PHYC90045 Introduction to Quantum Computing

Week 10

Lecture 19
Quantum Approximate Optimization Algorithm (QAOA), Variational Quantum Eigensolver (VQE), classical feedback

Lecture 20
Exponentials, and Quantum Optimization

Lab 10
Optimization problems

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Hybrid Quantum/Classical Optimization Algorithms

Physics 90045
Lecture 19

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Overview

This lecture we will talk about two algorithms to find the minimum energy of a quantum system:

- Quantum Approximate Optimization Algorithm (QAOA) algorithm
- Variational Quantum Eigen-solver (VQE) algorithm

Both algorithms are closely related, combining classical optimization with quantum mechanical states.

Kaye 8.5
Rieffel 13.4.2

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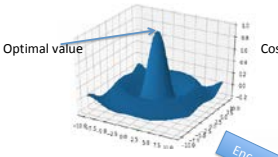
Review of last lecture



Encode

Ising coupling

local "field"

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

We can encode problems in the energy of the system, but we had no way of minimizing the energy. Today we will see a hybrid technique which allows us to minimize the energy of a quantum system.

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Recall Total Energy of the System

Consider a system that has an energy function:

$$E = J_{12} z_1 z_2 + J_{23} z_2 z_3 + J_{13} z_1 z_3 + B_1 z_1 + B_2 z_2 + B_3 z_3$$

where the z_i are +/-1, and the J's and B's are specific parameters defining the particular problem at hand.

To get ready to map to a QC, we write the total energy as the operator "H" (which physicists would call the "Hamiltonian") on a system of qubits as a sum of these terms with $z_i \rightarrow Z_i$ (where Zi is the Z operator on the ith qubit):

$$H = J_{12} Z_1 Z_2 + J_{23} Z_2 Z_3 + J_{13} Z_1 Z_3 + B_1 Z_1 + B_2 Z_2 + B_3 Z_3$$

Pairwise interactions between qubits

Bias on individual qubit

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Mapping the Spin Glass form to QC

Optimisation problems can often be cast into an equivalent "spin glass" form:

$$E = \sum_{i \neq j} J_{ij} z_i z_j + \sum_i B_i z_i$$

-> convert to a convenient form to map onto a quantum computer:

Ising coupling

local "field"

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

The Z_i are now operators defined as per our definitions with eigenvalues +/-1 (which can be mapped to binary variables 0/1)

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QUBO Problems

QUBO stands for "Quadratic Unconstrained Binary Optimization"

The cost function (which we want to minimize) is:

$$E(x_1, \ldots, x_n) = \sum_i c_i x_i + \sum_{i,j} Q_{ij} x_i x_j$$

Where x_i are Boolean (binary) variables, either 0 or 1.

NB. we will use x for binary, z for +/-1

Quadratic term

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Binary to energy

Typically when we write such energy functions we write in terms of the Z variables:

$$z_i$$ (lower case z)

But the binary variables in terms of 0 or 1:

$$x_i = 0 \quad \text{or} \quad x_i = 1$$

Can convert between x_i and Z_i using:

$$x_i \to \frac{z_i + 1}{2}$$

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Example: Number partitioning

Given a set, S, of numbers:

1, 3, 8, 10, 6, 5, 5

Is there a partition of this set of numbers into two disjoint subsets R and S − R, such that the sum of the elements in both sets is the same?

Yes (in this case): **{1, 8, 10}** and **{3, 6, 5, 5}**

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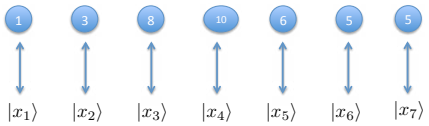
Graph Partitioning to QUBO

1, 3, 8, 10, 6, 5, 5



We assign a qubit to each number in the problem set.
The qubit being zero indicates it is one subset.
The qubit being one indicates it is in the other.

Qubits are $|0\rangle$ if they're in subset 0, $|1\rangle$ if they're in subset 1

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Number partitioning as a QUBO problem

1, 3, 8, 10, 6, 5, 5

As an optimization problem: We want

$$\sum_i w_i z_i = 0$$

The i^{th} number ± 1

Unfortunately if we just minimize this, all the qubits will end up with z_i=-1!

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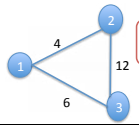
Number partitioning as a QUBO problem

But if we square, we should get a positive solution (or zero). We want to find the assignment of spins which has the minimum energy (ie. closest to zero):

$$H = \left(\sum_i w_i Z_i\right)^2 = \sum_{i \neq j} 2 w_i w_j Z_i Z_j + \sum_i w_i^2 I$$

Coupling is the product of numbers

Eg. For the set **{1, 2, 3}**:



$$H = 4Z_1Z_2 + 6Z_1Z_3 + 12Z_2Z_3 + 14I$$

Finding minimum energy state will solve the problem!

