Covalent

Quantum Machine Learning using Covalent

A QAOA application

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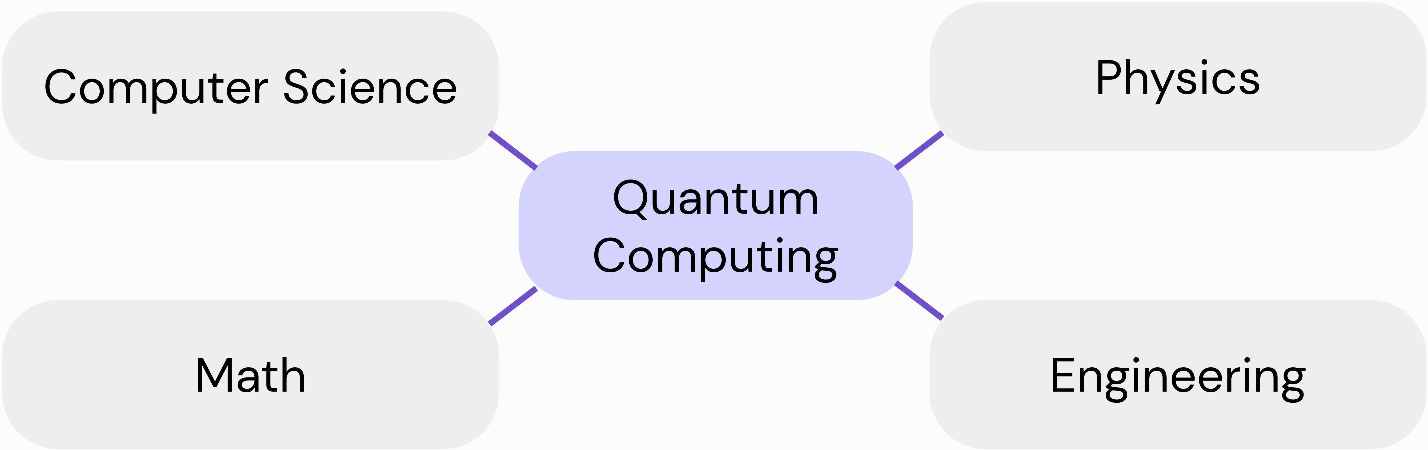
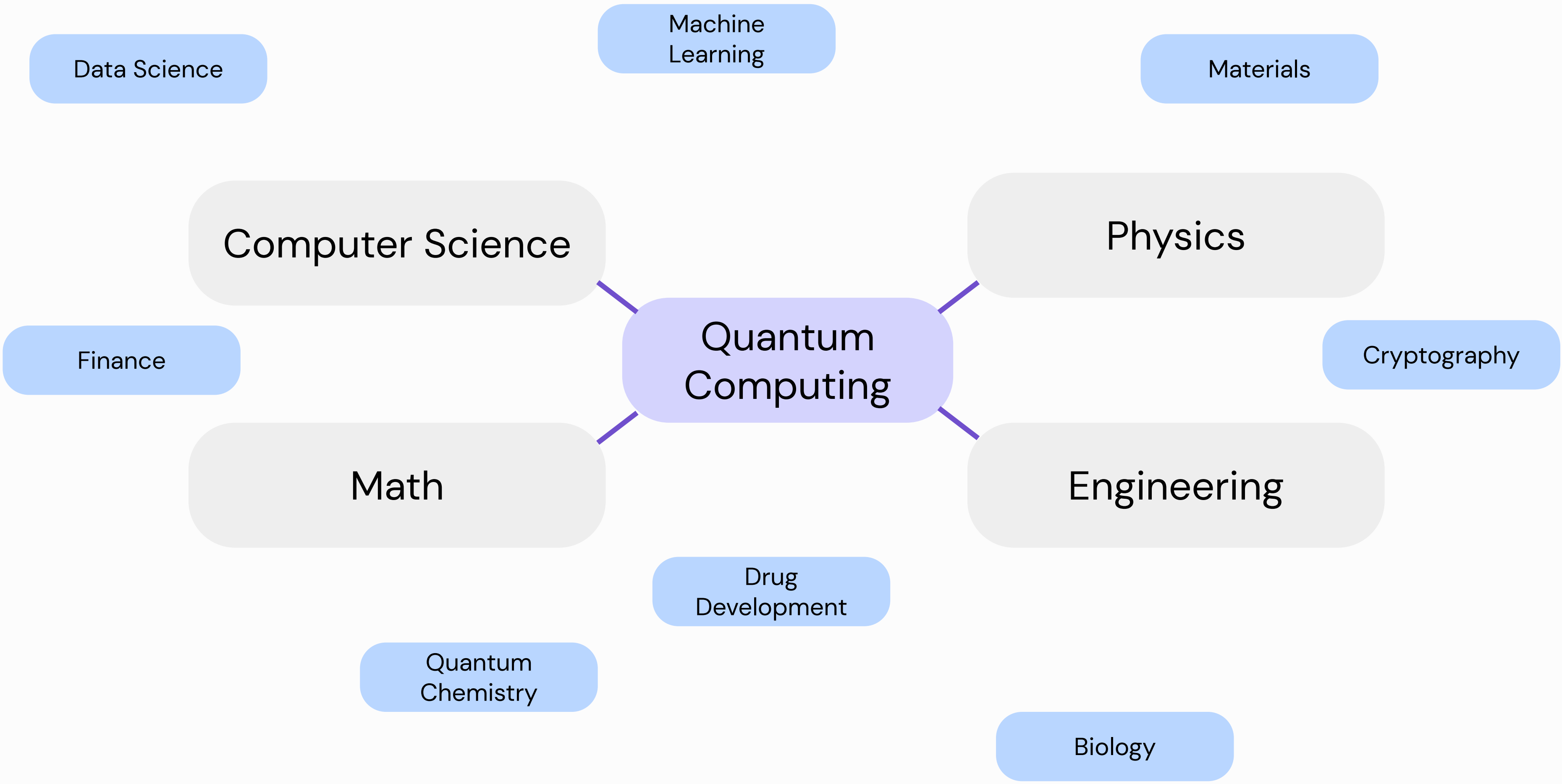
BSc, RPI, Dept. of Physics

Introduction to Quantum Computing


Computer Science
Physics
Quantum Computing
Math
Engineering


Data Science
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Cryptography
Math
Engineering
Drug Development
Quantum Chemistry
Biology

A Timeline of Quantum Computing

1994
Shor's Algorithm

2009
Yale creates first solid-state quantum processor

2011
D-Wave develops first commercial quantum annealer

2013
Google launches Quantum AI Labs

2017
Harvard builds 51-qubit quantum computer

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IBM builds 16-qubit quantum computer

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Agnostiq is founded

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Google claims quantum supremacy

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Amazon Braket becomes available

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Xanadu announces quantum supremacy

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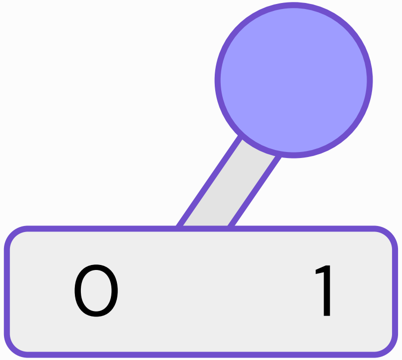
Classical Computers

Composed of **bits**, which can take on values of 0 or 1



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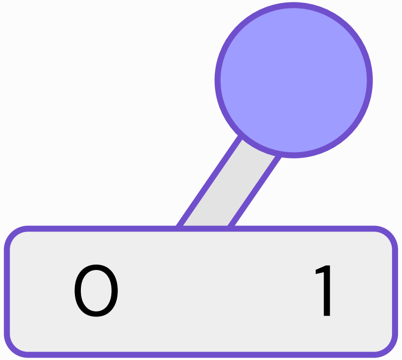

