CPEN 400Q Lecture 16
Solving combinatorial optimization problems with the Quantum Approximate Optimization Algorithm (part 2)

Friday 10 March 2023

Announcements

- Quiz 7 beginning of class Monday
- Assignment 2 due Monday March at 23:59
- Updated class schedule:
  - Monday March 13: in person
  - Friday March 17: pre-recorded "infotainment" lecture about compilation

We started exploring how optimization problems can be formulated as energy minimization problems:

$$\min_{\vec{x}} \ \text{cost}(\vec{x}) \quad \text{subject to constraints}(\vec{x})$$

Optimization	**Physical system**
$\vec{x}$	State of the system
$\text{cost}(\vec{x})$	Hamiltonian
Optimum $\vec{x^*}$	Ground state
$\text{cost}(\vec{x^*})$	Ground state energy

Last time

General adiabatic quantum computing:

1. Design a Hamiltonian $\hat{H}_c$ whose ground state represents the solution to our optimization problem
2. Prepare a system in a easy-to-prepare ground state of a mixer Hamiltonian $\hat{H}_m$
3. Perform adiabatic evolution to transform the system from the ground state of the "easy" Hamiltonian to the ground state of the problem Hamiltonian

Last time

What we will do:

1. Design a Hamiltonian $\hat{H}_c$ whose ground state represents the solution to our optimization problem
2. Prepare a system in a easy-to-prepare ground state of a mixer Hamiltonian $\hat{H}_m$
3. Run the quantum approximate optimization algorithm

QAOA is a gate-model algorithm that can obtain approximate solutions to combinatorial optimization problems.

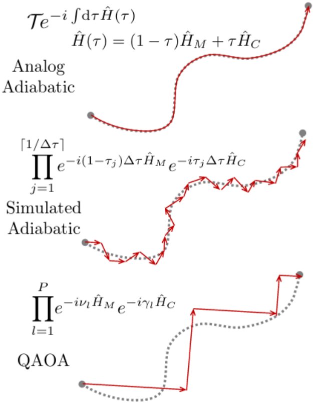
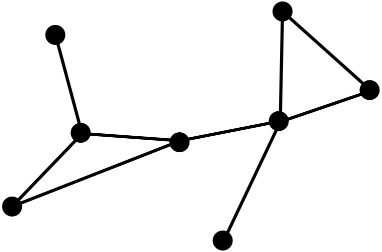
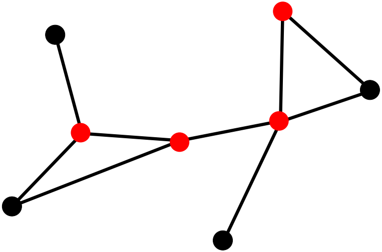


Image credit: G. Verdon, M. Broughton, J. Biamonte. *A quantum algorithm to train neural networks using low-depth circuits.* `https://arxiv.org/abs/1712.05304`

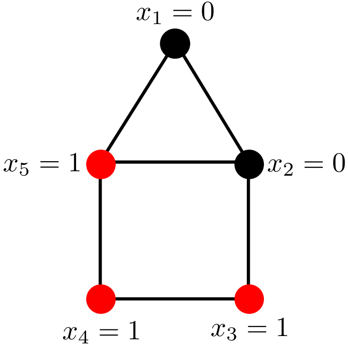
Last time

Minimum vertex cover: Given a graph $G = (V, E)$, what is the *smallest number of vertices* you can colour such that every edge in the graph is attached to at least one coloured vertex?





We turned this into an optimization problem over binary variables.



