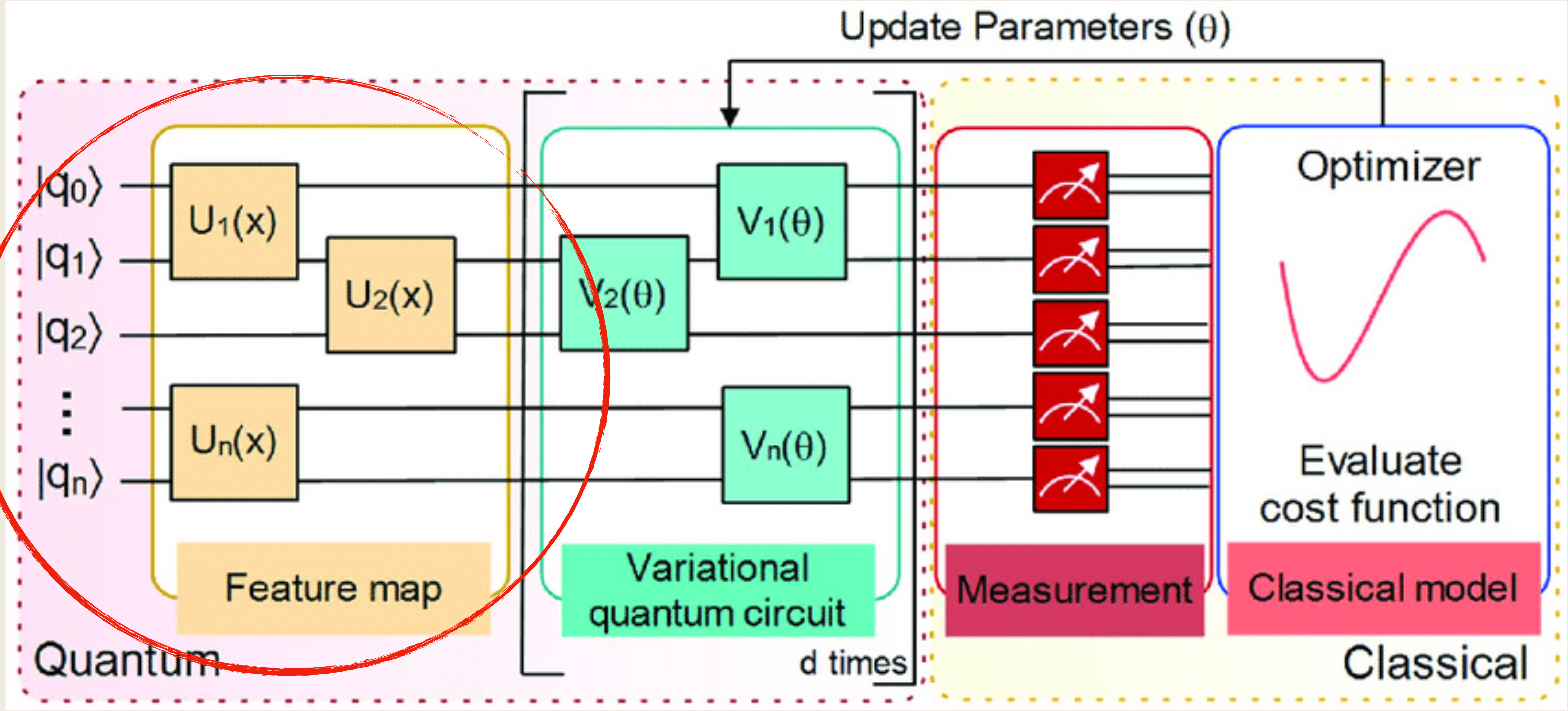
Plan with IceCube data

- Take set of IceCube data: tracks/cascades ($\nu_\mu CC/\nu_e CC$)
- Input into our QRAC
- Take states from QRAC, input them to train Variational Quantum Circuit
- First step, will be to investigate if VQC can classify tracks/cascades

