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QuantumNAS: Noise-Aware Search for Robust Quantum Circuits and the TorchQuantum Library

Hanrui Wang
MIT HAN Lab

[HPCA'22] QuantumNAS: Noise-adaptive search for robust quantum circuits

[DAC'22] QuantumNAT: Quantum Noise-Aware Training with Noise Injection, Quantization and Normalization

[DAC'22] QOC: Quantum On-Chip Training with Parameter Shift and Gradient Pruning

Torch Quantum

2022/06/28 EQuS

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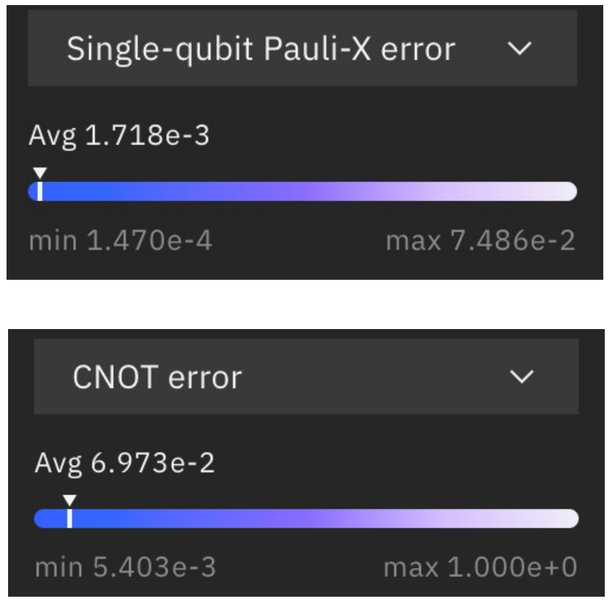
Outline

- Background
- QuantumNAS
- TorchQuantum Library
- Conclusion

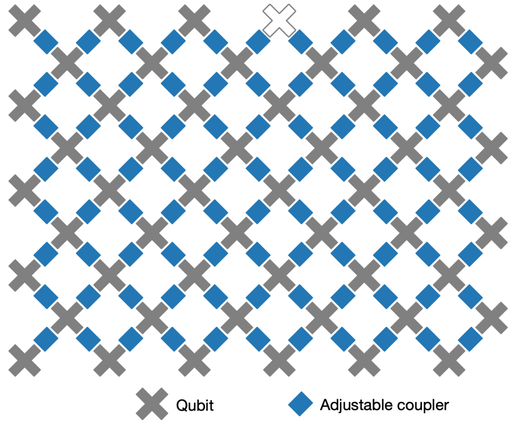
NISQ Era

- Noisy Intermediate-Scale Quantum (NISQ)
  - **Noisy**: qubits are sensitive to environment; quantum gates are unreliable
  - **Limited number** of qubits: tens to hundreds of qubits



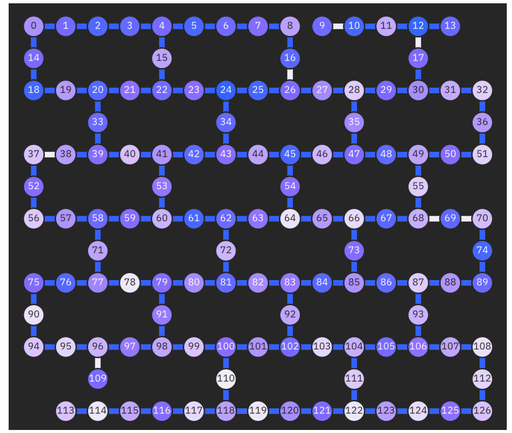
Gate Error Rate

https://quantum-computing.ibm.com/



Google Sycamore

https://www.nature.com/articles/s41586-019-1666-5

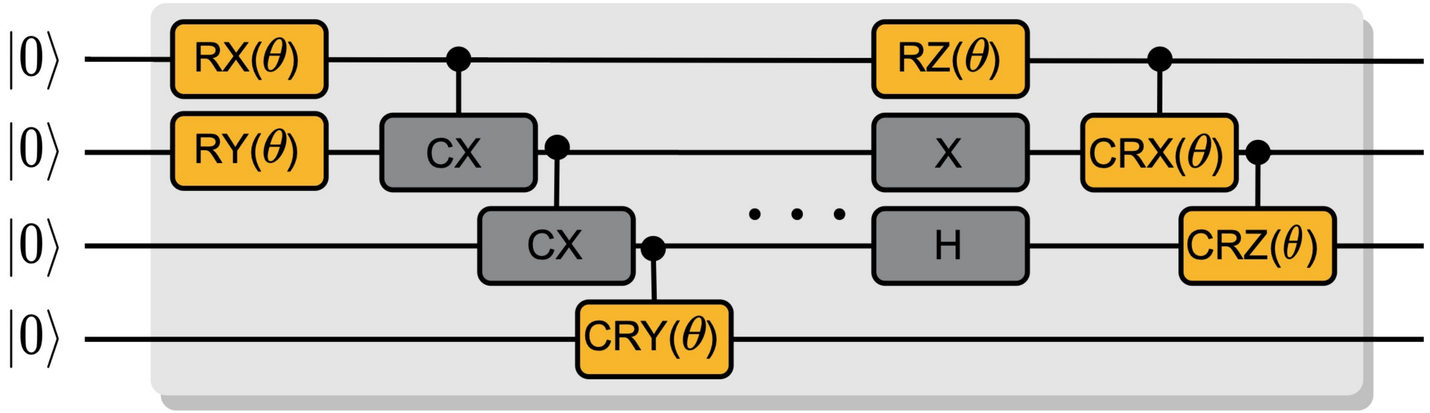


IBM Washington

https://quantum-computing.ibm.com/

Parameterized Quantum Circuits

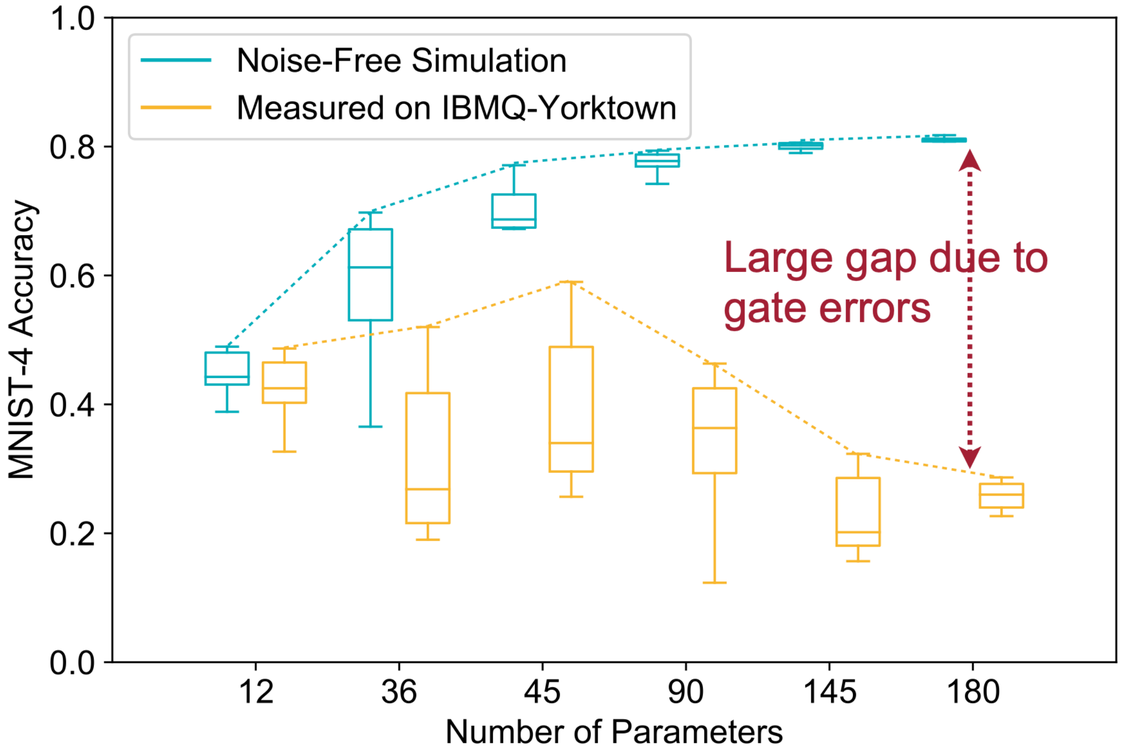
- Parameterized Quantum Circuits (PQC)
- Quantum circuit with fixed gates and parameterized gates



- PQCs are commonly used in **hybrid classical-quantum models** and show promises to achieve quantum advantage
  - Variational Quantum Eigensolver (VQE)
  - Quantum Neural Networks (QNN)
  - Quantum Approximate Optimization Algorithm (QAOA)

Challenges of PQC — Noise

- Noise **degrades** PQC reliability
- More parameters increase the noise-free accuracy but degrade the measured accuracy
- Therefore, circuit architecture is critical



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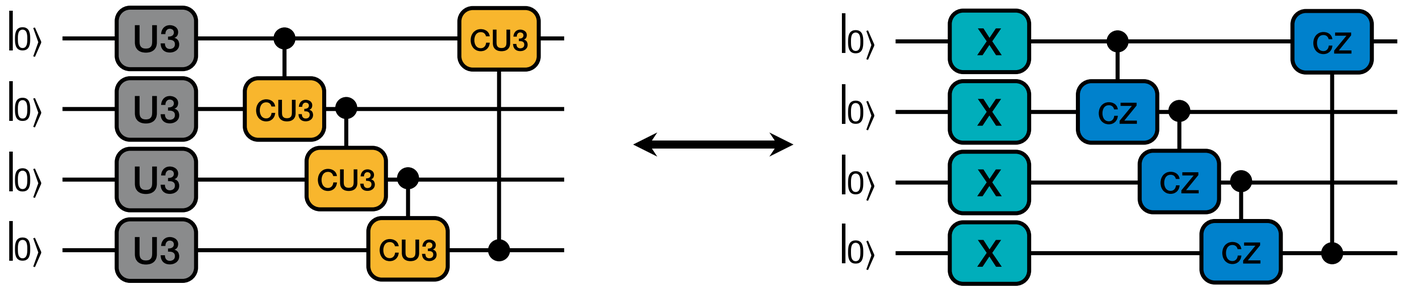
Challenges of PQC — Large Design Space

- Large design space for circuit architecture
  - Type of gates



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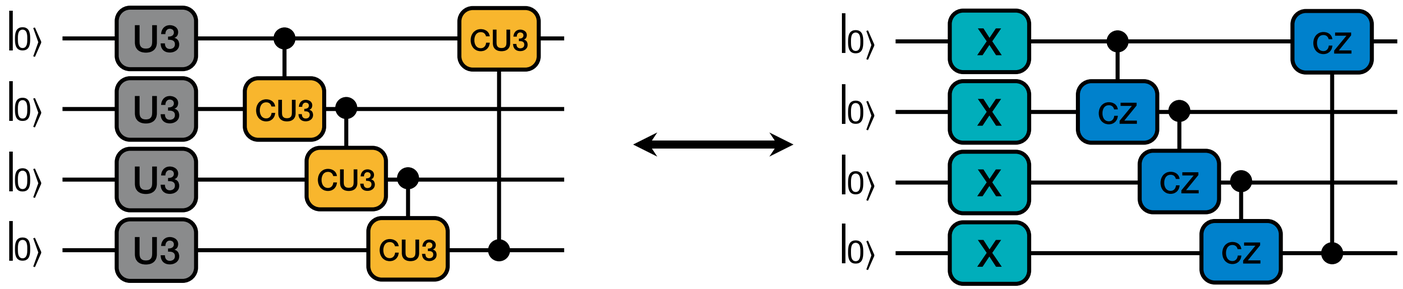

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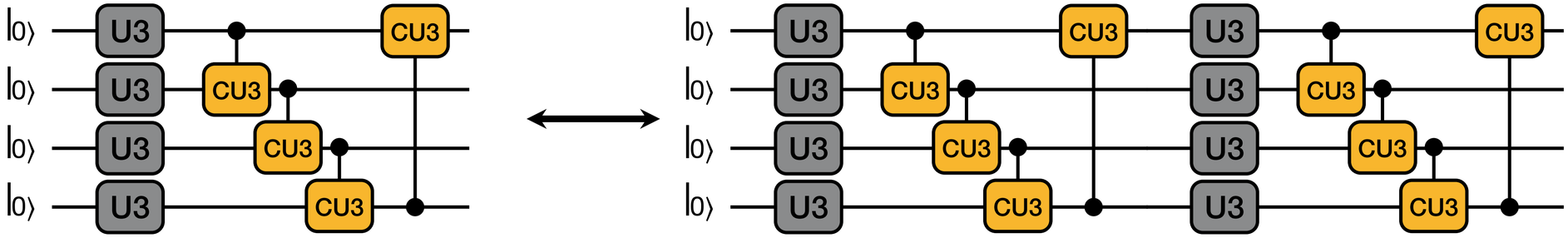

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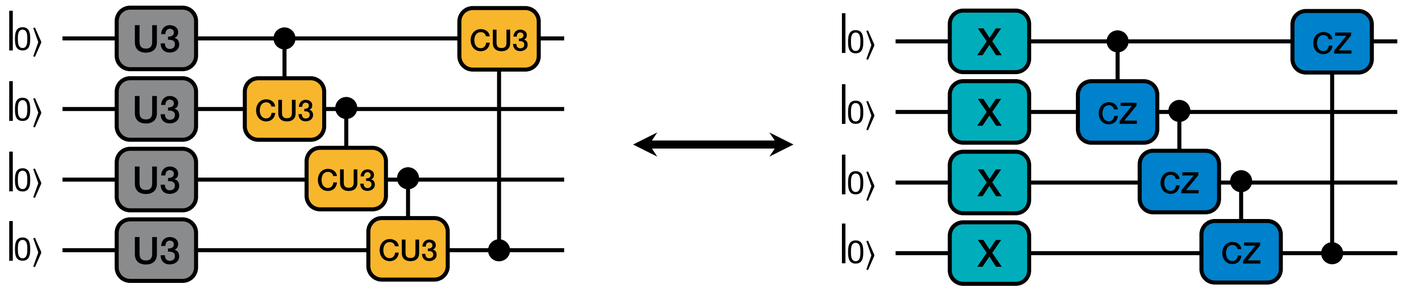

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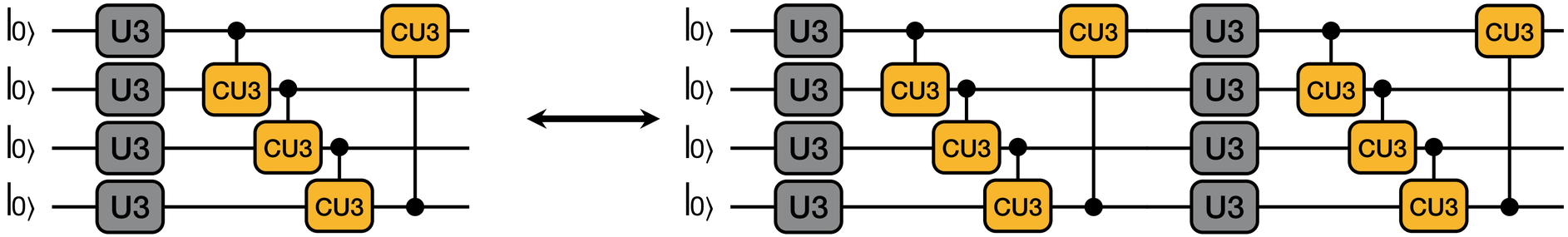
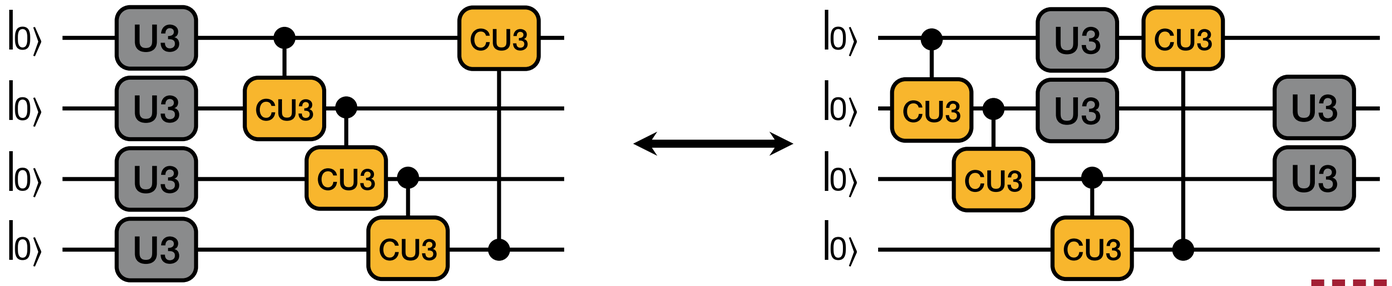