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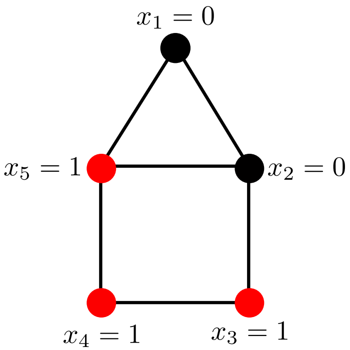
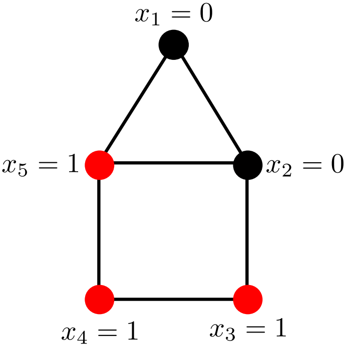


We defined a cost function term over a pair of vertices that is minimized for valid colourings:

Then for the whole graph,

Last time



We finished by adding a penalty term to minimize the number of coloured vertices:

The full cost function is:

- Convert cost functions of simple graph theory problems to Hamiltonians
- Distinguish between cost and mixer Hamiltonians and state the key requirements for the latter type
- Solve combinatorial optimization problems with QAOA in PennyLane

Game plan

1. Design a Hamiltonian $\hat{H}_c$ whose ground state represents the solution to our optimization problem
2. Prepare a system in a easy-to-prepare ground state of a mixer Hamiltonian $\hat{H}_m$
3. Run the quantum approximate optimization algorithm

Hamiltonian translation

Our full cost function over binary variables is

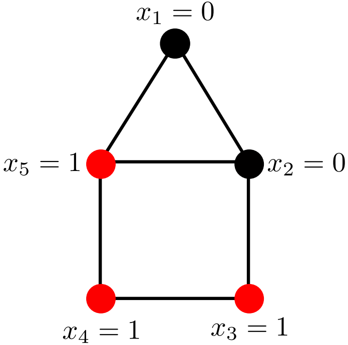
$$\min_{\vec{x}} \left(\sum_{ij \in E} (1 - x_i)(1 - x_j) + \sum_{i \in V} x_i \right)$$

Next steps:

1. Turn this into a Hamiltonian over qubits
2. Find its minimum energy

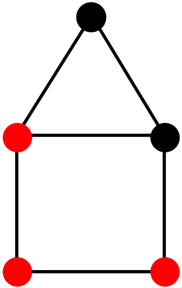
Hamiltonian translation

How should we do a mapping from this to qubits?



Hamiltonian translation

What should we use to represent cost?



Hamiltonian translation

Mathematically, we can make the mapping

This associates

- $x_i = 0$ to $z_i = 1$ (corresponds to $|0\rangle$)
- $x_i = 1$ to $z_i = -1$ (corresponds to $|1\rangle$)

A complete derivation of the cost function is provided as an appendix at the end of the lecture slides.

Hamiltonian translation

We will take the result:

Remember what the z_i represent; how can we express this cost function as a Hamiltonian?

$$\hat{H}_c = \sum_{ij \in E} (Z_i + Z_j + Z_i Z_j) - 2 \sum_{i \in V} Z_i$$

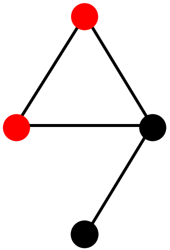
This makes sense:

More generally, we have weight the two term differently:

Hamiltonian translation

$$\hat{H}_c = \sum_{ij \in E} (Z_i + Z_j + Z_i Z_j) - 2 \sum_{i \in V} Z_i$$

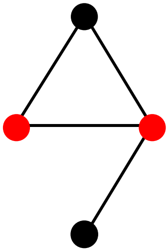
Try it: what is the energy of this *invalid* colouring?



Hamiltonian translation

$$\hat{H}_c = \sum_{ij \in E} (Z_i + Z_j + Z_i Z_j) - 2 \sum_{i \in V} Z_i$$

Try it: what is the energy of this *valid* colouring?



Game plan

1. Design a Hamiltonian $\hat{H}_c$ whose ground state represents the solution to our optimization problem
2. Prepare a system in a easy-to-prepare ground state of a mixer Hamiltonian $\hat{H}_m$
3. Run the quantum approximate optimization algorithm

Mixer Hamiltonians

We also need a *mixer* Hamiltonian. The mixer must have a special property: it *cannot commute* with the cost Hamiltonian.

$$\hat{H}_c = \sum_{ij \in E} (Z_i + Z_j + Z_i Z_j) - 2 \sum_{i \in V} Z_i$$

$\hat{H}_c$ is just a diagonal matrix, and its eigenstates are the computational basis states.