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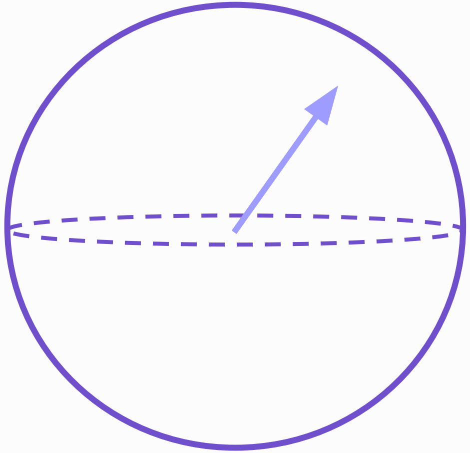
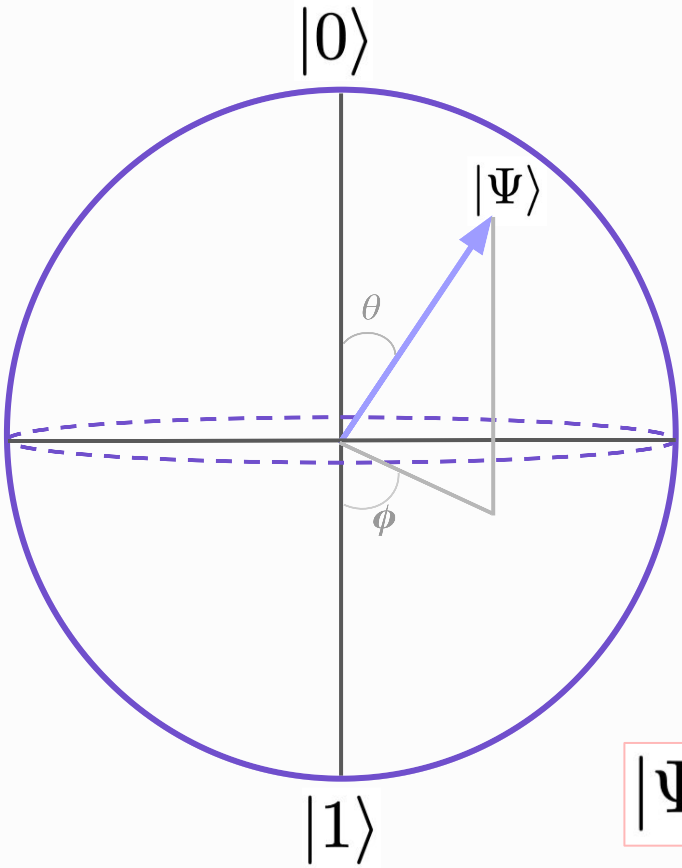


Bloch Sphere



$$|\Psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle$$

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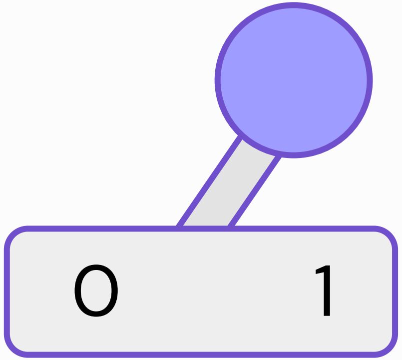

Deterministic measurements

Quantum Computers

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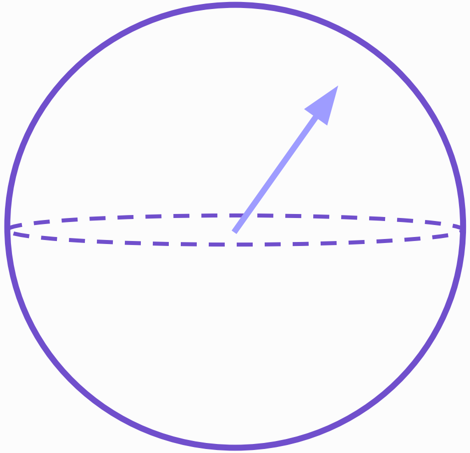
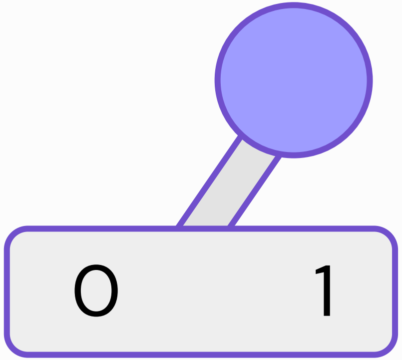


Probabilistic measurements

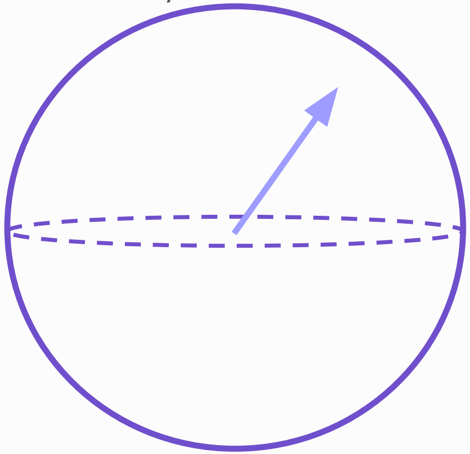
Classical Computers

If you have N bits, you have 2^N states that you can only execute 1 at a time (or in parallel)

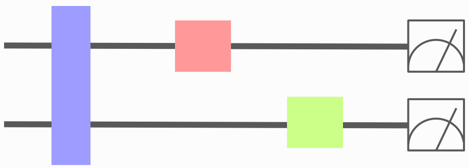


Quantum Computers

If you have N qubits, you can encode all 2^N components into one state simultaneously

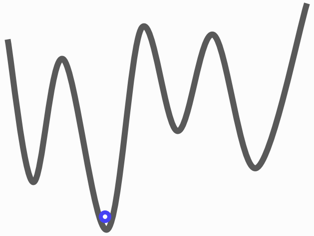


Types of Quantum Computers.



Gate-Based

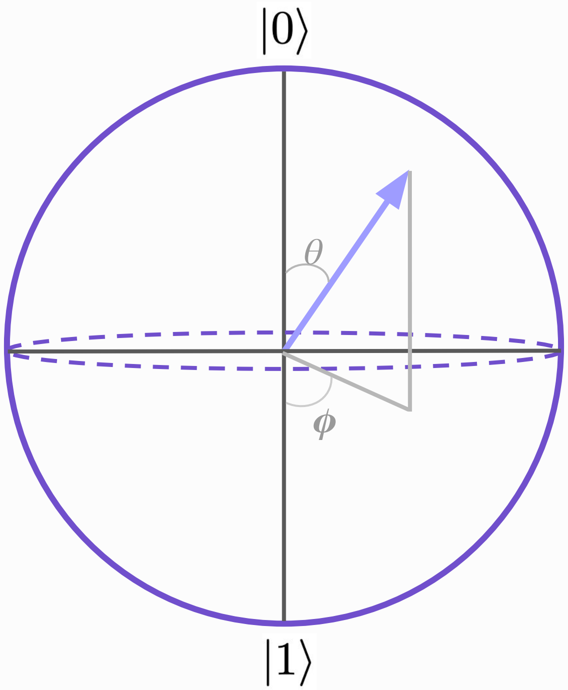
- Broad applications
- Apply gates, or circuit operations, to quantum state
- Universal computer



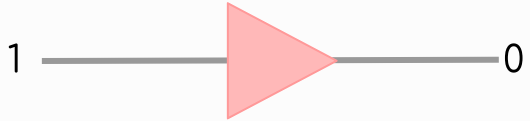
Quantum Annealers

- Search an energy landscape for the lowest-energy solution
- Problem encoded as a Hamiltonian
- Can only solve optimization problems