  - Position of gates



Goal of QuantumNAS

Automatically & efficiently search for noise-robust quantum circuit

Train one “SuperCircuit”, providing parameters to many “SubCircuits”

Solve the challenge of large design space

(1) Quantum noise feedback in the search loop
(2) Co-search the circuit architecture and qubit mapping

Solve the challenge of large quantum noise

QuantumNAS

- SuperCircuit Construction and Training
- Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

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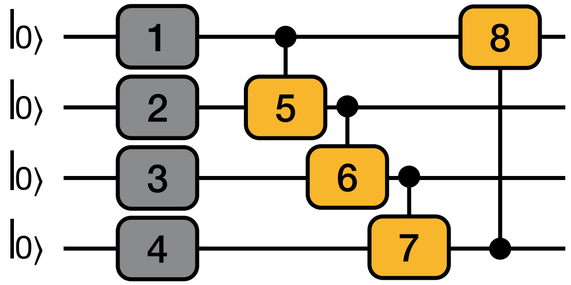

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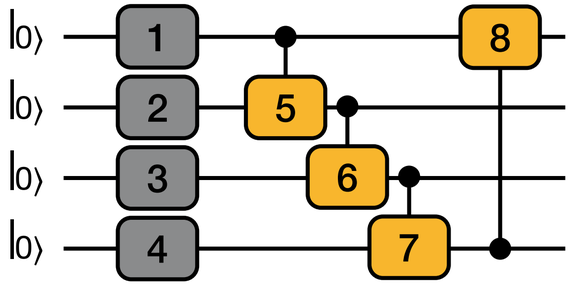
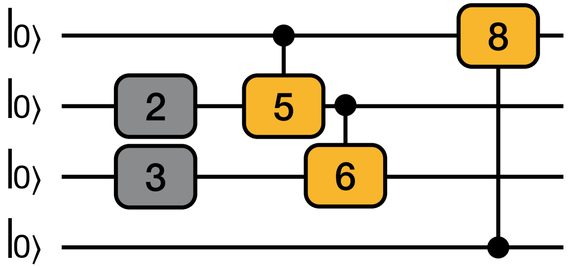
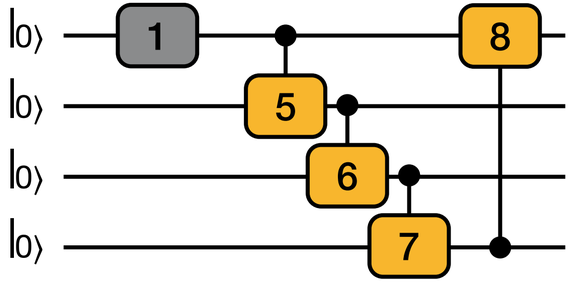
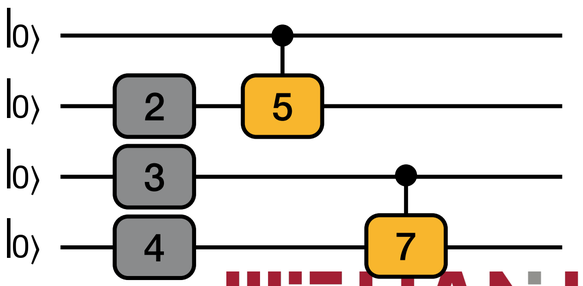


- Each candidate circuit in the design space (called SubCircuit) is a **subset** of the SuperCircuit







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SuperCircuit Construction

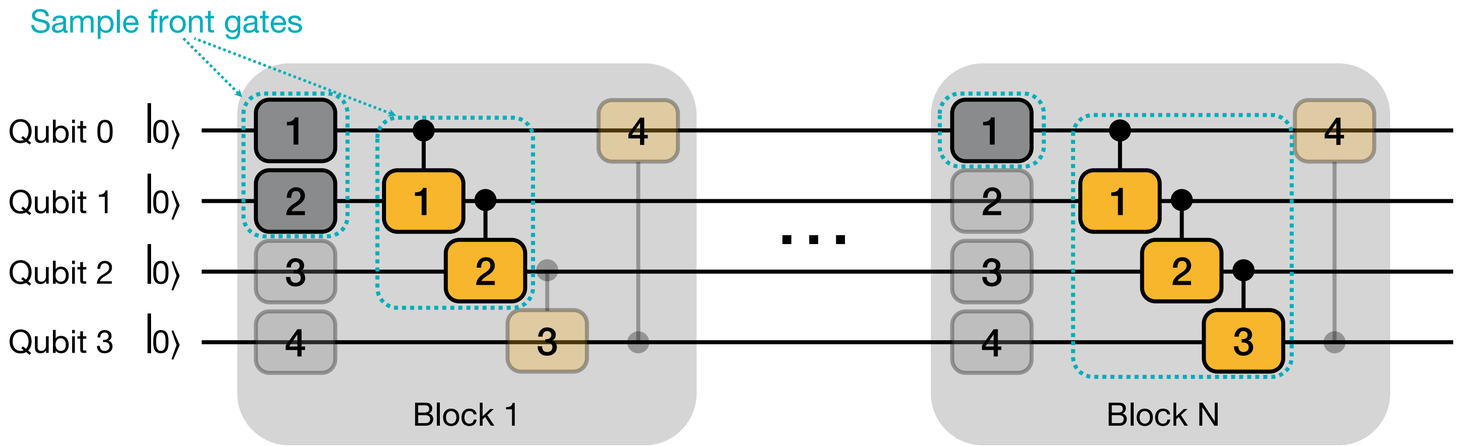
- Why use a SuperCircuit?
  - Enables **efficient** search of architecture candidates without training each
  - SubCircuit inherits parameters from SuperCircuit
  - With **inherited** parameters, we find some good SubCircuits, we find that they are **also good SubCircuits** with parameters **trained from-scratch** individually

SuperCircuit Training

- In one SuperCircuit Training step:
  - Sample a gate subset of SuperCircuit (a SubCircuit)
    - Front Sampling and Restricted Sampling
  - Only use the subset to perform the task and updates the parameters in the subset
  - Parameter updates are cumulative across steps

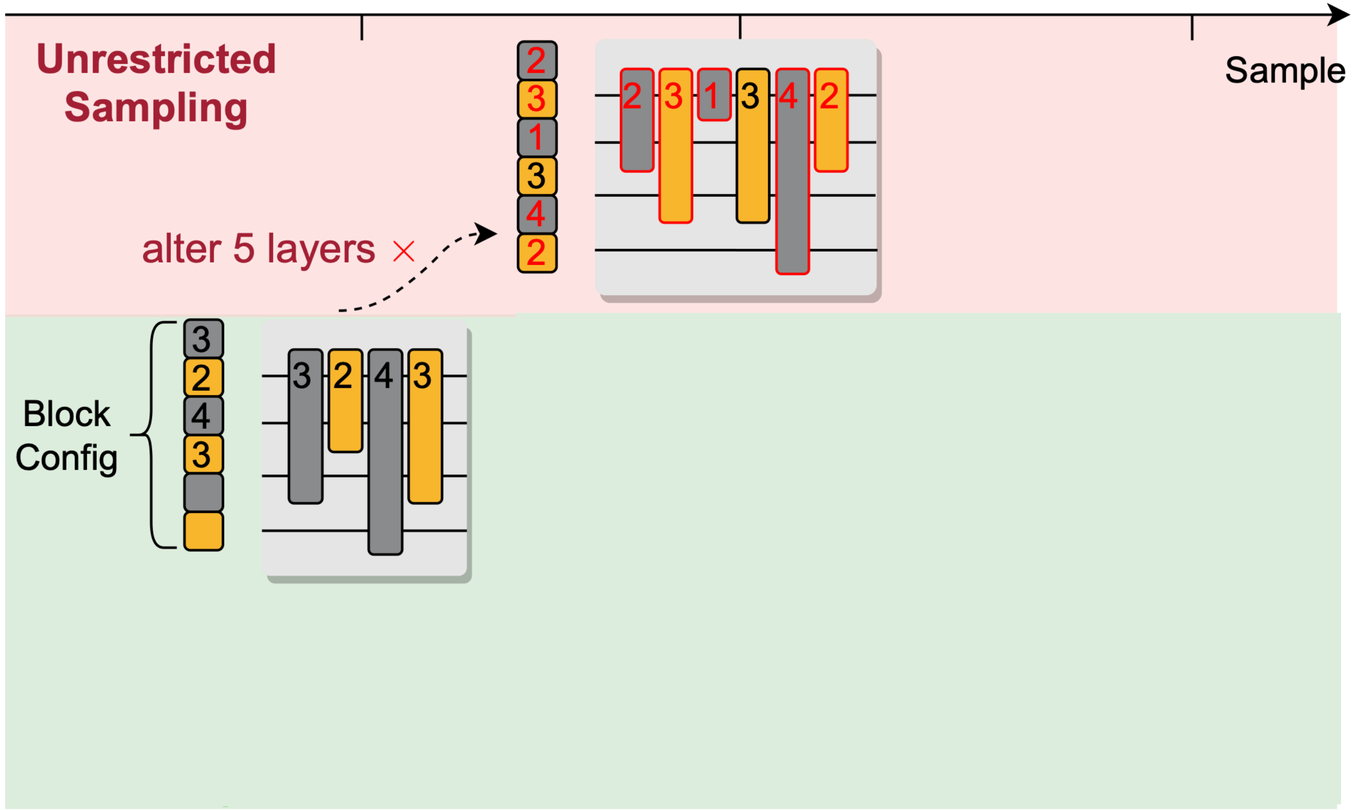
Front Sampling

- During sampling, we first sample total number of blocks, then sample gates within each block
  - Front sampling: Only the **front** several blocks and **front** several gates can be sampled to make SuperCircuit training more stable



Restricted Sampling

- Restricted Sampling:
  - Restrict the difference between SubCircuits of two consecutive steps
  - For example: restrict to at most 4 different layers



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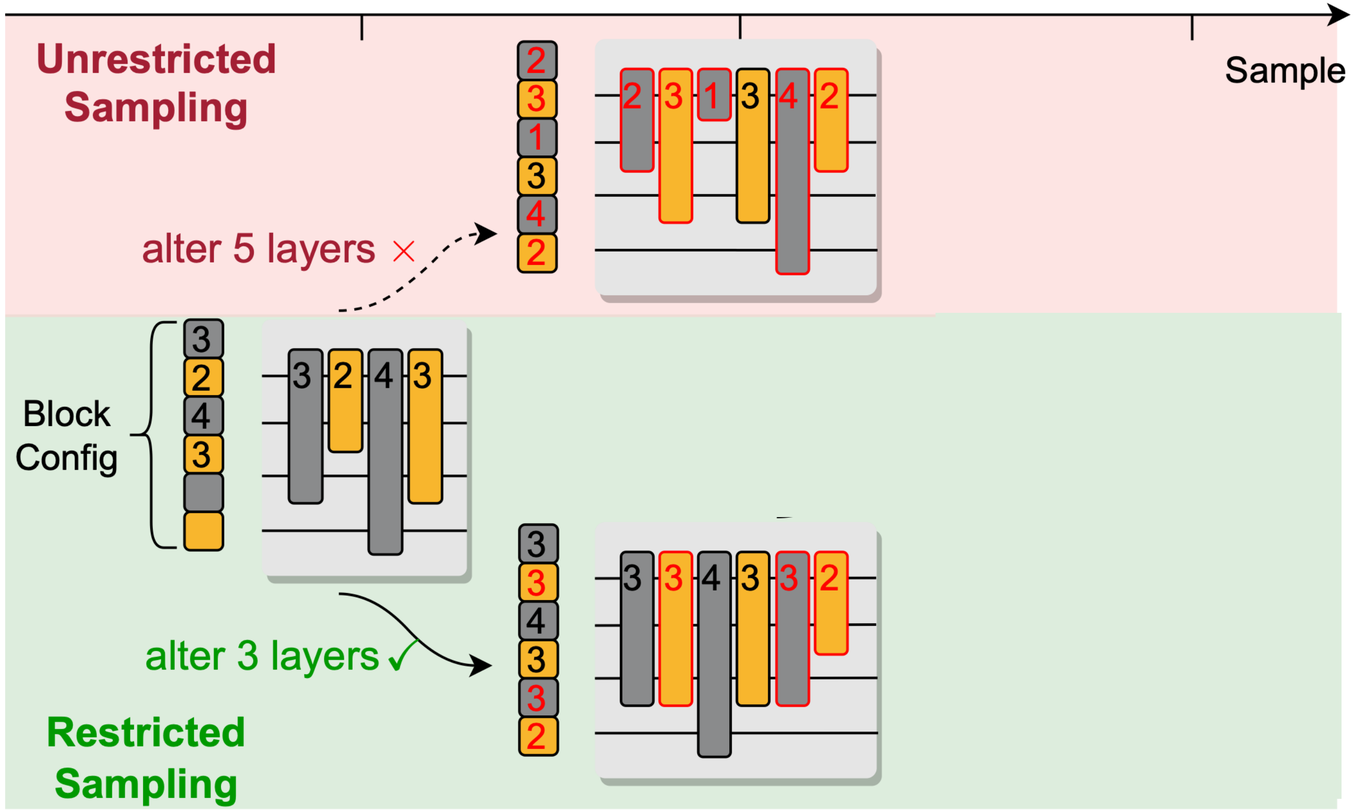