Mixer Hamiltonians

Any state can be expressed in terms of the computational basis:

Evolve this under the cost Hamiltonian:

Have we actually changed anything?

Original state:

New state:

Simply evolving under the cost Hamiltonian doesn't change the probability distribution of the state.

If $\hat{H}_m$ commutes with $\hat{H}_c$, then $\hat{H}_c$ and $\hat{H}_m$ have a shared set of eigenvectors so evolving under $\hat{H}_m$ doesn't affect the state either.

Need a mixer which *does not commute* with $\hat{H}_c$. Something like

Uniform superposition is an "easy to prepare" eigenstate of $\hat{H}_m$.

Game plan

1. Design a Hamiltonian $\hat{H}_c$ whose ground state represents the solution to our optimization problem
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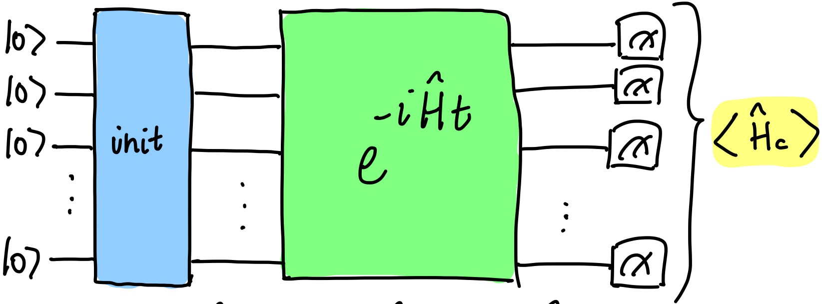
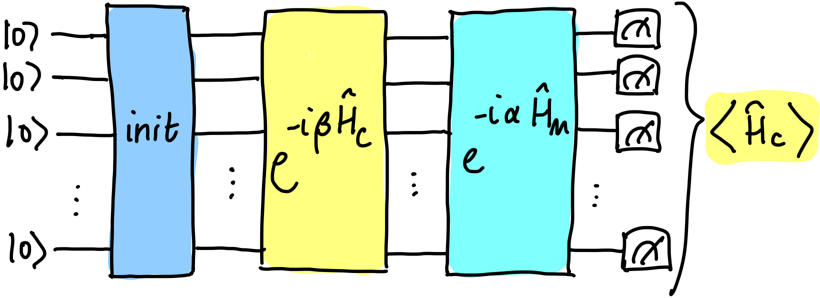
Initial idea: apply the unitary that evolves the Hamiltonian?



$$\hat{H} = \alpha \hat{H}_m + \beta \hat{H}_c$$

How do we implement this circuit?

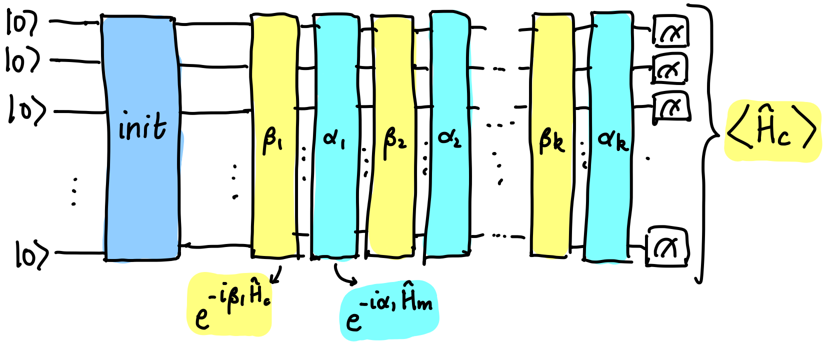
You might think that since $\hat{H}$ is a sum of terms...



But this is only true when $\hat{H}_c$ and $\hat{H}_m$ *commute*.

QAOA

QAOA does something similar to this but instead of applying each block for a fixed "time", "time" is a trainable parameter.



