

Quantum computing lecture 3:

Variational Algorithms

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12-1 PM, Apr 26, 2024

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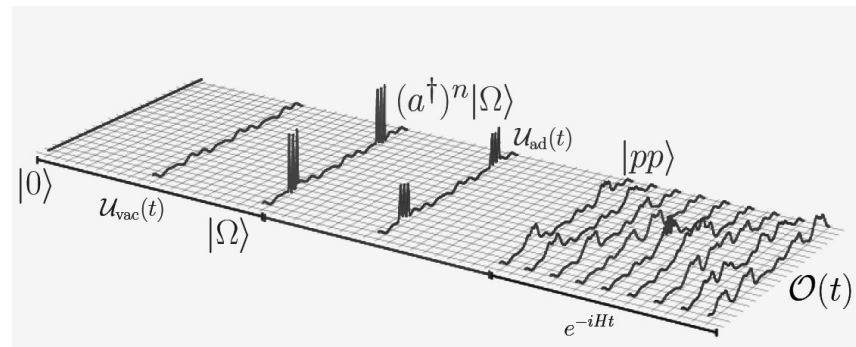


What we will learn

1. How to **simulate $\exp(-i H t)$** on quantum circuit?
2. How to perform measurement to extract any **observable $\langle O \rangle$** ?
3. How to study real world problems using **variational algorithms**?

1. What does simulation $\exp(-iHt)$ mean?

It literally means evolving some **quantum state** by applying an **Hamiltonian H** for a period of **time t** .



Hamiltonian as in Pauli matrices

The Hamiltonian H is usually expressed in terms of Pauli matrices, I, X, Y, Z

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \vec{\sigma} = (\sigma^0, \sigma^1, \sigma^2, \sigma^3) = (I, X, Y, Z)$$

such that the Hamiltonian is a linear combinations of products of these Pauli matrices

$$H = \sum_i c_i P_i$$

For example:

$$\begin{aligned} H_{ex} &= I_0 I_1 + X_0 X_1 + Y_0 Y_1 + Z_0 Z_1 \\ &= II + XX + YY + ZZ \end{aligned}$$

$$\exp(-iH_{ex}t) = \exp(-i[II + XX + YY + ZZ]t)$$

Trotter Formula

We learned that the **Trotter formula** could help us reduce the exponential of operator sums to individual exponential terms.

$$\exp(A + B) = \lim_{n \rightarrow \infty} \left(\exp(A/n) \exp(B/n) \right)^n$$

When A and B are commutative ($AB = BA$), the limit vanishes.

Our previous example becomes,

$$\begin{aligned} \exp(-iH_{ex}t) &= \exp(-i[II + XX + YY + ZZ]t) \\ &= \exp(-iIIt) \exp(-iXXt) \exp(-iYYt) \exp(-iZZt) \end{aligned}$$

But still, how do we time evolve any single Pauli term on the quantum circuit?

Single qubit simulation

Rotational operators take care single qubit Pauli terms (Taylor expansion)

$$e^{-iXt} = \cos(t)I - i \sin(t)X = \begin{pmatrix} \cos(t) & -i \sin(t) \\ -i \sin(t) & \cos(t) \end{pmatrix}$$

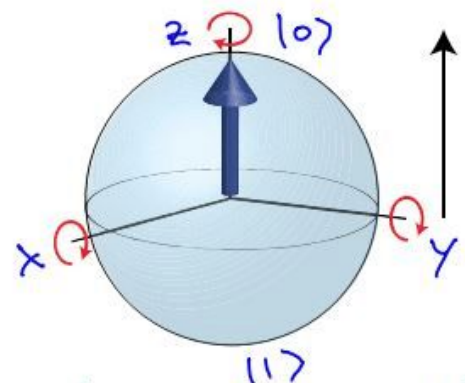
$$R_x(2t)$$

$$e^{-iYt} = \cos(t)I - i \sin(t)Y = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix}$$

$$R_y(2t)$$

$$e^{-iZt} = \cos(t)I - i \sin(t)Z = \begin{pmatrix} e^{-it/2} & 0 \\ 0 & e^{it/2} \end{pmatrix}$$

$$R_z(2t)$$



Rotational gates on Bloch sphere

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Exponential of Pauli operators

For multiple qubits, we need the following identity for any operator:

$$\exp(iAt) = \cos(t)I + i \sin(t)A, \quad \text{with } A^2 = I$$

Proof:

$$\begin{aligned} \exp(iAt) &= I + (iAt) + \frac{(iAt)^2}{2!} + \frac{(iAt)^3}{3!} + \frac{(iAt)^4}{4!} + \frac{(iAt)^5}{5!} + \dots \\ &= \underbrace{I + \frac{(iAt)^2}{2!} + \frac{(iAt)^4}{4!} + \dots}_{\text{even powers}} + \underbrace{(iAt) + \frac{(iAt)^3}{3!} + \frac{(iAt)^5}{5!} + \dots}_{\text{odd powers}} \\ &= I \left(1 - \frac{t^2}{2!} + \frac{t^4}{4!} + \dots \right) + iA \left(1 - \frac{t^3}{3!} + \frac{t^5}{5!} \dots \right) \\ &= I \cos(t) + iA \sin(t) \end{aligned}$$

Not surprisingly, this formula can be applied to any Pauli or Pauli product, since $X^2 = Y^2 = Z^2 = I$

Representation in Z-basis

We are familiar with the Z-basis or **computational basis**

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In fact any operations can be represented in this way:

$$\sigma_0 \equiv I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = |0\rangle\langle 0| + |1\rangle\langle 1|,$$

$$\sigma_1 \equiv X \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |1\rangle\langle 0| + |0\rangle\langle 1|,$$

$$\sigma_2 \equiv Y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = i|1\rangle\langle 0| - i|0\rangle\langle 1|,$$

$$\sigma_3 \equiv Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$$

Including the Control-Not gate!

$$\text{CNOT} = (|0\rangle\langle 0|)_0 \otimes I_1 + (|1\rangle\langle 1|)_0 \otimes X_1$$

Many qubits, Pauli-ZZ simulation

We start with $\exp(-iZZt)$, by claiming the following:

$$\exp(-iZ_0Z_1t) = \text{CNOT}_{0,1} \exp(-iZ_1t) \text{CNOT}_{0,1}$$

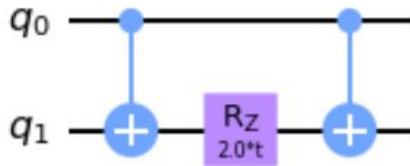
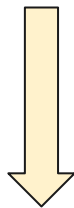
Proof:

$$\begin{aligned} RHS &= \left((|0\rangle\langle 0|)_0 \otimes I_1 + (|1\rangle\langle 1|)_0 \otimes X_1 \right) \times \left(I_0 \otimes \cos(t)I_1 - I_0 \otimes i \sin(t)Z_1 \right) \times \left((|0\rangle\langle 0|)_0 \otimes I_1 + (|1\rangle\langle 1|)_0 \otimes X_1 \right) \\ &= \left(\cos(t)(|0\rangle\langle 0|)_0 \otimes I_1 - i \sin(t)(|0\rangle\langle 0|)_0 \otimes Z_1 + \cos(t)(|1\rangle\langle 1|)_0 \otimes X_1 - i \sin(t)(|1\rangle\langle 1|)_0 \otimes X_1Z_1 \right) \\ &\quad \times \left((|0\rangle\langle 0|)_0 \otimes I_1 + (|1\rangle\langle 1|)_0 \otimes X_1 \right) \\ &= \cos(t)(|0\rangle\langle 0|)_0 \otimes I_1 - i \sin(t)(|0\rangle\langle 0|)_0 \otimes Z_1 + \cos(t)(|1\rangle\langle 1|)_0 \otimes \underbrace{X_1X_1}_{I_1} - i \sin(t)(|1\rangle\langle 1|)_0 \otimes \underbrace{X_1Z_1X_1}_{-Z_1} \\ &= \cos(t)(|0\rangle\langle 0| + |1\rangle\langle 1|)_0 \otimes I_1 - i \sin(t)(|0\rangle\langle 0| - |1\rangle\langle 1|)_0 \otimes Z_1 \\ &= \cos(t)I_1 \otimes I_0 - i \sin(t)Z_0 \otimes Z_1 = \exp(-iZ_0 \otimes Z_1t) = LHS \end{aligned}$$

Short proof: Pauli matrix are anticommutative.