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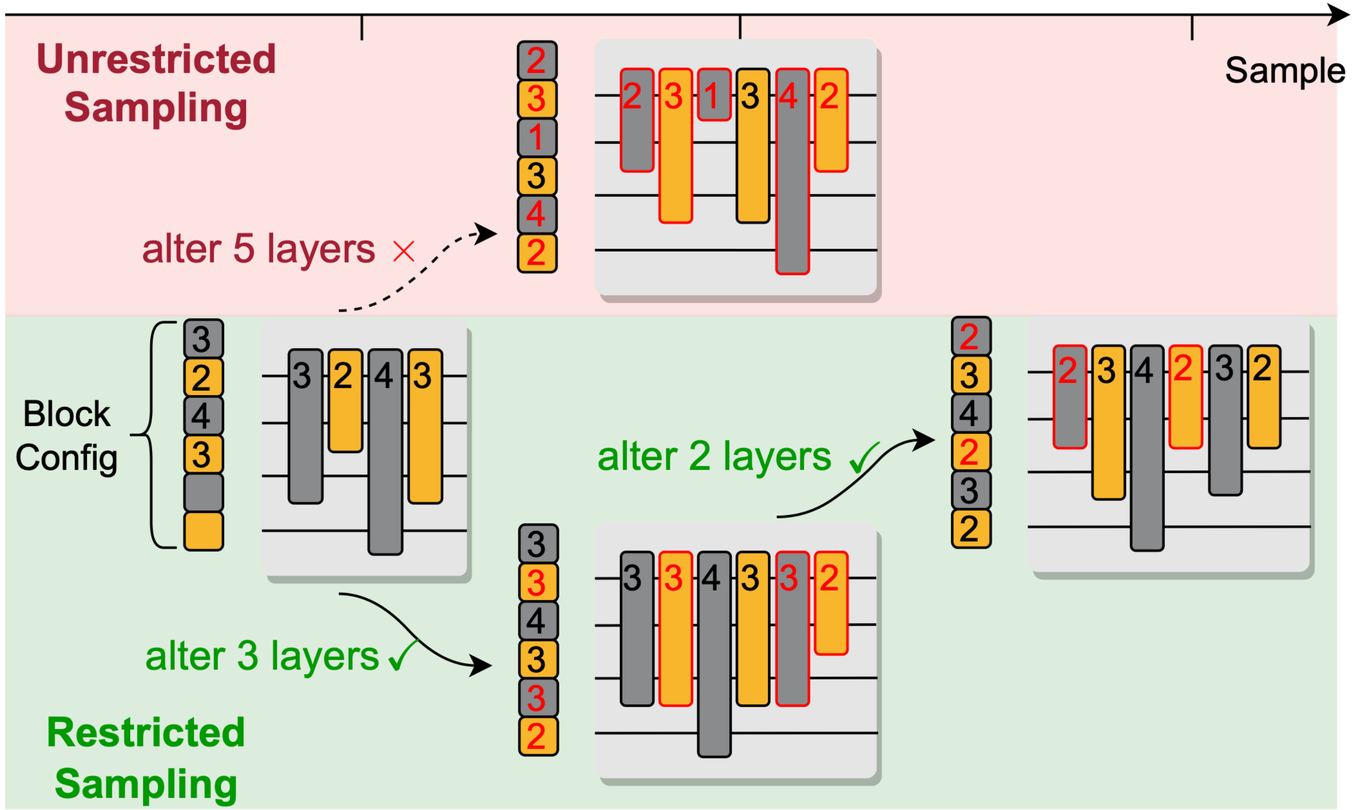
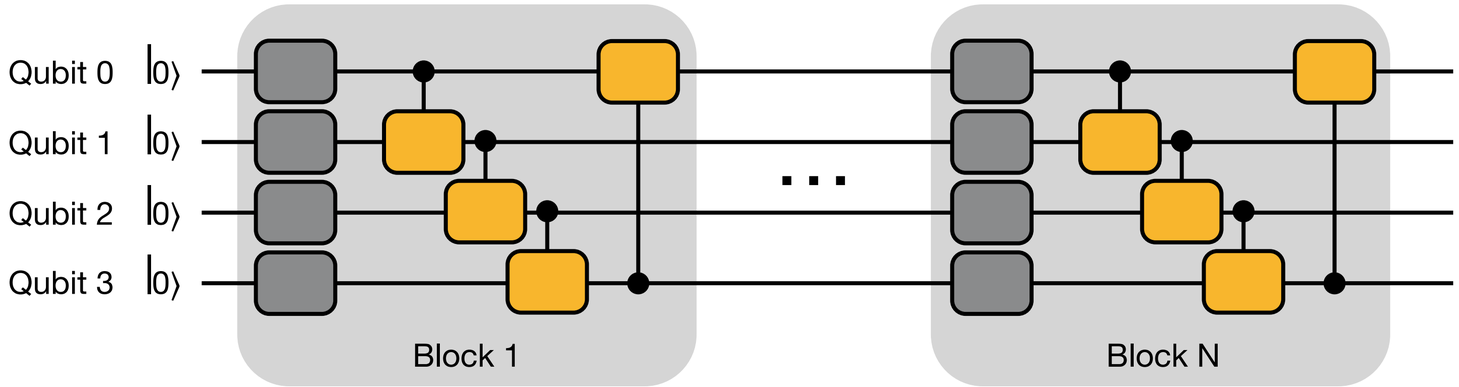


Train SuperCircuit for Multiple Steps

- In one SuperCircuit Training step: Sample and Train



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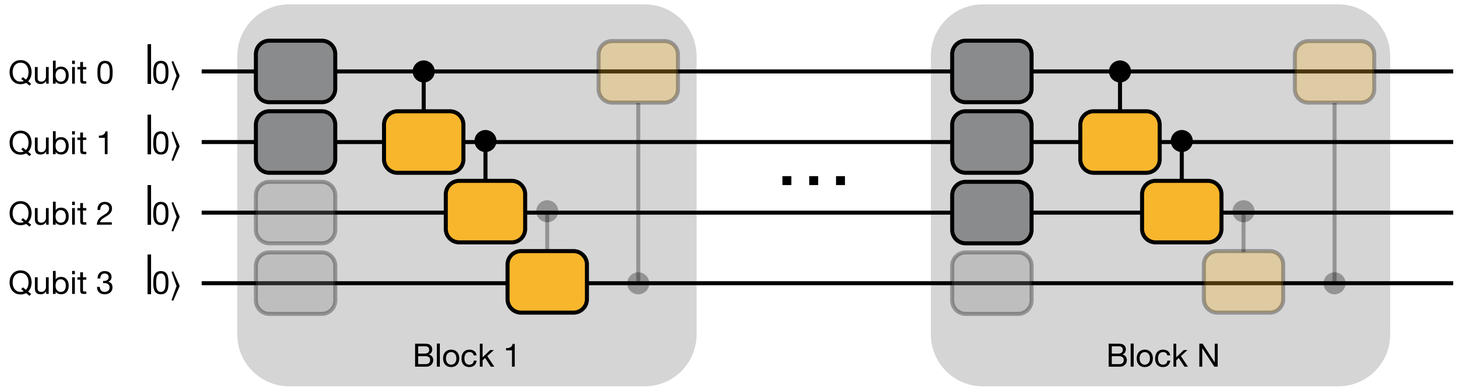

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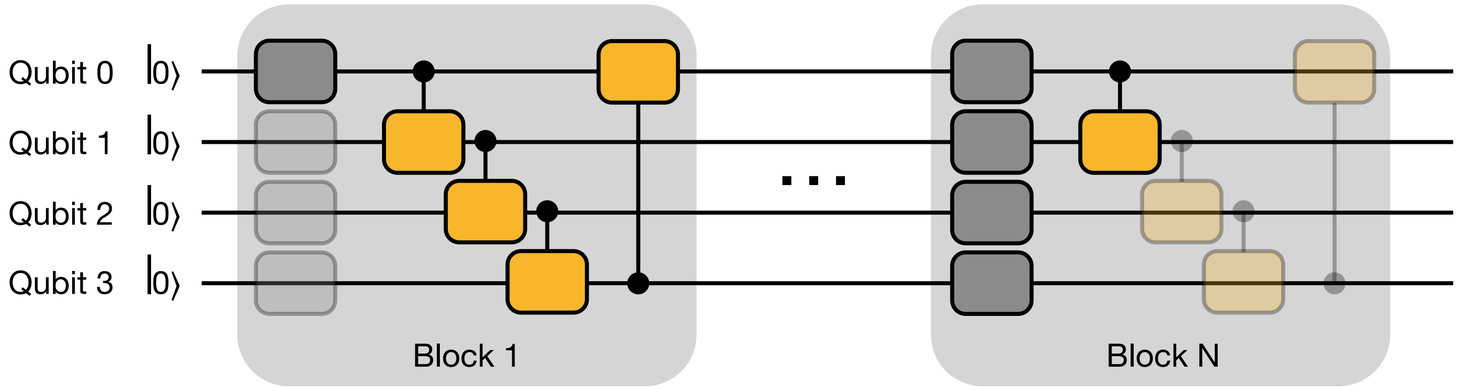

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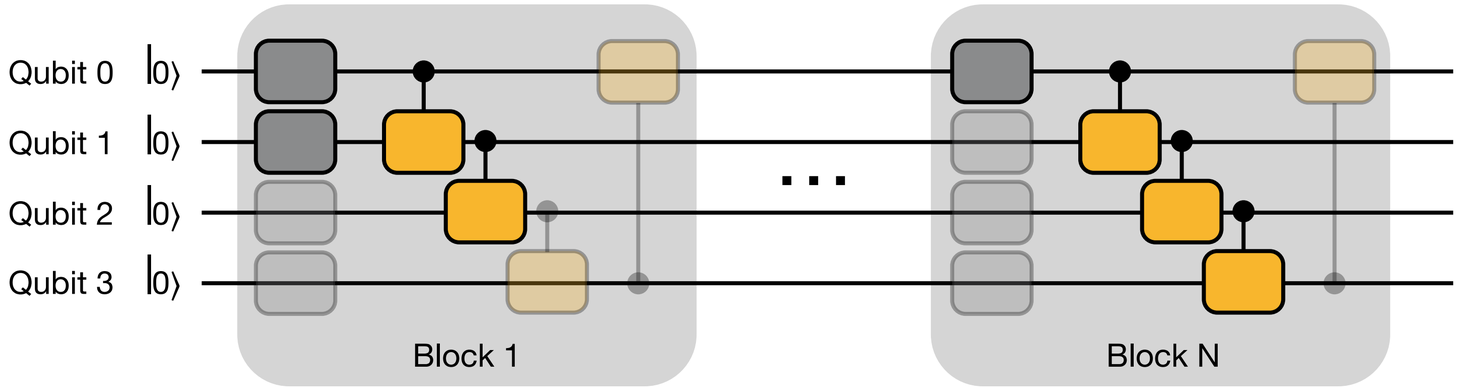

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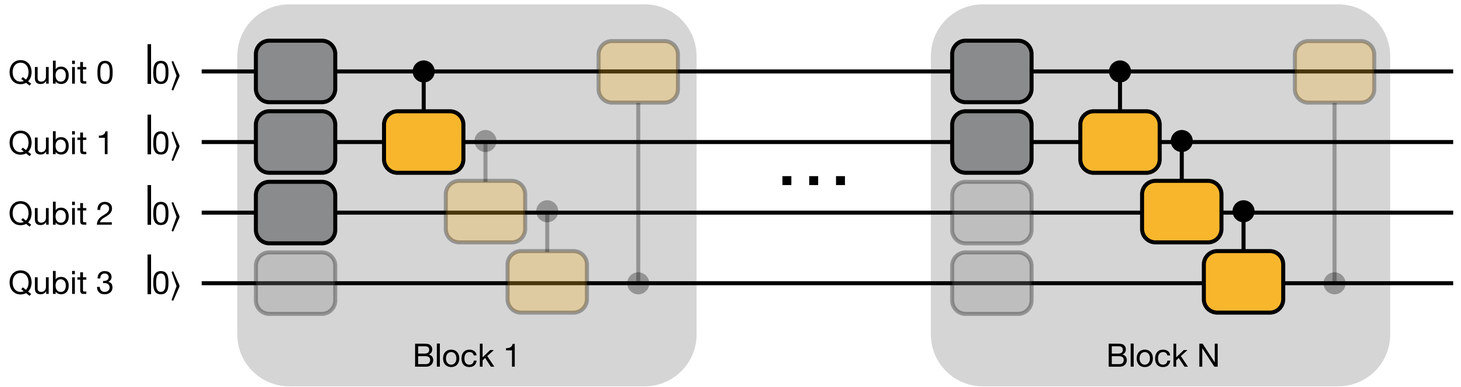

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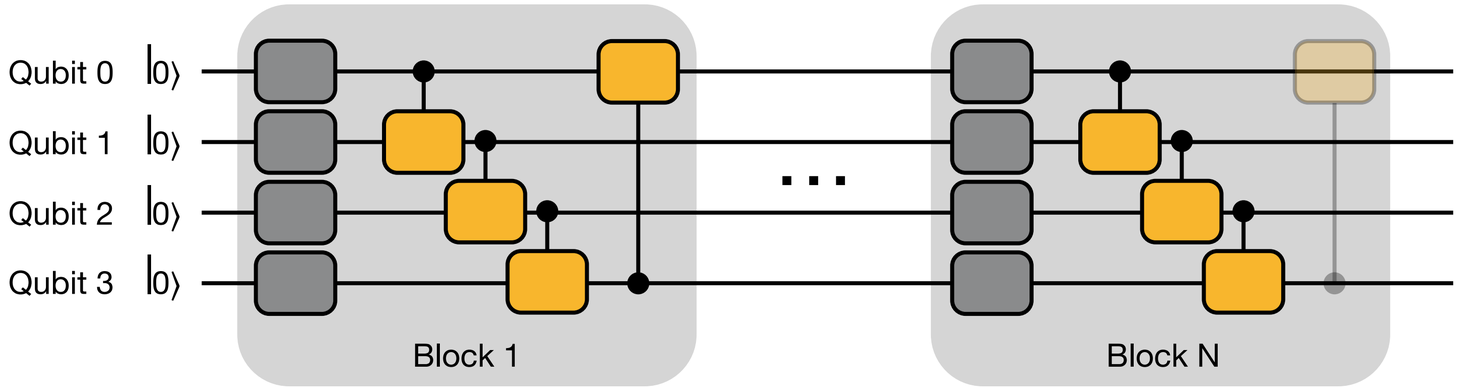

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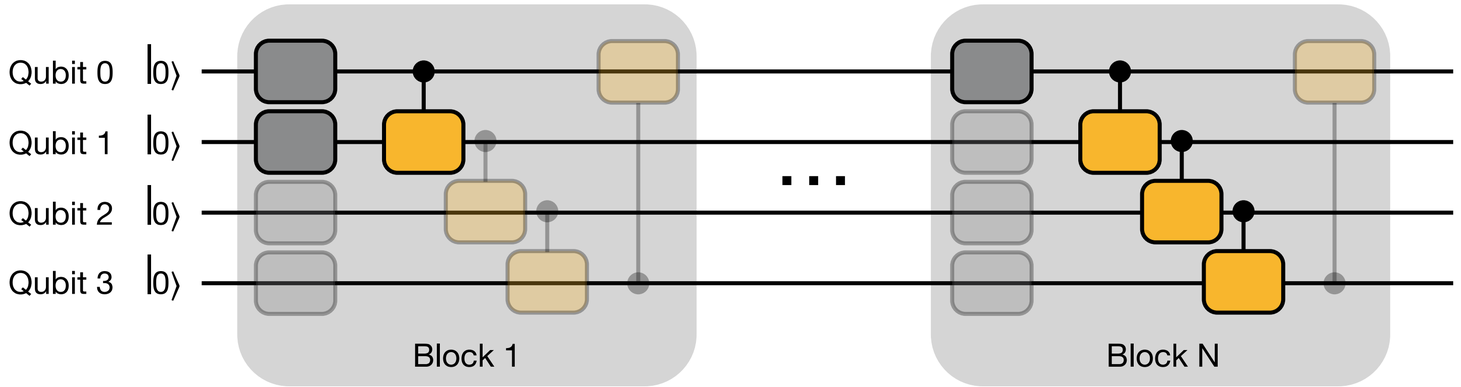

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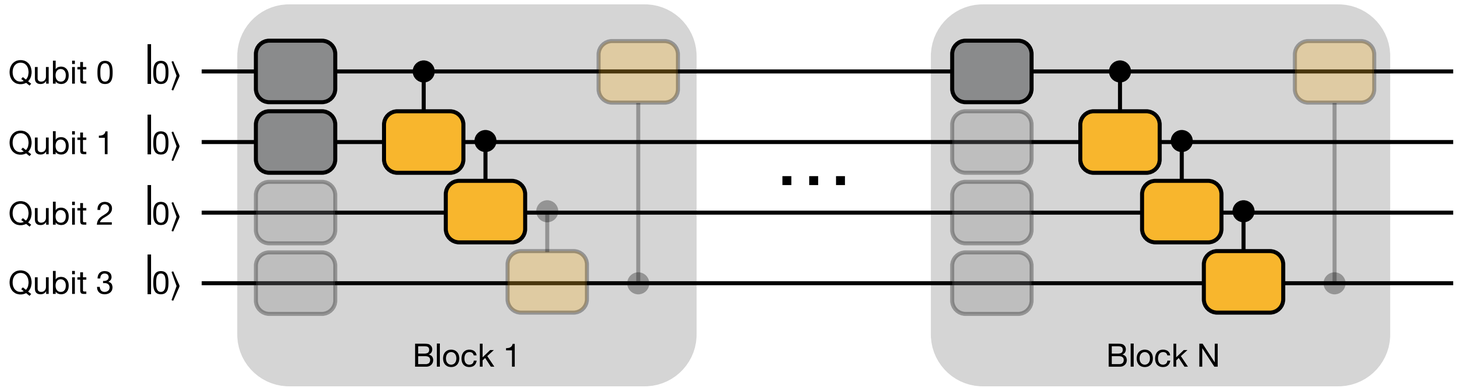

