จุฬาลงกรณ์มหาวิทยาลัย
CHULALONGKORN UNIVERSITY

Quantum Computing for Optimization Tasks

Prabhas Chongstitvatana

More Information

Search “Prabhas Chongstitvatana”

Go to me homepage

What is a quantum computer?

a computer that relies on special memory, "quantum bit", to perform massively parallel computing.

What is a quantum bit?

a basic unit of memory that uses superposition of "quantum" effect (entanglement) to store information.

a "qubit" stores the probability of information. It represents both "1" and "0" at the same time.

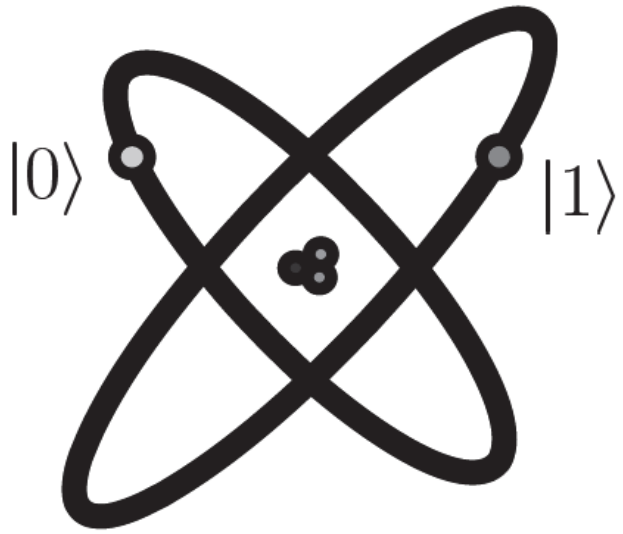
Quantum Bits (Qubits)

- Classical bits vs. Quantum bits
- Qubits are mathematical objects (similarly to 0/1 in classical bits)

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$

Prob. Prob.



What is the advantage?

It is very very fast compared to conventional computers

It has very large memory

Google quantum lab's paper

claim of 100,000,000x speed up

What is the Computational Value of Finite Range Tunneling?

Vasil S. Denchev,[1] Sergio Boixo,[1] Sergei V. Isakov,[1] Nan Ding,[1] Ryan Babbush,[1] Vadim Smelyanskiy,[1] John Martinis,[2] and Hartmut Neven[1]

[1] *Google Inc., Venice, CA 90291, USA*
[2] *Google Inc., Santa Barbara, CA 93117, USA*

(Dated: December 31, 2015)

Quantum annealing (QA) has been proposed as a quantum enhanced optimization heuristic exploiting tunneling. Here, we demonstrate how finite range tunneling can provide considerable computational advantage. For a crafted problem designed to have tall and narrow energy barriers separating local minima, the D-Wave 2X quantum annealer achieves significant runtime advantages relative to Simulated Annealing (SA). For instances with 945 variables, this results in a time-to-99%-success-probability that is $\sim 10^8$ times faster than SA running on a single processor core. We also compared physical QA with Quantum Monte Carlo (QMC), an algorithm that emulates quantum tunneling on classical processors. We observe a substantial constant overhead against physical QA: D-Wave 2X again runs up to $\sim 10^8$ times faster than an optimized implementation of QMC on a single core. We note that there exist heuristic classical algorithms that can solve most instances of Chimera structured problems in a timescale comparable to the D-Wave 2X. However, we believe that such solvers will become ineffective for the next generation of annealers currently being designed. To investigate whether finite range tunneling will also confer an advantage for problems of practical interest, we conduct numerical studies on binary optimization problems that cannot yet be represented on quantum hardware. For random instances of the number partitioning problem, we find numerically that QMC, as well as other algorithms designed to simulate QA, scale better than SA and better than the best known classical algorithms for this problem. We discuss the implications of these findings for the design of next generation quantum annealers.

v3 [quant-ph] 30 Dec 2015

I. INTRODUCTION

Simulated annealing (SA) [1] is perhaps the most widely used algorithm for global optimization of pseudo-Boolean functions with little known structure. The objective function for this general class of problems is

