Introduction to Quantum Computing
Lecture 21: Variational Quantum Algorithms I

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This Lecture

1. Noisy Intermediate Scale Quantum Devices and Near-Term Quantum Algorithms
2. Variational Quantum Algorithms: What & How (4 steps)
3. Step 1: Hamiltonian Problem with an Example (Max-Cut)

Noisy Intermediate Scale Quantum Devices and

Near-Term Quantum Algorithms

NISQ Devices: Limitations

Noisy Intermediate-Scale Quantum (NISQ) Devices

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  Time that quantum information can be stored

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Main Question:

Can NISQ devices offer **computational advantage** and **how**?

NISQ Devices: Where we are

Superconducting hardware

- Number of Qubits: ≈ 100 (IBM's "*Osprey*" has 433 and plans to announce by the end of the year "Condor" with 1121 qubits)
- Circuit depth: ≈ 100 : 20 cycles of 5 gates
- Quality of gates (a bit outdated):

  1-qubit gate error: 1.6×10^{-3}

  2-qubit gate error: 6.2×10^{-3}

  Measurement error: 3.2×10^{-2}

From "Quantum supremacy using a programmable superconducting processor", Frank Arute, Kunal Arya, $[\cdots]$, John M. Martinis, Nature volume 574, 505 (2019)

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- Heuristics with **potential speed-ups**

  (to be examined case-by-case)

Variational Quantum Algorithms: What & How (4 steps)

VQA: The Mathematical Task

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There exist variations:

- Find the minimum eigenvector (called "ground state")
- Find other eigenvalues or eigenvectors
- Find the expectation value ("energy") of a quantum state $|\psi\rangle$

$$\langle\psi| \mathcal{H} |\psi\rangle$$

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How to use this to solve everyday problems?

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  QMA is to BQP, what NP is to P

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- The k-local Hamiltonian problem is:

  Find the **ground state energy** of a Hamiltonian $\mathcal{H} = \sum_i \mathcal{H}_i$ where each $\mathcal{H}_i$ acts on at most k-qubits.

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- We can use VQA to solve all problems in NP and BQP!

- But is it really practical? (not always: time, prob of success)

Applications: Why is this task useful

- Optimisation
- Quantum Chemistry
- Quantum Simulation
- Many-body Physics
- Quantum Machine Learning

VQA: four steps

Step 1 Hamiltonian Encoding

Express your desired problem as the ground state of a suitable qubit-Hamiltonian $\mathcal{H}$

Step 2 Energy estimation (the only quantum part)

Given copies of a state $|\psi\rangle$, estimate its energy $\langle\psi|\mathcal{H}|\psi\rangle$

VQA: four steps

Step 3 Choice of Ansatz

A family of parametrised quantum states $|\psi(\vec{\theta})\rangle$ where one of its members approximates best the ground state

Step 4 Classical optimiser

A classical optimiser that finds the values $\vec{\theta}^*$ that minimise the cost $C(\vec{\theta}) := \langle\psi(\vec{\theta})| \mathcal{H} |\psi(\vec{\theta})\rangle$, ie $\vec{\theta}^* := \arg\min_{\vec{\theta}} C(\vec{\theta})$

Step 1: Hamiltonian Problem with an Example (Max-Cut)

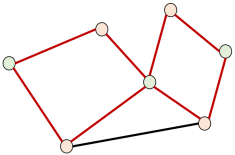
The Max-Cut Problem

- Given Graph $G = (V, E)$

  with vertices $v \in V$ and edges $e = (v_1, v_2) \in E$
- Partition vertices to two sets S, T

  where $S \cup T = V$ and $S \cap T = \emptyset$
- Cut is the number of edges between the two sets S, T

  (# of red edges)



The Max-Cut Problem

Task: Select S, T such that the Cut is maximised

$$\max_{(S,T)} \#(s,t) \in E \mid s \in S \wedge t \in T$$

- Decision version of Max-Cut is NP-complete
- Max(Min)-Cut has applications in Flow Networks including circuit optimisation (VLSI design), computer vision and others
- Version that edges have a weight w_e and one maximises the total weight of the cut edges exists (similar analysis):

$$\max_{(S,T)} \sum_{(s,t)} w_{(s,t)} \mid (s,t) \in E \ \wedge \ s \in S \wedge t \in T$$

Towards a Quantum Solution for Max-Cut

- Need to use our tool (ground state energy of a Hamiltonian)
- In general one can take any classical algorithm that solves Max-Cut and replace an expensive sub-routine with a Hamiltonian problem
- Natural map of this problem to a (simple) Hamiltonian