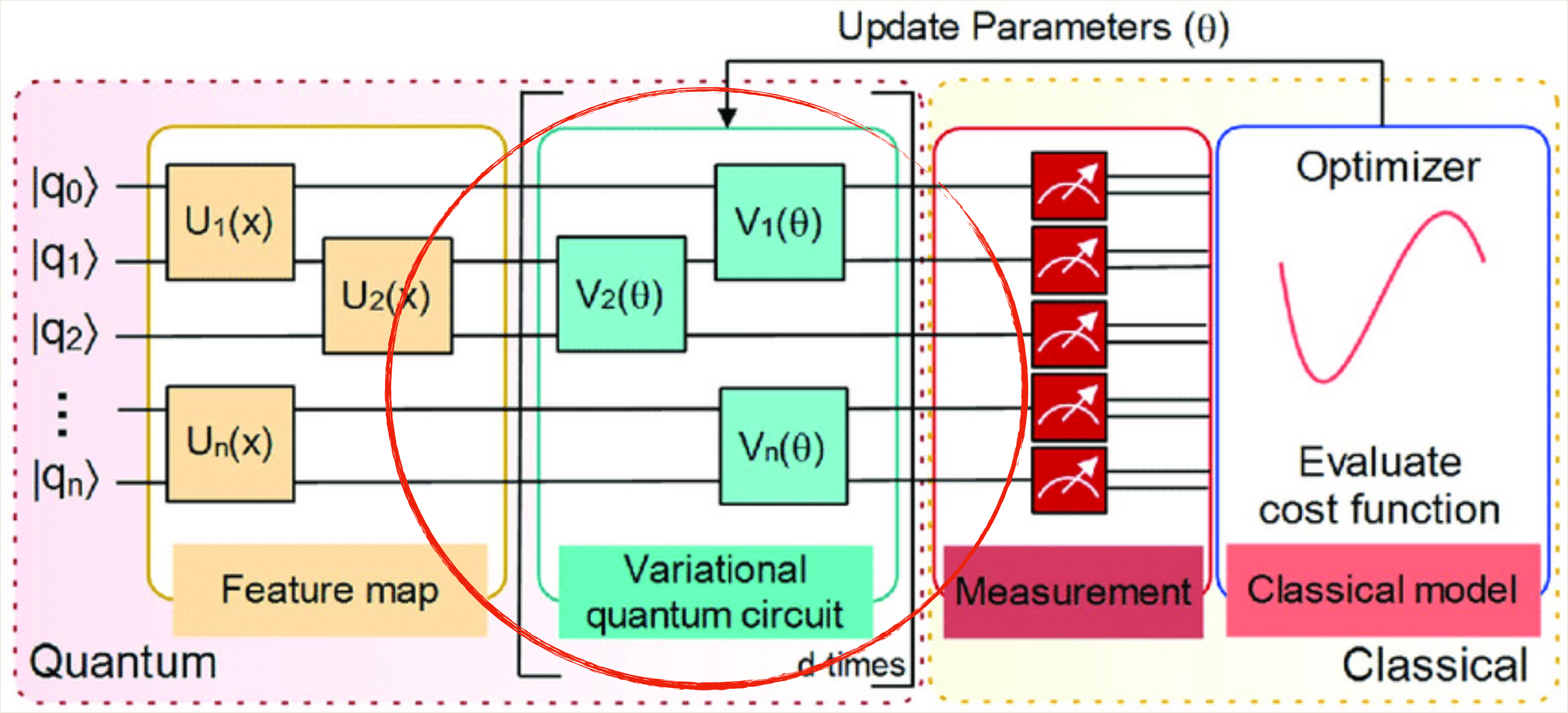




Variational Quantum Circuit

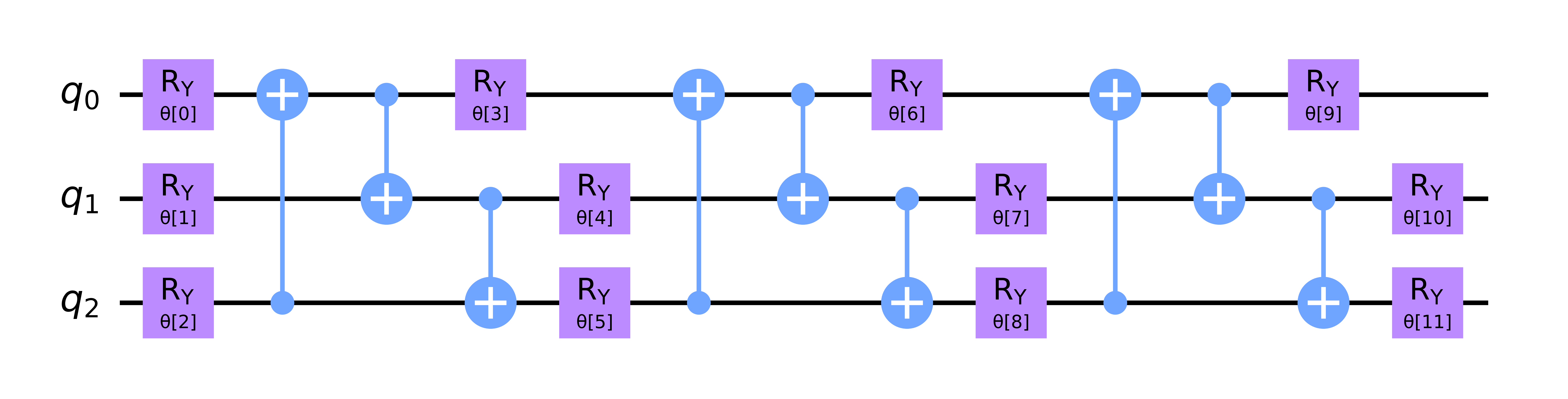


Variational Quantum Circuit



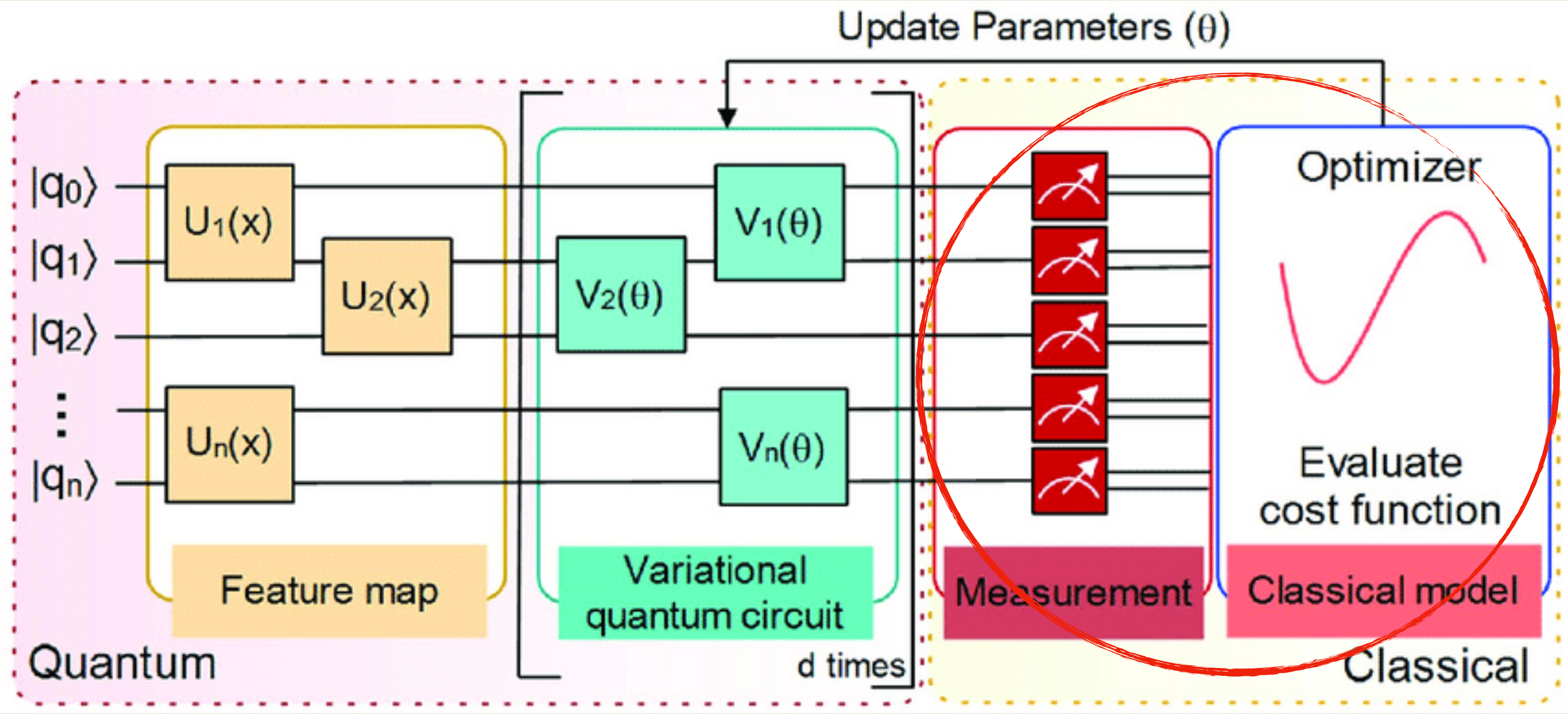
Model Circuit

- Is the variational part, where machine learning happens, called the "ansatz"
- The ansatz is parameterized by a set of free parameters θ that will be updated during training
- The structure of the ansatz, entanglement, type of rotations, number of parameters, number of gates, are all tunable



A 3 qubit example of a "RealAmplitudes" ansatz from qiskit.

Variational Quantum Circuit



Loss Function

- Default: is cross-entropy loss

$$\text{CrossEntropyLoss}(predict, target) = -\sum_{i=0}^{N_{\text{classes}}} target_i * log(predict_i).$$

  - The difference between the ideal distribution (the true labels/target) and the measured distribution
- Calculated across a batch of samples, and the average is taken across the batch to obtain the final loss value for that iteration
- Others like MSE are also used
- Inherently a classical operation