standard time-dependent Hamiltonian used for QA is

$$H(t) = -A(t)\sum_{j=1}^{N}\sigma_j^x + B(t)H_{\mathrm{P}}\ , \qquad (2)$$

where H_{P} is written as in Eq. (1) but with the spin vari-

Example of quantum computers

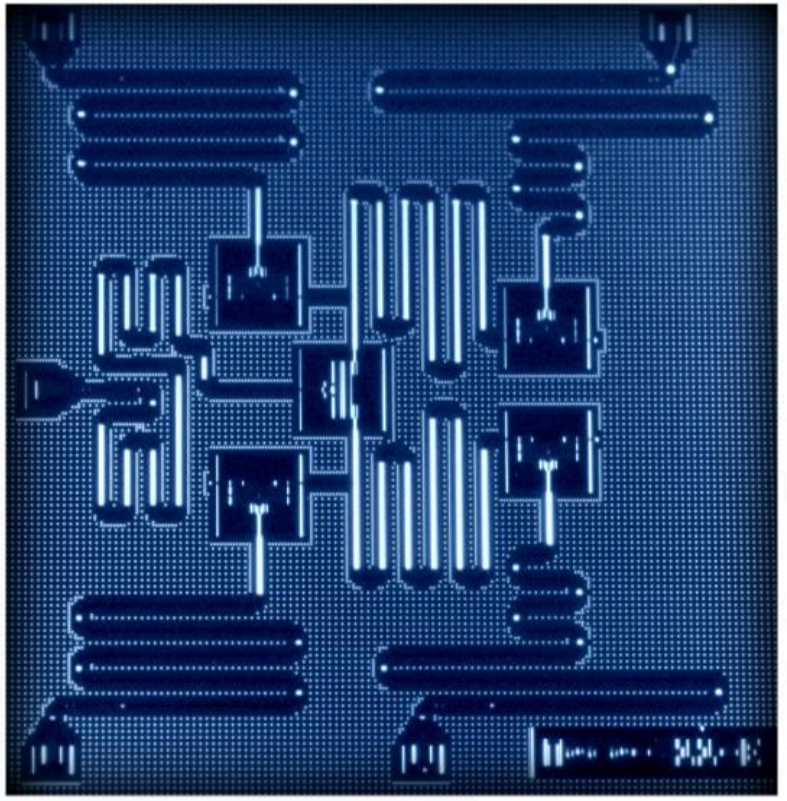
IBM 5 and 50 qubits

D-wave two, quantum annealing

IBM 50 qubits quantum computer

IBM System One in Japan

IBM 5 qubits processor



Google Nasa, D-Wave 2x machine

STEPHEN

Impact of quantum computer on industry

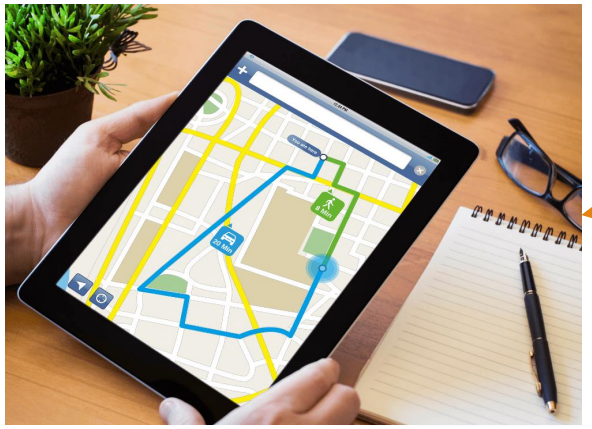
Four industry (near future)

- Pharmaceuticals
- Chemicals
- Automotive
- Finance

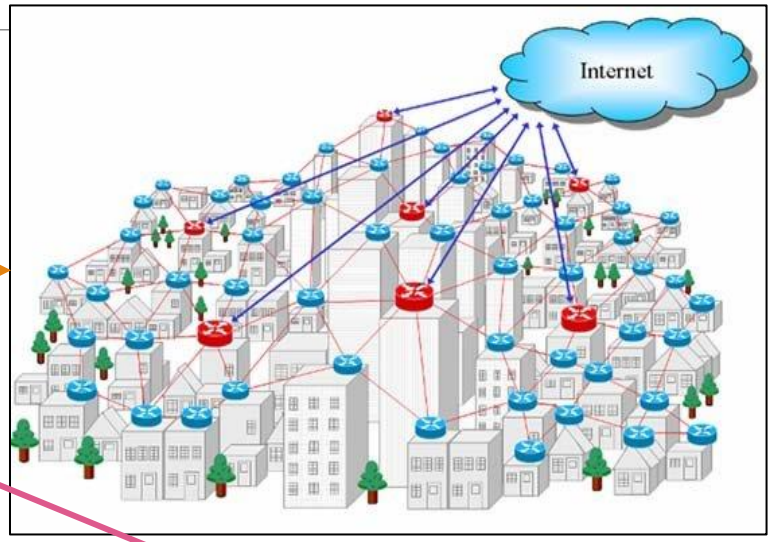
Four use cases

- Quantum Simulation
- Quantum AI and Machine learning
- Quantum Optimization
- Quantum Factorization

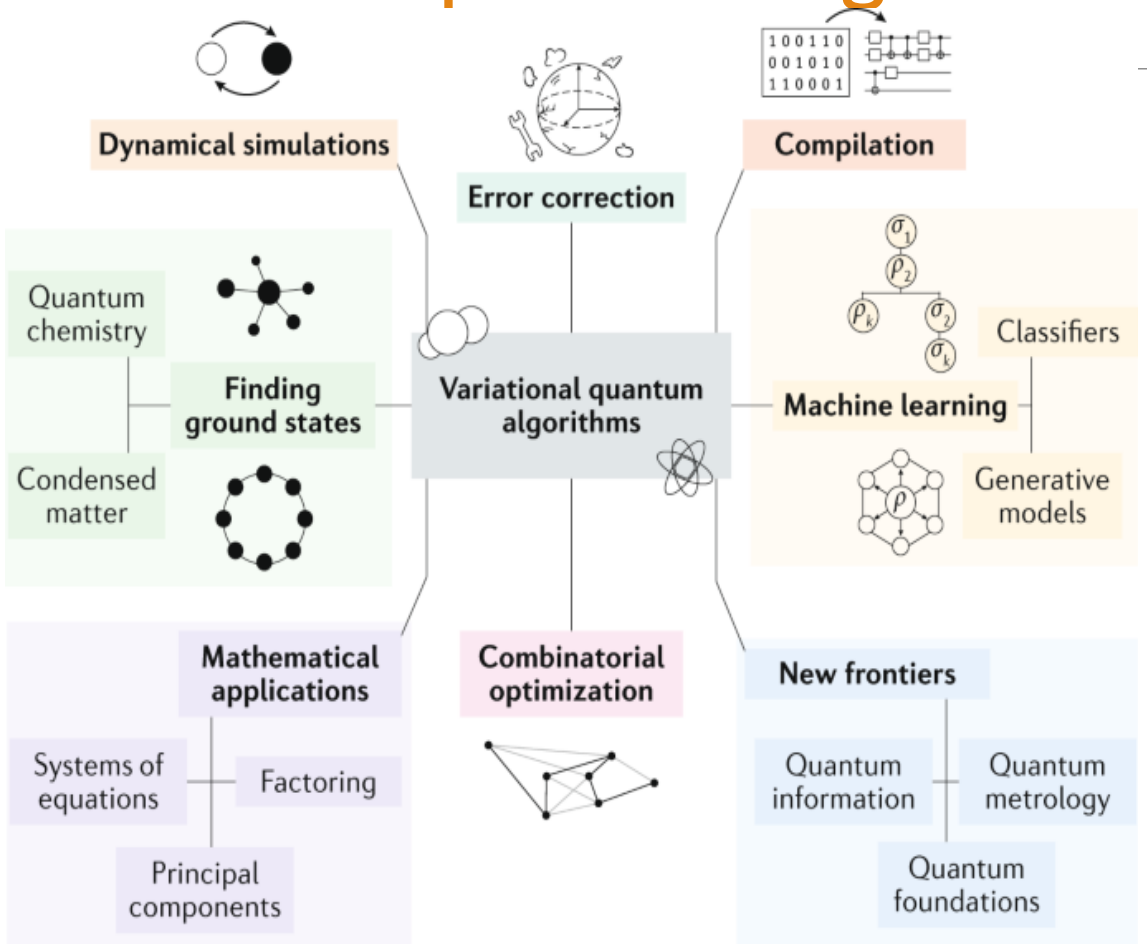
Toward solving optimization problems with a quantum computer



