Introduction to Quantum Machine Learning and Neural Networks (Part 2)

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Warm-up:
Quantum Encoding

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Basis Encoding

- Encode data as computational basis states
- Examples:
  - Bit string:
    $x = (1, 0, 1) \rightarrow |101\rangle$
  - Number as binary:
    $6 = 4 + 2 + 0 = 1 \cdot 2^2 + 1 \cdot 2^1 + 0 \cdot 2^0 = 110_2 = |110\rangle$
- Typically one qubit per feature

Pros

- Simple
- Implementation is straightforward

Cons

- Poor for continuous data
- No natural notion of similarity

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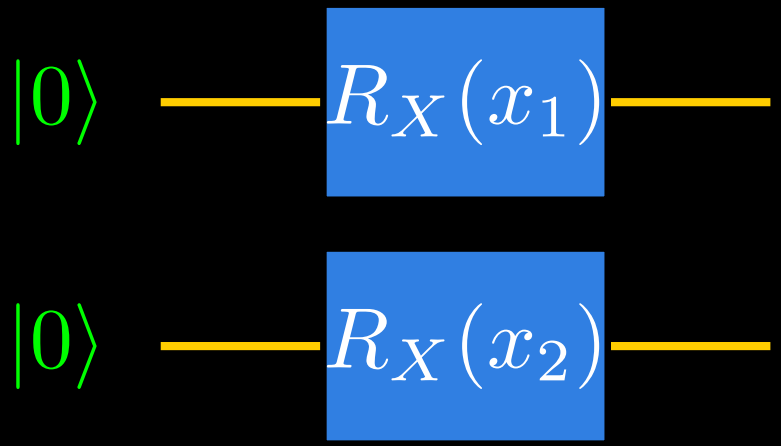
Angle Encoding

- Suppose $x = (x_1, x_2)$
- Angle encoding:

$$x \to R_X(x_1)\,|0\rangle \otimes R_X(x_2)\,|0\rangle$$



Pros

- Natural for continuous data
- Efficient and hardware friendly
- Effective with shallow circuits

Cons

- One rotation per feature
- Limited expressivity without entangling layers
- Capturing global correlations requires deep circuits

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Amplitude Encoding

- Encode features as state amplitudes
- Example:
  - $x \rightarrow \sum_i \frac{x_i}{\|x\|} |i\rangle$

Pros

- Most compact
- Full vector stored as single state

Cons

- State preparation is expensive
- Difficult to implement in practice

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Example: Amplitude Encoding

- Scheme:
  - $x \to \sum_i \frac{x_i}{\|x\|} |i\rangle$
  - $|i\rangle$ is i in binary
- Suppose $x = (x_0, x_1, x_2, x_3) = (1, 2, -1, 1)$
- Normalize x:

$$\|x\| = \sqrt{1^2 + 2^2 + (-1)^2 + 1^2} = \sqrt{7}$$

- Encode:

$$|\psi(x)\rangle = \tfrac{1}{\sqrt{7}} |00\rangle + \tfrac{2}{\sqrt{7}} |01\rangle - \tfrac{1}{\sqrt{7}} |10\rangle + \tfrac{1}{\sqrt{7}} |11\rangle$$

- Cost: $\lfloor \log_2(n) \rfloor + 1$ qubits (the bit length of n)