Let's implement this, and find parameters that minimize the cost.

Next time

Content:

- Density matrices and mixed states
- Noise in quantum computing

Action items:

1. Explore PennyLane's built-in QAOA module
2. Assignment 2
3. Work on final project

Recommended reading:

- Original QAOA paper `https://arxiv.org/abs/1411.4028`
- PennyLane Intro to QAOA tutorial
  `https://pennylane.ai/qml/demos/tutorial_qaoa_intro.html`
- Qiskit QAOA tutorial
  `https://qiskit.org/textbook/ch-applications/qaoa.html`

Full derivation: Hamiltonian translation

In order

We will make the mapping

$$x_i \to \frac{1}{2}(1 - z_i), \quad , z_i \in \{-1, 1\}$$

This associates $x_i = 0$ to $z_i = 1$ (corresponds to $|0\rangle$), and $x_i = 1$ to $z_i = -1$ (corresponds to $|1\rangle$).

Full derivation: Hamiltonian translation

Let's expand our cost function and make this substitution.

$$\sum_{ij \in E} (1 - x_i)(1 - x_j) + \sum_{i \in V} x_i$$

$$\sum_{ij \in E} (1 - x_i - x_j + x_i x_j) + \sum_{i \in V} x_i$$

Full derivation: Hamiltonian translation

$$\sum_{ij\in E}(1 - x_i - x_j + x_i x_j) + \sum_{i\in V} x_i$$

Substitute:

$$\sum_{ij\in E}\left(1 - \frac{1}{2}(1 - z_i) - \frac{1}{2}(1 - z_j) + \frac{1}{4}(1 - z_i)(1 - z_j)\right) + \sum_{i\in V}\frac{1}{2}(1 - z_i)$$

Expand:

$$\sum_{ij\in E}\left(1 - \frac{1}{2} + \frac{1}{2}z_i - \frac{1}{2} + \frac{1}{2}z_j + \frac{1}{4} - \frac{1}{4}z_i - \frac{1}{4}z_j + \frac{1}{4}z_i z_j\right) + \sum_{i\in V}\frac{1}{2}(1 - z_i)$$

Collect:

$$\sum_{ij\in E}\left(\frac{1}{4} + \frac{1}{4}z_i + \frac{1}{4}z_j + \frac{1}{4}z_i z_j\right) + \sum_{i\in V}\frac{1}{2}(1 - z_i)$$

Full derivation: Hamiltonian translation

$$\sum_{ij\in E}\left(\frac{1}{4}+\frac{1}{4}z_i+\frac{1}{4}z_j+\frac{1}{4}z_iz_j\right)+\sum_{i\in V}\frac{1}{2}(1-z_i)$$

Consider now that: the total number of edges and vertices are constant - they will provide only an "offset" to the cost, and the values of the variables don't matter.

$$\sum_{ij\in E}\left(\frac{1}{4}z_i+\frac{1}{4}z_j+\frac{1}{4}z_iz_j\right)-\sum_{i\in V}\frac{1}{2}z_i$$

And finally, the absolute value doesn't matter, so we can rescale:

$$\sum_{ij\in E}(z_i+z_j+z_iz_j)-2\sum_{i\in V}z_i$$

Can also weight the terms differently depending on which constraint is more important (i.e., if you care more about just getting a valid colouring, weight the first one more).

$$\gamma \sum_{ij \in E} (z_i + z_j + z_i z_j) - 2\lambda \sum_{i \in V} z_i$$

To turn this into a Hamiltonian, recall that

- Each z_i represents an expectation value of Z_i
- Computing expectation values is linear

Full derivation: Hamiltonian translation

$$\gamma \sum_{ij \in E} (z_i + z_j + z_i z_j) - 2\lambda \sum_{i \in V} z_i$$

$$\hat{H} = \gamma \sum_{ij \in E} (Z_i + Z_j + Z_i Z_j) - 2\lambda \sum_{i \in V} Z_i$$

Next time: we will look at the actual QAOA that can find the optimal configuration / minimum energy.