Optimization problems



Variational quantum algorithms



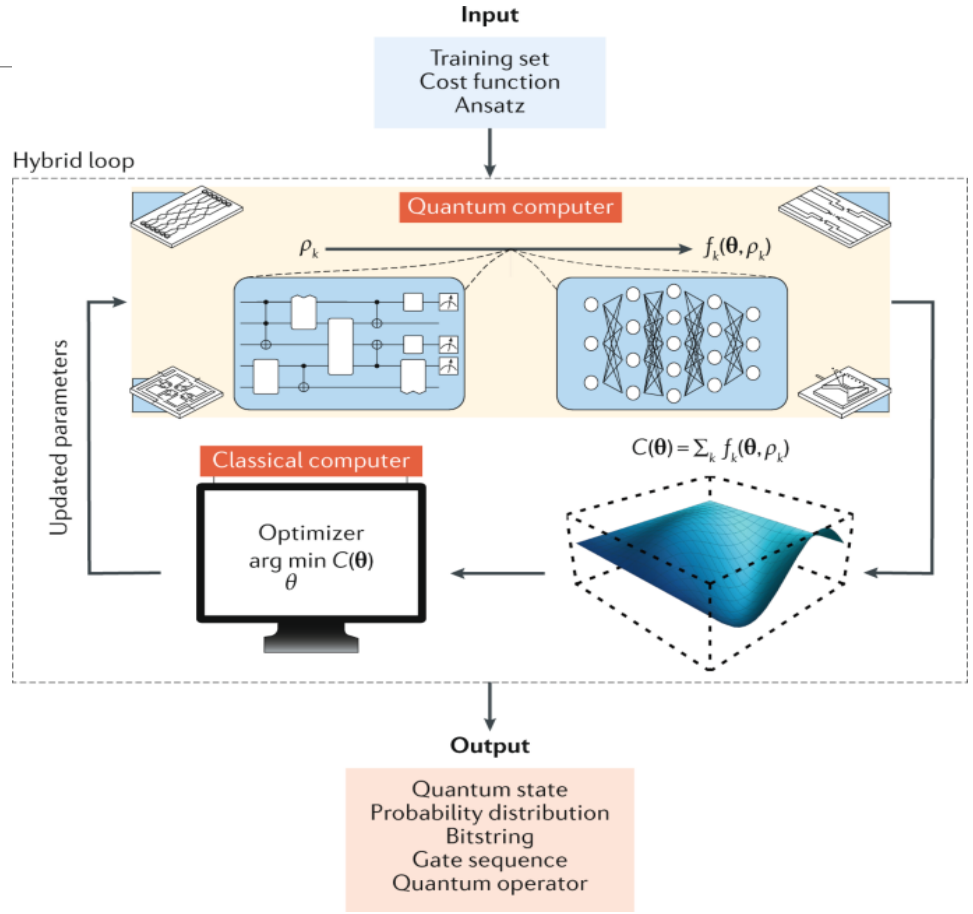


Photo https://media.springernature.com/m685/springer-static/image/art%3A10.1038%2Fs42254-021-00348-9/MediaObjects/42254_2021_348_Fig1_HTML.png and https://media.springernature.com/lw685/springer-static/image/art%3A10.1038%2Fs42254-021-00348-9/MediaObjects/42254_2021_348_Fig2_HTML.png