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XOR Example

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XOR

Classic Machine Learning Example

- Requires a non-linear separator
- Not solvable by a (single-layer) perceptron

Input	Output
0 & 0	0
0 & 1	1
1 & 0	1
1 & 1	0

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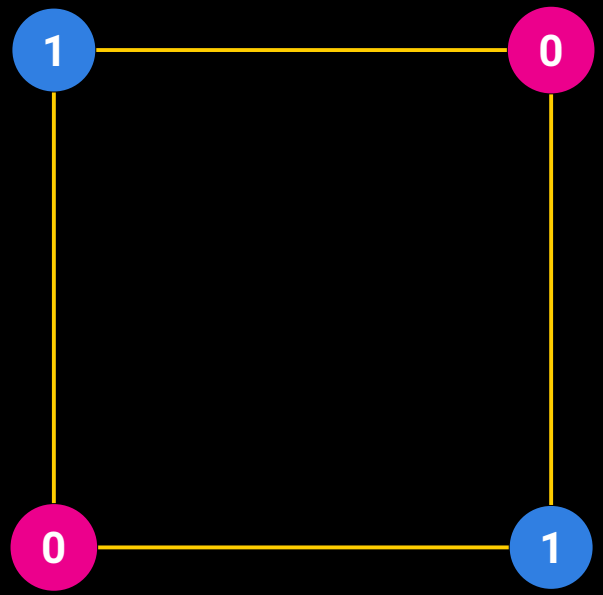
XOR - Visualization

Classic Machine Learning Example

- Requires a non-linear separator
- Not solvable by a (single-layer) perceptron



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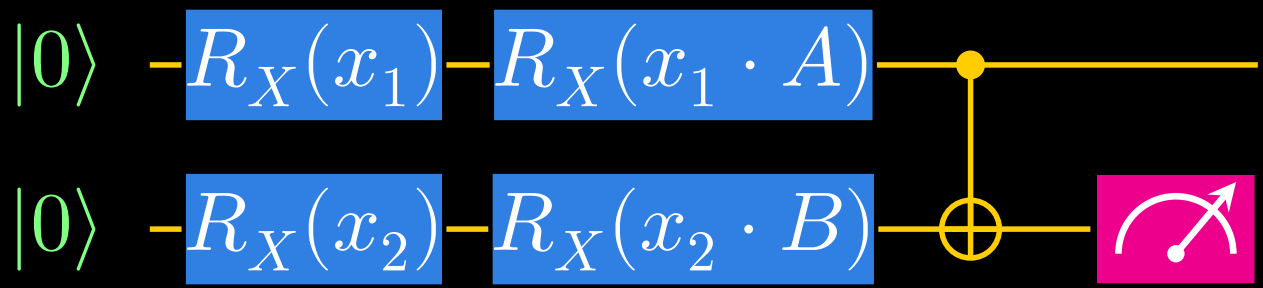
XOR - MATLAB Implementation

Adapted from

`https://www.mathworks.com/help/matlab/math/solve-xor-problem-using-quantum-neural-network.html`



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Completing the Model

A Quantum Machine Learning model has three components:

- Encoding (already covered)
- Circuit (transforms the state)
- Measurement (produces output)

Our Next Question:

What do the circuit and measurement add to the model?

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Quantum Machine Learning Pipeline

$$x \to |\psi(x)\rangle \to U(\theta)\,|\psi(x)\rangle \to \text{measurement} \to f(x, \theta)$$

- Encoding defines the representation
- Circuit transforms that representation
- Measurement extracts information

Together, these define the model $f(x, \theta)$

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Parametrized Quantum Circuits

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Parametrized Quantum Circuits

- A quantum circuit with tunable parameters θ
- Applies a unitary transformation:

$$U(\theta)\,|\psi(x)\rangle$$

- Parameters control gate operations
- The circuit structure determines what transformations are possible