Many qubits, Pauli-ZZ simulation

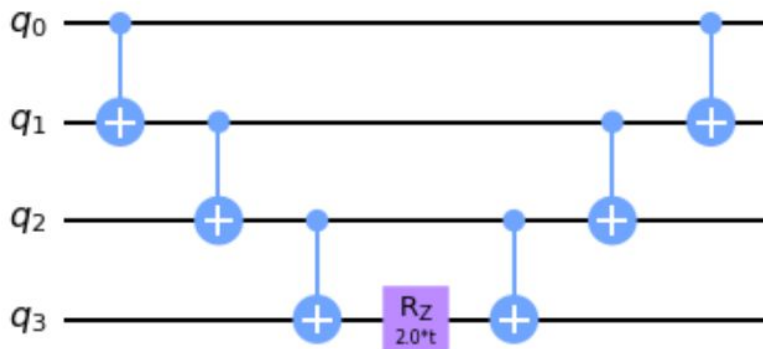
$$\exp(-iZ_0Z_1t) = \text{CNOT}_{0,1} \exp(-iZ_1t) \text{CNOT}_{0,1}$$



Many qubits, Pauli-ZZ...Z simulation

The results can be generalized to $\exp(-i ZZ\dots Z t)$, where the circuit is **a tower of control gates**

For example, $\exp(-i ZZZZ t)$ becomes



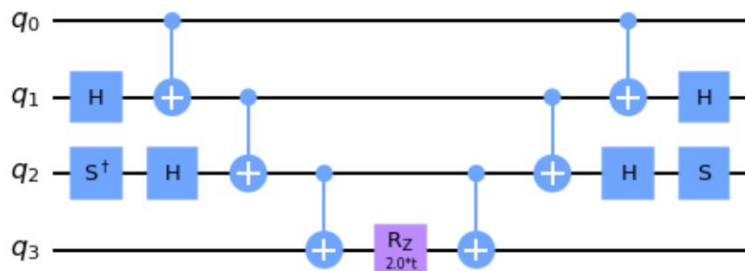
Many qubits, any Pauli simulation

The results can be generalized to $\exp(-i P t)$ for any Pauli string P by finding a unitary matrix $\sigma_k^j = U_k Z U_k^\dagger$

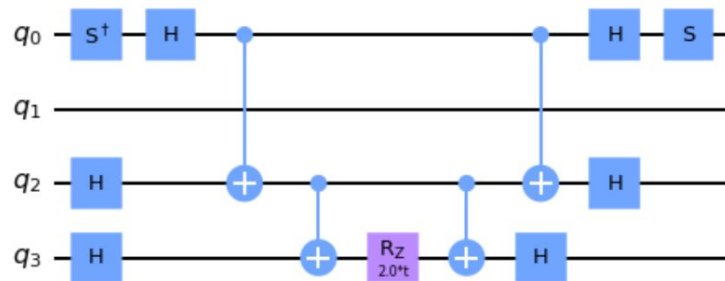
$$X = H Z H^\dagger, \quad Y = (S H) Z (S H)^\dagger$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad S = \sqrt{Z} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

because $U_k \exp(-i P t) U_k^\dagger = U_k (\cos(t) I - i \sin(t) P) U_k^\dagger = \cos(t) I - i \sin(t) (U_k P U_k^\dagger)$ for each qubit k



$$\exp(-i Z_3 X_2 Y_1 Z_0 t)$$



$$\exp(-i Y_3 I_2 X_1 X_0 t)$$



Qiskit Lab

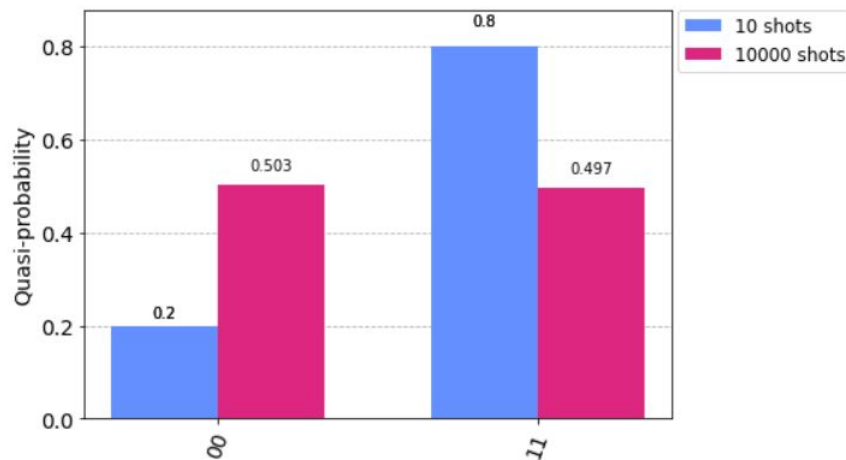
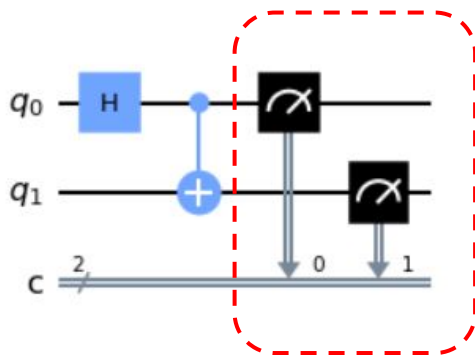
Today, you will have a chance to verify these basic simulation strategies in Qiskit.

You will learn how to construct Hamiltonian using simple Python commands and build quantum circuit automatically.

2. How to extract **observable** $\langle O \rangle$ from measurement?

Firstly, what is measurement?

By quantum mechanics, measurement **collapse** the wavefunction (in a sense, we lost the full information of the state). Therefore, we must measure/sample the quantum state **many times (shots)** to partially reconstruct the state.





Observable

- What is observable?

Quantity of interests that can be measured. For example, energy of the state.

- How are observables constructed?

Formally, it is the expectation value of an operator $\langle O \rangle = \langle \psi | \hat{O} | \psi \rangle$

On the quantum circuit, it is computed as a certain weighted sum of probabilities in the computational basis.