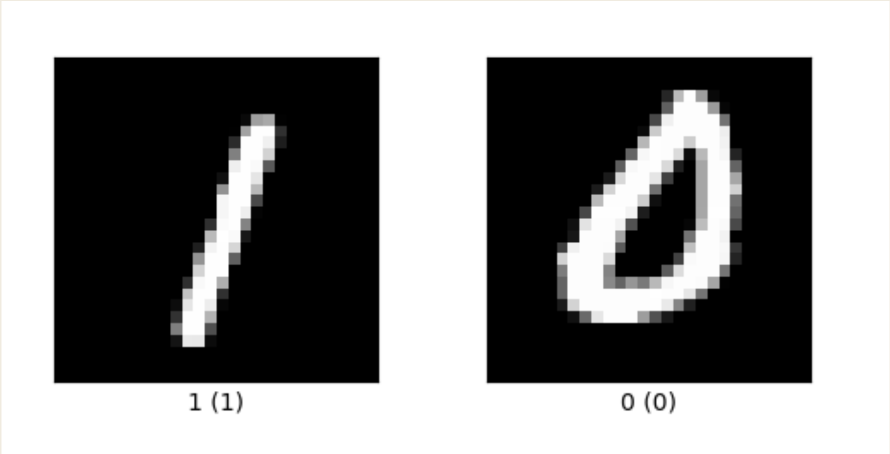
Optimization

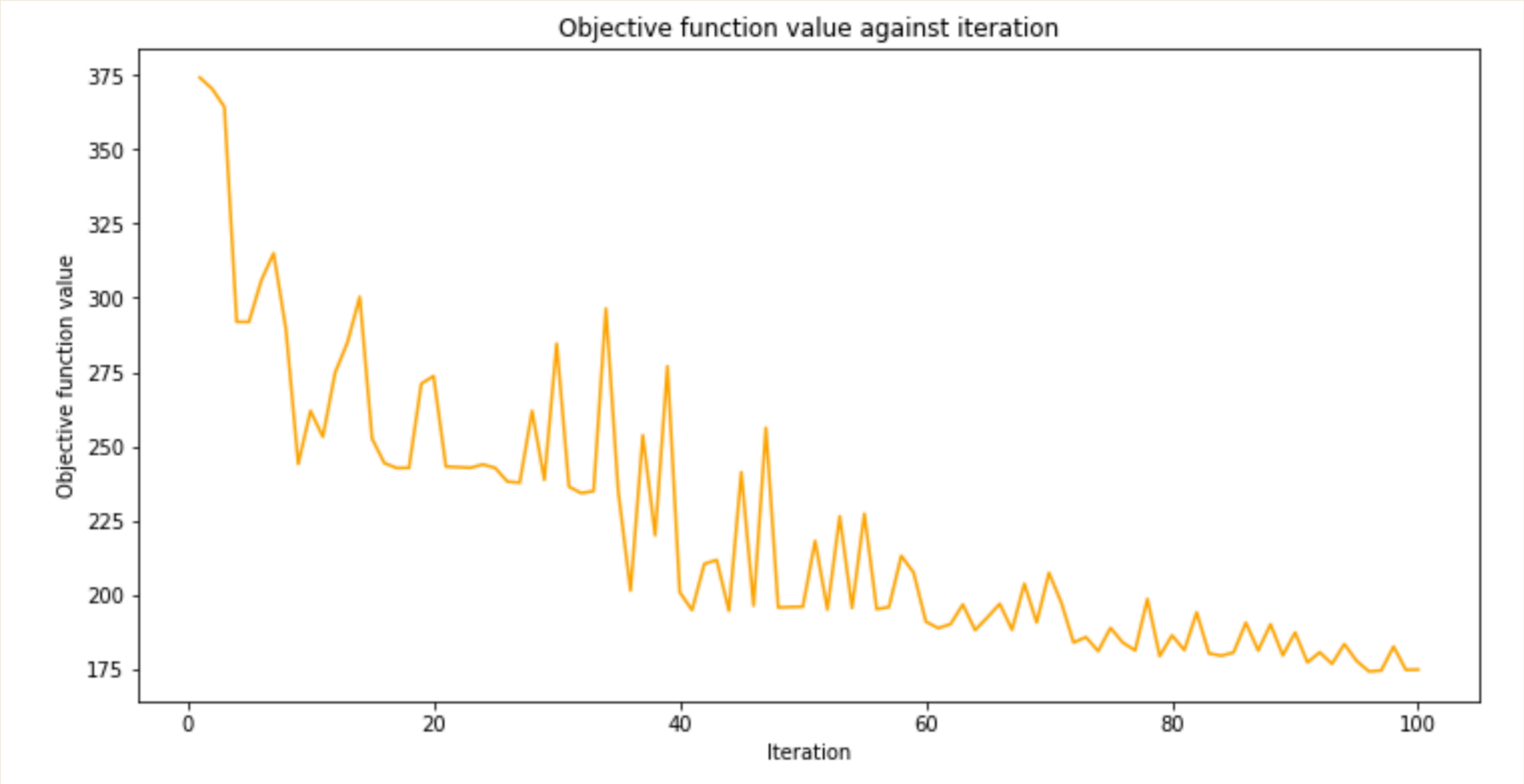
- Optimization performed using classical algorithms: COBYLA, ADAM, SPSA, etc.
  - Numerical Differentiation has been the norm for a while using parameter-shift differentiation
  - It's unclear how intermediate derivatives could be stored/reused inside a quantum computation
- Investigating if we can use quantum optimization techniques like quantum annealing
- A lot is still unknown about what is optimal, more of an art to test
- "There is often little theoretical motivation for any given optimizer, although recent work has been to analyze the training dynamics of QVCs (VQCs)"

arXiv:2202.01389v3

Proof of Concept using Qiskit

- MNIST: image classification 0s and 1s
- Input image via amplitude encoding into 8 qubit VQC
- ~about 100 tunable parameters
- Iterations are a hyper parameter
- COBYLA, cross-entropy loss function
- Training score: 97%
- Testing score: 98%





What's next?

- Comparing VQC structure with amplitude encoding of IceCube simulation data with QRAC encoding
- Takes ~16 qubits to encode largest IceCube events via amplitudes
- Need larger quantum computers than publicly available (applied for ORNL grant)
- Now have access to ~100 qubit QCs
- Choose optimal qubits in target QCs, implement custom feature maps, testing ansatz types, optimizations, loss functions etc.
- Transition away from Qiskit to PennyLane (a QML framework)