Connection to CML

Parameters act like the weights in a neural network

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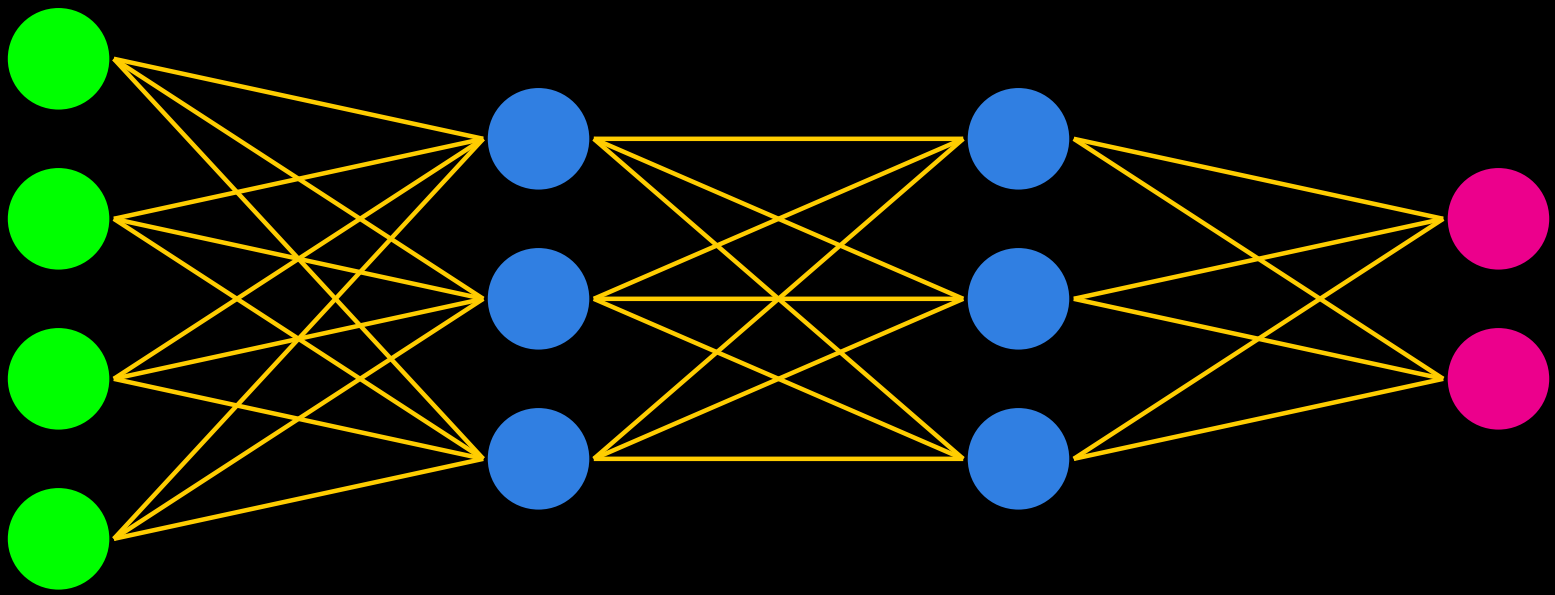
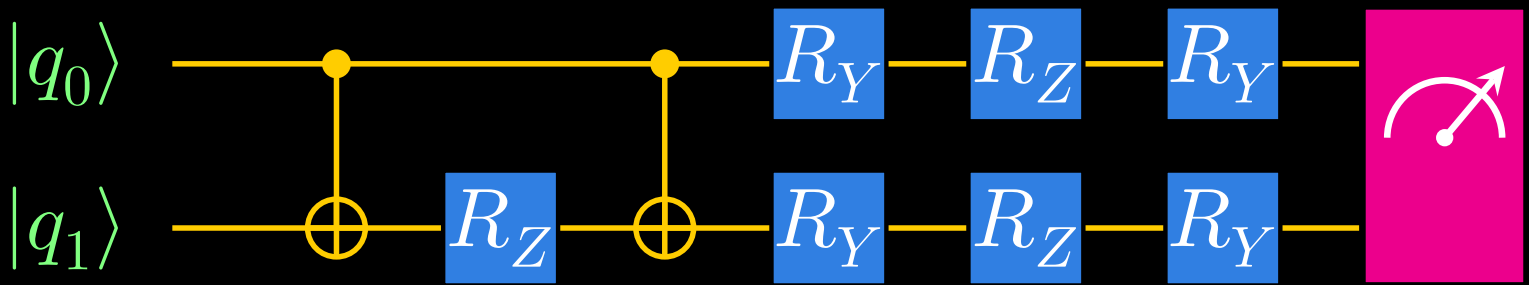
Classical & Quantum Neural Nets