Quantum variational eigensolver

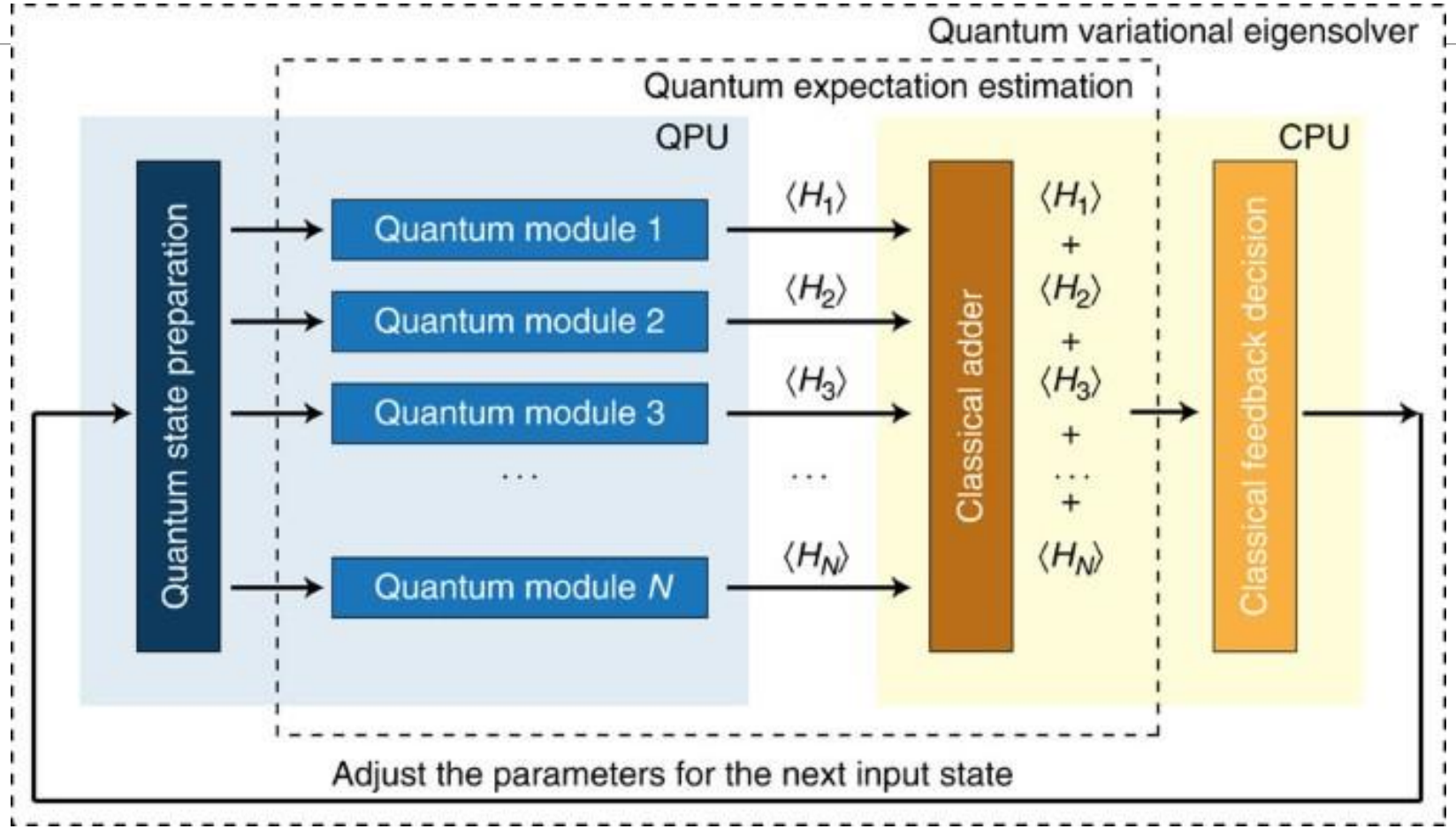
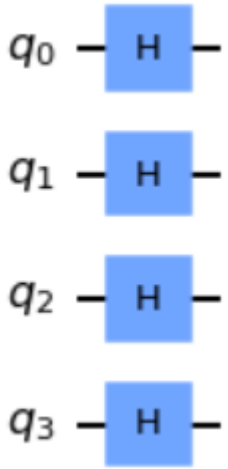
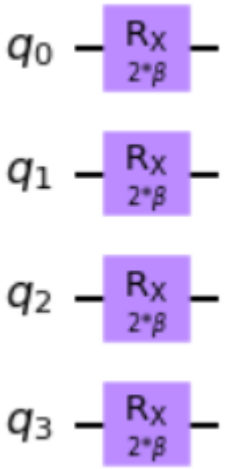


Photo https://media.springernature.com/m685/springer-static/image/art%3A10.1038%2Fncomms5213/MediaObjects/41467_2014_Article_BFncomms5213_Fig1_HTML.jpg

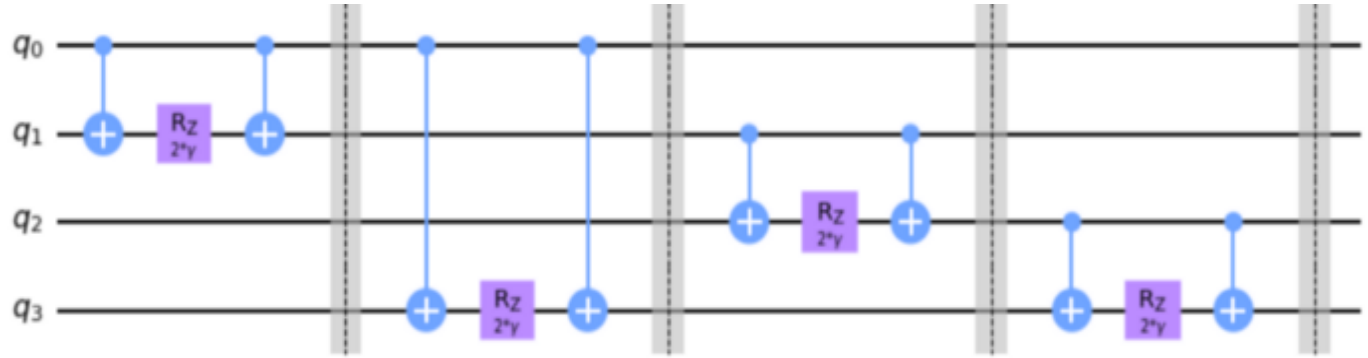
Quantum approximate optimization algorithm (QAOA)