Pauli-Z based observable

For example, $\hat{O}_1 = \frac{1}{2}I_0Z_1$ $|\psi\rangle = \sum_i c_i |i\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle$

Then
$$\begin{aligned}\hat{O}_1 |\psi\rangle &= \frac{1}{2} \left(c_{00}IZ|00\rangle + c_{01}IZ|01\rangle + c_{10}IZ|10\rangle + c_{11}IZ|11\rangle \right) \\ &= \frac{1}{2} \left(c_{00}|00\rangle - c_{01}|01\rangle - c_{10}|10\rangle + c_{11}|11\rangle \right)\end{aligned}$$
$$\begin{aligned}\langle\psi|\hat{O}_1|\psi\rangle &= \frac{1}{2}(|c_{00}|^2 - |c_{01}|^2 - |c_{10}|^2 + |c_{11}|^2) \\ &= \frac{1}{2}(P(00) - P(01) - P(10) + P(11))\end{aligned}$$

$Z|0\rangle = |0\rangle$
 $Z|1\rangle = -|1\rangle$

linear combo of probabilities

Obviously, this generalizes to any linear combinations of Pauli-Z observables

Any Pauli observable

What about Pauli-X, Pauli-Y based observables?

Just like the simulation problem, the trick is to append quantum gates that move the calculations to computational basis!

$$X = H^\dagger Z H, \quad Y = H_y^\dagger Z H_y \qquad H_y = H S^\dagger$$

For example,

$$\begin{aligned} \langle \psi | I_0 X_1 Y_2 Z_3 | \psi \rangle &= \langle \psi | I_0 (H^\dagger Z H)_1 (H_y^\dagger Z H_y)_2 Z_3 | \psi \rangle \\ &= \langle \psi | H_1 (H_y)_2 | I_0 Z_1 Z_2 Z_3 | H_1 (H_y)_2 | \psi \rangle \\ &= \langle \psi' | I_0 Z_1 Z_2 Z_3 | \psi' \rangle \end{aligned}$$

We see that any Pauli observables are just the same as Pauli-Z based observables by **appending basis transformation gates**.



Qiskit Lab

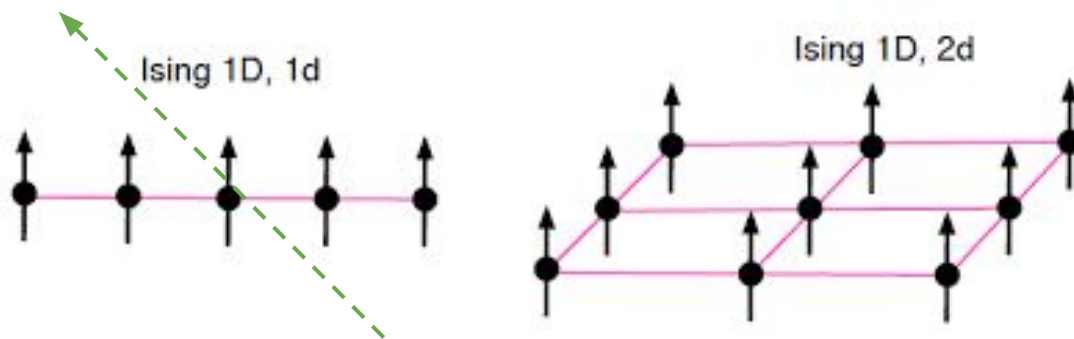
Today, you will have a chance to compute observables in Qiskit. In practice, all these probabilities arithmetics will be grouped and combined to minimize the number of operations.

Often observables are linear combination of Pauli's themselves, so one would need many different quantum circuits to compute the observable. Optimizing (minimizing) the number of circuits is itself an NP-hard problem...

Let us appreciate all the work done by Qiskit under the hood :)

Qiskit Lab

Today in the lab, we will study the real-time evolution of the famous Ising model with an arbitrary external field.



Despite of analytical solutions. They are both intractable to simulate when the system scales.

The 1D case is already intractable with just 100 sites (more than number of atoms in the universe). The 2D model is usually evolved with Monte Carlo using Metropolis algorithm.

Qiskit Lab

Specifically, the 1D Ising model Hamiltonian (discretized to mimic the continuum, PBC, local coupling)

$$H(\vec{\sigma}) = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j - \sum_j h_j \sigma_j$$

How to encode the problem onto qubits?

- What are quantum states?
- What are the Hamiltonian operator?

Hint:

$$Z |0\rangle = +1 |0\rangle$$

$$Z |1\rangle = -1 |1\rangle$$

Qiskit Lab

Specifically, the 1D Ising model Hamiltonian (discretized to mimic the continuum, PBC, local coupling)

$$H(|\psi\rangle) = - \sum_{\langle i,j \rangle} J_{ij} Z_i Z_j - \sum_j h_j Z_j$$

Note: we will deal with a slightly different form in the lab

How to encode the problem onto qubits?

- What are quantum states? $0 \mapsto |0\rangle, 1 \mapsto |1\rangle$
- What are the Hamiltonian operator? $\sigma_i \mapsto Z_i$

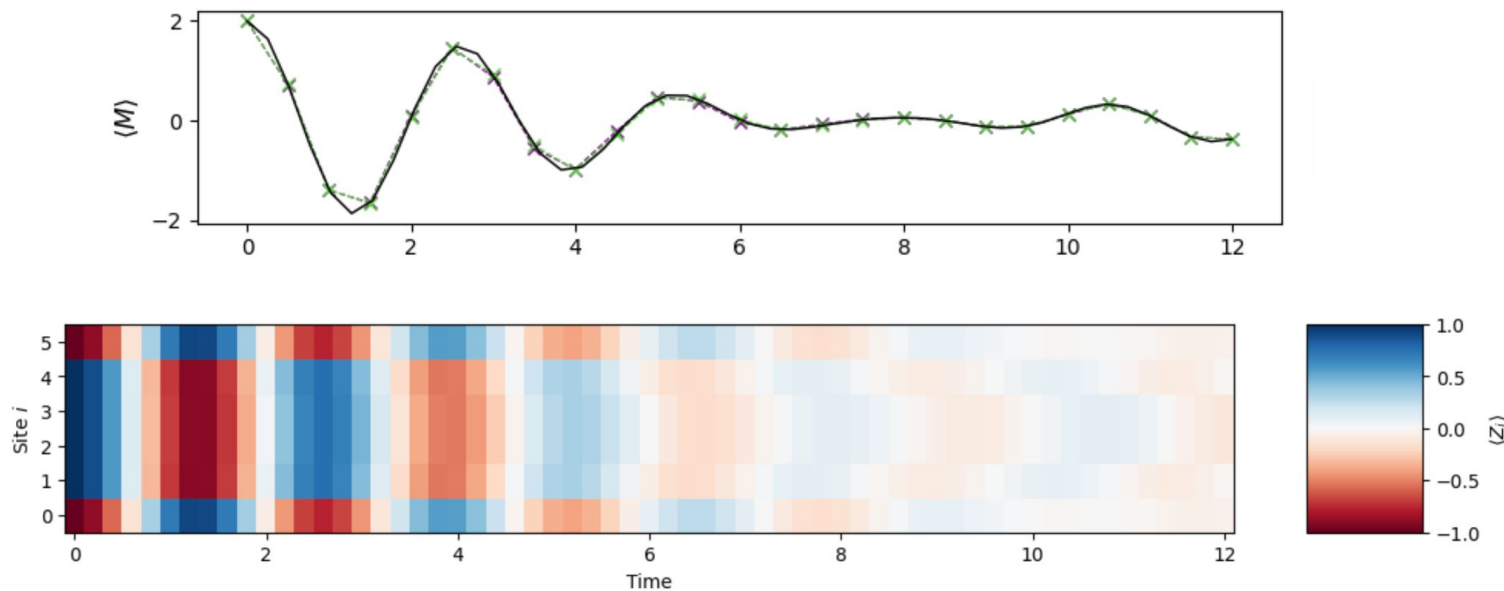
Hint:

$$Z|0\rangle = +1|0\rangle$$

$$Z|1\rangle = -1|1\rangle$$

Qiskit Lab

Taking the 1D example, we analyze its global property (total magnetization) and local property (spin distribution) evolve over time.