Parametrized transformations of data





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Output from Quantum Model

- After applying the circuit, the state is:

$$U(\theta)\,|\psi(x)\rangle$$

- We measure an observable O
- Output is an expectation value:

$$f(x,\theta) = \langle\psi(x)|U^{\dagger}(\theta)OU(\theta)|\psi(x)\rangle$$

Connection to Classical

This is the quantum version of $f(x, W)$

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Quantum ML Models

- A QML model is defined by:
  - Encoding $x \to |\psi(x)\rangle$
  - Circuit $U(\theta)$
  - Measurement O

Key Point

All three together define the hypothesis class

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Quick Check-in

If we fix the encoding but change $U(\theta)$,
are we using the same model?

No!

Changing the circuit changes the transformation and thus the hypothesis class.

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Variational Quantum Algorithms

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Shifting to Algorithms

- We've discussed:
  - How to encode data
  - A parametrized quantum model $f(x, \theta)$
- What kinds of computations are possible?

Variational Quantum Algorithms

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Variational Quantum Algorithms

Elements of a VQA:

- Hybrid of quantum and classical methods
- Parametrized quantum circuits
- Circuit parameters are optimized using a classical algorithm

Hybrid System

Quantum computer evaluates the function,
classical computer optimizes the function

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Variational Computation Loop

- Initialize parameters θ
- Prepare quantum state
- Apply circuit $U(\theta)$
- Measure to compute cost $C(\theta)$
- Update θ using a classical optimizer
- Repeat

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Quantum Learning

Recall

"Learning" is optimization

- Define a cost function

$$C(f(x, \theta), y)$$

- $C(\theta)$ is computed via measurements on a quantum device
- Find

$$\min_{\theta} C(\theta)$$

- Circuit structure completes the model design
- Optimization determines the best parameters

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Quick Check-in

What role does the quantum computer play in the learning loop?

Answer

The quantum computer evaluates the model by computing $C(\theta)$

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Why a Hybrid Approach?

- Current quantum hardware is limited:
  - Noisy
  - Small number of qubits (∼100-1000)
  - Noisy Intermediate-Scale Quantum (NISQ) era
- Fully quantum algorithms are difficult to run on hardware
- This approach enables learning on near-term quantum devices

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Variational Quantum Eigensolvers (VQE)

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Variational Quantum Eigensolver

- Standard NISQ routine
- **Goal**: find the lowest energy state of a quantum system
- Corresponds to finding the ground state of a Hamiltonian H

Main Benefit

Many problems in physics, chemistry, and materials science can be expressed as finding the ground state of a Hamiltonian

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Setting Up a VQE

- We want to compute the minimum energy:

$$E_0 = \min_{\theta} \langle \psi(\theta) | H | \psi(\theta) \rangle$$

  - $|\psi(\theta)\rangle$ is prepared using a parametrized circuit
  - H is the Hamiltonian of the system

- Optimal parameter values $\hat{\theta}$ approximate the ground state of H

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The VQE Loop

- Prepare an initial state $|\psi(\theta)\rangle$
- Measure the expectation value

