CPEN 400Q / EECE 571Q Lecture 13
Introducing variational algorithms

Tuesday 1 March 2022

Announcements

- Assignment 3 available
  - second-last assignment
  - please read grading details
  - due Friday 11 March 23:59
- Meetings *next week* for project prototypes (schedule selection starting tomorrow)

Quiz 6 after class today.

Last time

We learned about RSA, implemented Shor's algorithm, and used it to decompose numbers into their prime factors.

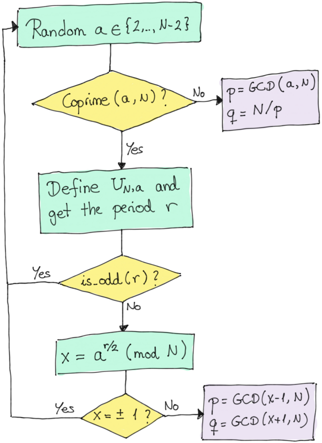


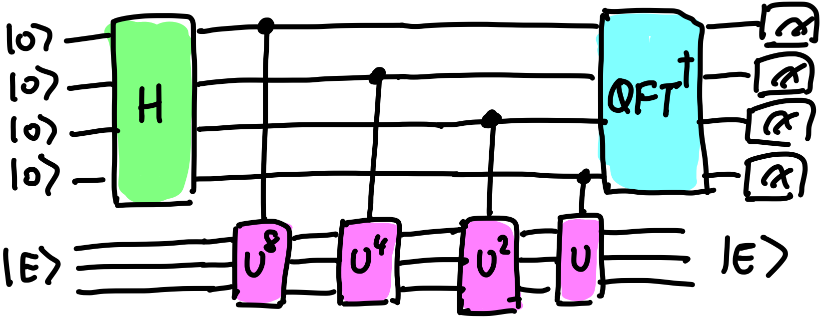
Image credit: Xanadu Quantum Codebook node S.4

Learning outcomes

- Describe the main structural elements of a variational quantum algorithm
- Compute gradients of variational circuit parameters using the parameter-shift rule
- Find optimal parameters of a variational circuit in PennyLane

Why variational algorithms?

Consider an algorithm like QPE...



Why variational algorithms?

"Full-size algorithms" like QPE, Shor, Grover, etc.:

- Use many qubits
- Require dense qubit *connectivity*
- Have high circuit depth

Today's quantum computers today aren't really suitable for these...

Why variational algorithms?

[A NISQ-era device, for exemplary purposes]

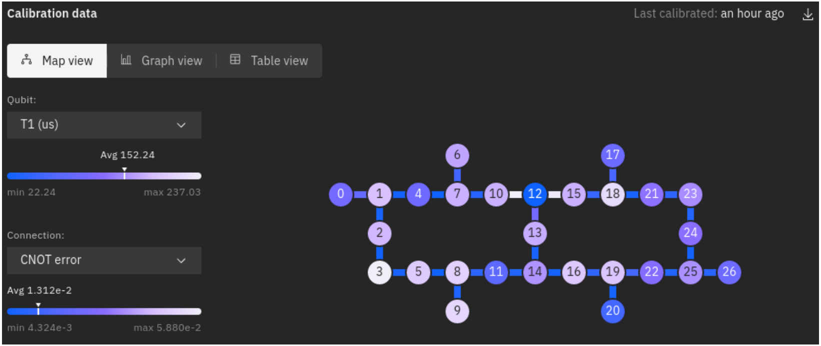


Image credit: IBM Q Auckland, screen capture 2022-03-01.

`https://quantum-computing.ibm.com/services?services=systems&system=ibm_auckland`

Why variational algorithms?

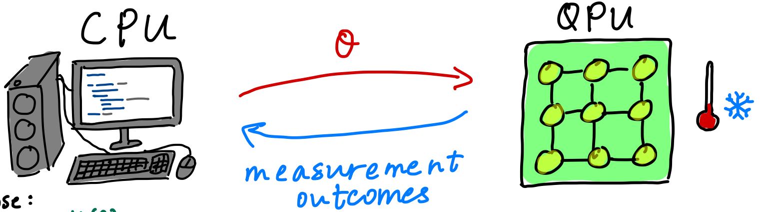
What *can* we do with a NISQ device?