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- In general one can take any classical algorithm that solves Max-Cut and replace an expensive sub-routine with a Hamiltonian problem
- Natural map of this problem to a (simple) Hamiltonian
- Assign to each vertex v a spin $s_v \in \{+1, -1\}$
- Those with $s_i = +1$ define the one set (say S) those with $s_i = -1$ define the other set (say T)

Towards a Quantum Solution for Max-Cut

- Consider the cost $\mathcal{H}(\vec{s})$ (energy) of a configuration $\vec{s} := (s_1, \cdots, s_n)$

  Split the edges to three sets:

  E^{+1} edges between vertices that both have $s = +1$

  E^{-1} edges between vertices that both have $s = -1$

  E^{C} edges between vertices with different spins (the "cut")

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$$\begin{aligned} \mathcal{H}(\vec{s}) &= \sum_{(i,j)\in E(G)} s_i s_j \qquad (1) \\ &= \sum_{(i,j)\in E^{+1}(G)} s_i s_j + \sum_{(i,j)\in E^{-1}(G)} s_i s_j + \sum_{(i,j)\in E^{C}(G)} s_i s_j \end{aligned}$$

Towards a Quantum Solution for Max-Cut

- Note that $s_i s_j = 1$ for E^{+1}, E^{-1} while $s_i s_j = -1$ for E^C:

$$\begin{aligned}
\mathcal{H}(\vec{s}) &= \sum_{(i,j)\in E^{+1}(G)} 1 + \sum_{(i,j)\in E^{-1}(G)} 1 - \sum_{(i,j)\in E^{C}(G)} 1 \\
&= \sum_{(i,j)\in E^{+1}(G)} + \sum_{(i,j)\in E^{-1}(G)} + \sum_{(i,j)\in E^{C}(G)} 1 - 2 \sum_{(i,j)\in E^{C}(G)} 1 \\
&= \sum_{(i,j)\in E(G)} -2 \sum_{(i,j)\in E^{C}(G)} \\
&= |E| - 2\mathrm{Cut}(G) \qquad (2)
\end{aligned}$$

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\end{aligned} \tag{2}$$

- The greater the $\mathrm{Cut}(G)$ the smaller the energy $\mathcal{H}(\vec{s})$
- Minimising Energy = Solving Max-Cut!

Towards a Quantum Solution for Max-Cut

- Map each spin s_i to a qubit $|x_i\rangle$, where $+1 \to |0\rangle$; $-1 \to |1\rangle$
- The cost function (Hamiltonian) changes
  $\mathcal{H}(\vec{s}) = \sum_{(i,j)\in E} s_i s_j \to \mathcal{H}(\vec{x}) := \sum_{(i,j)\in E} (-1)^{x_i + x_j}$

  $\to \hat{\mathcal{H}}(\vec{x}) := \sum_{(i,j)\in E} Z_i \otimes Z_j$

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  Check: For each edge $(i,j) \in E$ we have
  $Z_i \otimes Z_j |x_i\rangle \otimes |x_j\rangle = (-1)^{x_i+x_j} |x_i\rangle \otimes |x_j\rangle$

  As earlier, if edge of same type $\rightarrow$ even parity there a $+1$ contribution (comp states remain invariant)

  If edge of different type (i.e. counts in "cut") $\rightarrow$ odd parity and contributes as -1 (comp states remain invariant)

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  If edge of different type (i.e. counts in "cut") $\rightarrow$ odd parity and contributes as -1 (comp states remain invariant)
- Taking all terms together:
  $\sum_{(i,j)\in E} Z_i \otimes Z_j |x_1 \cdots x_n\rangle = (|E| - 2\mathrm{Cut}(G)) |x_1 \cdots x_n\rangle$

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- The smallest eigenvalue of $\hat{\mathcal{H}}(\vec{x})$ gives the maximum $\mathrm{Cut}(G)$
- Special case of an Ising Hamiltonian (important class)

$$\mathcal{H}(\vec{x}) = -\sum_{(i,j)} J_{ij} Z_i \otimes Z_j - \mu \sum_i h_i Z_i$$

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Next Lecture:

- How to compute the cost/energy of a quantum state $C(\psi) := \langle\psi| \mathcal{H} |\psi\rangle$

- How to approximate the minimum without brute-forcing the full Hilbert space

References

Variational Quantum Algorithms Reviews

1. *Variational quantum algorithms*, Cerezo, Marco, et al. Nature Reviews Physics (2021): 1-20.
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3. *Quantum optimization using variational algorithms on near-term quantum devices*, Moll, Nikolaj, et al. Quantum Science and Technology 3.3 (2018): 030503.