Quantum computing history

We have really come a long way in past 40 years!

Feynman, “Simulating Physics with Computers” (1981)

Toffoli Gate
(1980)

Shor’s Algo
(1994)

Error Correction
(1995)

Variational Eigensolver
(2014)

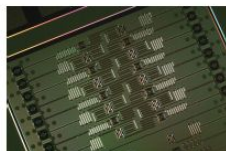
Quantum Machine Learning
(2017)

Currently, we are in the **Noisy Intermediate-Scale Quantum (NISQ)** era...

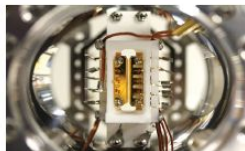
Preskill, Quantum, 2 (2018)



Google



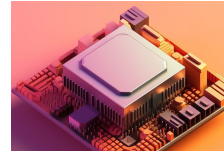
IBM



Rigetti



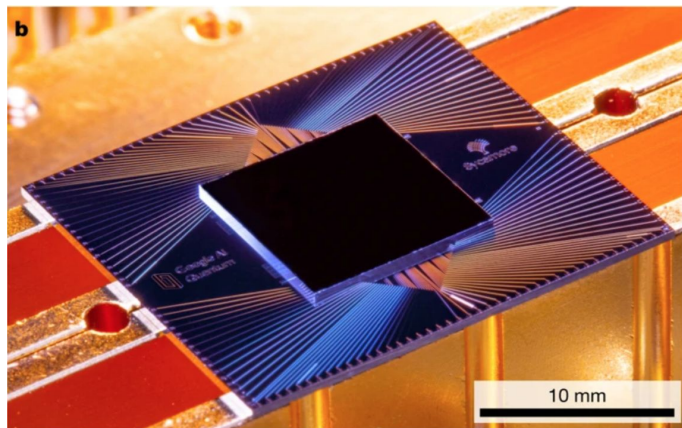
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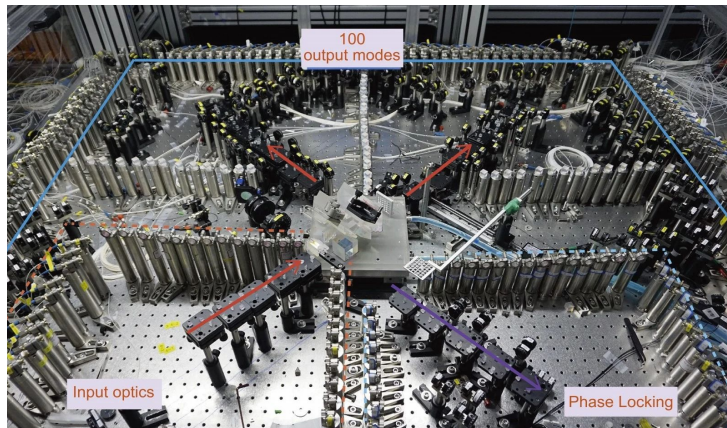
USTC



Towards Quantum Advantage



Google AI Quantum 1910.11333 (2019)



UTSC, Jian-Wei Pan's group, Science 370, 1460 (2020)

Natural science
Optimization
Finance

Telecommunication
Quantum machine learning
...

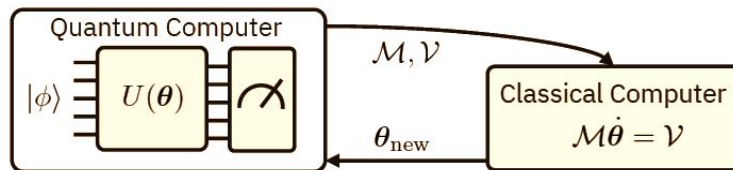
3. Variational algorithms

Perhaps the most successful applications of quantum computing is the variational algorithm.

Based on the **Variational Principle** $\langle \psi_{\text{guess}} | H | \psi_{\text{guess}} \rangle \geq \langle E_0 \rangle = \langle \psi_0 | H | \psi_0 \rangle$

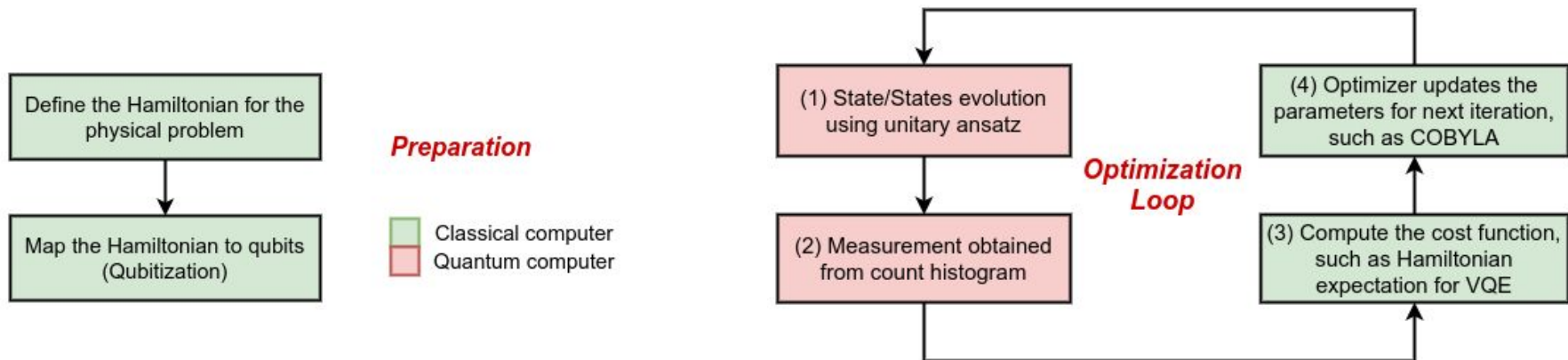
By tweaking the **ansatz (guess wavefunction)**, we can obtain the ground state energy of the Hamiltonian.

Optimal circuit (i.e. solution) to the chemistry or physics problem is obtained by collaboration between quantum device and CPU.



VQE (Variational Quantum Eigensolver)

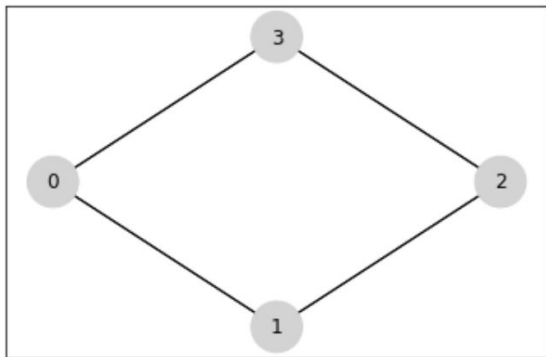
The simplest variational algorithm is VQE



Now, we look at an interesting problem that we can solve with VQE

Maxcut problem (maximum cut)

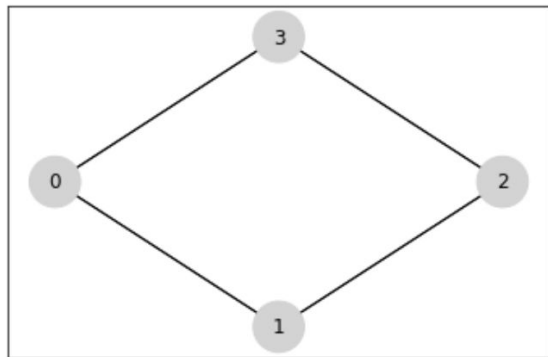
Given a graph of n nodes, how do we cut the graph into two partitions such that the number of edges between the two partitions are maximized?