Suitable algorithms should:

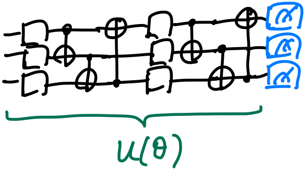
- Not be too long
- Fit the processor architecture well
- Use a quantum computer to do something non-trivial
- Still solve an interesting problem

Variational algorithms

Feature an iterative exchange between classical and quantum devices. (Sometimes called “hybrid” quantum-classical algorithms)

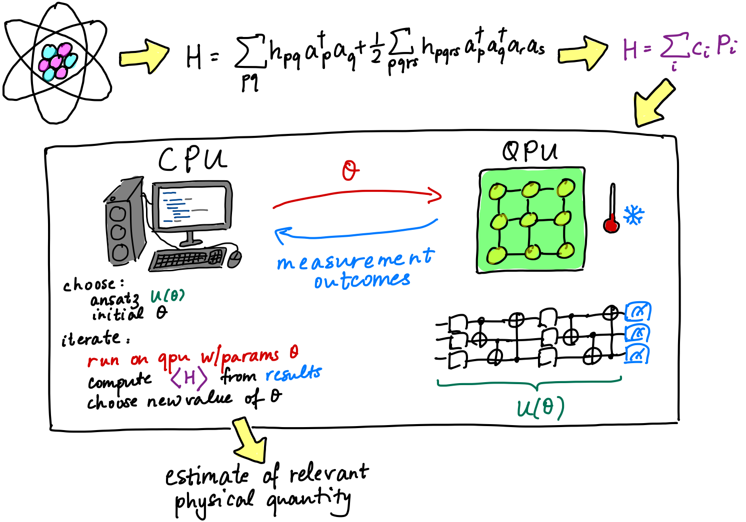


choose:
    ansatz $U(\theta)$
    initial θ
iterate:
    run on qpu w/params θ
    compute cost from results
    choose new value of θ



Variational algorithms

Useful in many domains: quantum chemistry, quantum machine learning, optimization, etc.



Variational algorithms

We will cover in the rest of the course:

- The basics of setting up and running variational algorithms
  - Quantum gradients
  - Parametrized quantum circuits and variational ansaetze
  - Cost functions
- A number of common variational algorithms
  - Variational quantum classifier (VQC)
  - Variational quantum eigensolver (VQE)
  - Quantum approximate optimization algorithm (QAOA)
- Challenges and solutions for running such algorithms on noisy quantum hardware

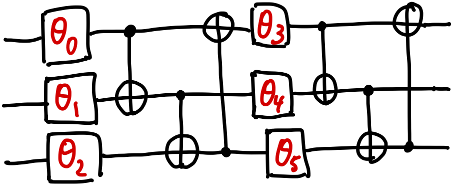
Parametrized quantum circuits

Some quantum operations depend on real-valued *parameters*.

These can be passed as arguments to a quantum function.

```
def circuit(x, y, z):
    qml.RX(x, wires=0)
    qml.RY(y, wires=1)
    qml.RZ(z, wires=2)
```

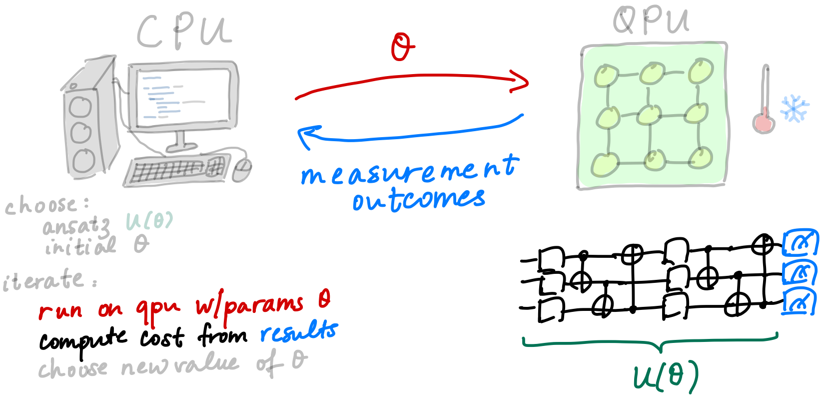
We call these **parametrized quantum circuits**.




```
def parametrized_circuit(theta):
    qml.RX(theta[0], wires=0)
    qml.RX(theta[1], wires=1)
    qml.RX(theta[2], wires=2)
    qml.CNOT(wires=[0, 1])
    qml.CNOT(wires=[1, 2])
    qml.CNOT(wires=[2, 0])
    qml.RX(theta[3], wires=0)
    qml.RX(theta[4], wires=1)
    qml.RX(theta[5], wires=2)
    qml.CNOT(wires=[0, 1])
    qml.CNOT(wires=[1, 2])
    qml.CNOT(wires=[2, 0])
```

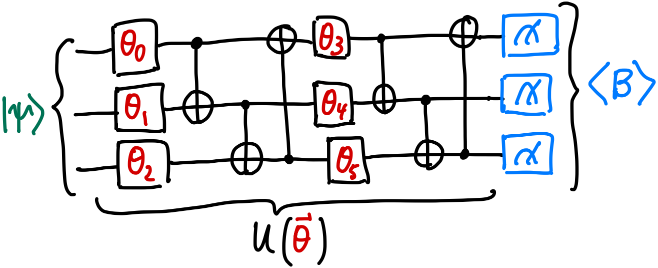
Parametrized quantum circuits

Parametrized circuits are used to assist in evaluation of a cost function which represents a particular problem.