Preparing an initial state



The mixing unitary



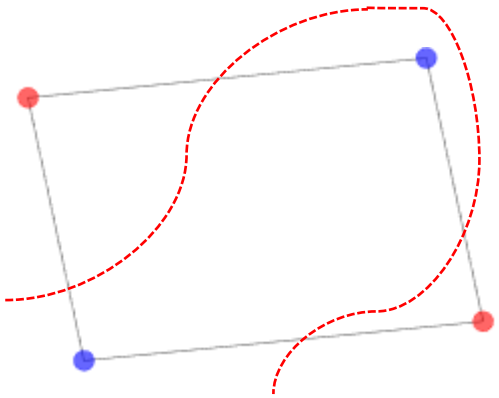
The problem unitary

$$|\psi(\boldsymbol{\beta},\boldsymbol{\gamma})\rangle = \underbrace{U(\boldsymbol{\beta})U(\boldsymbol{\gamma})\cdots U(\boldsymbol{\beta})U(\boldsymbol{\gamma})}_{p \text{ times}}|\psi_0\rangle$$

$$U(\boldsymbol{\beta}) = e^{-i\boldsymbol{\beta}H_B} \text{ and } U(\boldsymbol{\gamma}) = e^{-i\boldsymbol{\gamma}H_P}$$

where H_B is the mixing Hamiltonian and H_P is the problem Hamiltonian.

Goal: find $(\boldsymbol{\beta_{opt}}, \boldsymbol{\gamma_{opt}})$ to get $\langle\psi(\boldsymbol{\beta_{opt}}, \boldsymbol{\gamma_{opt}})|H_P|\psi(\boldsymbol{\beta_{opt}}, \boldsymbol{\gamma_{opt}})\rangle$



The max-cut problem

Photo https://qiskit.org/textbook/ch-applications/qaoa.html

Quantum gates

Operator	Gate(s)	Matrix
Pauli-X (X)		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

Common quantum logic gates by name (including abbreviation), circuit form(s) and the

Quantum approximate optimization algorithm (QAOA)

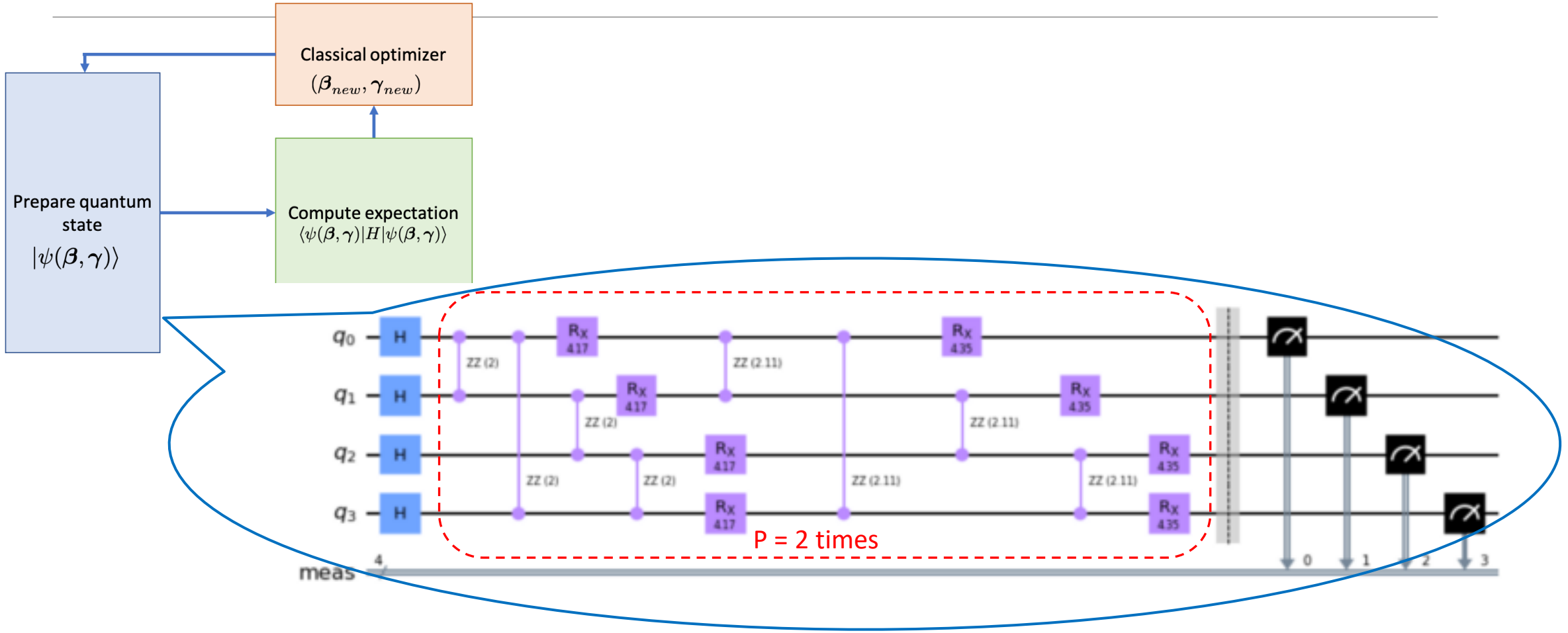


Photo https://qiskit.org/textbook/ch-applications/qaoa.html

Quantum-inspired evolutionary algorithm

- One approach to tackle the optimization problem is to use evolutionary algorithms such as Genetic algorithms (GAs) and Compact genetic algorithm (cGA).

- Quantum-inspired genetic algorithms: the algorithms are still executed in the classical computers but took some of the ideas of quantum phenomena and translate them into classical analogue.