$$\langle\psi(\theta)|H|\psi(\theta)\rangle$$

- Use a classical optimizer to update θ
- Repeat until the system converges

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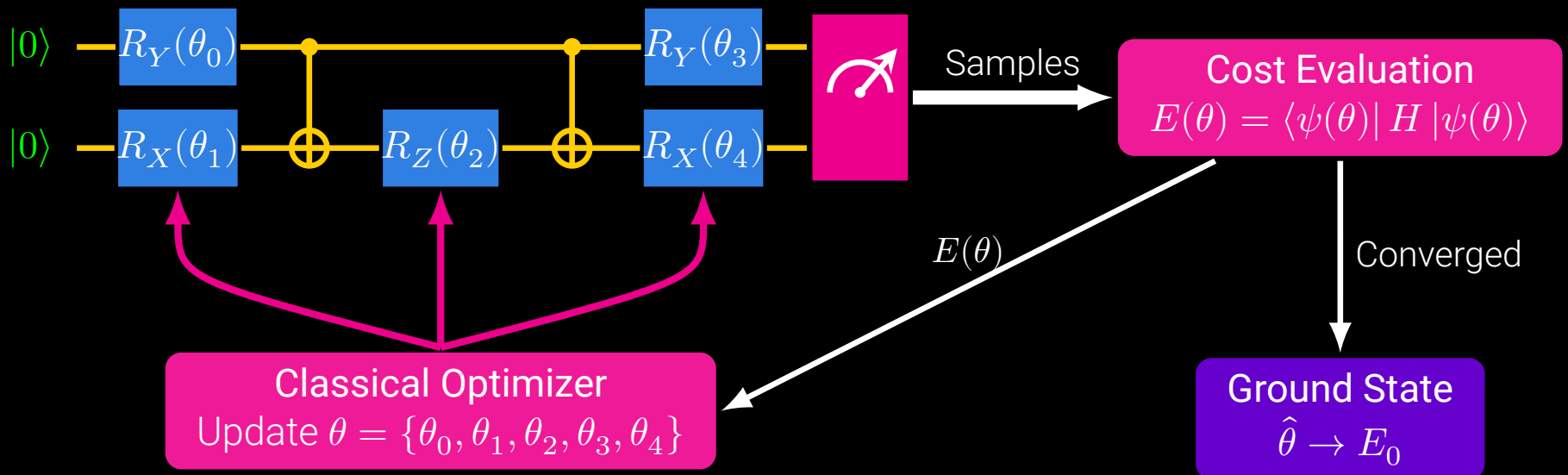
The VQE Loop - Diagram

1. State Preparation & Measurement



2. Classical Optimization Loop

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Quick Check-in

What is the cost function in VQE?

Answer

The expected energy:

$$\langle \psi(\theta) | H | \psi(\theta) \rangle$$

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VQE - MATLAB Implementation

- Pauli operators

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Construct H as a combination

$$H = 0.2I \otimes I + 0.05I \otimes Z + 0.05Z \otimes I + 0.7Z \otimes Z + 0.15X \otimes X - 0.05Y \otimes Y$$

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Quantum Approximate Optimization Algorithm (QAOA)

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From VQE to QAOA

- VQE uses a general-purpose quantum circuit
- Designed for problems like finding ground states

Next Question

What if we design the circuit specifically for an optimization problem?

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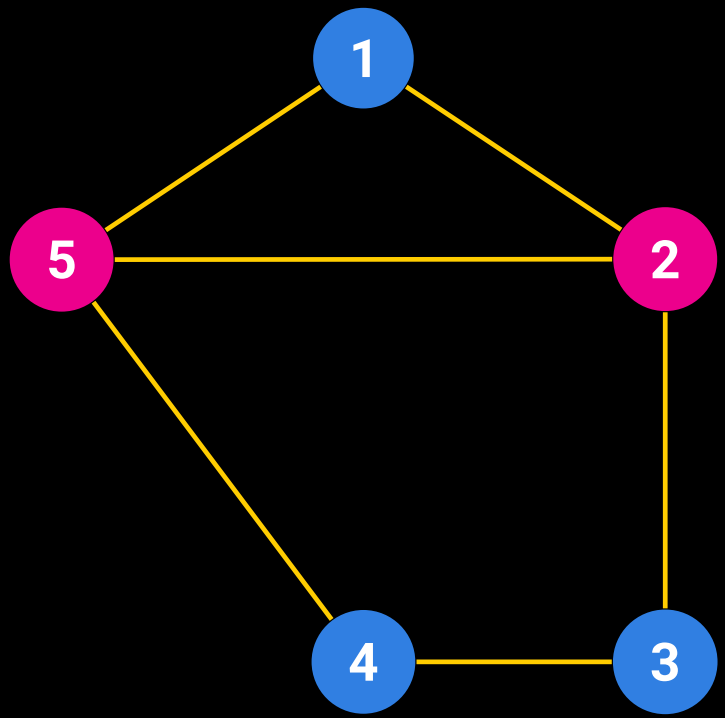
Quantum Approximate Optimization Algorithm