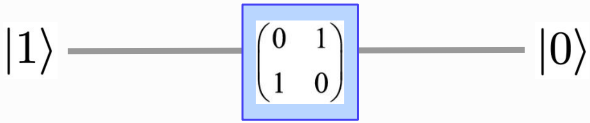
Quantum Gates



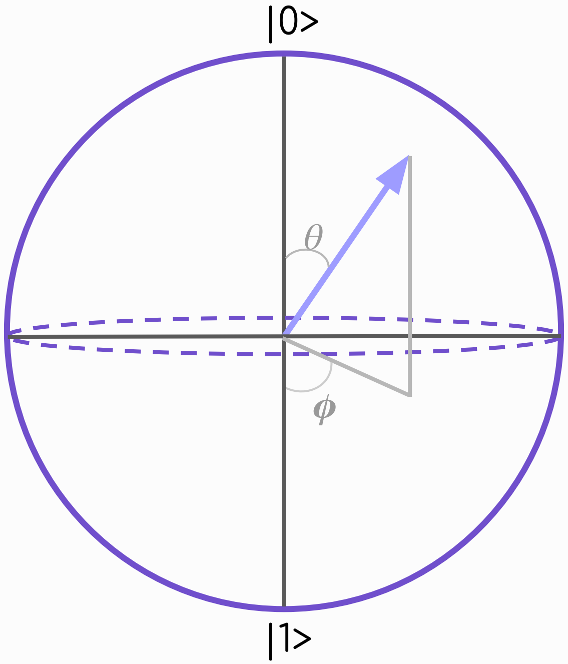
- Classical NOT Gate



- Pauli X Gate



Quantum Gates



- Pauli X Gate

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

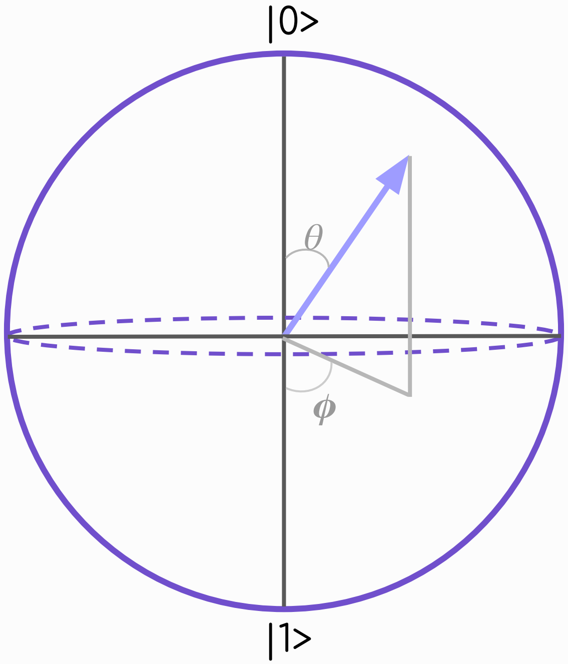
- Pauli Y Gate

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- Pauli Z Gate

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Quantum Gates



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- Hadamard Gate

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

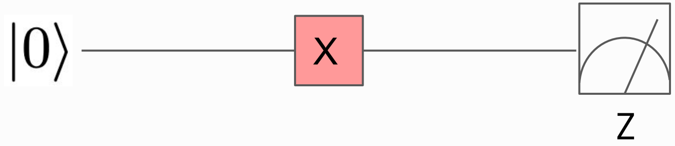
- Controlled NOT Gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

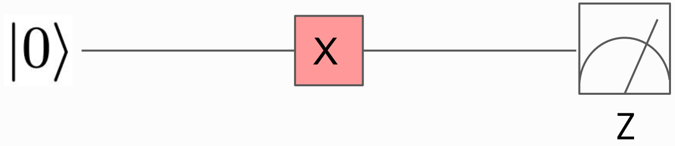
- Toffoli Gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Building a Quantum Circuit

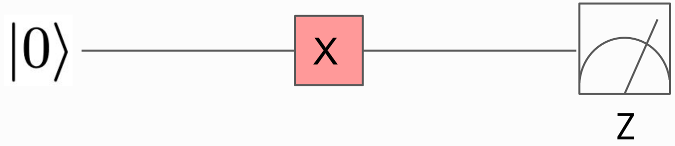


Building a Quantum Circuit



$$\begin{bmatrix}1\\0\end{bmatrix} \qquad \begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} \qquad \begin{bmatrix}0&1\end{bmatrix}\begin{bmatrix}1&0\\0&-1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}$$

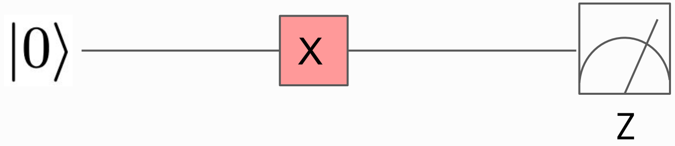
Building a Quantum Circuit



$$\begin{bmatrix}1\\0\end{bmatrix} \qquad \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} \qquad \begin{bmatrix}0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix}$$

$$|0\rangle \qquad \sigma_x \, |0\rangle = |1\rangle \qquad \langle 1| \, \sigma_z \, |1\rangle$$

Building a Quantum Circuit

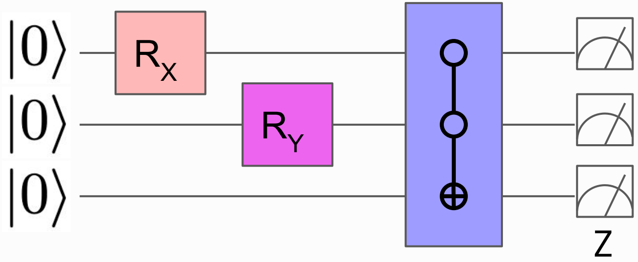



```
import pennylane as qml

dev1 = qml.device("default.qubit", wires=1)

@qml.qnode(dev1)
def circuit():
    qml.PauliX(wires=0)
    return qml.expval(qml.PauliZ(0))
```

Building a Quantum Circuit




```python
import pennylane as qml
dev1 = qml.device("default.qubit", wires=3)
@qml.qnode(dev1)
def circuit(params):
    qml.RX(params[0], wires=0)
    qml.RY(params[1], wires=1)
    qml.Toffoli(wires=[0,1,2])
    return qml.expval(qml.PauliZ(0)),
qml.expval(qml.PauliZ(1)), qml.expval(qml.PauliZ(2))
```

Introduction to Quantum Machine Learning

Machine Learning

- A model is developed to describe and make predictions about data
- Model parameters are tuned using a training dataset
- The model is assessed by making predictions about a test dataset

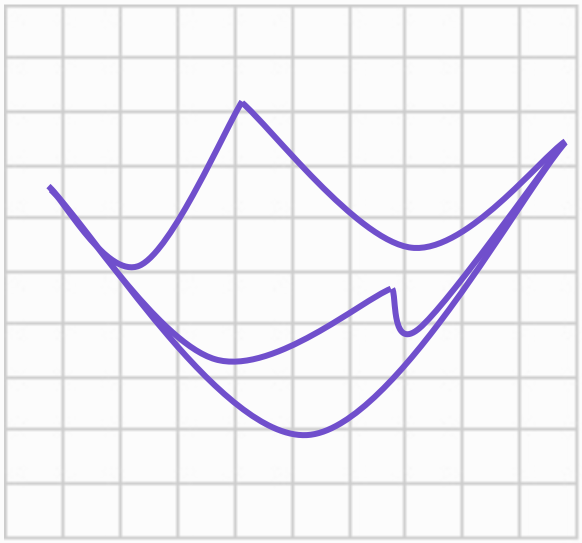
Machine Learning

A model is developed to describe and make predictions about data

Model parameters are tuned using a training dataset

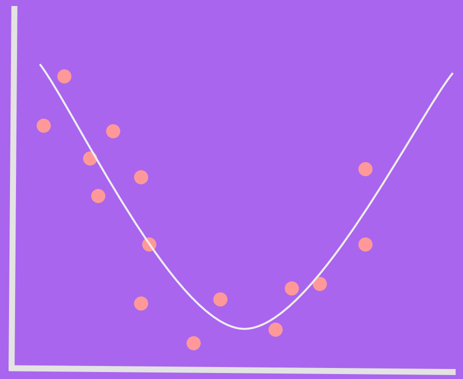
The model is assessed by making predictions about a test dataset