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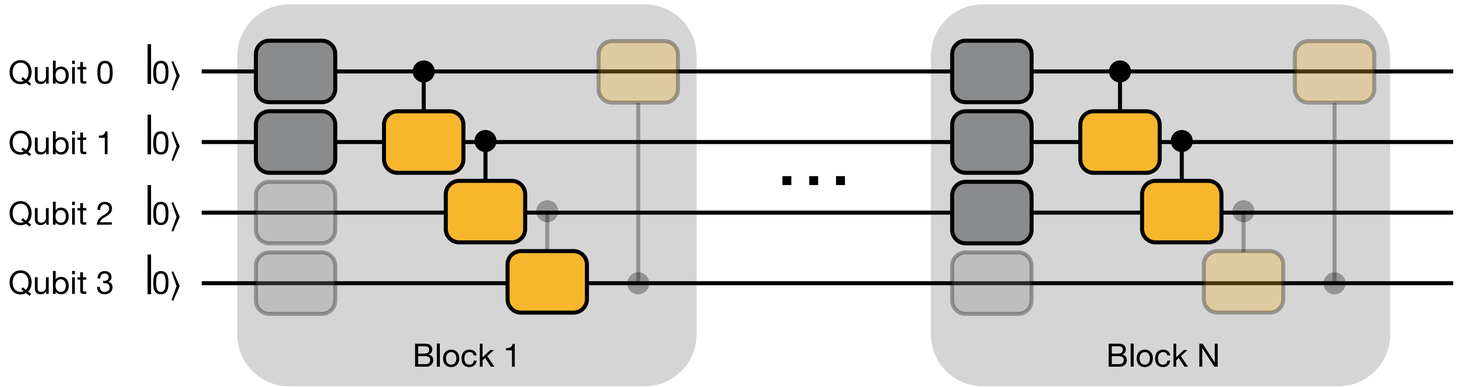

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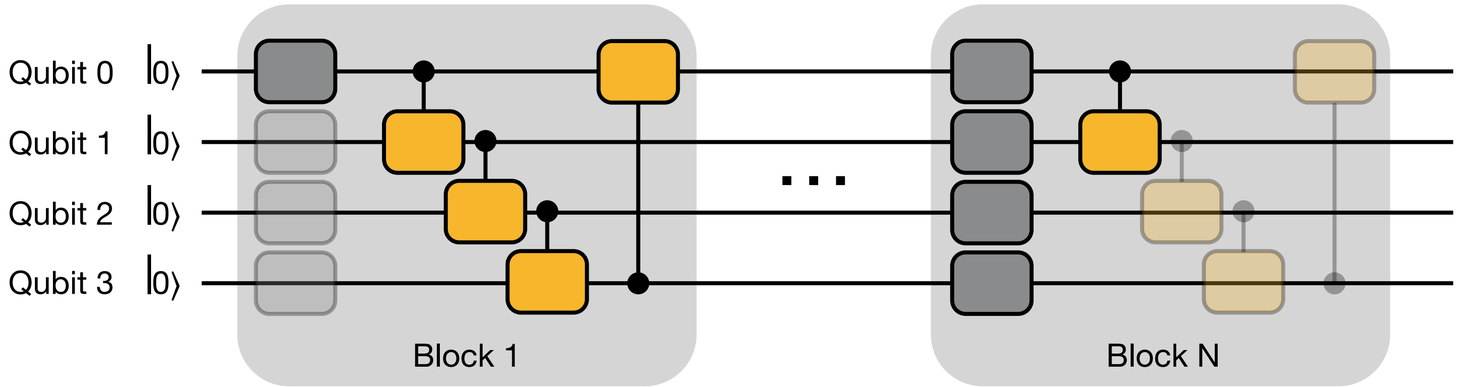

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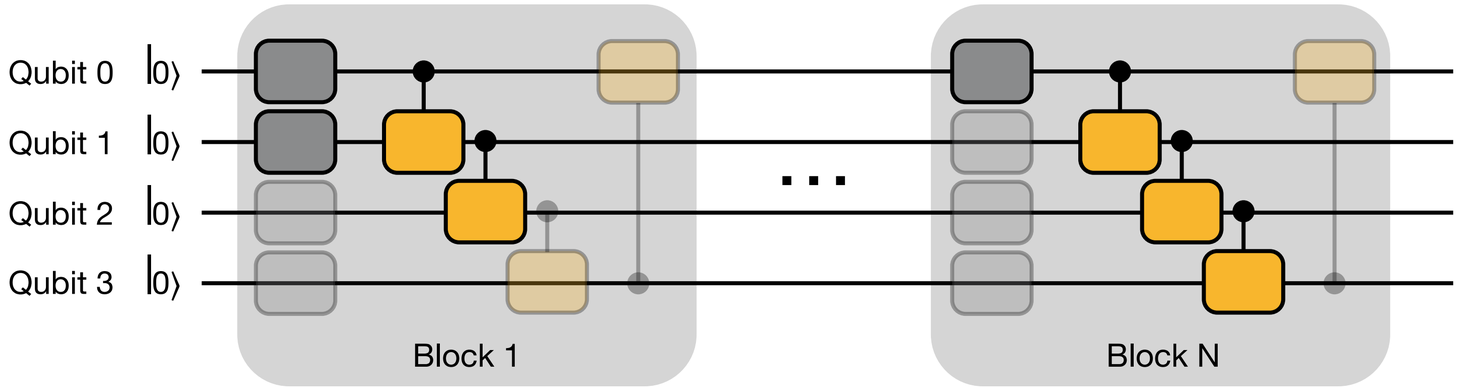

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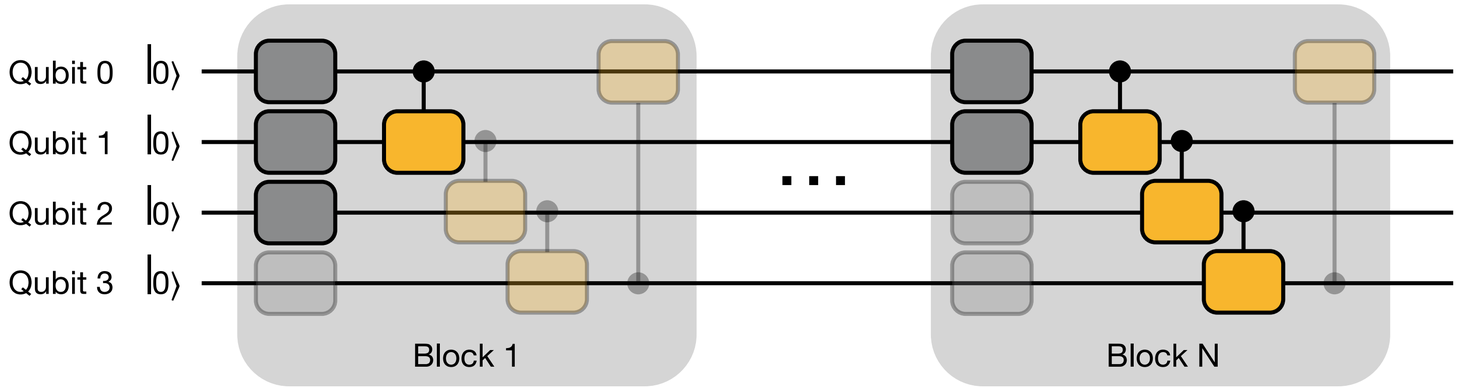

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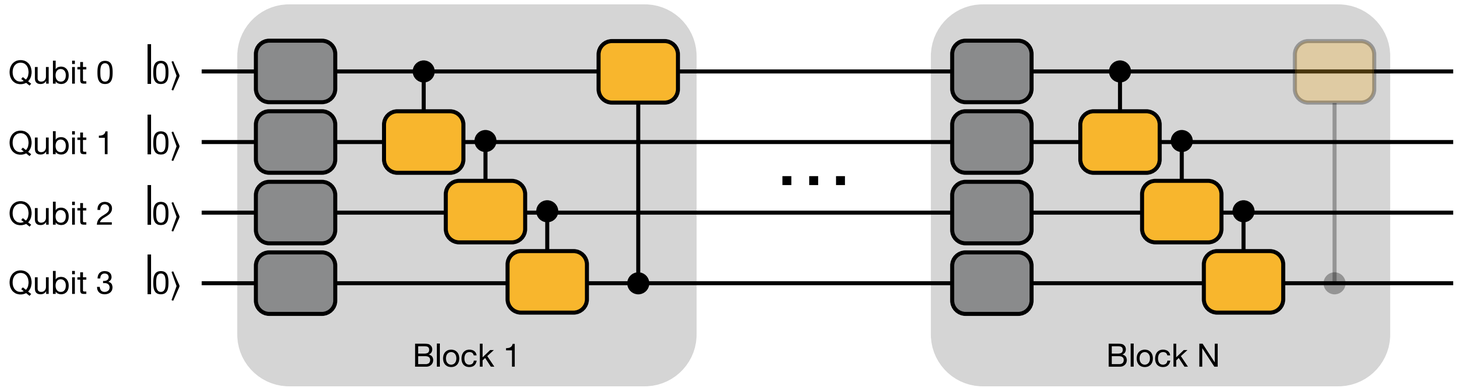

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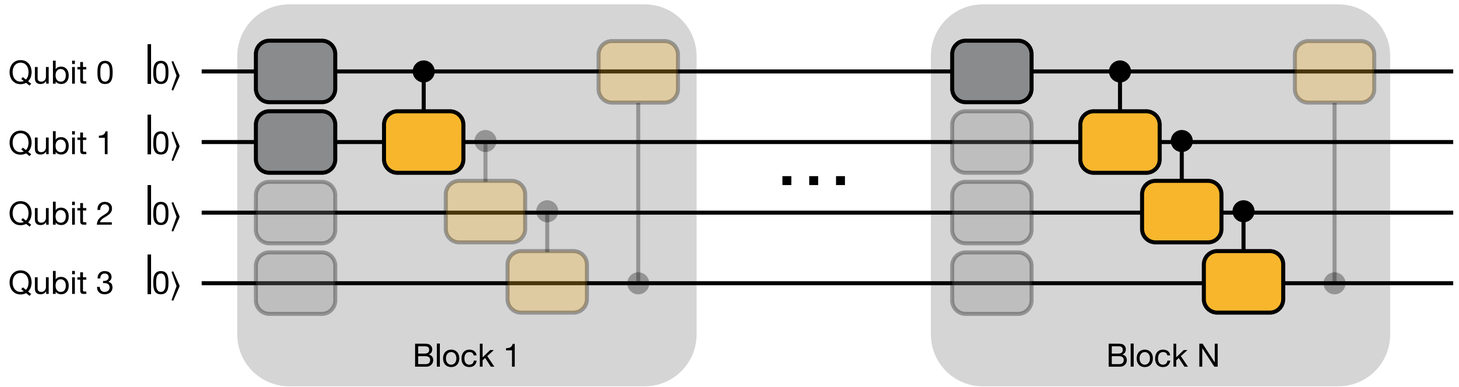

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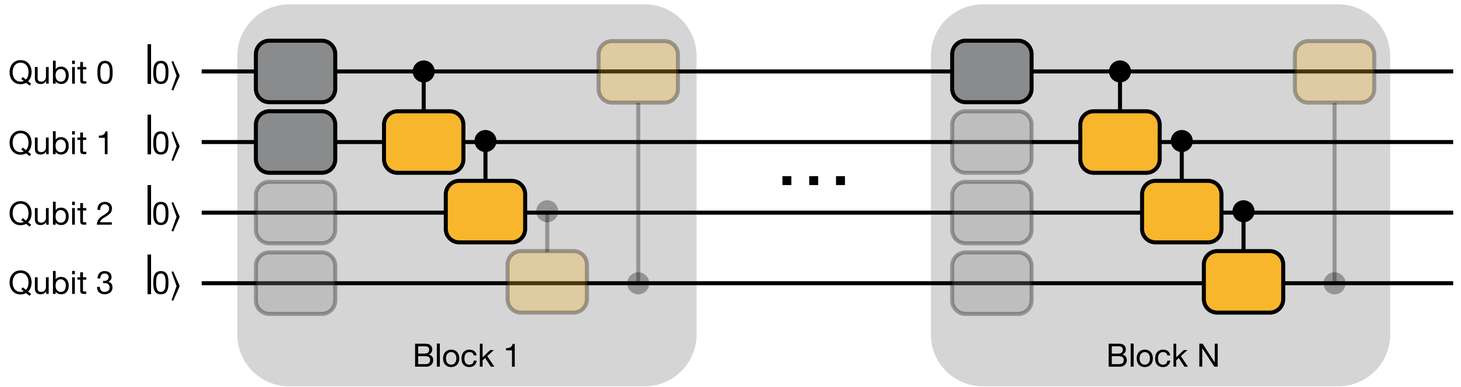

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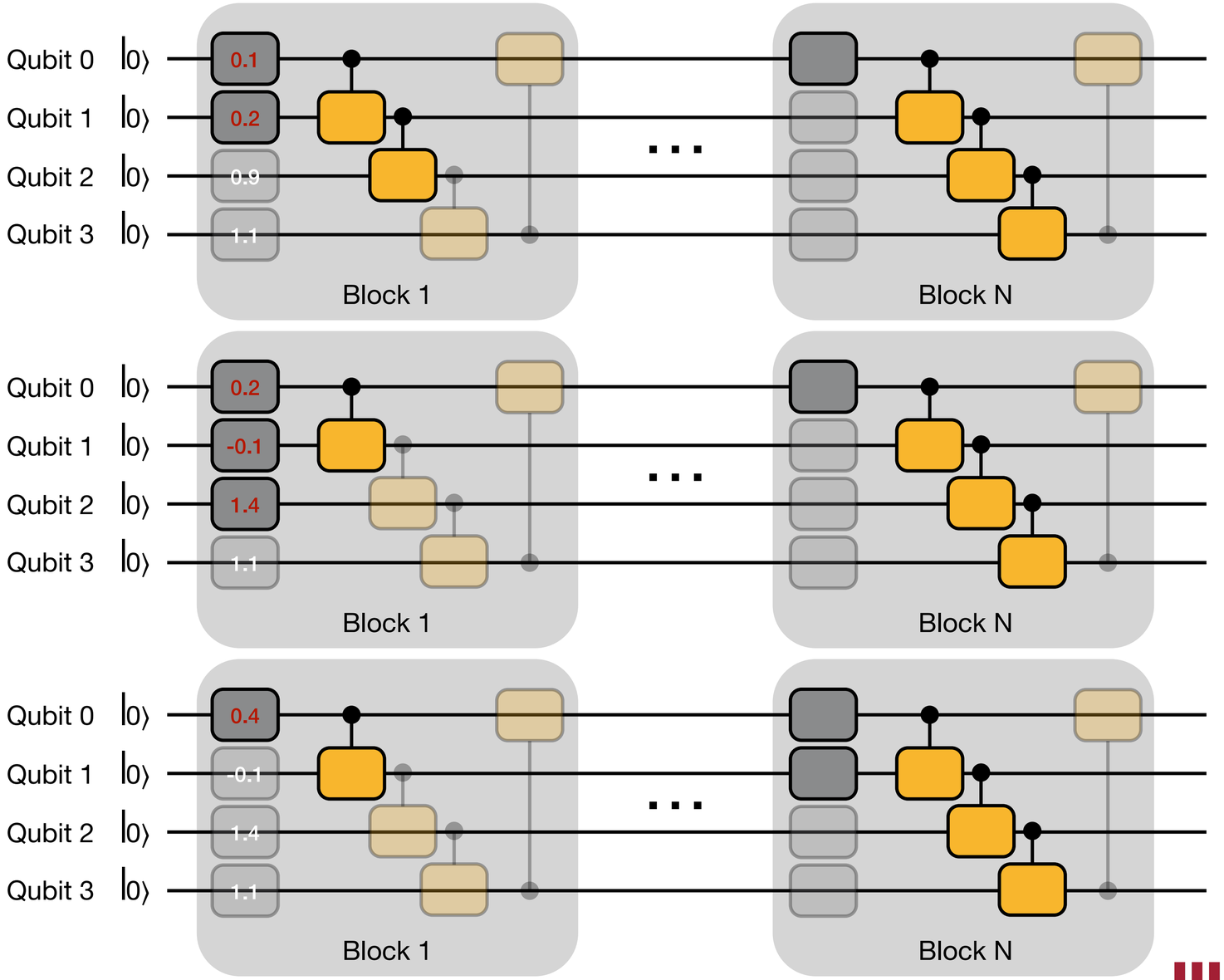