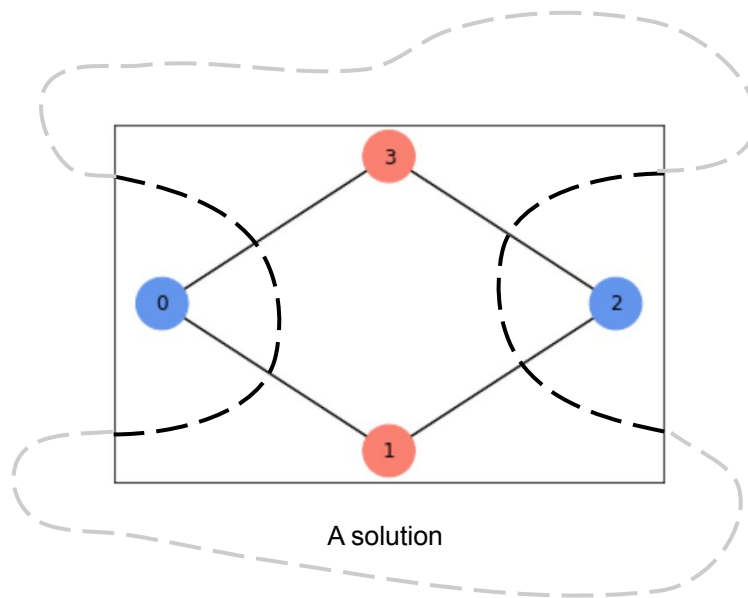
Initial Problem

Maxcut problem (maximum cut)

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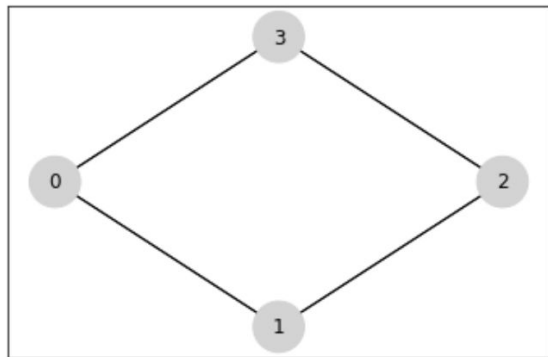
Initial Problem



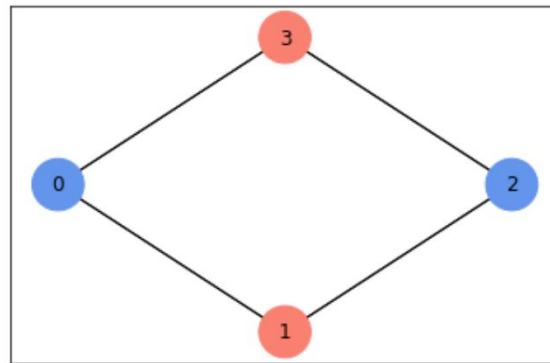
A solution

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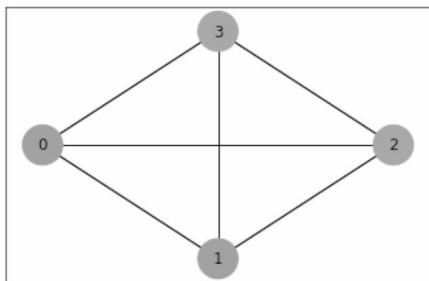
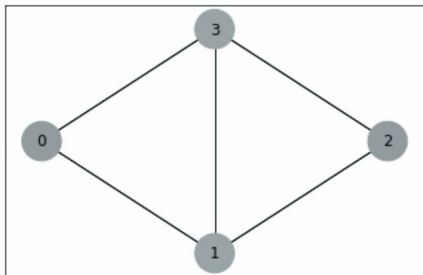
Initial Problem



A solution

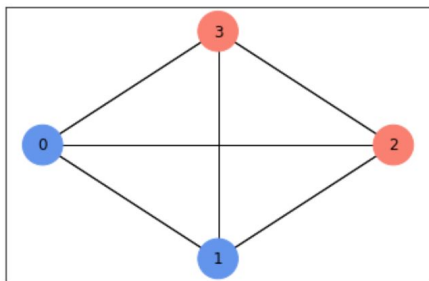
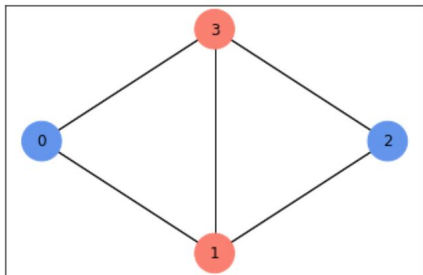
Why Maxcut? It represents an universal problem; involving lots of active research

Maxcut problem is **NP-Hard**!