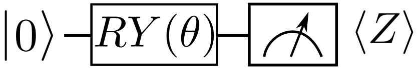
We are trying to *find optimal values* for these parameters in order to minimize the cost, which represents the solution to the problem.

Expectation values are often used to construct a cost function.



$$\min_{\vec{\theta}} \langle B\rangle = \min_{\vec{\theta}} \langle\psi| U^\dagger(\vec{\theta}) B U(\vec{\theta}) |\psi\rangle$$

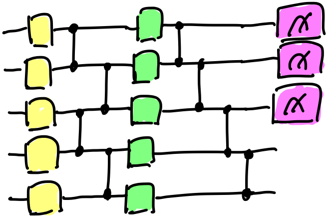
Example: find the value of θ which minimizes $\langle Z \rangle$.

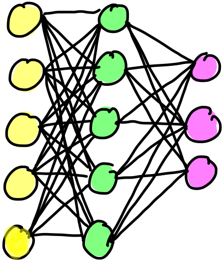


Easy to solve by hand ($\theta^* = \pi$). How can we *train* the quantum circuit to learn the optimal value?

Training variational quantum circuits

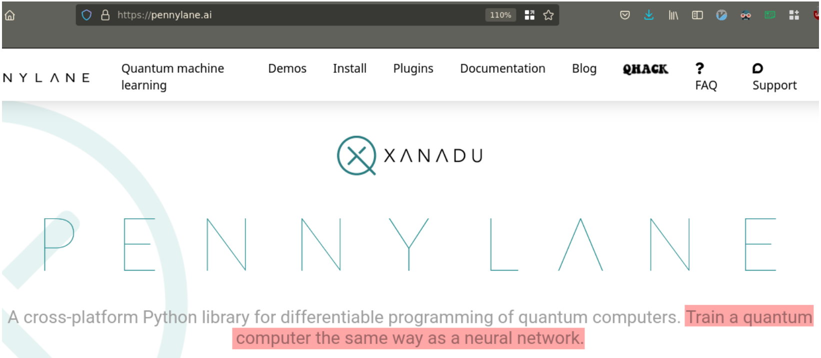
Working with variational quantum circuits is a lot like working with neural networks (architecture and layer design, training to determine optimal weights, etc.)





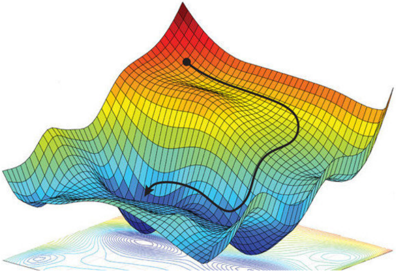
Variational circuits are often termed *quantum neural networks*.

Training variational quantum circuits



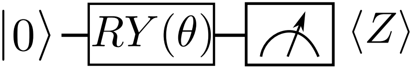
Training variational quantum circuits

Circuits can be trained using standard optimization techniques *on a classical computer* such as gradient descent.



... but how do we compute the gradient of a quantum circuit?

Image credit: A. Amini, A. P. Soleimany, S. Karaman, D. Rus. *Spatial Uncertainty Sampling for End-to-End Control*. NIPS 2017.

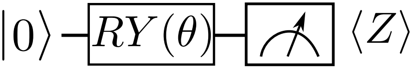


Key point: the expectation values measured at the end are *functions* of the variational parameters, i.e.,

$$\langle Z\rangle = f(\theta)$$

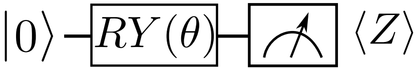
We can compute such functions, then differentiate them.

Gradients of quantum circuits



Let's compute the analytical expression for $\langle Z\rangle$:

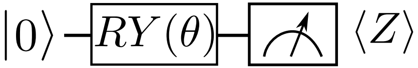
$$
\begin{aligned}
\langle Z\rangle &= \langle 0|RY^\dagger(\theta)\cdot Z\cdot RY(\theta)|0\rangle\\
&= \langle 0|RY(-\theta)\cdot Z\cdot RY(\theta)|0\rangle\\
&= \langle 0|RY(-\theta)\cdot Z\cdot [\cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle]\\
&= \langle 0|RY(-\theta)[\cos(\theta/2)|0\rangle - \sin(\theta/2)|1\rangle]\\
&= \langle 0|[\cos(\theta/2)(\cos(-\theta/2)|0\rangle + \sin(-\theta/2)|1\rangle)\\
&\qquad - \sin(\theta/2)(-\sin(-\theta/2)|0\rangle + \cos(-\theta/2)|1\rangle)]
\end{aligned}
$$