ICECUBE SOUTH POLE NEUTRINO OBSERVATORY

Qiskit

PENNYLANE

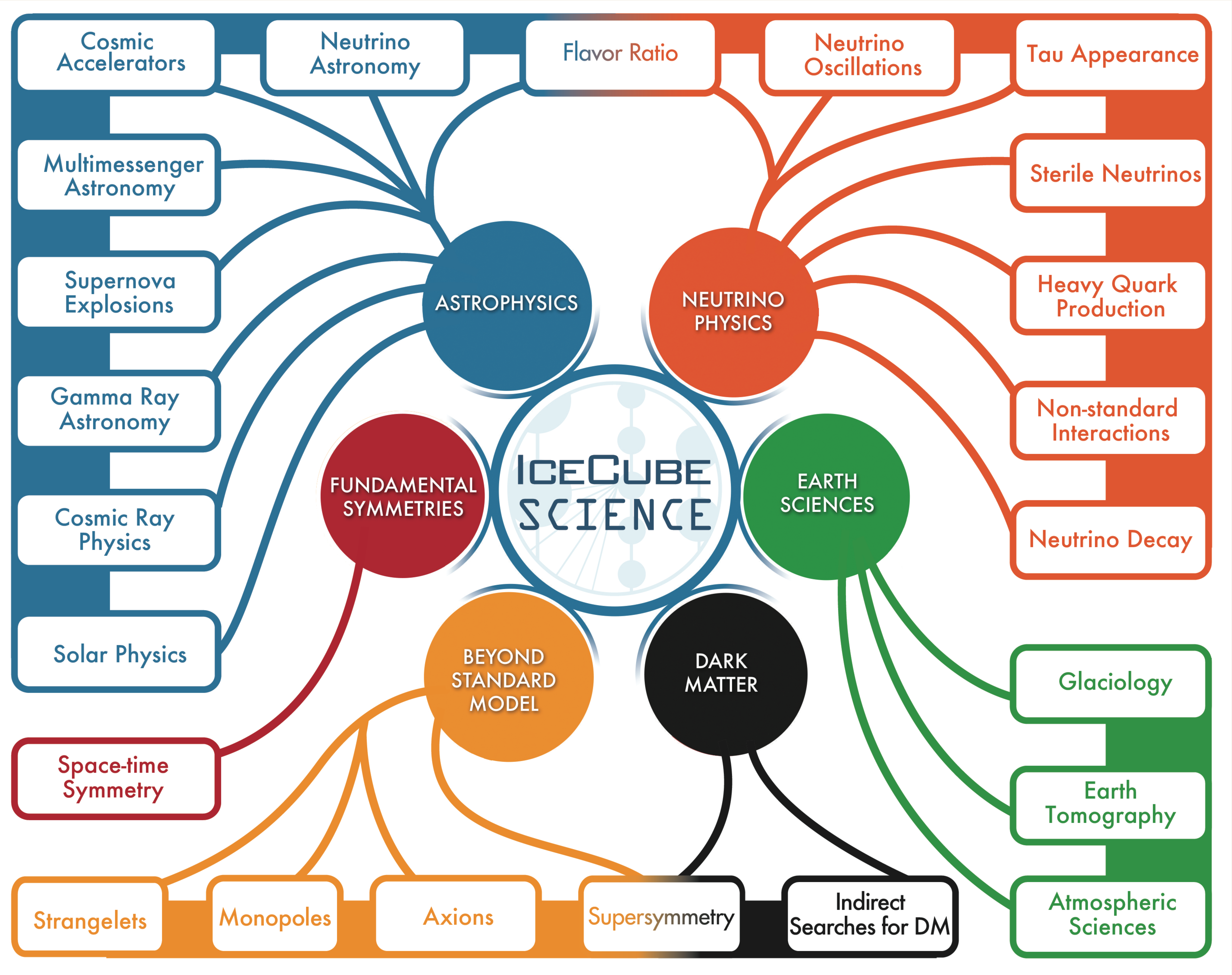
Conclusion/Takeaway

- ML in neutrino physics has been very successful the past two decades and will continue to contribute
- Yet with concerns about the streetlight effect and increasing data loads in next generation experiments/observatories, we might need new tools
- QC can take advantage of additional degrees of freedom to enhance data compression
- QCML is still a burgeoning field; much is still unknown about optimizations, actual quantum speedups, feasibility on current NISQ computers, etc.
- ***"The question on whether quantum computers can really play a role in identifying practical ML applications is still wide open, and it is unlikely to be decided by theoretical proofs…"***