- A variational algorithm for combinatorial optimization
- Example: MaxCut for graph partitioning
- Uses a structured, problem-specific circuit



Key Idea

Build the circuit from the structure of the problem

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The QAOA Circuit

- Alternates between two operators:
  - Problem Hamiltonian H_C
  - Mixer Hamiltonian H_B

$$U(\gamma, \beta) = e^{-i\beta H_B} e^{-i\gamma H_C}$$

- Parameters: (γ, β)

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How QAOA Works

- Start from an initial state

$$H^{\otimes n} \left|0\right\rangle^{\otimes n}$$

- Apply alternating operators:
  - $e^{-i\gamma H_C}$ encodes the problem
  - $e^{-i\beta H_B}$ explores possible solutions
- Measure to estimate solution quality
- Optimize parameters (γ, β)

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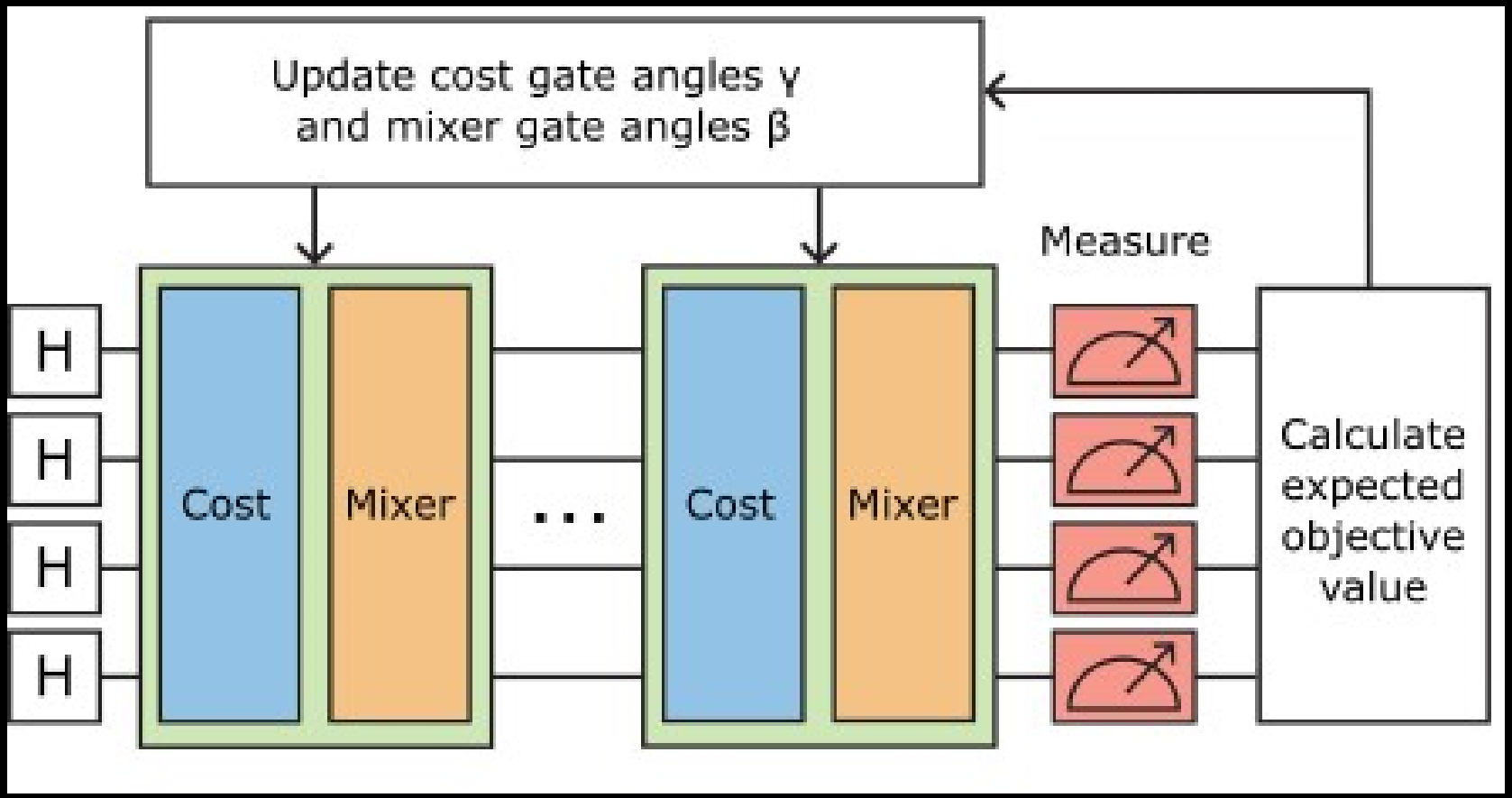
QAOA Circuit