Optimizing a cost function



Machine Learning Example

A model is developed to describe and make predictions about data



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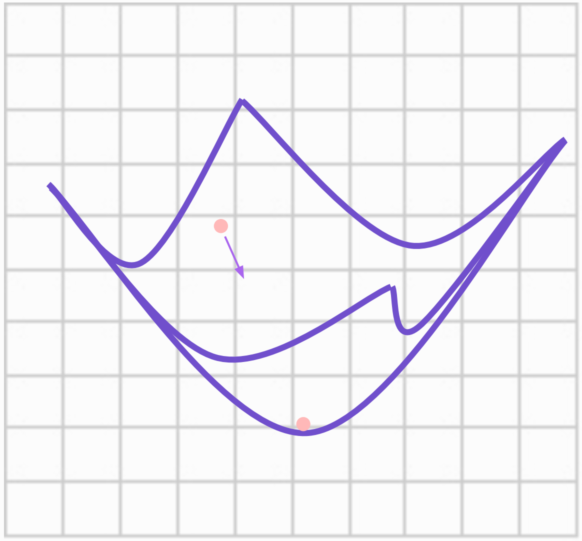
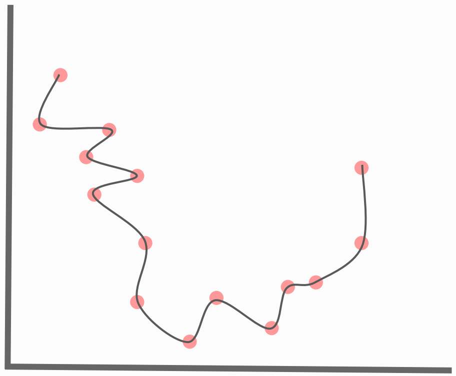
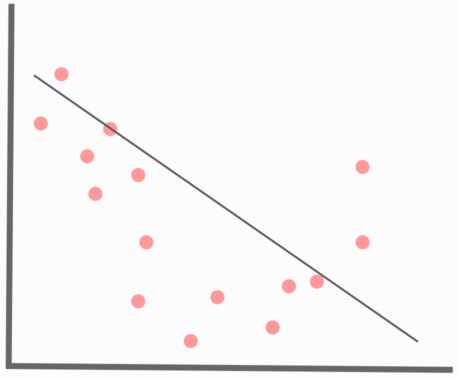


Machine Learning Example





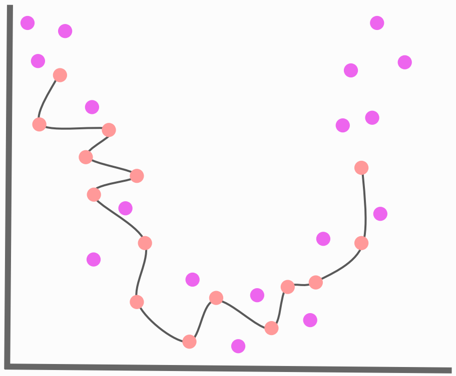
Overfitting

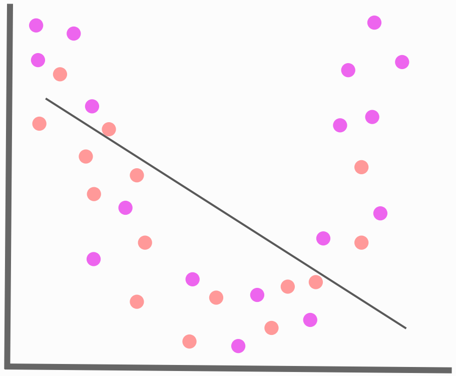
Model is too tailored to the training data and does not generalize to test data

Underfitting

Model is too general and does not well represent the training or test data

Machine Learning Example





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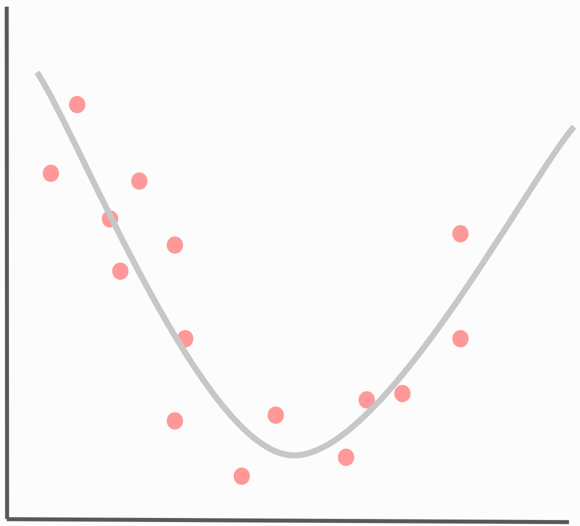
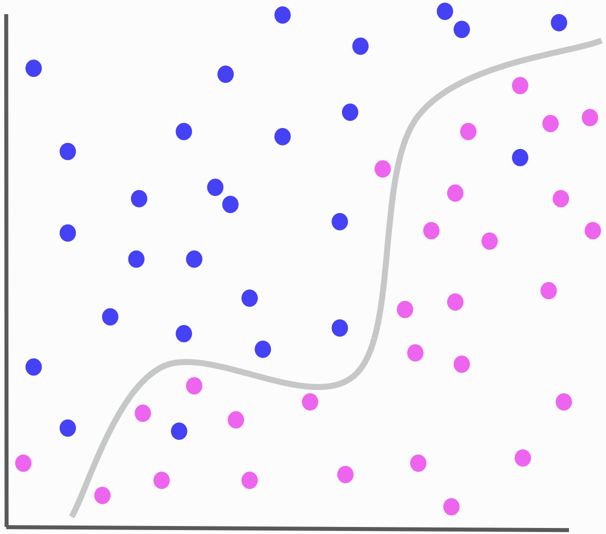
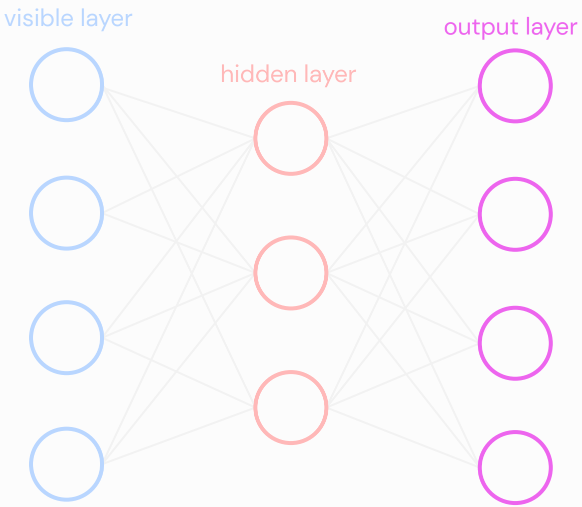
Regression