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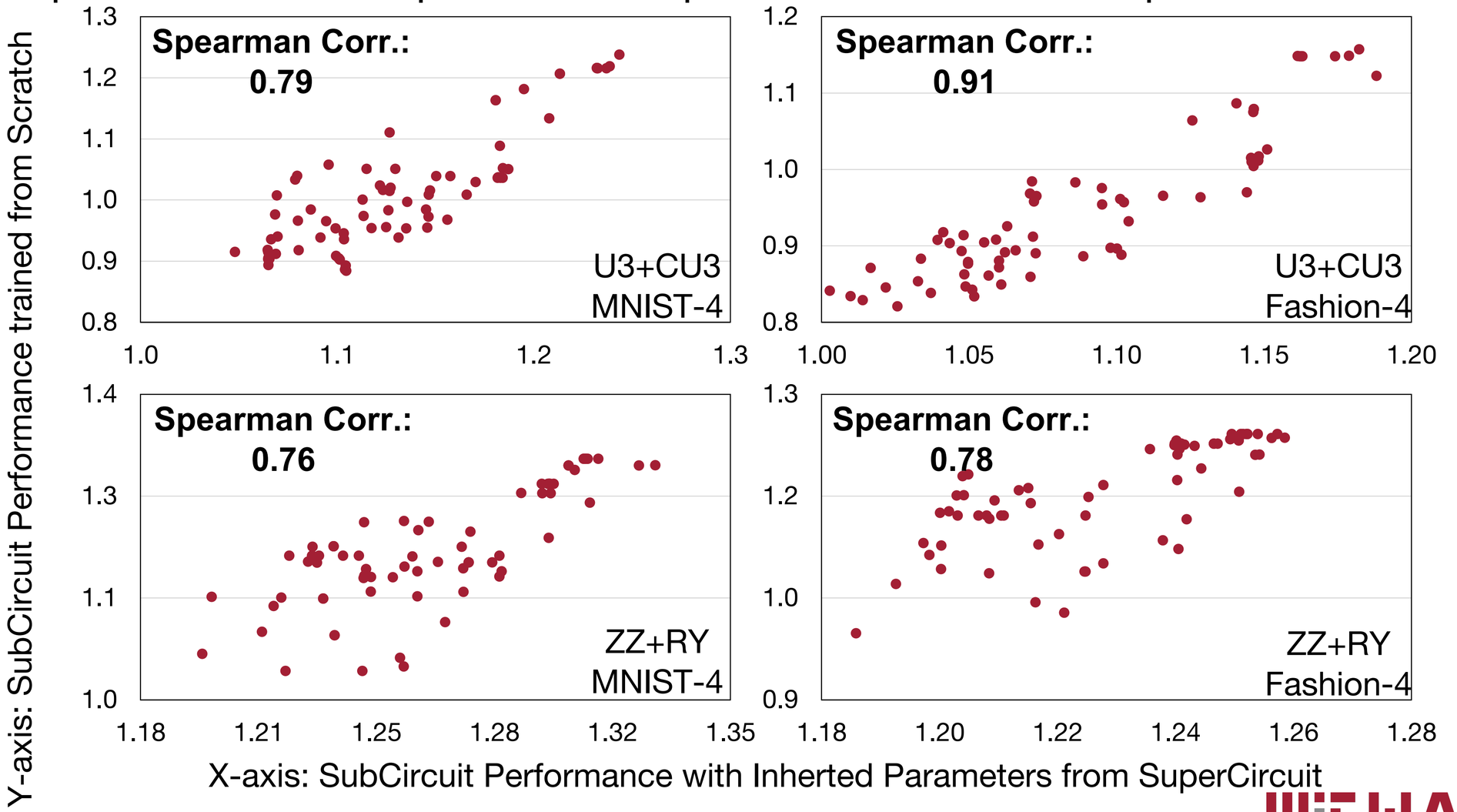
How Reliable is the SuperCircuit?

- Inherited parameters from SuperCircuit can provide accurate relative performance



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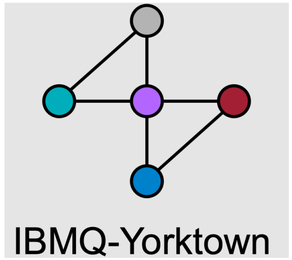
Noise-Adaptive Evolutionary Co-Search

- Search the best SubCircuit and its qubit mapping on target device



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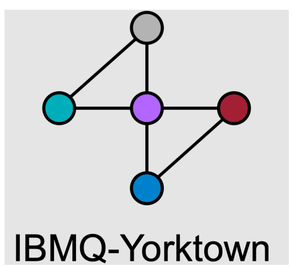
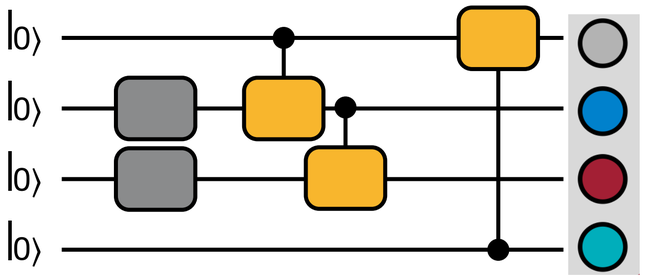
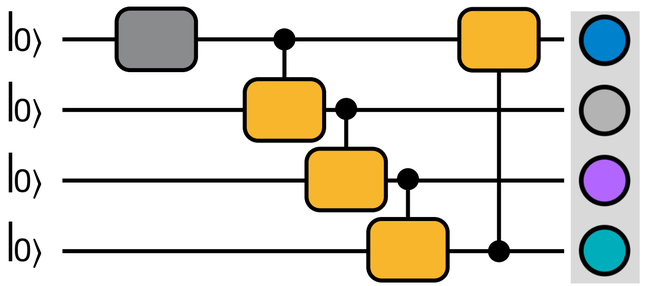
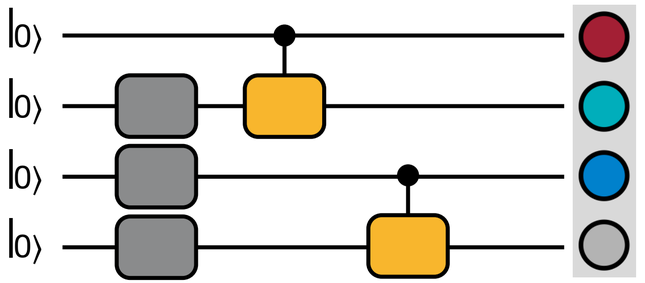








Evolutionary Search Engine
Mutation
Crossover

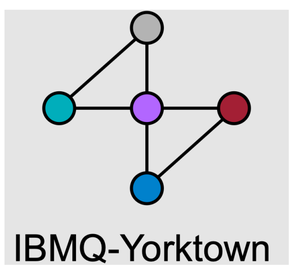
SubCircuit and Qubit Mapping pairs

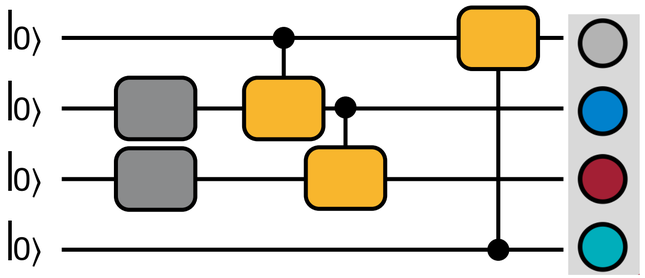
Parameters from SuperCircuit

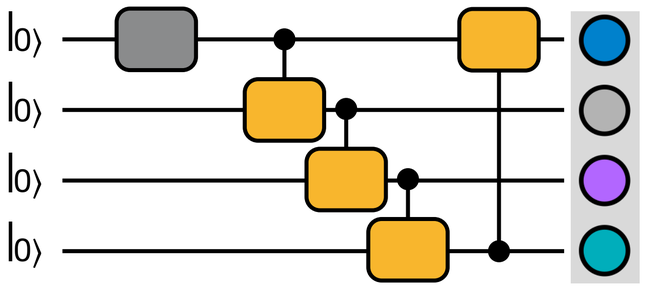
Simulate with noise model
Or
Directly run on real QC device

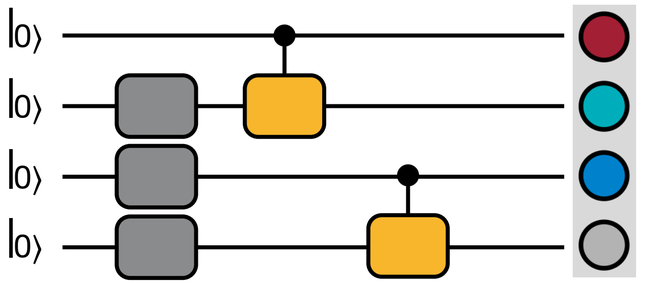
Noise-Adaptive Evolutionary Co-Search

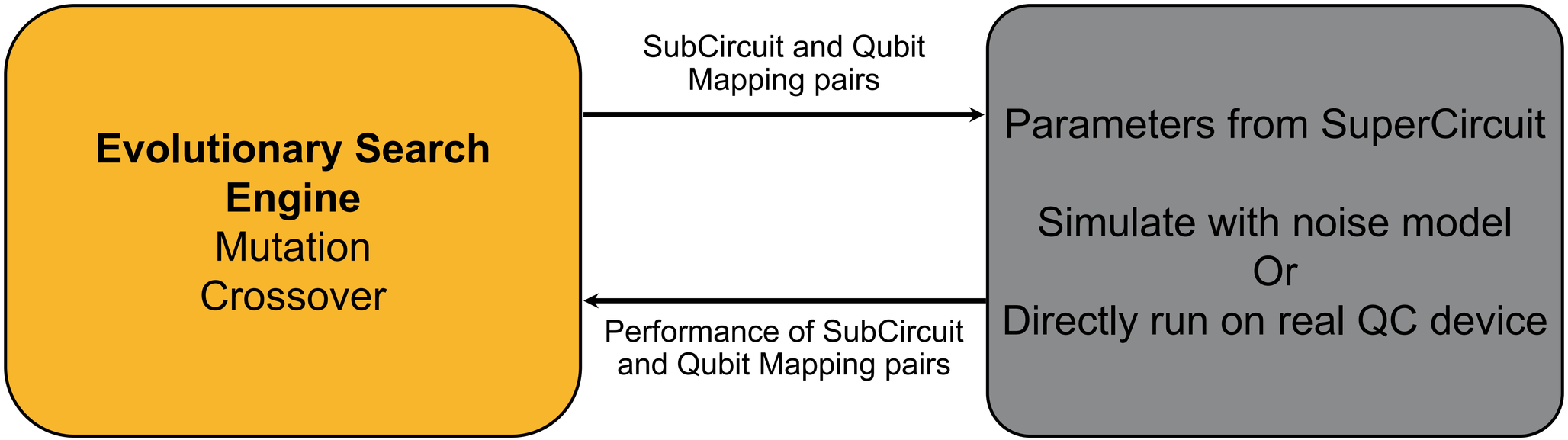
- Search the best SubCircuit and its qubit mapping on target device





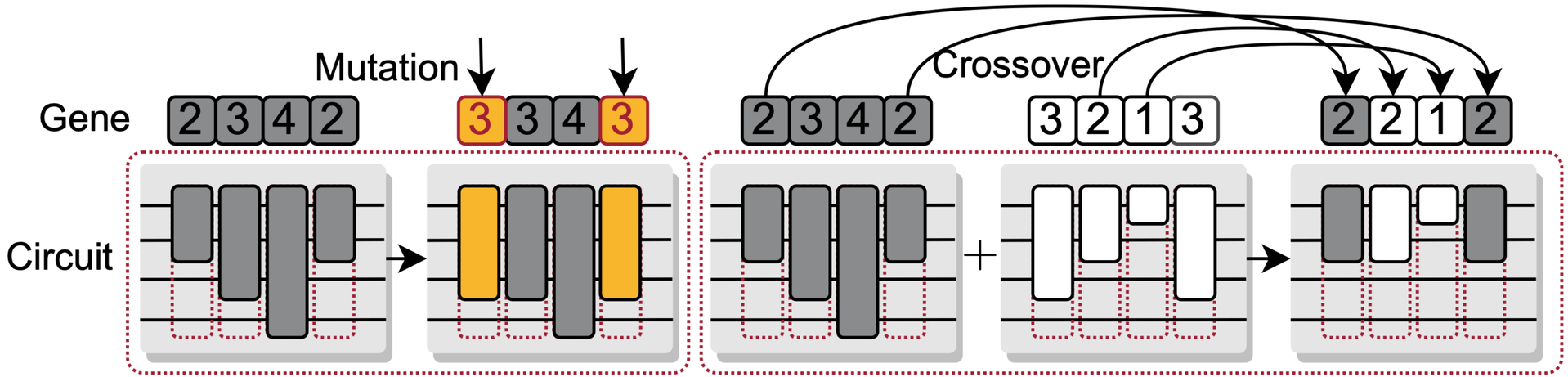






Mutation and Crossover

- Mutation and crossover create new SubCircuit candidates



QuantumNAS

- SuperCircuit Construction and Training
- Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

QuantumNAS

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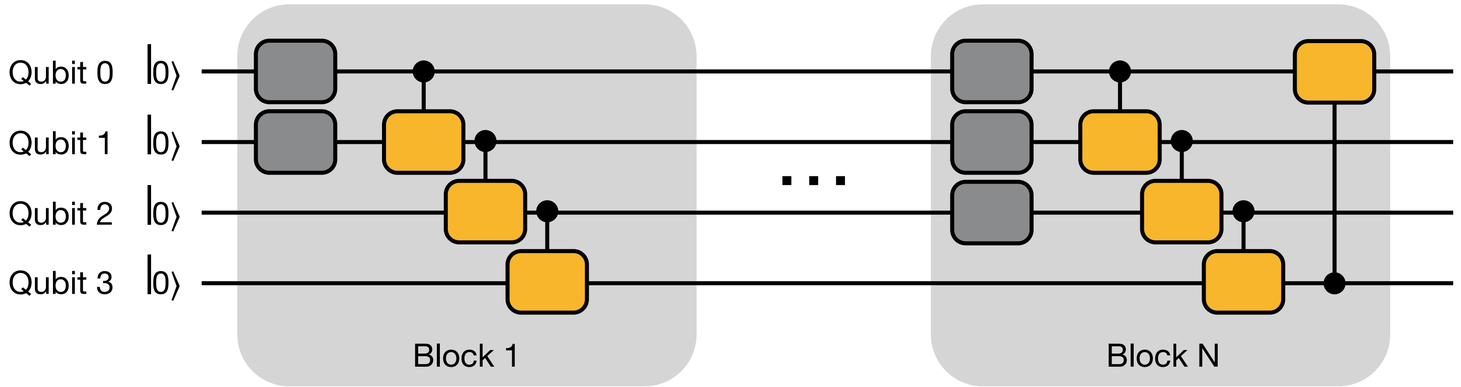
Iterative Pruning

- Some gates have parameters close to 0
  - Rotation gate with angle close to 0 has small impact on the results
- Iteratively prune small-magnitude gates and fine-tune the remaining parameters



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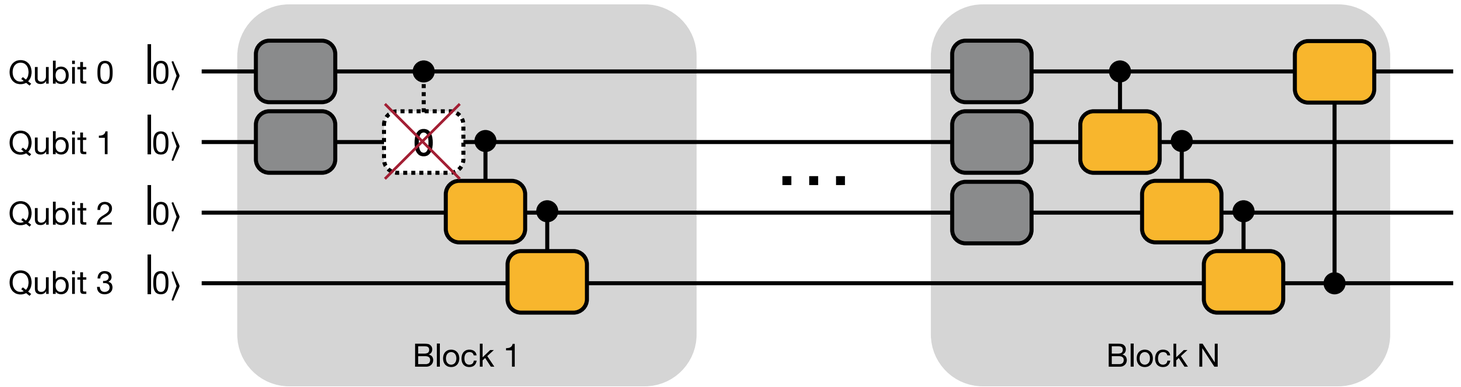