Based on the Perspective Manuscript by M. Schuld and N. Killoran, PRX Quantum 3, 030101 (2022)

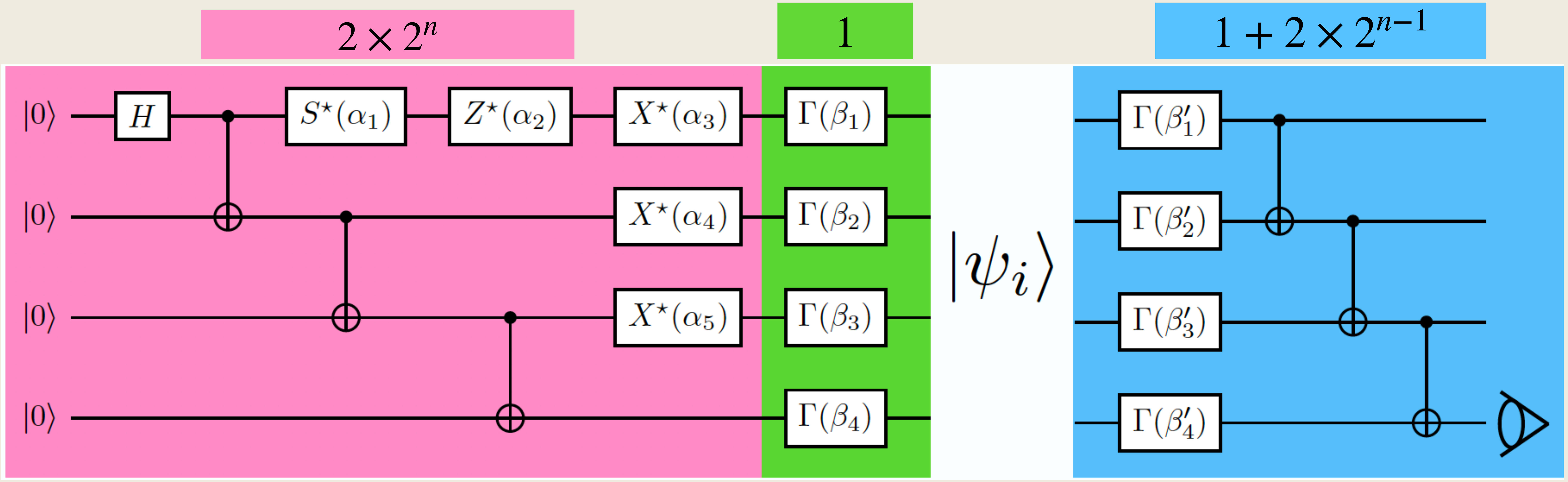
Gracias! Thank you! Preguntas? Questions?