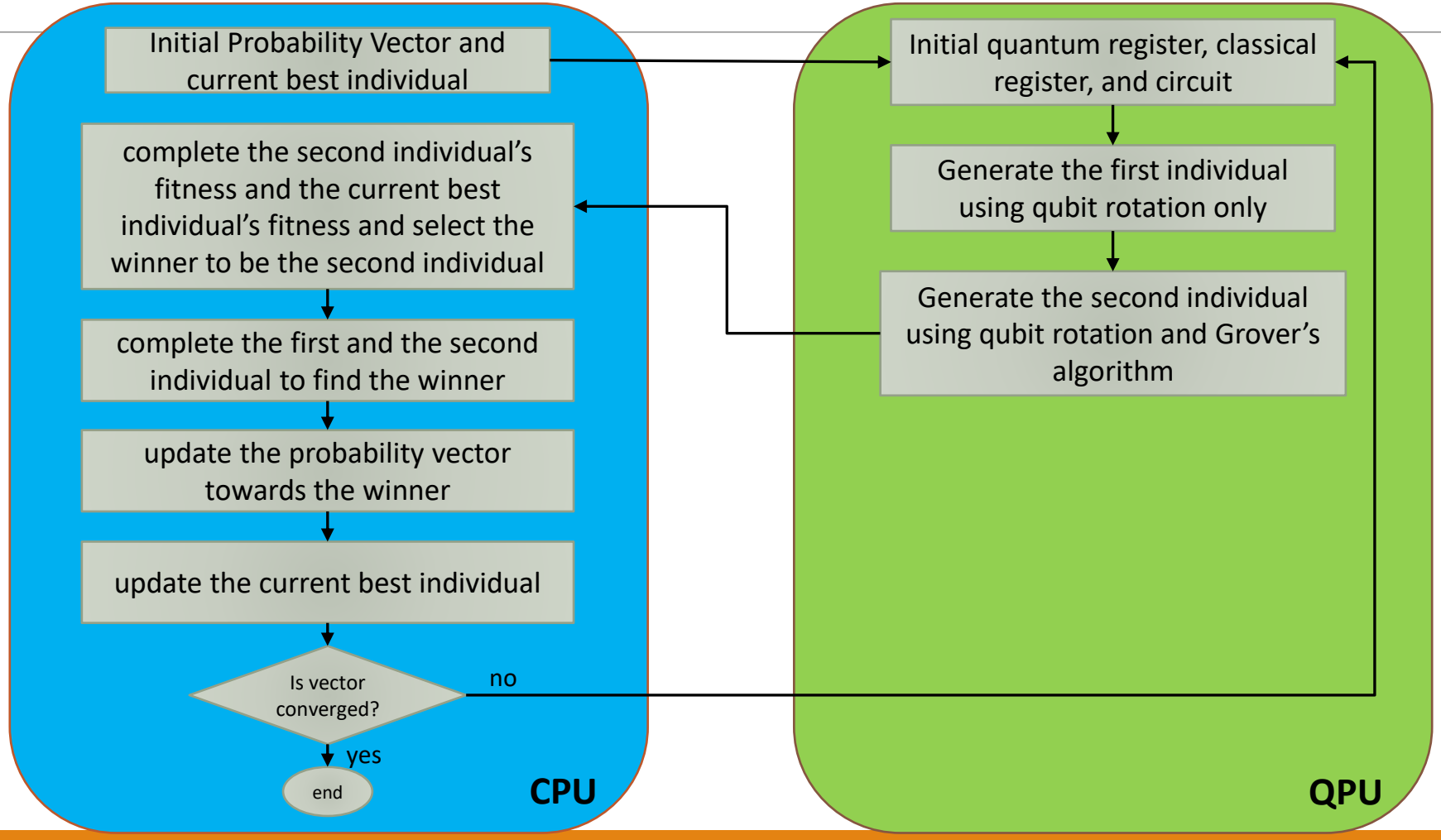
Quantum-assisted genetic algorithms

- Quantum-assisted genetic algorithms perform mutation operator while crossover and population update are on the classical side.

- Compact genetic algorithm represents the population as a a probability distribution in a quantum register. The quantum variable is then updated toward the winner via qubit rotation

- Redefining the GA in the context of quantum computation by creating a population with superposition of all states.

Grover-assisted Compact Genetic Algorithm (cGA*)



The schematic of Grover-assisted compact genetic algorithm.

Grover's Search Algorithm

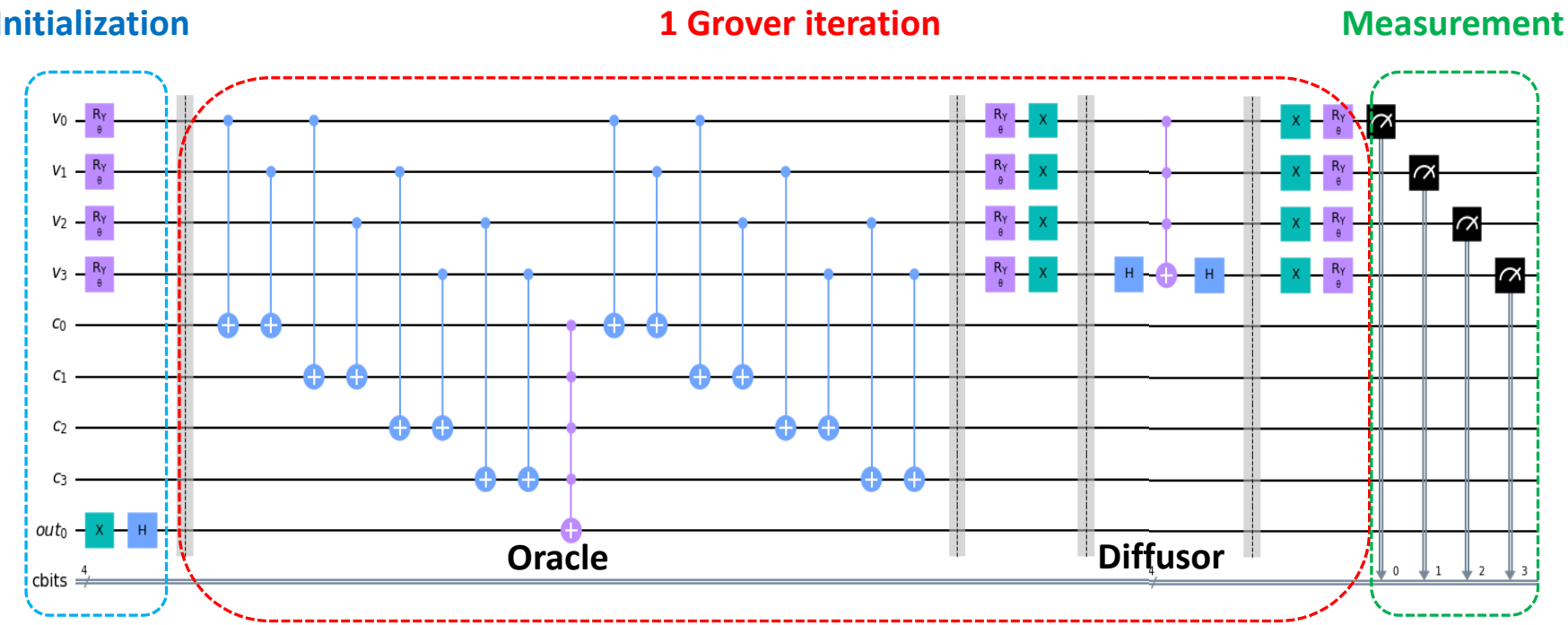
- "For what value of *x* does *f(x)* = *k*, for some number *k*?"
- A quantum computer allows us to calculate *f(x)* for a superposition of all values of *x* at the same time
- We use the result to increase the amplitude of the good values of *x* and repeat until we have a high probability of reading out the value we want.
- If there are *N* possible values for *x*, we will have to try half of them (*N/2*) on average before finding the answer.
- Grover's algorithm uses entanglement and interference to grow those probability amplitudes faster than a simple linear check of all possible values. Instead of *N/2* tries, around $\sqrt{N}$ calculations will be enough.