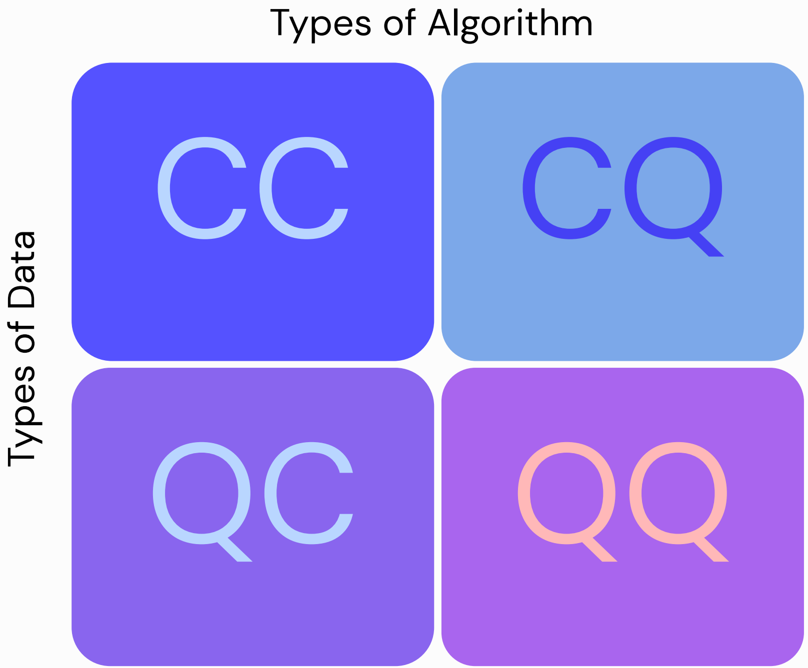
Classification



Neural Networks



Quantum Machine Learning



Quantum Machine Learning

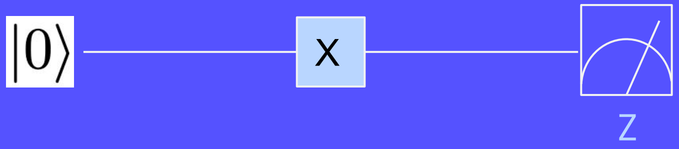
Types of Algorithm

Types of Data

CQ

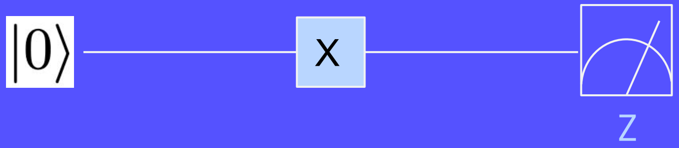
classical data with quantum algorithms

Parameterized Quantum Circuits



This circuit does not have tunable parameters

Parameterized Quantum Circuits



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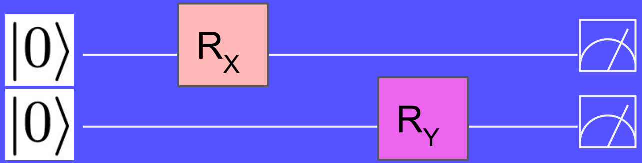

The input angles in R_X and R_Y are tunable parameters

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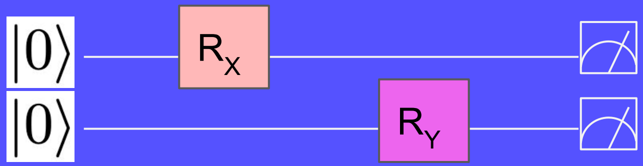


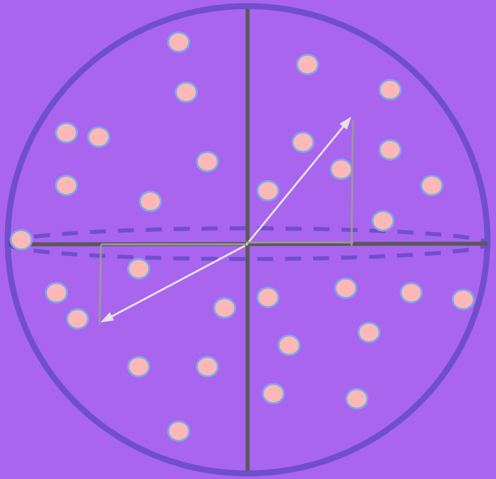
The input angles in R_X and R_Y are tunable parameters

A quantum circuit with tunable parameters consists of unitary operations $U(\theta)$ performed on n qubits

Parameterized Quantum Circuits

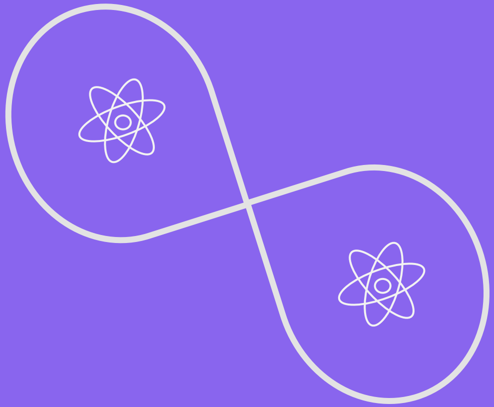
Expressibility

We want our quantum circuit to be able to span a wide subset of Hilbert Space!



Entanglement

Entangled qubits are difficult to simulate using a classical simulator.



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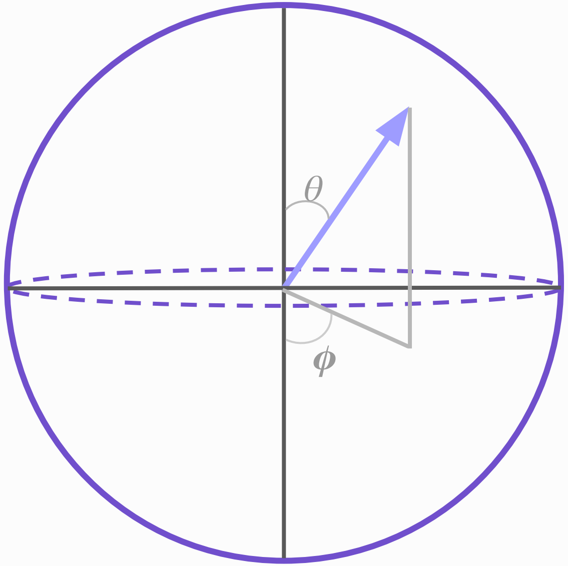

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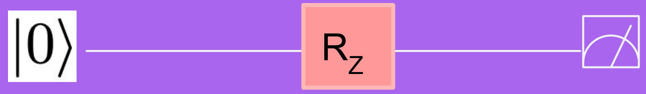

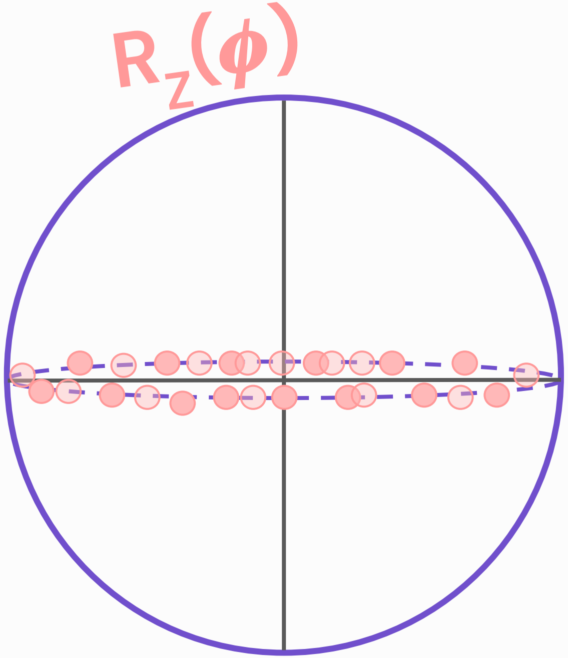

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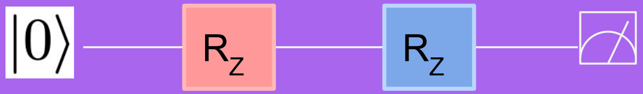