Let's compute the analytical expression for $\langle Z\rangle$:

$$
\begin{aligned}
\langle Z\rangle &= \langle 0|[\cos(\theta/2)(\cos(-\theta/2)|0\rangle + \sin(-\theta/2)|1\rangle) \\
&\qquad - \sin(\theta/2)(-\sin(-\theta/2)|0\rangle + \cos(-\theta/2)|1\rangle)] \\
&= \langle 0|[\cos(\theta/2)(\cos(\theta/2)|0\rangle - \sin(\theta/2)|1\rangle) \\
&\qquad - \sin(\theta/2)(\sin(\theta/2)|0\rangle + \cos(\theta/2)|1\rangle)] \\
&= \langle 0|\,[\cos^2(\theta/2)|0\rangle - \cos(\theta/2)\sin(\theta/2)|1\rangle \\
&\qquad - \sin^2(\theta/2)|0\rangle - \sin(\theta/2) cos(\theta/2)|1\rangle] \\
&= \cos^2(\theta/2) - \sin^2(\theta/2) \\
&= \cos(\theta)
\end{aligned}
$$

Gradients of quantum circuits



In order to train the circuit, we can use gradient descent; just compute the derivative of the function!

$$\langle Z\rangle = \cos(\theta)$$
$$\frac{\partial\langle Z\rangle}{\partial\theta} = -\sin(\theta)$$

But obviously, we don't want to do this by hand... use automatic differentiation instead! PennyLane will do this for us.

`qml.grad` is a *transform*: apply to a QNode to obtain a function that computes the *gradient* of that QNode.

```
@qml.qnode(dev)
def pqc(theta):
    qml.RY(theta, wires=0)
    return qml.expval(qml.PauliZ(0))

grad_fn = qml.grad(pqc)
grad_fn(theta)
```

Easy to do in software, but what about on hardware?

To train using gradient descent, then we'd have to:

1. guess an initial value for θ
2. run a circuit that computes the gradient at θ
3. use those results to produce an updated value for θ
4. repeat 2-3 until converged

You don't actually need a different circuit: you can use a circuit to compute its own gradient by running the circuit multiple times at different values, and combining the results.

Our circuit implements the function

$$f(\theta) = \cos(\theta)$$

The gradient of this function is

$$\frac{\partial f(\theta)}{\partial \theta} = -\sin(\theta)$$

Consider the following:

$$\frac{1}{2}\left(\cos(\theta + \pi/2) - \cos(\theta - \pi/2)\right)$$

The parameter-shift rule

Let's simplify this by noting that

$$\cos(\theta + \pi/2) = -\sin(\theta)$$
$$\cos(\theta - \pi/2) = \sin(\theta)$$

Then:

$$\begin{aligned}\frac{1}{2}\left(\cos(\theta + \pi/2) - \cos(\theta - \pi/2)\right) &= \frac{1}{2}\left(-\sin(\theta) - \sin(\theta)\right) \\ &= -\sin(\theta) \\ &= \frac{\partial f(\theta)}{\partial \theta}\end{aligned}$$

$$\frac{\partial f(\theta)}{\partial \theta} = \frac{1}{2}\left(\cos(\theta + \pi/2) - \cos(\theta - \pi/2)\right)$$

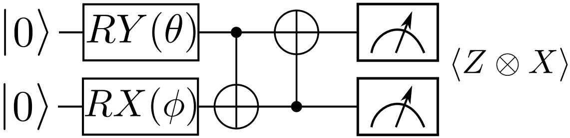
This is an example of a parameter-shift rule: we can compute gradients with respect to parameters of a circuit by evaluating them at shifted versions of those parameters!

More generally, for all single-qubit rotation gates $U(\theta)$,

$$\frac{\partial f(\theta)}{\partial \theta} = \frac{1}{2}\left(f(\theta + \pi/2) - f(\theta - \pi/2)\right)$$

where $f(\theta)$ is the function implemented by the *whole circuit*, with every other parameter held constant.

Let's try an example with more than one parameter.



Next time

Content:

- Embedding data in variational circuits
- The variational quantum classifier

Action items:

1. Assignment 3 (can do all problems)
2. Start working on prototype implementation for project

Recommended reading:

- QML glossary entries (`https://pennylane.ai/qml/glossary.html`):
  - Quantum differentiable programming
  - Parameter-shift rules
  - Quantum gradients
  - Variational circuit
- `https://arxiv.org/abs/2012.09265v2` (review paper)