The Stages of Grover's Search Algorithm

1. Initialization : All qubits are set to be in superposition. All states have the amplitude $1/\sqrt{N}$
2. Oracle : The oracle function marks the state *x'* that satisfies the condition *f(x')* = 1 by performing a phase flip.
3. Amplification : phase flips the amplitudes around the average amplitude. The flip causes the target state's amplitude to increase and the others to decrease.
4. Measurement : The qubits are read, and output given.

Grover iteration (repeat oracle and amplification stages) requires approximately $\frac{\pi}{4}\sqrt{\frac{N}{t}}$ where *N* is the number of states and *t* is the number of target solutions.

Grover-assisted Compact Genetic Algorithm (cGA*)



The quantum circuit of Grover's search algorithm.

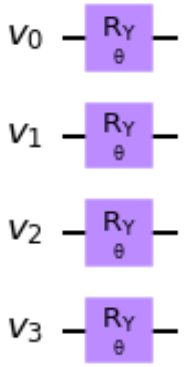
Grover-assisted Compact Genetic Algorithm (cGA*)

An arbitrary single-qubit state

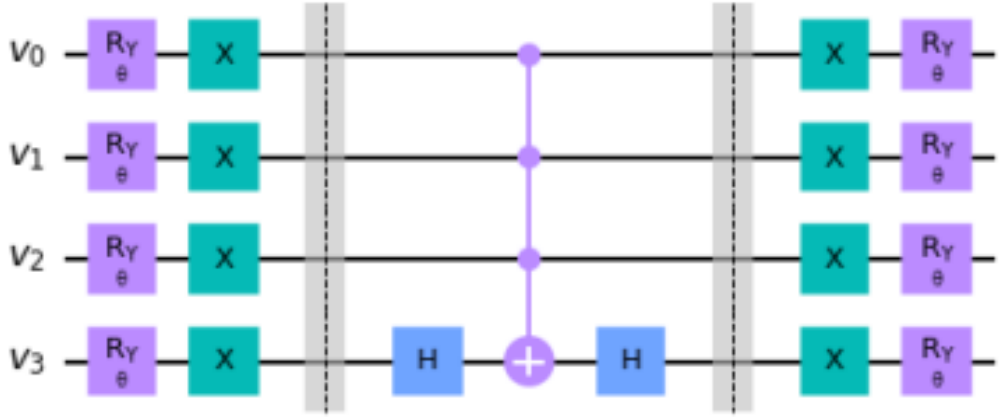
$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

The qubit rotation for angle(θ)

$$angle(\theta) = (probability(p) - 0.5) \times \pi$$



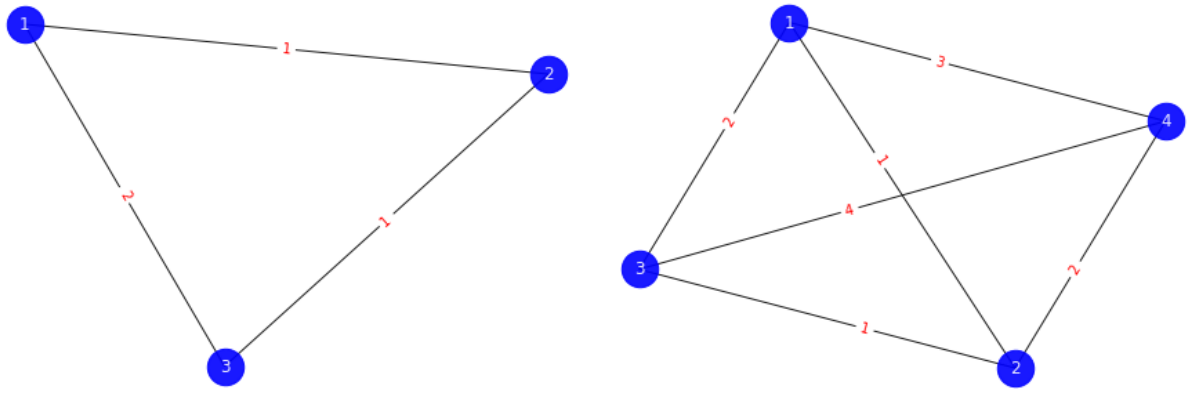
A circuit to initial the state based on the probability which encoding problem with 4 qubits.