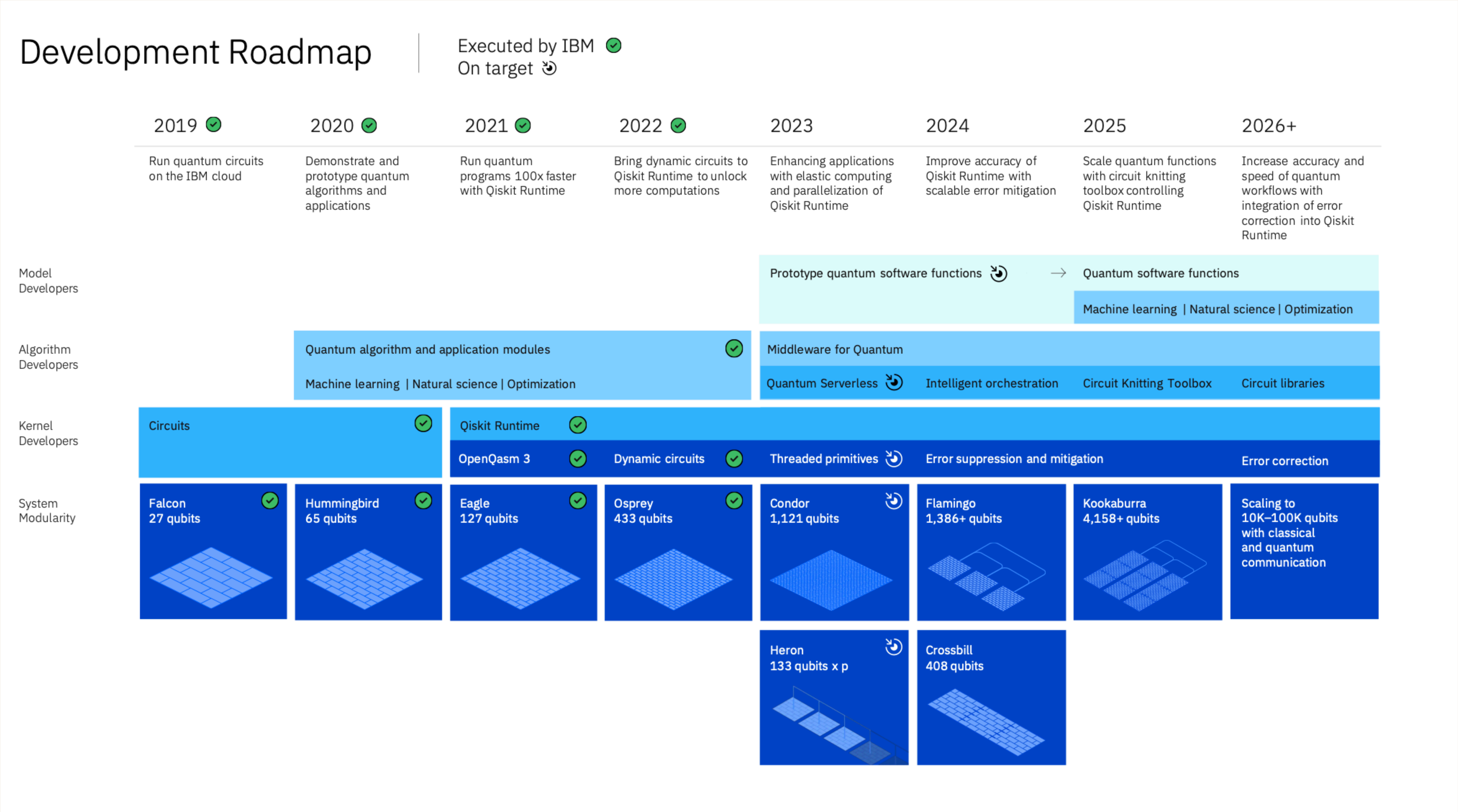
New arm of hectopus:
Quantum Computing!



Measuring Context Eigenstates

- The values for one context are all related. Only need to calculate one “fingerprint” and figure out mapping
- Scales like 4^N
- For 12 qubits this can be done in a few hours and stored in 2 MB




Development Roadmap
Executed by IBM
On target
2019
2020
2021
2022
2023
2024
2025
2026+
Run quantum circuits on the IBM cloud
Demonstrate and prototype quantum algorithms and applications
Run quantum programs 100x faster with Qiskit Runtime
Bring dynamic circuits to Qiskit Runtime to unlock more computations
Enhancing applications with elastic computing and parallelization of Qiskit Runtime
Improve accuracy of Qiskit Runtime with scalable error mitigation
Scale quantum functions with circuit knitting toolbox controlling Qiskit Runtime
Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers
Prototype quantum software functions
Quantum software functions
Machine learning | Natural science | Optimization
Algorithm Developers
Quantum algorithm and application modules
Machine learning | Natural science | Optimization
Middleware for Quantum
Quantum Serverless
Intelligent orchestration
Circuit Knitting Toolbox
Circuit libraries
Kernel Developers
Circuits
Qiskit Runtime
OpenQasm 3
Dynamic circuits
Threaded primitives
Error suppression and mitigation
Error correction
System Modularity
Falcon 27 qubits
Hummingbird 65 qubits
Eagle 127 qubits
Osprey 433 qubits
Condor 1,121 qubits
Flamingo 1,386+ qubits
Kookaburra 4,158+ qubits
Scaling to 10K–100K qubits with classical and quantum communication
Heron 133 qubits x p
Crossbill 408 qubits

Overview

- Introduction to Quantum Computing
- Application of QC to HEP
- QCML in HEP
- QCML for neutrino astronomy
- Variational Quantum Circuits
- Conclusion