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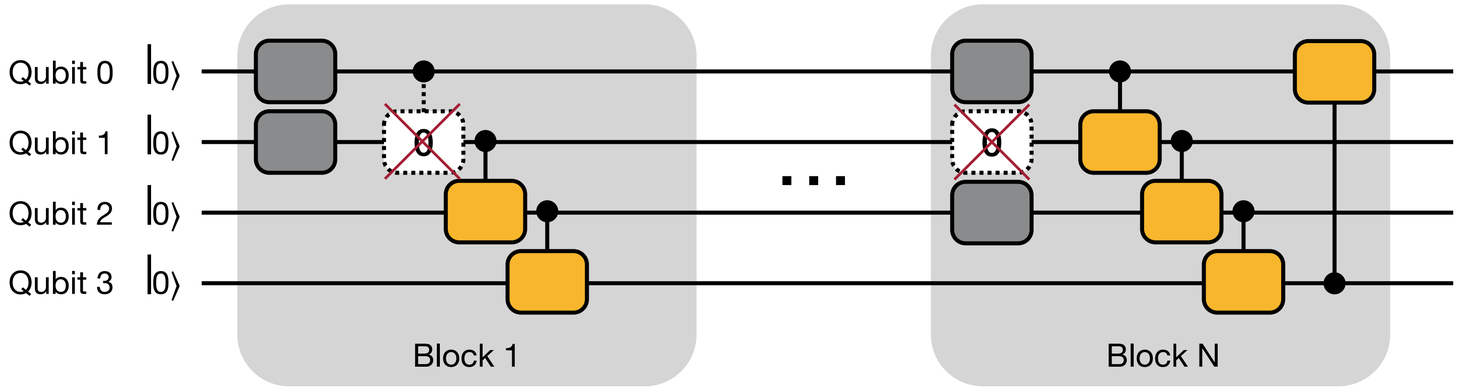

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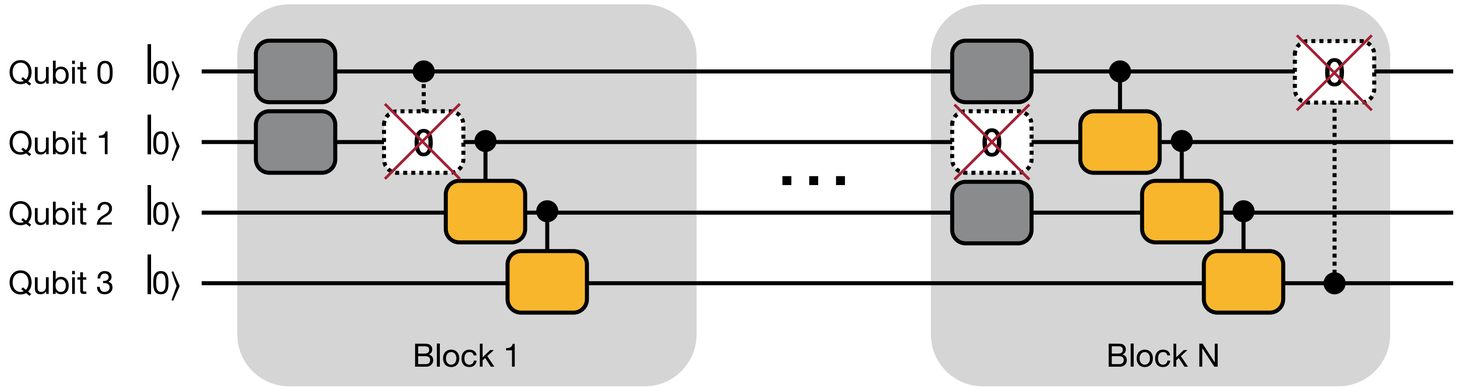

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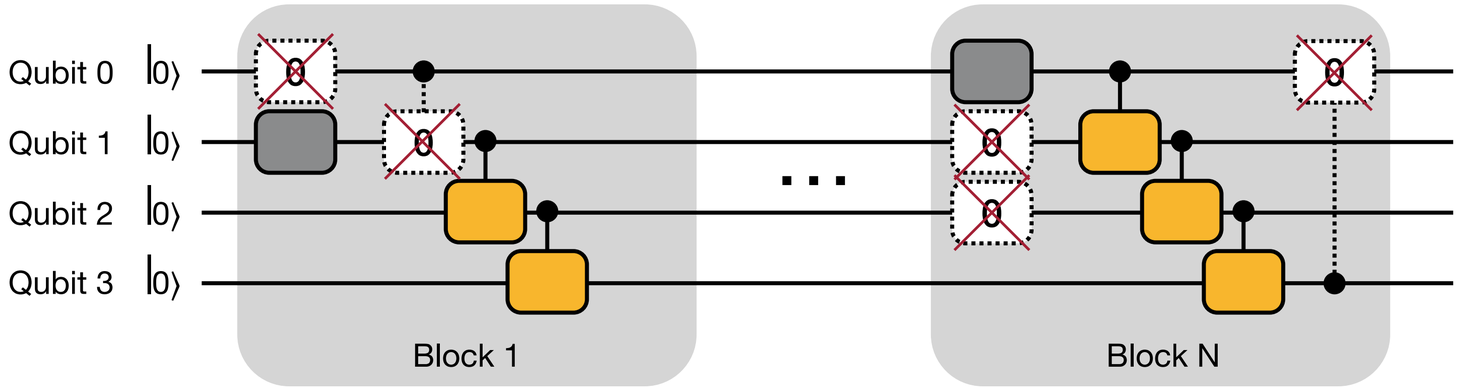
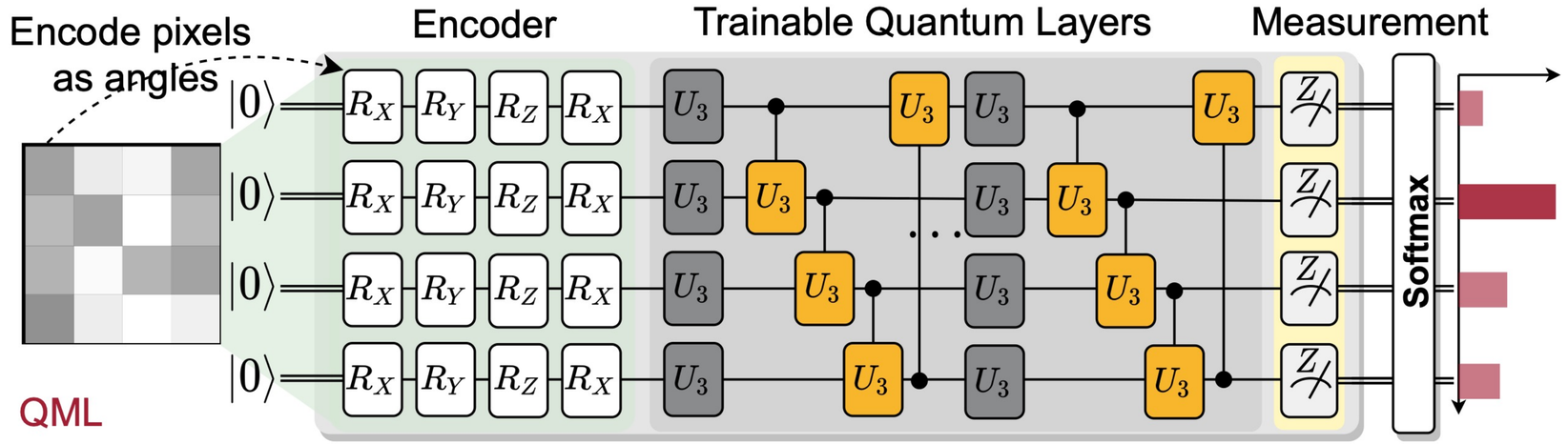


Evaluation Setups: Benchmarks and Devices

- Benchmarks
  - QML classification tasks: MNIST 10-class, 4-class, 2-class, Fashion 4-class, 2-class, Vowel 4-class
  - VQE task molecules: H2, H2O, LiH, CH4, BeH2
- Quantum Devices
  - IBMQ
  - #Qubits: 5 to 65
  - Quantum Volume: 8 to 128

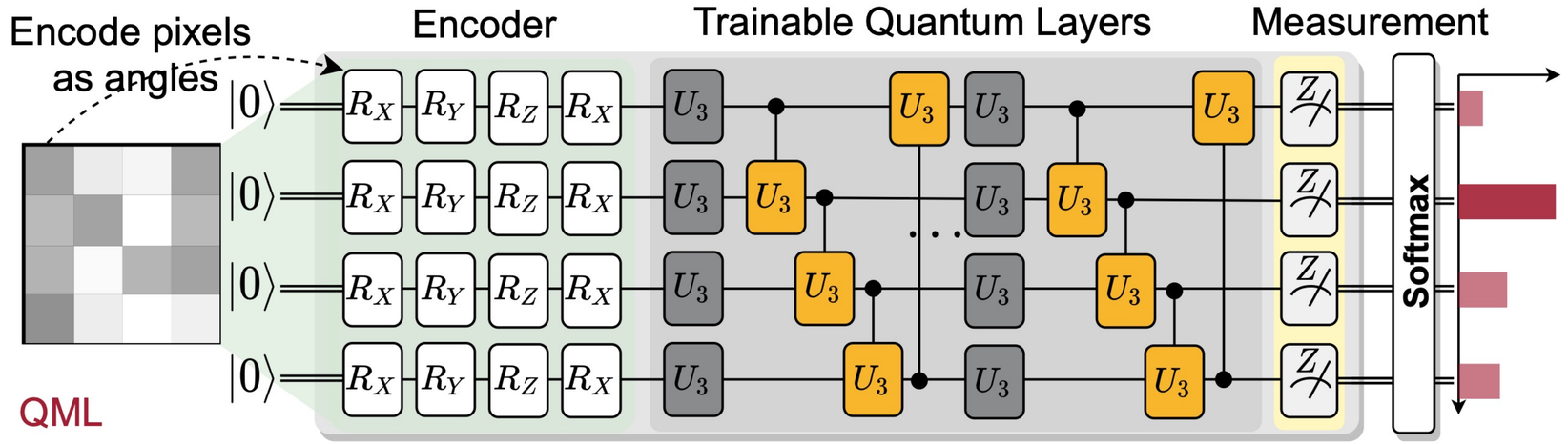
Benchmarks: QNN and VQE

- Quantum Neural Networks: classification

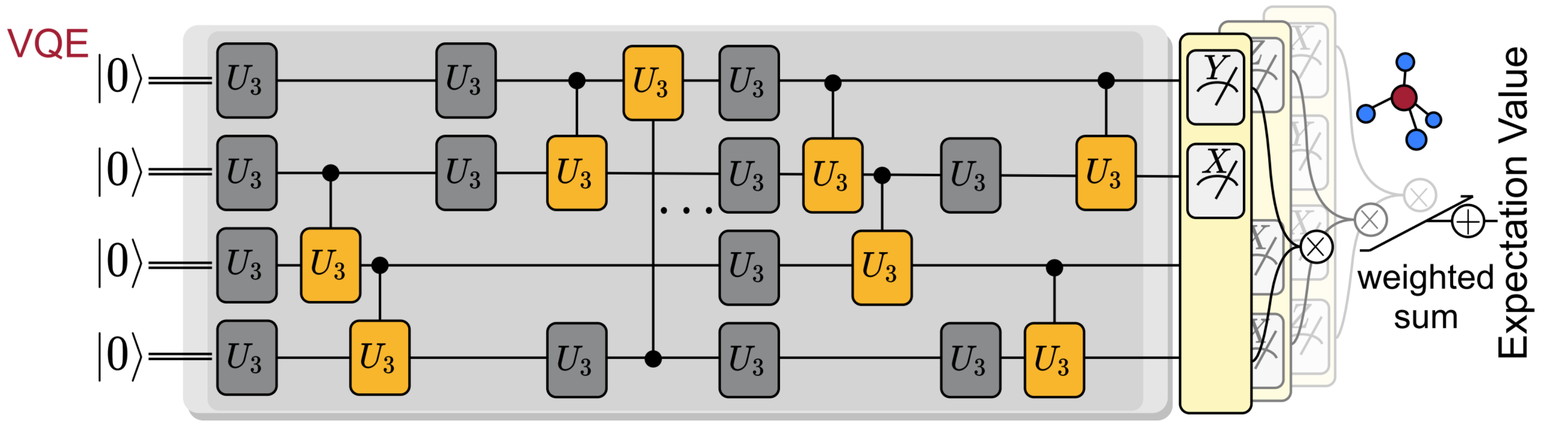


Benchmarks: QNN and VQE

- Quantum Neural Networks: classification

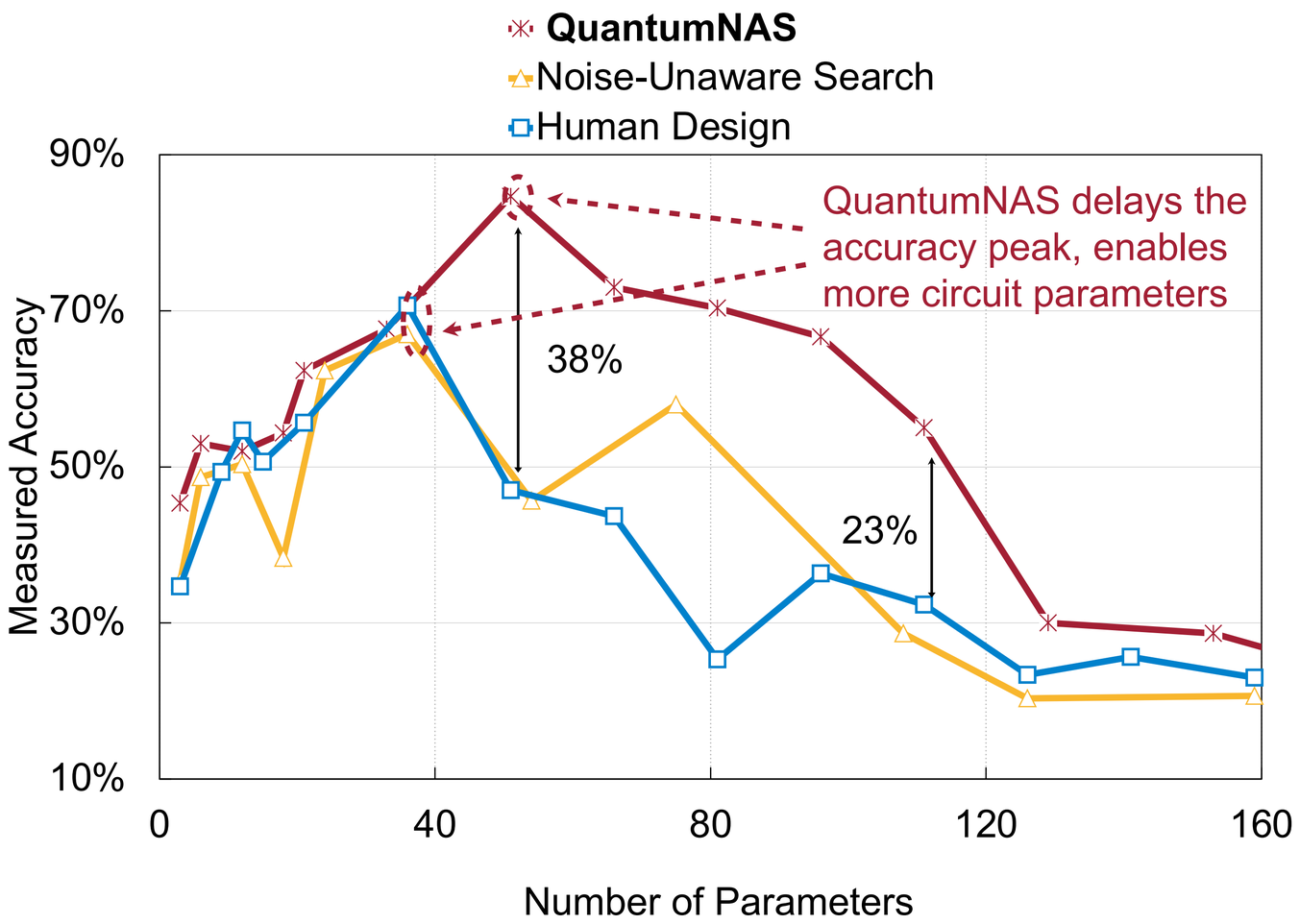


- Variational Quantum Eigensolver: finds the ground state energy of molecule Hamiltonian