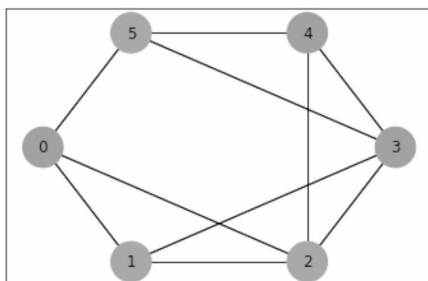
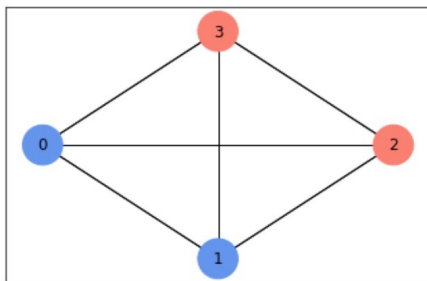
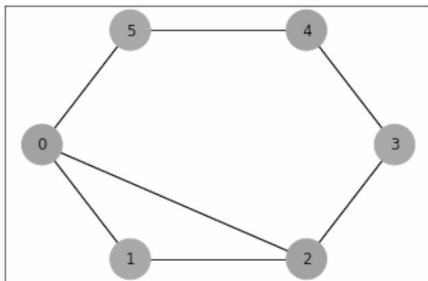
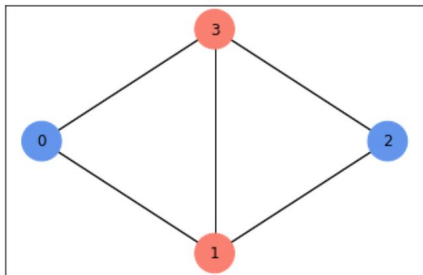
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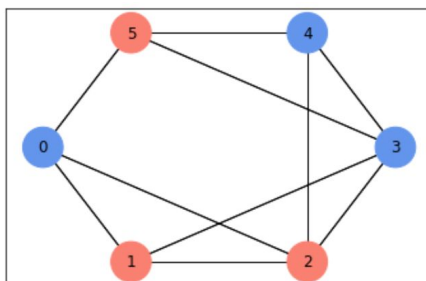
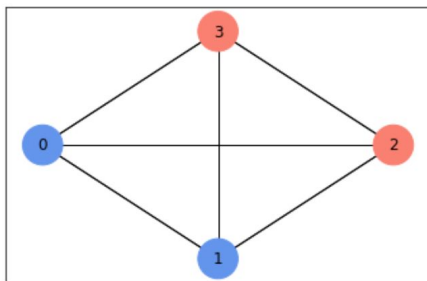
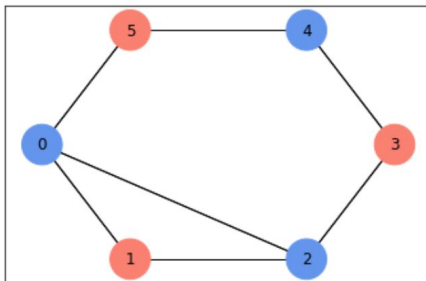
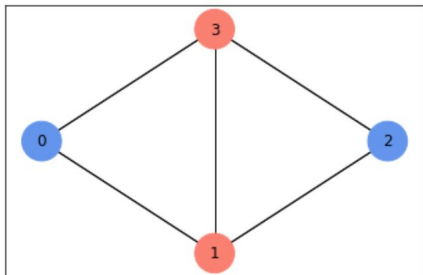
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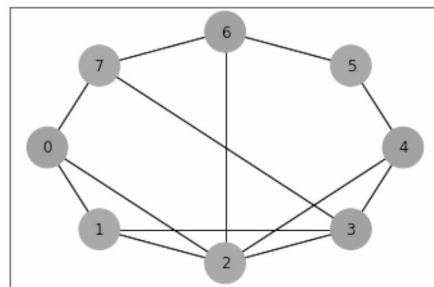
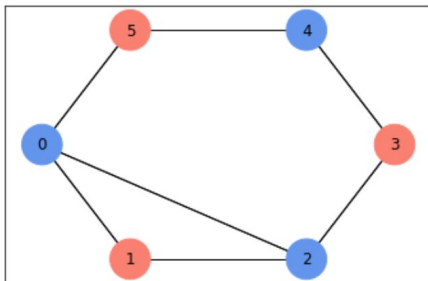
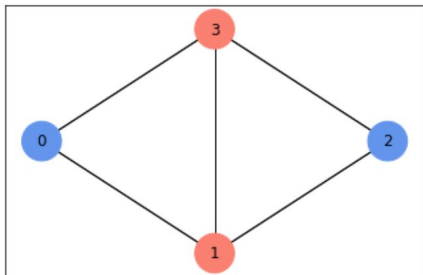
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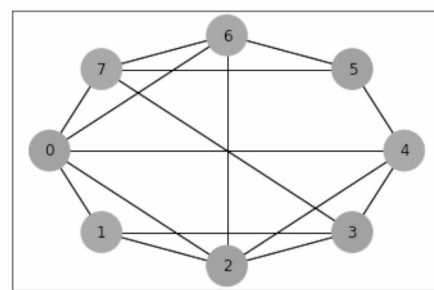
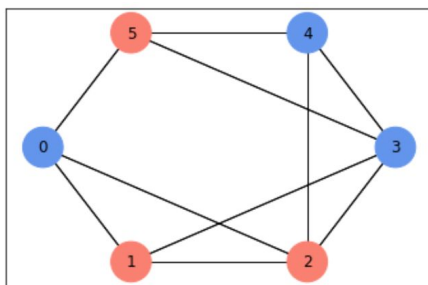
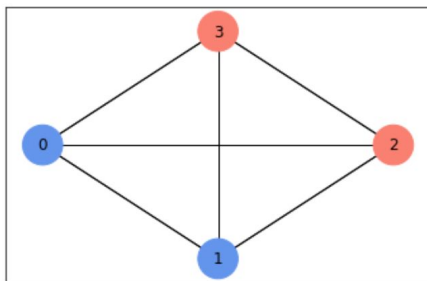


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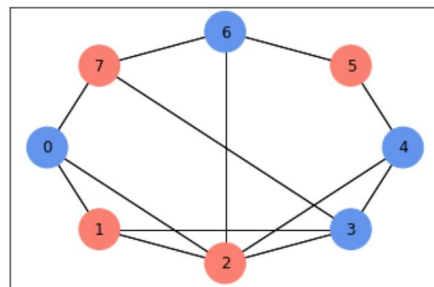
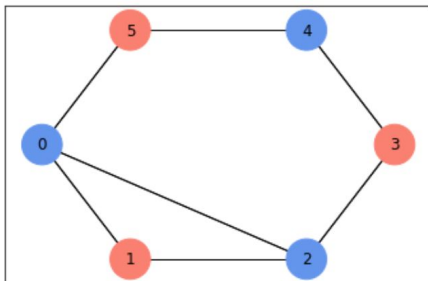
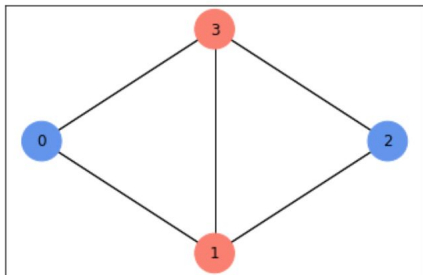
Maxcut problem is **NP-Hard**!



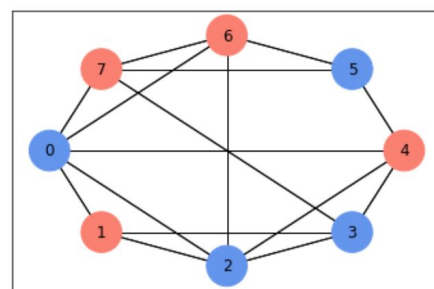
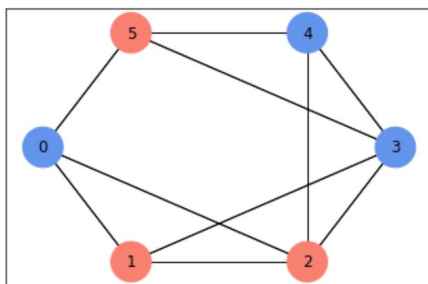
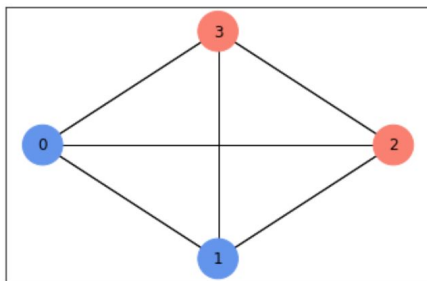
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Maxcut problem is **NP-Hard**!