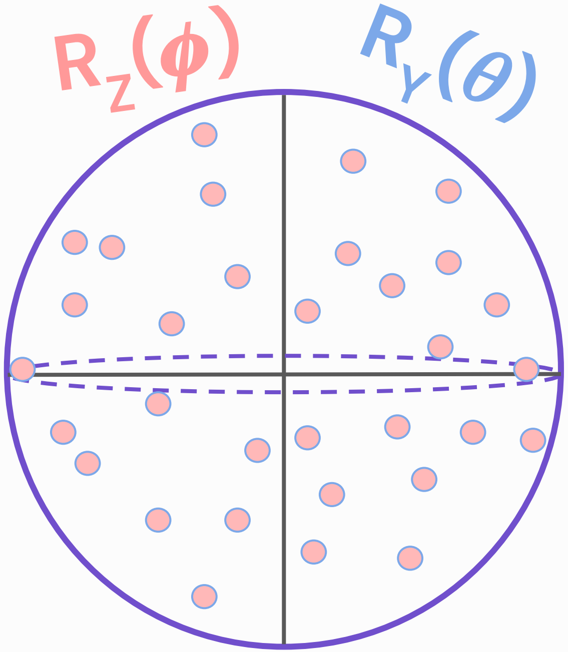

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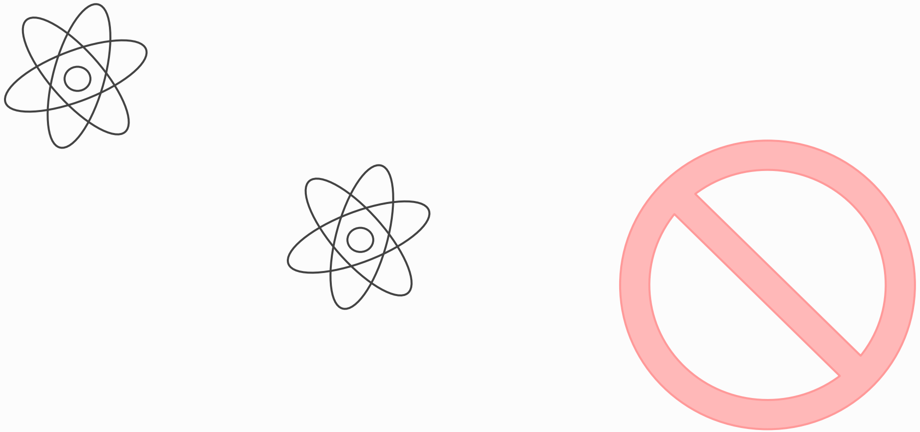

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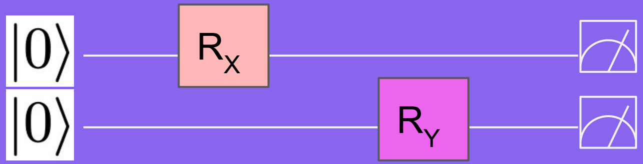

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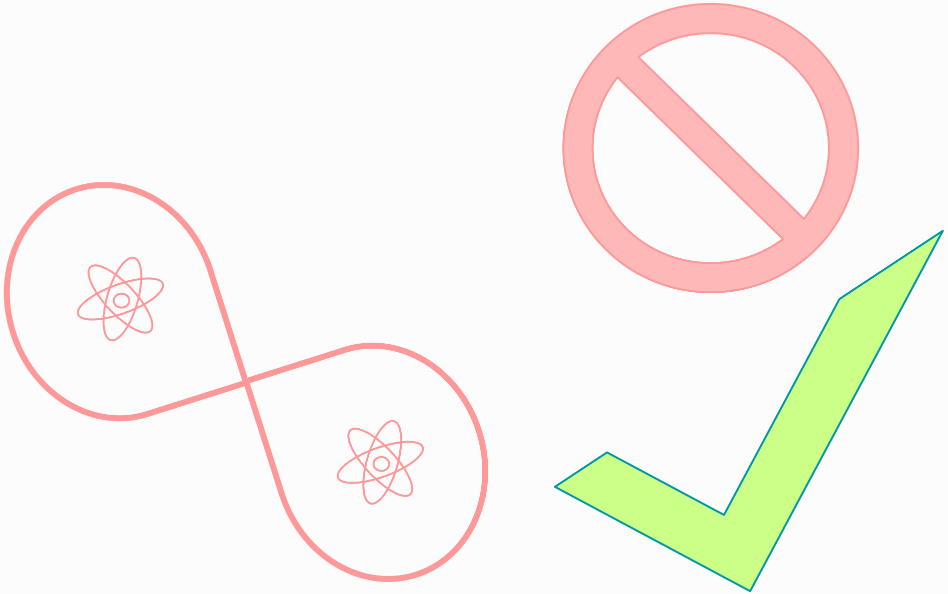

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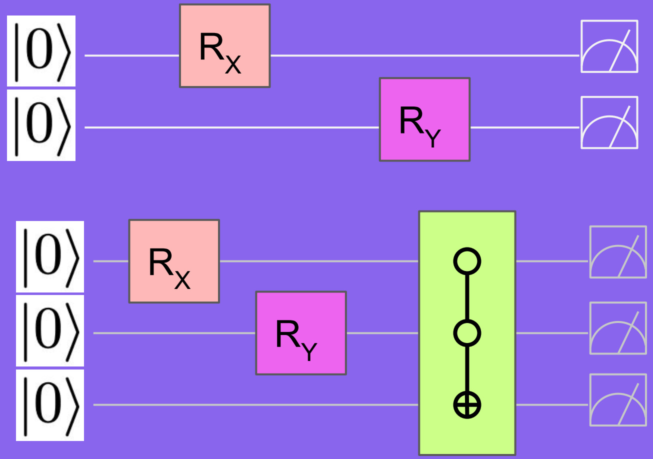


Limitations in the NISQ Era.

Coherence Time

The time a qubit is able to maintain its quantum state before it breaks down due to noise

Qubit Connectivity

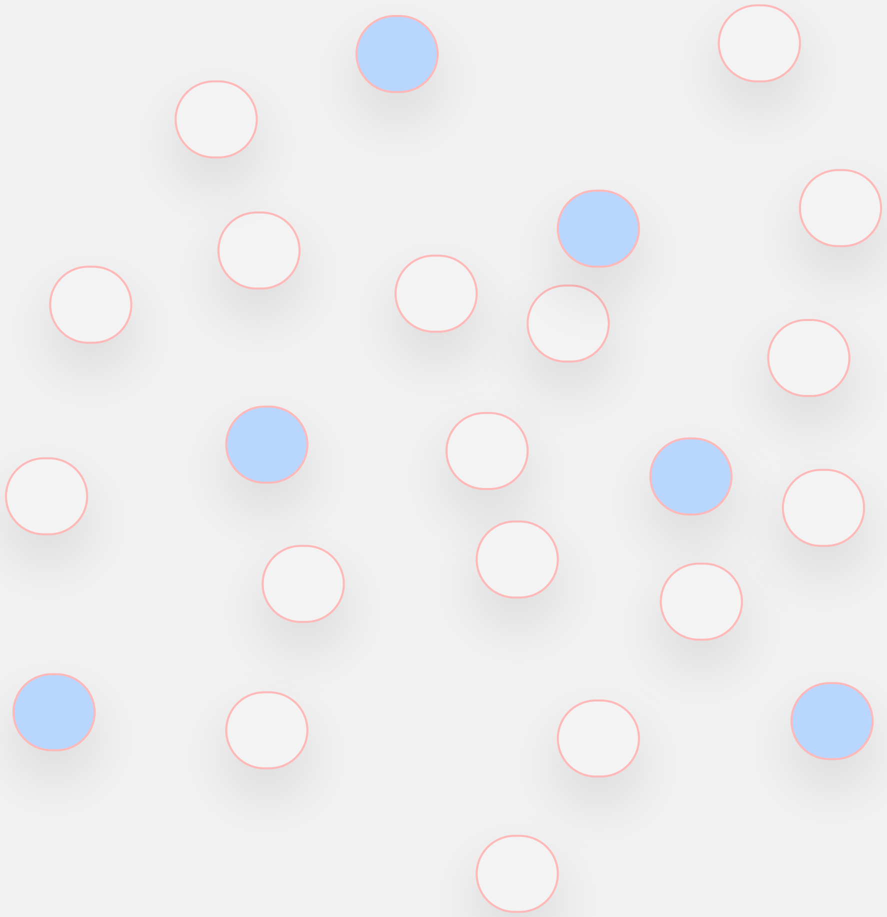
In today's quantum computers, not all qubits are able to interact with each other