QML Results

- 4-classification: MNIST-4 U3+CU3 on IBMQ-Yorktown



Torch Quantum

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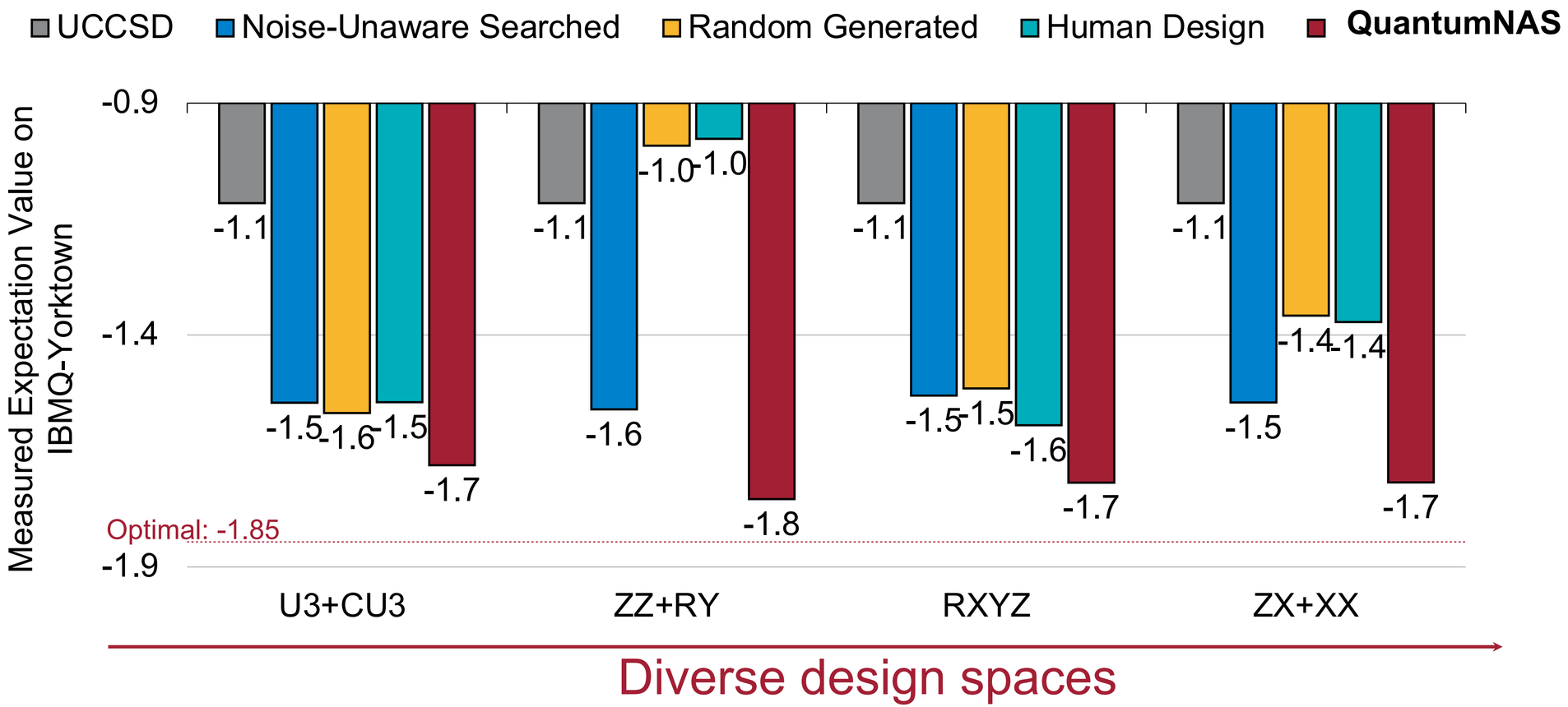
Consistent Improvements on Diverse Design Spaces

- H2 in different design spaces on IBMQ-Yorktown



Scalable to Large #Qubits

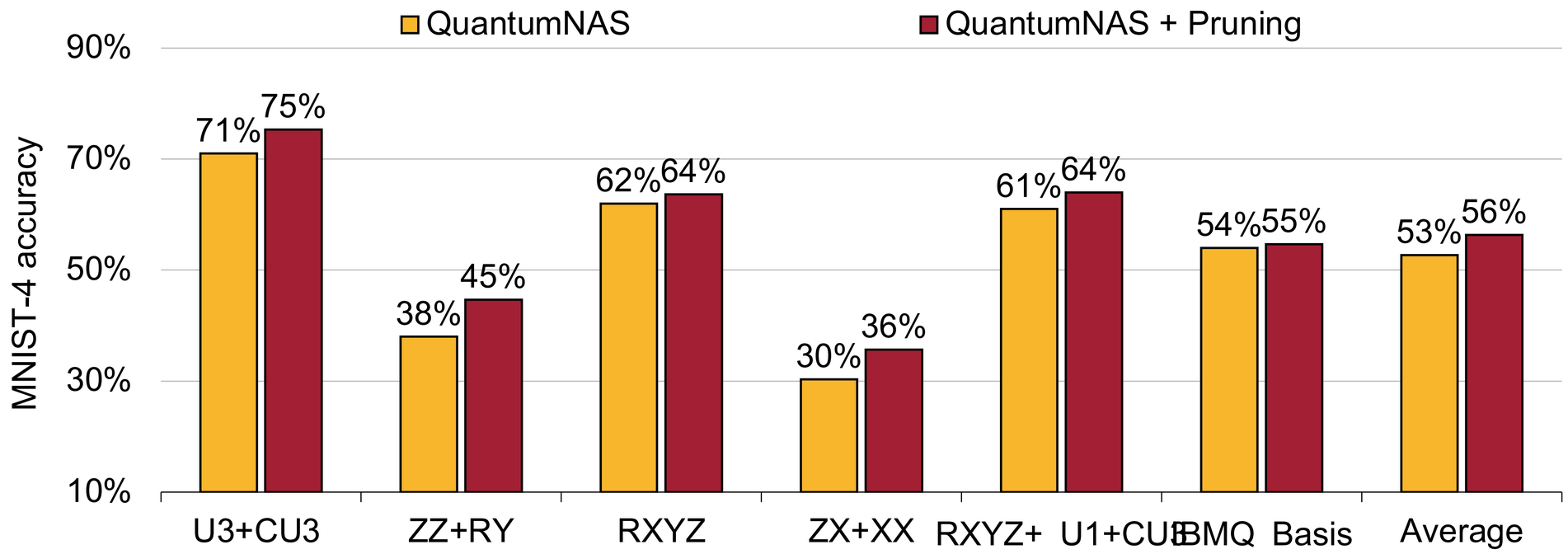
- On large devices
- MNIST-10 accuracy

More Qubits

Method	Noise-Unaware Searched	Random	Human	**QuantumNAS**
Melbourne (15Q, 8QV, use 15Q)	11%	10%	15%	**32%**
Guadalupe (16Q, 32QV, use 16Q)	14%	12%	10%	**15%**
Montreal (27Q, 128QV, use 21Q)	13%	7%	14%	**16%**
Manhattan (65Q, 32QV, use 21Q)	11%	11%	15%	**18%**

Effective of Quantum Gate Pruning

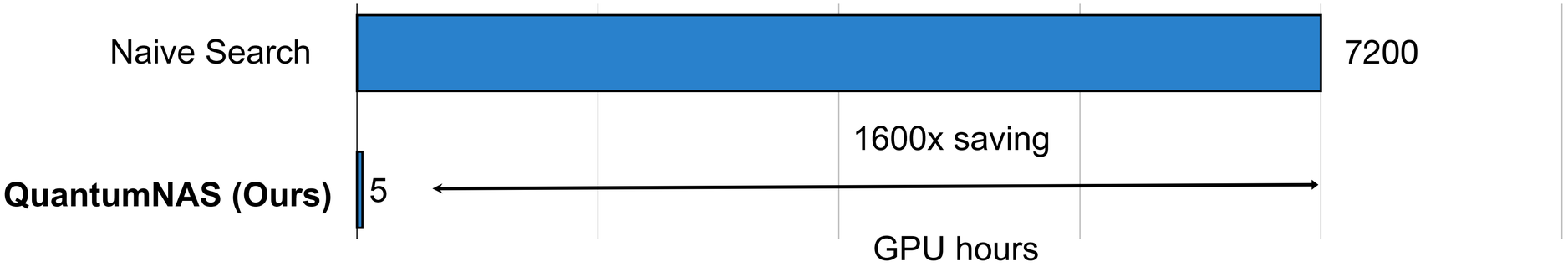
- For MNIST-4, Quantum gate pruning improves accuracy by 3% on average



Time Cost

- On 1 Nvidia Titan RTX 2080 ti GPU

#qubits \ Step	SuperCircuit Training	Noise-Adaptive Co-search	SubCircuit Training	Deployment on Real QC
4 Qubits	0.5h	3h	0.5h	0.5h
15 Qubits	5h	5h	5h	1h
21 Qubits	20h	10h	15h	1h



Torch Quantum

Open-source: TorchQuantum

- TorchQuantum — An open-source library for differentiable quantum simulation

  https://github.com/mit-han-lab/torchquantum

TorchQuantum

- Features
  - Easy construction and simulation of quantum circuits in **PyTorch**
  - **Dynamic** computation graph for easy debugging
  - **Gradient** support via autograd
  - **Batch** mode inference and training on CPU/GPU.
  - Easy **deployment** on real quantum devices such as IBMQ
  - Easy **hybrid** classical-quantum model construction
  - (coming soon) **pulse-level** simulation
  - Tutorials, videos and example projects of QML and using ML to optimize quantum computer system problems
- Will be on **QCE** (Quantum Computing Engineering) tutorials

Open-source: TorchQuantum

- Statevector

```
_state = torch.zeros(2 ** self.n_wires, dtype=C_DTYPE)
_state[0] = 1 + 0j
```

- Quantum Gates

```
'cnot': torch.tensor([[1, 0, 0, 0],
                      [0, 1, 0, 0],
                      [0, 0, 0, 1],
                      [0, 0, 1, 0]], dtype=C_DTYPE),
```

Torch Quantum

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Open-source: TorchQuantum

- Quantum Gates

```
def crx_matrix(params):
    theta = params.type(C_DTYPE)
    co = torch.cos(theta / 2)
    jsi = 1j * torch.sin(-theta / 2)

    matrix = torch.tensor([[1, 0, 0, 0],
                           [0, 1, 0, 0],
                           [0, 0, 0, 0],
                           [0, 0, 0, 0]], dtype=C_DTYPE, device=params.device
                          ).unsqueeze(0).repeat(co.shape[0], 1, 1)
    matrix[:, 2, 2] = co[:, 0]
    matrix[:, 2, 3] = jsi[:, 0]
    matrix[:, 3, 2] = jsi[:, 0]
    matrix[:, 3, 3] = co[:, 0]

    return matrix.squeeze(0)
```

- Matrix-vector multiplication: torch.einsum and torch.bmm

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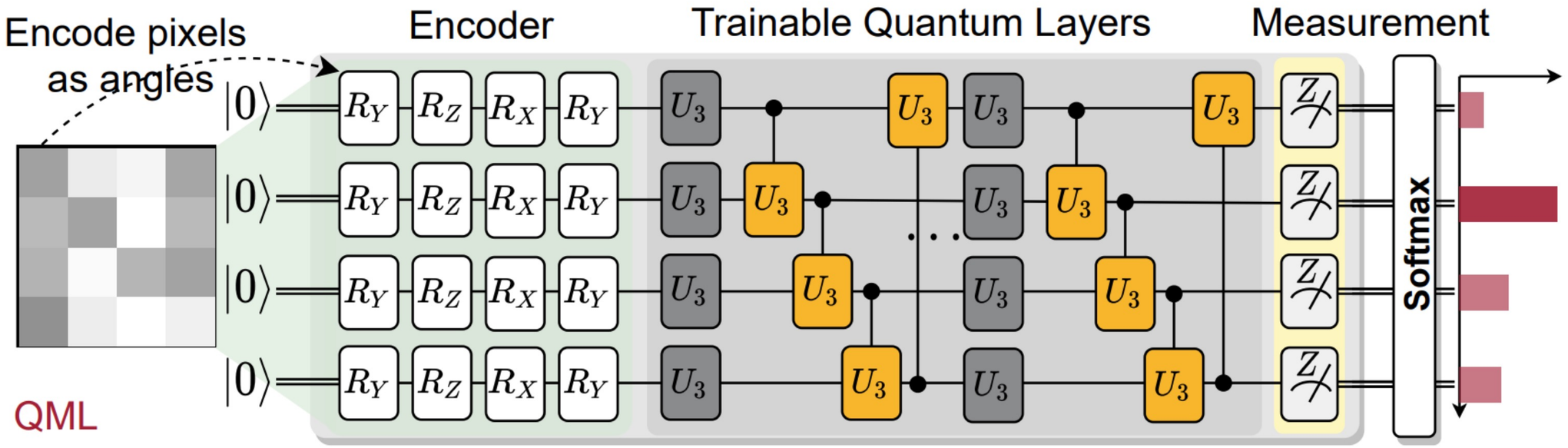
MNIST Example with QNN



MNIST Example

Initialize a quantum device

Specify encoder gates

Specify trainable gates

```
import torch.nn as nn
import torch.nn.functional as F
import torchquantum as tq
import torchquantum.functional as tqf

class QFCModel(nn.Module):
  def __init__(self):
    super().__init__()
    self.n_wires = 4
    self.q_device = tq.QuantumDevice(n_wires=self.n_wires)
    self.measure = tq.MeasureAll(tq.PauliZ)

    self.encoder_gates = [tqf.rx] * 4 + [tqf.ry] * 4 + \
                         [tqf.rz] * 4 + [tqf.rx] * 4
    self.rx0 = tq.RX(has_params=True, trainable=True)
    self.ry0 = tq.RY(has_params=True, trainable=True)
    self.rz0 = tq.RZ(has_params=True, trainable=True)
    self.crx0 = tq.CRX(has_params=True, trainable=True)
```

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MNIST Example

Reset statevector

Encode classical pixels

Apply the trainable gates

Apply some non-trainable gates

Measure to get classical values

```
def forward(self, x):
  bsz = x.shape[0]
  # down-sample the image
  x = F.avg_pool2d(x, 6).view(bsz, 16)

  # reset qubit states
  self.q_device.reset_states(bsz)

  # encode the classical image to quantum domain
  for k, gate in enumerate(self.encoder_gates):
    gate(self.q_device, wires=k % self.n_wires, params=x[:, k])

  # add some trainable gates (need to instantiate ahead of time)
  self.rx0(self.q_device, wires=0)
  self.ry0(self.q_device, wires=1)
  self.rz0(self.q_device, wires=3)
  self.crx0(self.q_device, wires=[0, 2])

  # add some more non-parameterized gates (add on-the-fly)
  tqf.hadamard(self.q_device, wires=3)
  tqf.sx(self.q_device, wires=2)
  tqf.cnot(self.q_device, wires=[3, 0])
  tqf.qubitunitary(self.q_device0, wires=[1, 2], params=[[1, 0, 0, 0],
                                                         [0, 1, 0, 0],
                                                         [0, 0, 0, 1j],
                                                         [0, 0, -1j, 0]])

  # perform measurement to get expectations (back to classical domain)
  x = self.measure(self.q_device).reshape(bsz, 2, 2)

  # classification
  x = x.sum(-1).squeeze()
  x = F.log_softmax(x, dim=1)

  return x
```

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MNIST Example

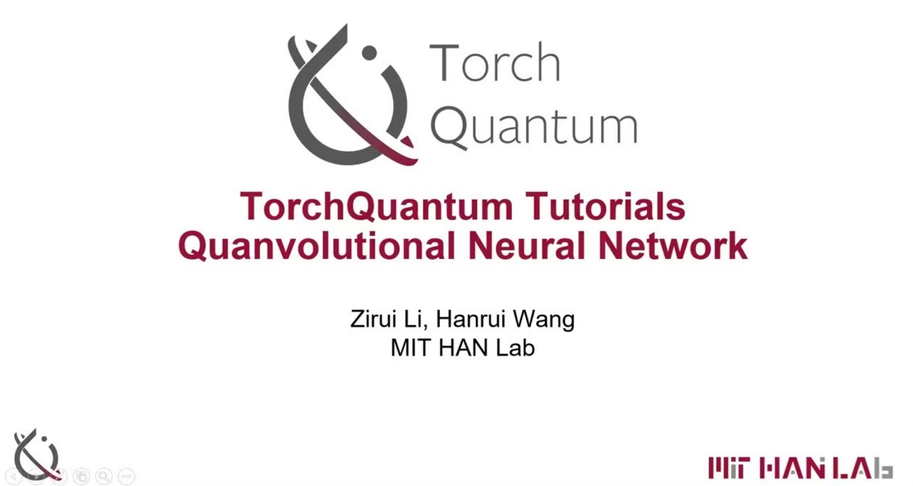
Initialize a QiskitProcessor

The ‘forward’ will be run on real QC

```
# then try to run on REAL QC
backend_name = 'ibmqx2'
print(f"\nTest on Real Quantum Computer {backend_name}")
processor_real_qc = QiskitProcessor(use_real_qc=True,
                                    backend_name=backend_name)
model.set_qiskit_processor(processor_real_qc)
valid_test(dataflow, 'test', model, device, qiskit=True)
```

Examples and tutorials

- Tutorial Colab and videos



Thank you for listening!