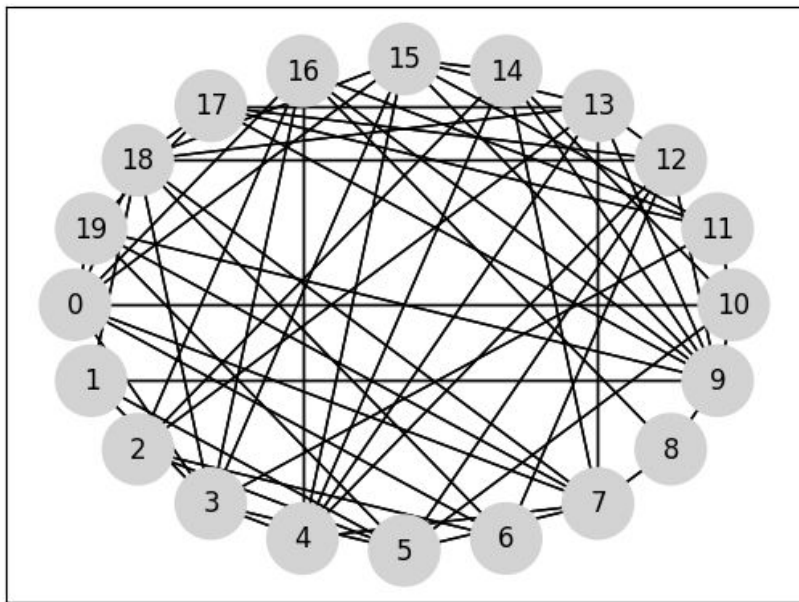


...



Maxcut problem is **NP-Hard**!

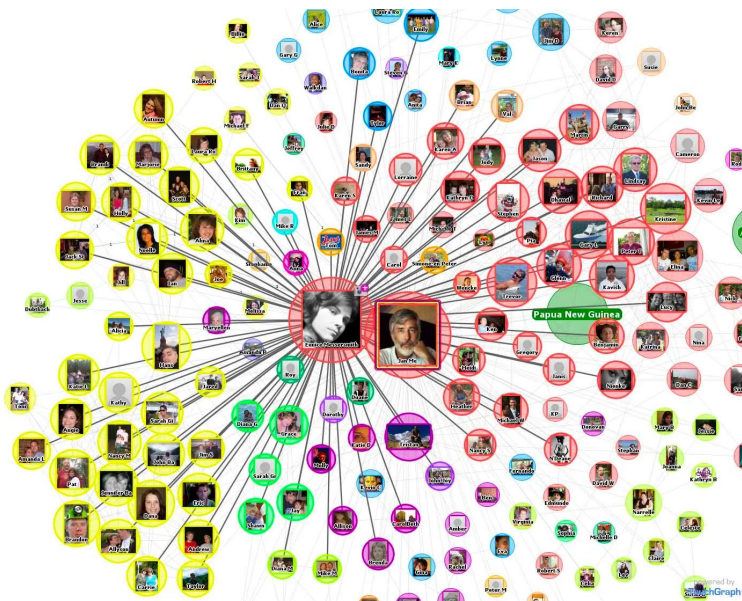
Eventually, bruteforce solutions $\mathcal{O}(n!)$ for large graphs becomes impractical...



$n = 20$ is already so slow to compute...



Yet, Maxcut problem is so universal & important



Images are from Google Search

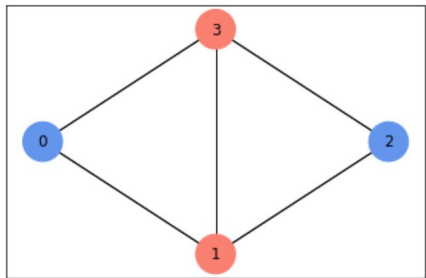
Maxcut problem, binary encoding

How to leverage quantum computing to solve Maxcut problems?

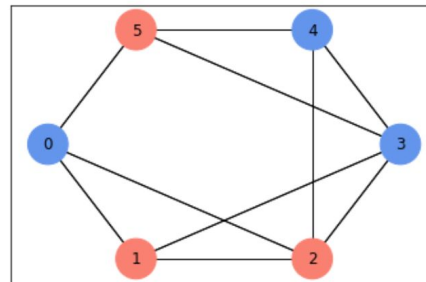
We represent a solution to the n -node Maxcut using binary sequence,

$$\mathbf{x} = x_0 x_1 x_2 \cdots x_{n-1} = |x_0\rangle |x_1\rangle |x_2\rangle \cdots |x_{n-1}\rangle$$

where $x_i = 0$ indicates node- i in **Partition 0 (red)**, and $x_i = 1$ indicates node- i in **Partition 1 (blue)**.



$$\mathbf{x} = 1010 = |1\rangle_0 |0\rangle_1 |1\rangle_2 |0\rangle_3$$



$$\mathbf{x} = 100110 = |100110\rangle$$

Maxcut problem Hamiltonian

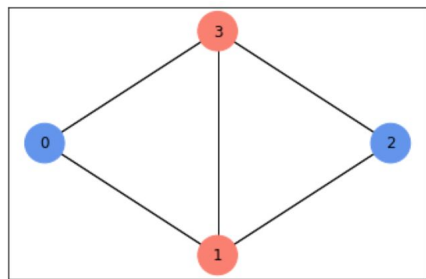
With these binary variables, we can build a problem Hamiltonian for any Maxcut problem

$$H(\mathbf{x}) = \sum_{i,j} w_{ij} x_i (1 - x_j)$$

$$w_{ij} = \begin{cases} 1, & \text{if edge}(i, j) \in G \\ 0, & \text{if edge}(i, j) \notin G \end{cases}$$

where w_{ij} is connectivity (adjacency matrix).

We claim a solution to the maxcut problem must **maximize this Hamiltonian!**



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

$$\mathbf{x} = 1010 = |1\rangle_0 |0\rangle_1 |1\rangle_2 |0\rangle_3$$

$$\begin{aligned} w_{01}x_0(1-x_1) &= w_{01} \cdot 1 \cdot (1-0) = 1 \\ w_{03}x_0(1-x_3) &= w_{03} \cdot 1 \cdot (1-0) = 1 \\ w_{10}x_1(1-x_0) &= w_{10} \cdot 0 \cdot (1-1) = 0 \\ w_{12}x_1(1-x_2) &= 0 \\ w_{13}x_1(1-x_3) &= 0 \\ w_{21}x_2(1-x_1) &= 1 \\ w_{23}x_2(1-x_3) &= 1 \\ w_{30}x_3(1-x_0) &= 0 \\ w_{31}x_3(1-x_1) &= 0 \\ w_{32}x_3(1-x_2) &= 0 \end{aligned}$$

$$H(\mathbf{x}) = 4$$

Maxcut problem qubit encoding

To map the Hamiltonian to quantum circuit, we use

$$x_i \rightarrow \frac{I - Z}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Why?