Covalent

The Quantum Approximation Optimization Algorithm

QAOA

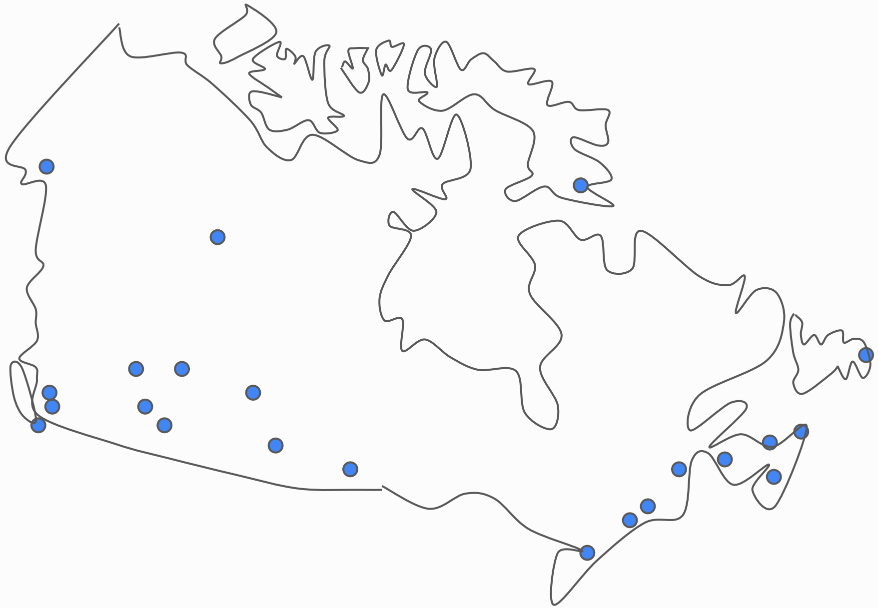
- Combinatorial optimization problems are computationally expensive to solve exactly
- QAOA is a mathematical method to find approximate solutions
- It is simple to implement and can be run on NISQ devices



Combinatorial Optimization Example

The Traveling Salesman Problem

Given a list of cities and the distance between each pair of cities, what is the shortest possible route that visits each city exactly once and returns home at the end?



QAOA problems involve...

$$Z \in \{0,1\}^n$$

Bit String Z

- Elements in the string are binary-valued
- n is the total number of elements

$$C_\alpha = \begin{cases} 1, & \text{if z satisfies clause } C_\alpha \\ 0, & \text{otherwise.} \end{cases}$$

Clause C

- For all elements in Z, if the element satisfies C_α it is given a value of 1

$$C(z) = \sum_{\alpha=1}^{m} C_\alpha(z)$$

Clause Satisfaction

- m is the total number of clauses
- The greater the value of C(z), the better the overall clause satisfaction

Hamiltonians

$$U(H,t) = e^{-iHt/\hbar}$$

- Using a Hamiltonian to construct a quantum circuit
- Hamiltonians can be evolved using the time evolution operator

Cost Hamiltonian

The expectation value of the cost hamiltonian is the cost function to be optimized.

Mixer Hamiltonian

A layer to increase the mix the quantum state so the angles ɣ and β can be optimized.

Cost Hamiltonian

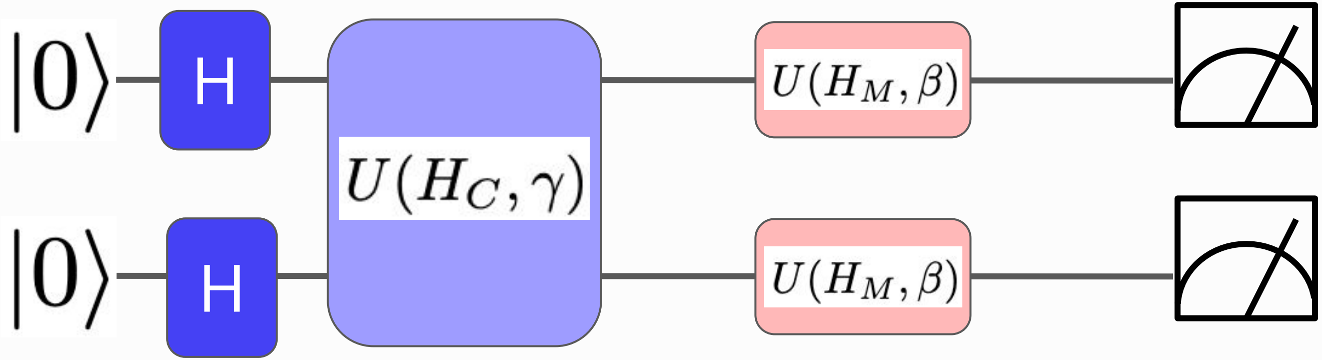
The expectation value of the cost hamiltonian is the cost function to be optimized.

$$U(H_C, \gamma) \equiv e^{-i\gamma C}$$

Mixer Hamiltonian

A layer to increase the complexity of the quantum circuit.

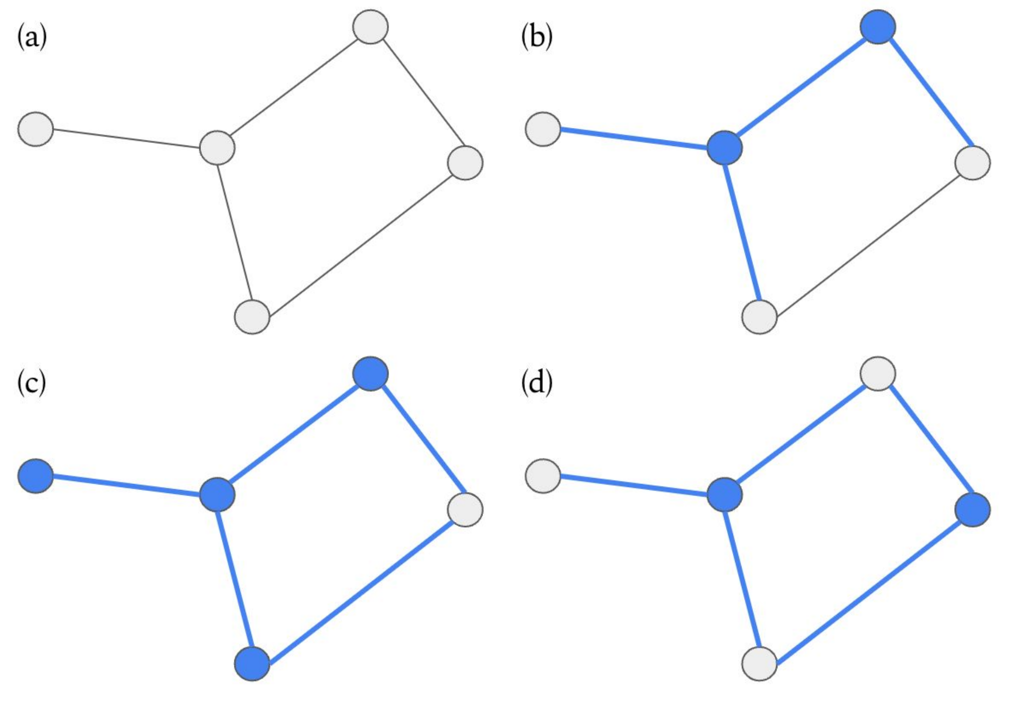
$$U(H_M, \beta) \equiv e^{-i\beta\sigma_x}$$


$|0\rangle$
$|0\rangle$
H
H
$U(H_C, \gamma)$
$U(H_M, \beta)$
$U(H_M, \beta)$

The Minimum Vertex Cover Problem

A combinatorial optimization problem to find the minimum number of vertices needed to cover all edges in a graph

There are no exact solutions to the minimum vertex cover problem that can be found in polynomial time



Solving QAOA Problems with Quantum Circuits

1. Define a cost and a mixer hamiltonian
2. Construct the cost and mixer layers
3. Construct a circuit by alternating cost and mixer layers
4. Use classical techniques to optimize the circuit parameters
5. Get the approximate solutions by measuring the circuit output

Define a cost and a mixer hamiltonian

```
from pennylane import qaoa

cost_h, mixer_h = qaoa.min_vertex_cover(graph, constrained=False)
```

Construct the cost and mixer layers

```
def qaoa_layer(gamma, alpha):
    qaoa.cost_layer(gamma, cost_h)
    qaoa.mixer_layer(alpha, mixer_h)
```

Construct a circuit by alternating cost and mixer layers

```python
import pennylane as qml
wires = range(4)
depth = 2

def circuit(params, **kwargs):
    for w in wires:
        qml.Hadamard(wires=w)
    qml.layer(qaoa_layer, depth, params[0], params[1])
```