- Take home
  - **TorchQuantum:** fast open-source **library** for quantum simulation
  - **QuantumNAS:** framework to search for **noise-robust** circuit architecture

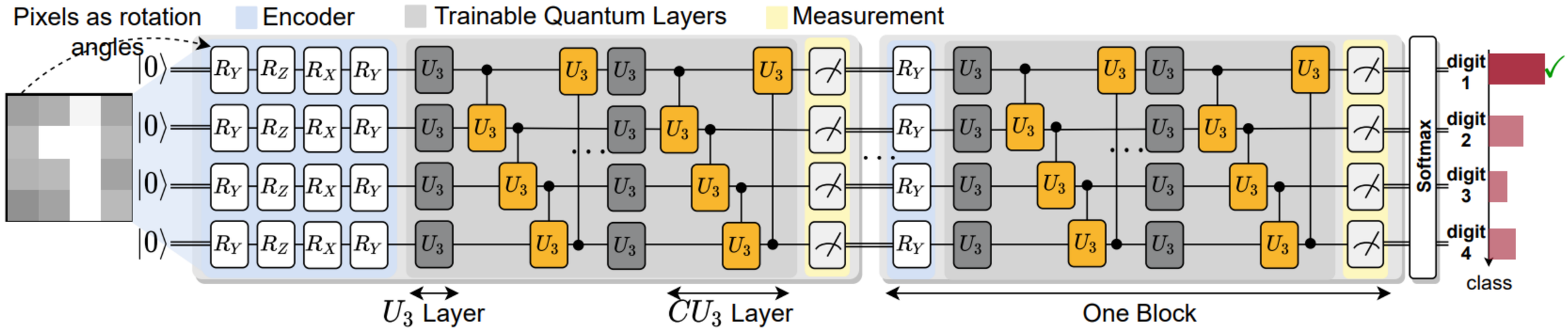
Torch Quantum

https://github.com/mit-han-lab/torchquantum

qmlsys.mit.edu

QuantumNAT

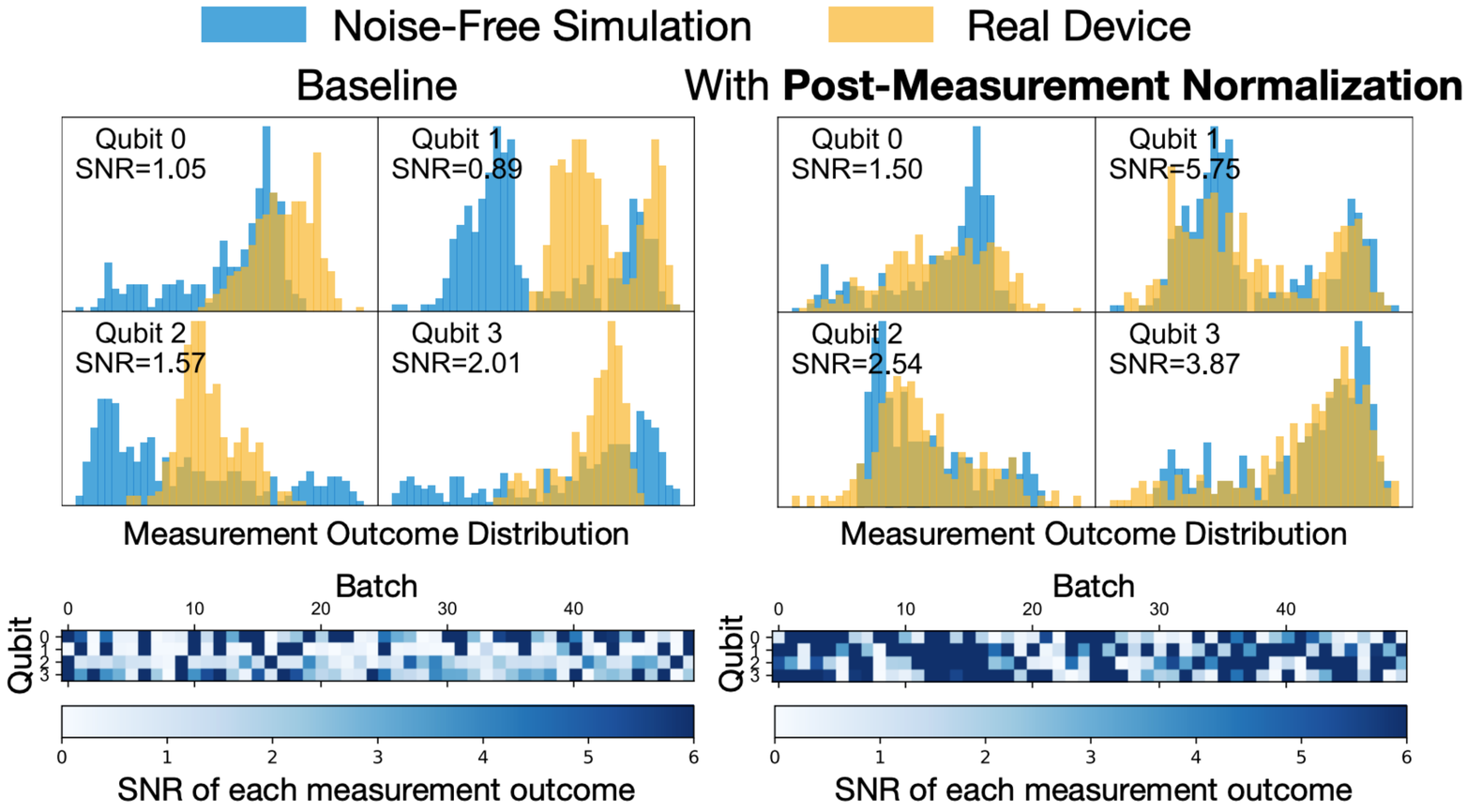
- **QuantumNAS: find the circuit architecture robust to noise**
- **QuantumNAT: further make the parameter robust to noise**



[DAC'22] Wang et, at, QuantumNAT: Quantum Noise-Aware Training with Noise Injection, Quantization and Normalization

Post-Measurement Normalization

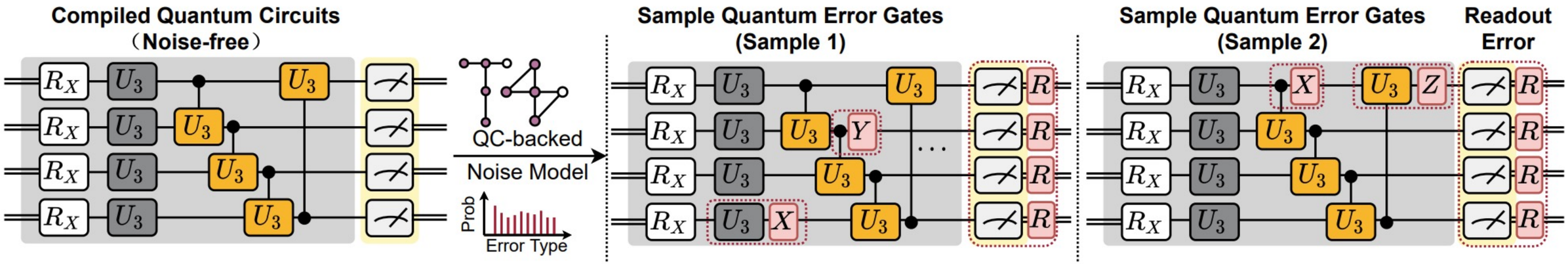
- **Normalize the measurement outcomes on the batch dimension**



2nd block output of a 3-block model, IBMQ-Quito

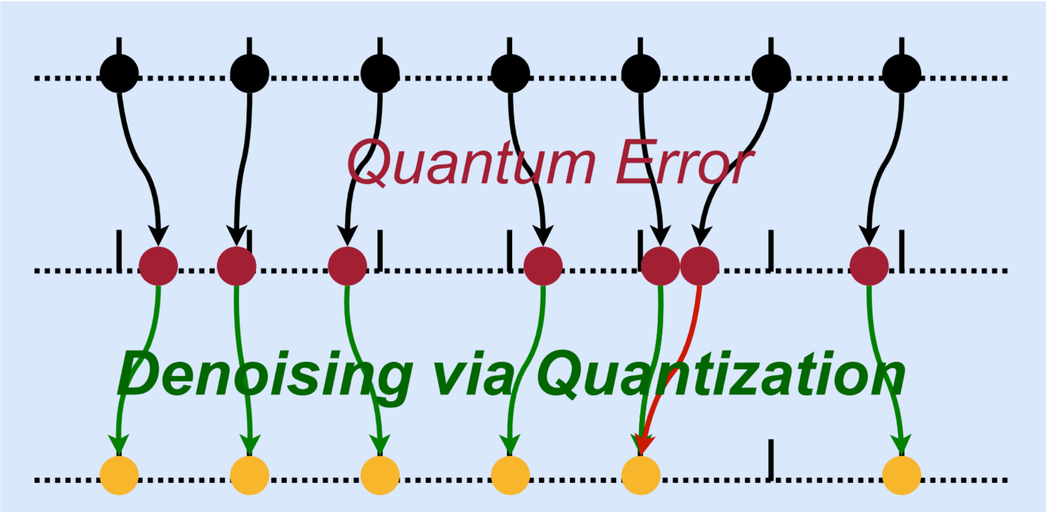
Noise Injection

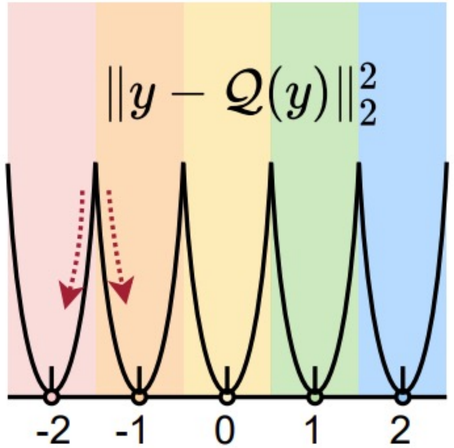
- **Insert noise gate during training, according to the noise model**
- **For each step, sample new positions for noise gates**



Post-Measurement Quantization

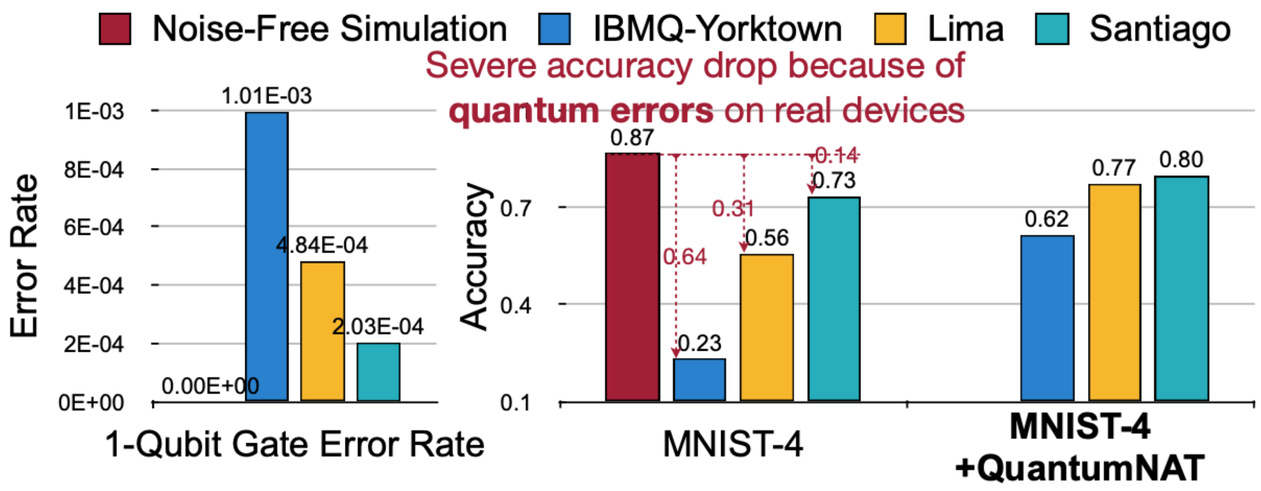
- **Quantization provides denoising effects**
- **Quadratic penalty loss to encourage measurement outcomes close to quantization centroids**

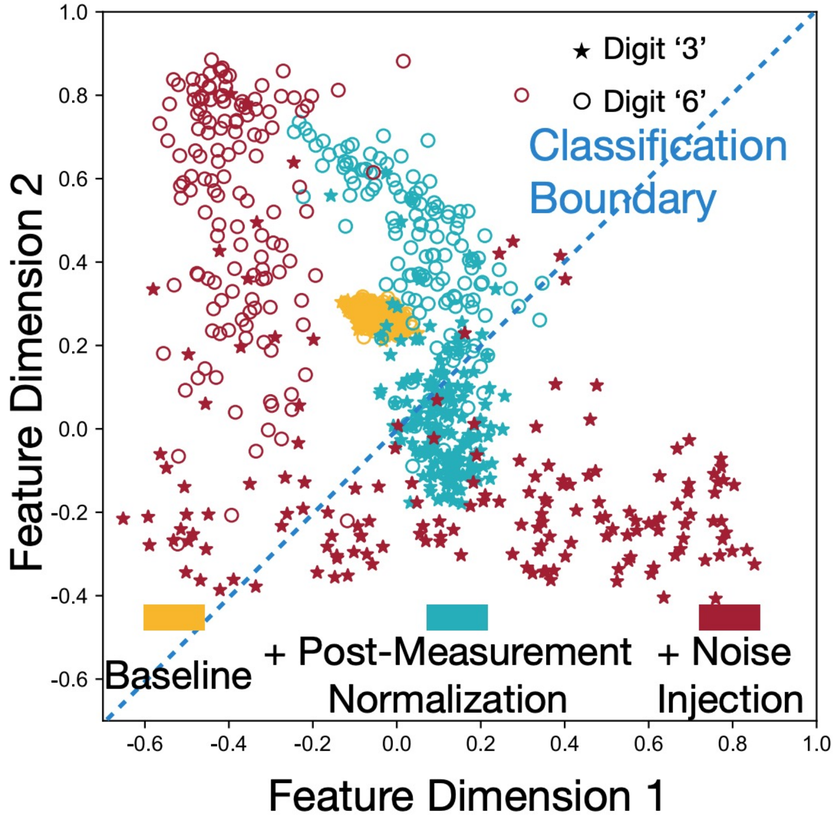




Evaluation

- **On classification tasks with QNN**

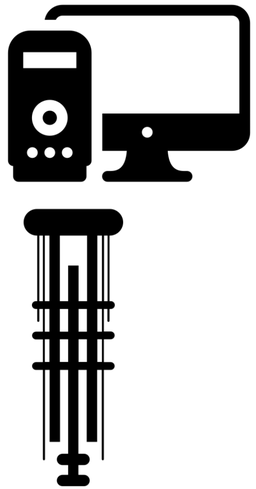




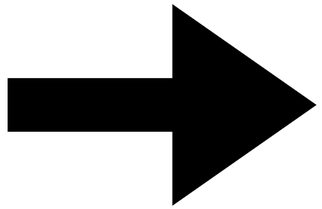
QOC (Quantum On-Chip Training)

Train on classical

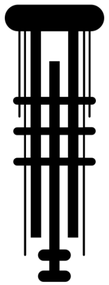
Deploy on quantum



Scalability ↑



Train & Deploy on quantum



[DAC'22] Wang et, at, QOC: Quantum On-Chip Training with Parameter Shift and Gradient Pruning