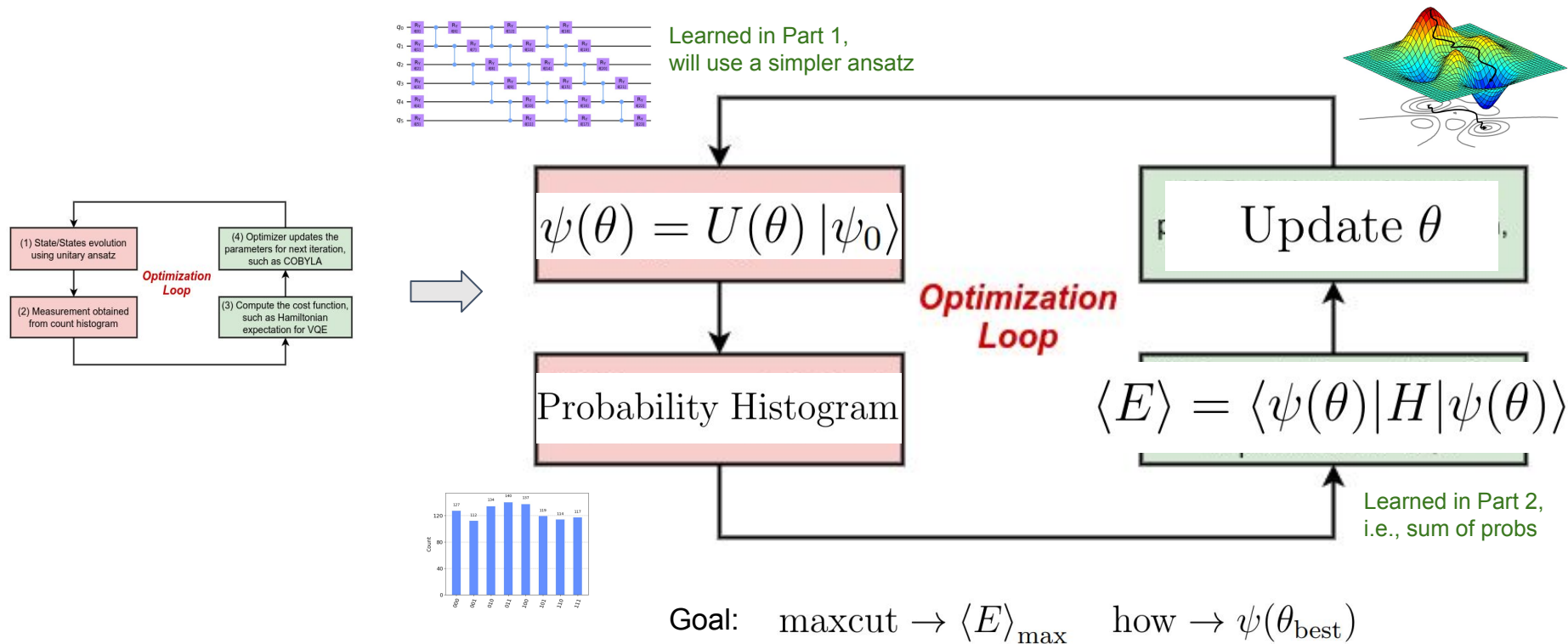
Check its eigenvalue
and eigenvector

Then, the **Maxcut Hamiltonian** becomes a sum of Pauli-Z and Pauli-ZZ operators (i.e., Ising Hamiltonian)

$$H \rightarrow \sum_{ij} w_{ij} \frac{I_i - Z_i}{2} \left(I - \frac{I_j - Z_j}{2} \right) = \sum_i c_i Z_i + \sum_{ij} d_{ij} Z_i Z_j$$

Our task today is to find optimal solution to this Maxcut Hamiltonian using VQE.

VQE to Maxcut, overview





Qiskit Lab

Today, you will build a VQE algorithm in Qiskit from scratch, and then we will test our algorithm on the Maxcut problem. I hope you have a taste of quantum computing techniques to real life problems.

The game does not simply stop here...

1. We can use problem-inspired ansatz, such as QAOA (quantum approximate optimization algorithm), where quantum speedup over classical algorithm is proven in some cases.
 2. We can add weights on edges, constraints on the graph, and essentially describe many problems using this Ising model, such as Traveling Salesman, Knapsack, Satisfiability problem, Social networks...
- ...

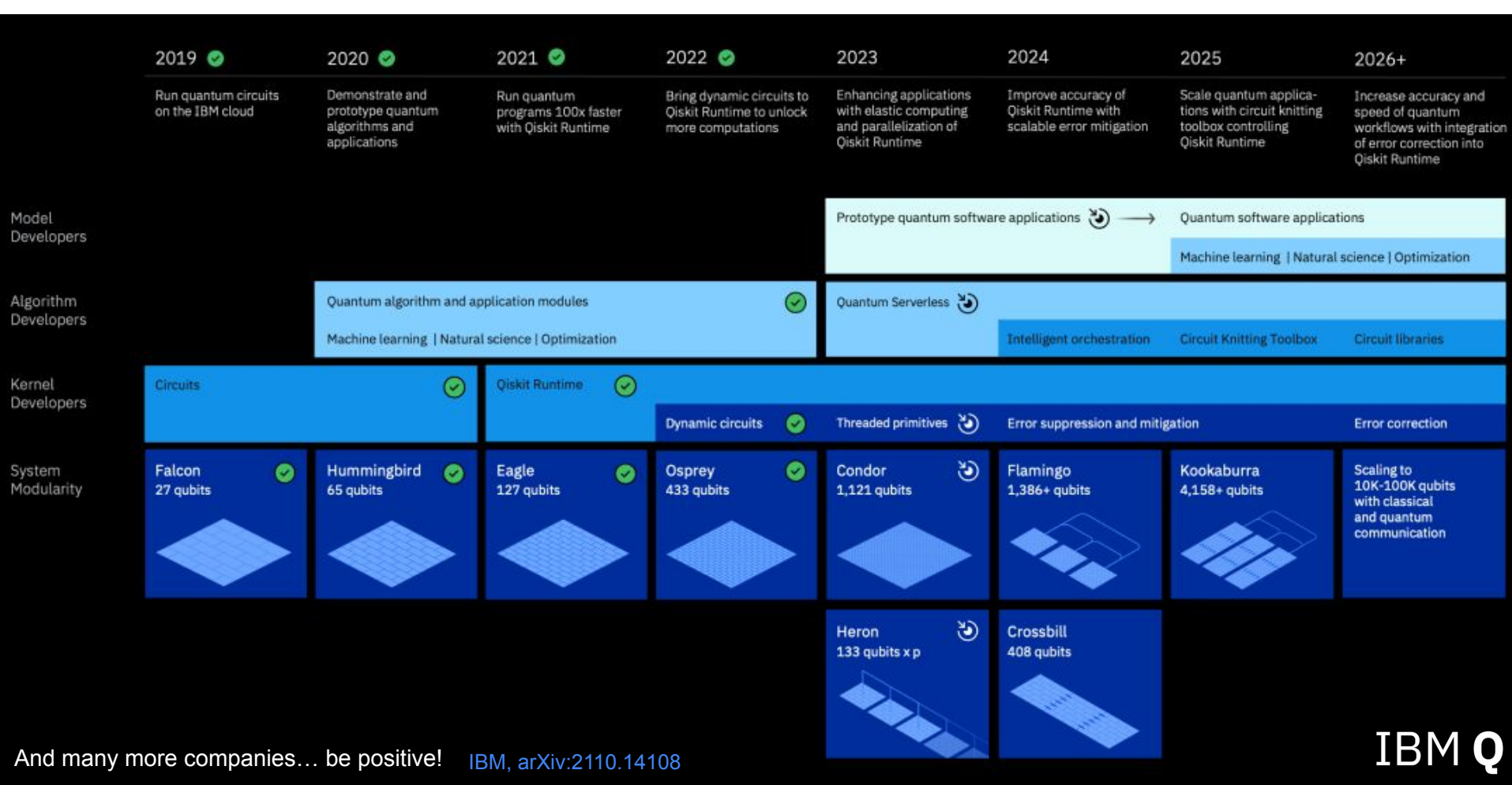


Why quantum computing?

“Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical”

Richard Feynman





And many more companies... be positive! [IBM, arXiv:2110.14108](#)