Use classical techniques to optimize the circuit parameters

```
dev = qml.device("lightning.qubit", wires=qubits)

@qml.qnode(dev)
def cost_function(params):
    circuit(params)
    return qml.expval(cost_h)

optimizer = qml.GradientDescentOptimizer()
steps = 70
params = np.array([[0.5, 0.5], [0.5, 0.5]],
requires_grad=True)
```

Get the approximate solutions by measuring the circuit output

```
for i in range(steps):
    params = optimizer.step (cost_function, params)

print params
```

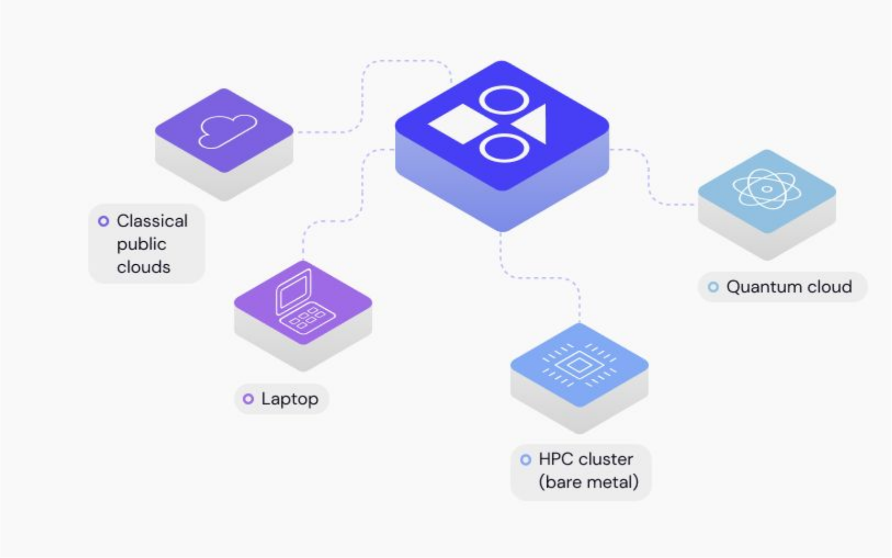
Covalent

covalent.xyz

Covalent is an open source workflow orchestration platform for quantum and high performance computing.

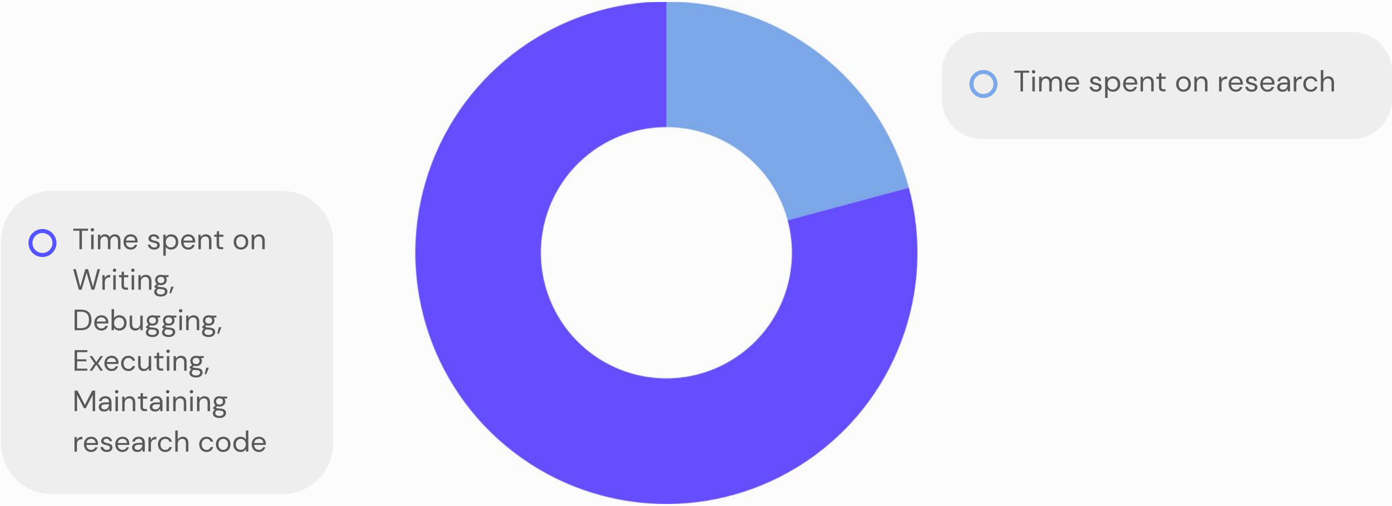
Covalent is designed to make your experiments:

- Modular
- Scalable
- Reproducible



Why does Covalent exist?

Computational research

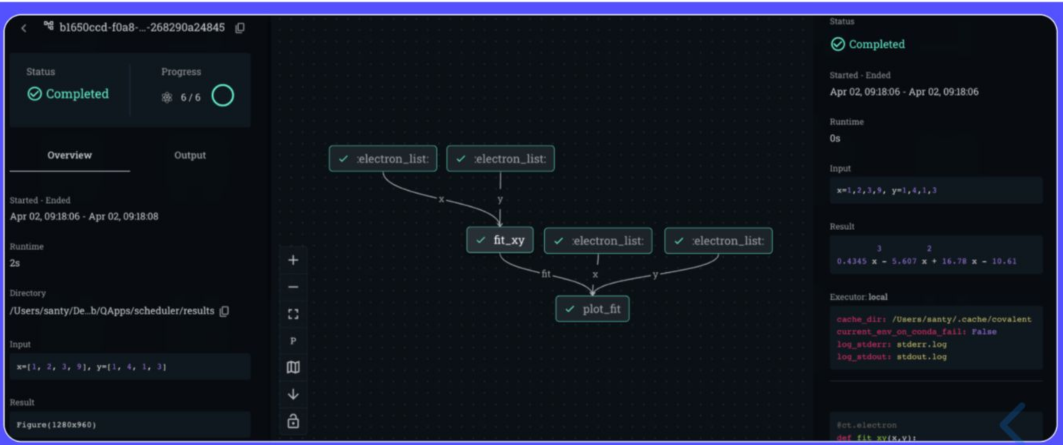


Real–time monitoring

Visual overview	Status/Error updates	Checkpoints	Meta-data	Parameter	Interactive
Visualize an share your workflow to transfer knowledge as fast as possible	*Get real time Updates on errors and completion*	*Stores anything and everything automatically without a single line of code*	*Maintains details from environment to hardwares used*	*Never forget the hyper-parameters that worked*	*Start/stop/manage your HPC jobs right from the UI*

Beautiful and interactive UI

bring your workflows to life!



Modularize your experiments.

@ct.electron

Define a cost and a mixer hamiltonian

@ct.electron

Construct a circuit by alternating cost and mixer layers

@ct.electron

Construct the cost and mixer layers

@ct.electron

Use classical techniques to optimize the circuit parameters

@ct.electron

Get the approximate solutions by measuring the circuit output

Modularize your experiments.

@ct.electron

Define a cost and a mixer hamiltonian

@ct.electron

Construct a circuit by alternating cost and mixer layers

@ct.electron

Construct the cost and mixer layers

@ct.electron

Use classical techniques to optimize the circuit parameters

Can dispatch specific electrons to remote devices

@ct.electron

Get the approximate solutions by measuring the circuit output

Modularize your experiments.

@ct.electron

Define a cost and a mixer hamiltonian

@ct.electron

Construct a circuit by alternating cost and mixer layers

@ct.electron

Construct the cost and mixer layers

@ct.electron

Use classical techniques to optimize the circuit parameters

@ct.electron

Get the approximate solutions by measuring the circuit output

@ct.lattice

Call all electrons in the desired order to create the workflow

Covalent

Thank You

covalent.xyz

agnostiqHQ/covalent

@covalentxyz

Initializing the Slurm Executor

```
wget https://repo.anaconda.com/miniconda/Miniconda3-py38_4.12.0-Linux-x86_64.sh

sh ./Miniconda3-py38_4.12.0-Linux-x86_64.sh

pip install pennylane==0.23.0
pip instal cloudpickle
pip install covalent
```