A diffuser circuit which encoding problem with 4 qubits.

Travelling Salesman Problem

- Find a shortest route that a salesman visits every city exactly once and returns to the starting point.
- Define an oracle to recognize all feasible solutions.
- TSP is mapped to an Ising model with scales $(N-1)^2$ spins are required, where N is the number of cities, and we designate city 1 to appear first in the route.



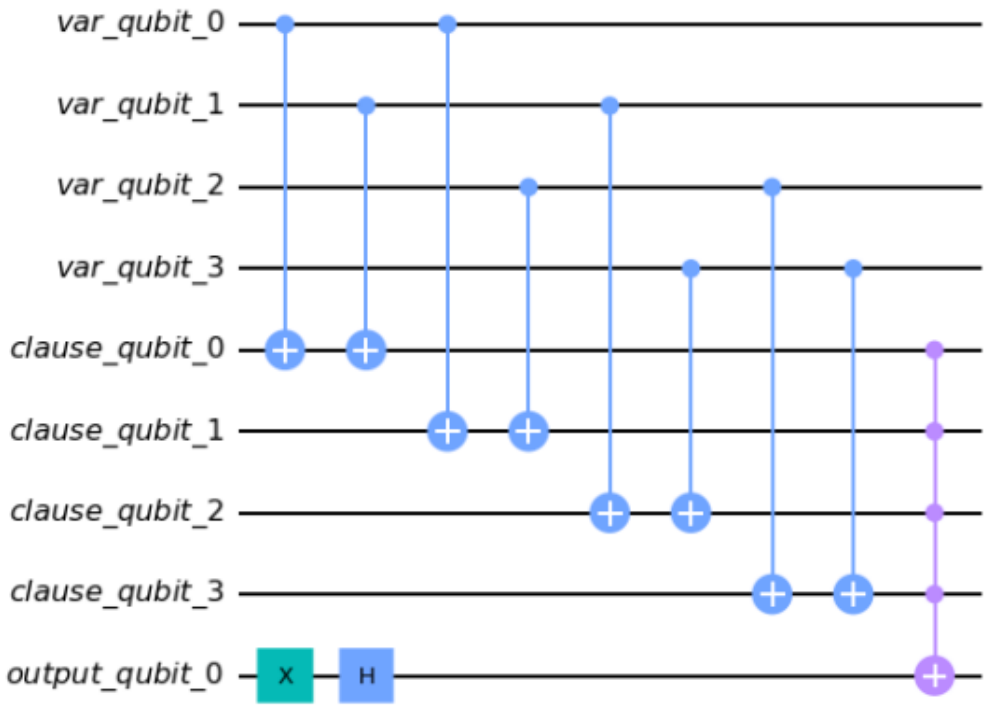
The TSP 3 cities and 4 cities.

	1	2	3
1	1	0	0
2	0	1	0
3	0	0	1

Matrix represents the route $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$.

Travelling Salesman Problem

- The oracle to check a feasible solution on the quantum state:



An example of oracle circuit for TSP 3 cities.

the oracle to verify a solution of TSP 3-city,

we need to check all 4 clauses include:
$(X_{2,2}, X_{2,3})$, $(X_{2,2}, X_{3,2})$, $(X_{2,3}, X_{3,3})$, and $(X_{3,2}, X_{3,3})$.

Travelling Salesman Problem

- Classical optimizer:
  - the graph is fully connected.
  - three components in a single objective function to be minimized, and we get the following:

$$\text{Energy} = \sum_{i,j} w_{i,j} \sum_{p} X_{i,p} X_{j,p+1} + B \sum_{p} \left(1 - \sum_{i} X_{i,p}\right)^2 + B \sum_{i} \left(1 - \sum_{p} X_{i,p}\right)^2$$

Total distance

The constraints to check a feasible path

where *B* is the weight of the penalty term, it has a large enough weight to avoid an infeasible solution.

Experiment results

- TSP is mapped to an Ising model with $(n-1)^2$ spins, where *n* is the number of cities
- The total cost of quantum state preparation is $O(n^2-1)$.
- The total quantum complexity is $O(I\frac{\pi}{4}\sqrt{\frac{n}{t}})$, where *I* is the circuit depth for Grover iteration at first, *n* is the number of cities, and *t* is the number of solutions from oracle.

#Cities	#Qubits	#Ancilla qubits	#CNOT	Circuit depth
3	$(n-1)^2$	$2(n-1)$	$57g$	$2+99g$
4	$(n-1)^2$	$2(n-1)$	$315g$	$1+549g$

n is the number of cities, and *g* is the number of Grover iterations.

Observation

- Increasing the number of shots aids in obtaining a probability distribution of results, mitigating stochastic errors.

- Quantum algorithms we have today only offer modest speed-ups over their classical counterparts.

- Quantum algorithms don’t seem to offer exponential speedups for black box optimization problem. However, it’s possible that there may be some exponential speedup in cases where you know a bit more about the problem.

Reference

K. Suksen, N. Benchasattabuse and P. Chongstitvatana, "Compact Genetic Algorithm with Quantum-Assisted Feasibility Enforcement," ECTI TRANSACTIONS ON COMPUTER AND INFORMATION TECHNOLOGY, Vol.16, No.4, December 2022, pp.422-435.

DOI: 10.37936/ecti-cit.2022164.247821

More Information

Search “Prabhas Chongstitvatana”

Go to me homepage

Q & A