MathWorks:
https://www.mathworks.com/help/matlab/math/max-cut-with-qaoa.html

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Quick Check-in

What determines the structure of the QAOA circuit?

Answer

The optimization problem itself (via H_C and H_B)

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QAOA Example: Max-Cut

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VQE vs QAOA

VQE	QAOA
General-purpose circuit	Problem-specific circuit
Physics-based problems	Combinatorial optimization problems
Flexible ansatz	Structured, layered ansatz
Minimize energy $\langle\psi\|H\|\psi\rangle$	Maximize objective $\langle H_C\rangle$

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The Training Problem

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Computing Gradients

- Training requires gradients of the cost function:

$$\frac{\partial C(\theta)}{\partial \theta_i}$$

- We cannot perform backpropagation through a quantum circuit
- Instead, we use the parameter-shift rule

Parameter-Shift Rule

$$\frac{\partial C}{\partial \theta_i} = \frac{1}{2}[C(\theta_i + s) - C(\theta_i - s)]$$

for a fixed shift s

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Parameter-Shift Rule

- Most quantum circuits use rotation gates

$$R_X(\theta) = e^{-i\frac{\theta}{2}X} \qquad R_Y(\theta) = e^{-i\frac{\theta}{2}Y} \qquad R_Z(\theta) = e^{-i\frac{\theta}{2}Z}$$

- Choosing $s = \frac{\pi}{2}$ gives a special result

Exact Derivative for Rotation Gates

$$\frac{\partial C}{\partial \theta} = \frac{1}{2}\left[C\left(\theta + \frac{\pi}{2}\right) - C\left(\theta - \frac{\pi}{2}\right)\right]$$

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Cost of Gradient Computation

- Each gradient requires multiple circuit evaluations
- For p parameters:

$$\text{Number of evaluations} \sim O(p)$$

- Each evaluation requires repeated measurements (sampling)

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Barren Plateaus

- In some circuits, gradients become very small
- As system size increases:

$$\nabla_\theta C(\theta) \approx 0$$

- Optimization becomes extremely difficult

Key Idea

In high-dimensional quantum systems, the landscape can become nearly flat

Why This Matters

Even though the model is expressive, it may not be trainable

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How Do You Get Started?

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Getting Started

- Learn the language
  - Linear algebra
  - Bra-ket (Dirac) notation
  - Quantum circuits
- Python - most common programming language for quantum computing
- Machine learning resources
  - MATLAB Tutorials
  - IBM Qiskit
  - PennyLane

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Any Questions?

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Thank you!

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