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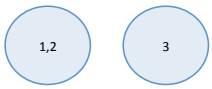
Solution for our Number Partitioning

$$H = 4Z_1Z_2 + 6Z_1Z_3 + 12Z_2Z_3 + 14I$$

Two degenerate solutions: $|110\rangle$ $|001\rangle$



$$E = 4 - 6 - 12 + 14 = 0$$

And of course, they correctly partition the numbers: 1+2 = 3

Other combinations go worse, eg, $|111\rangle$

$$E = 4 + 6 + 12 + 14 = 36$$

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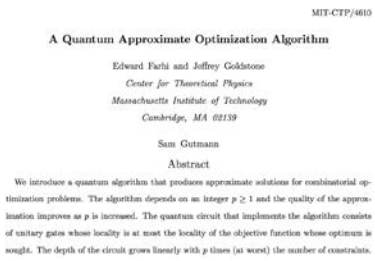
QAOA Overview

QAOA = "Quantum Approximate Optimization Algorithm"



MIT-CTP/4610

A Quantum Approximate Optimization Algorithm

Edward Farhi and Jeffrey Goldstone
Center for Theoretical Physics
Massachusetts Institute of Technology
Cambridge, MA 02139

Sam Gutmann

Abstract

We introduce a quantum algorithm that produces approximate solutions for combinatorial optimization problems. The algorithm depends on an integer $p \geq 1$ and the quality of the approximation improves as p is increased. The quantum circuit that implements the algorithm consists of unitary gates whose locality is at most the locality of the objective function whose optimum is sought. The depth of the circuit grows linearly with p times (at worst) the number of constraints.

Farhi, Goldstone and Gutman, 2014

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Structure of Algorithm

QUI/Quantum Computer

(1) Prepare a trial state $|\psi(\theta)\rangle$

on the quantum computer, where θ represents angles in phase and X rotations.

(2) **Measure** the solution in z basis to obtain the energy, E.

(3) For small depth circuits can analytically calculate optimal values for θ. Original paper found these for a MAX-CUT problem.

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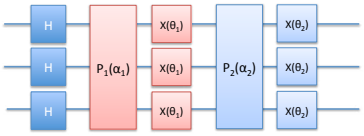
QAOA Trial state

The QAOA trial state has a particular form:

$$R_x(\theta_k)P(\alpha_k)\dots R_x(\theta_2)P(\alpha_2)R_x(\theta_1)P(\alpha_1)\,|+\rangle^{\otimes n}$$

X-rotations on every qubit

Phase gate, closely related to the problem Hamiltonian/Energy



Preparation of a trial state, k=2 steps

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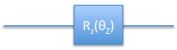
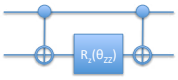
Phase gates in QAOA

For every Z term in the Hamiltonian:



$$H = E_Z Z$$

For every ZZ term in the Hamiltonian:



$$H = E_{ZZ} ZZ$$

Angles all proportional to their term in the Hamiltonian:

$$\theta_{ZZ} = \alpha E_{ZZ} \qquad \theta_Z = \alpha E_Z$$ etc

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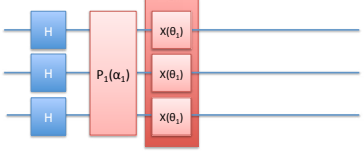
X-rotations

The QAOA trial state has a particular form:

$$R_x(\theta_k)P(\alpha_k)\dots R_x(\theta_2)P(\alpha_2)R_x(\theta_1)P(\alpha_1)\,|+\rangle^{\otimes n}$$

X-rotations on every qubit



Preparation of a trial state, k=1 steps

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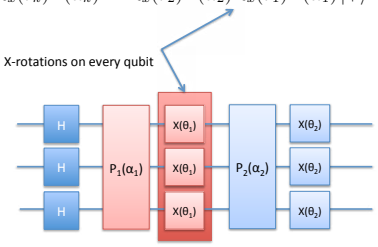
X-rotations

The QAOA trial state has a particular form:

$$R_x(\theta_k)P(\alpha_k)\dots R_x(\theta_2)P(\alpha_2)R_x(\theta_1)P(\alpha_1)\,|+\rangle^{\otimes n}$$



Preparation of a trial state, k=2 steps

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Measuring the energy

The Hamiltonian of a QUBO problem can be expressed as a sum of several terms:

Ising coupling — local "field"

$$H = \sum_{i \neq j} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

For example:

$$H = B_1 Z_1 + B_2 Z_2 + J_{12} Z_1 Z_2$$

A better approximation to the ground state (depending on the number of steps, k, and the choice of angles) will have a higher probability of measuring the minimum energy, and the lowest energy state.

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Measure to find energy

Measure Z:

In the QUI you can look directly at probabilities rather than measure and building statistics!

Unlike for QEC codes, you don't need to add an extra qubit to measure correlations. Eg. For ZZ you can just multiply yourself for a given state!

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Multiple measurements

Original function we would like to minimize:

$$H = B_1 Z_1 + B_2 Z_2 + J_{12} Z_1 Z_2$$

Take many samples, to determine:

$$\langle H \rangle = B_1 \langle Z_1 \rangle + B_2 \langle Z_2 \rangle + J_{12} \langle Z_1 Z_2 \rangle$$

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Structure of Algorithm

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(1) Prepare a trial state $|\psi(\theta)\rangle$

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(2) **Measure** the solution in z basis to obtain the energy, E.

(3) For small depth circuits can analytically calculate optimal values for θ. Original paper found these for a MAX-CUT problem. **However, prohibitative to calculate analytically for larger depth circuits.**

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Structure of Algorithm

QUI/Quantum Computer

(1)Prepare a trial state $|\psi(\theta)\rangle$

on the quantum computer, where θ can be any adjustable gate parameter.

(2) **Measure** the expectation value of the energy, E.

Repeat these steps until the value of the energy converges

(3) Use a **classical optimization** technique such as the Nelder–Mead simplex method, determine new values of θ that decrease E.

Classical

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VQE overview

VQE = Variational Quantum Eigensolver

We need not confine ourselves to Ising/Z terms. Many interesting quantum systems have a Hamiltonian, H, which includes terms in X and Y (and might not even come from a qubit system at all!).

Or perhaps we have a Hermitian matrix, and we just want to find the smallest eigenvalue. How do we do that?

1) Pick a convenient basis to express H
2) Write out the total energy, H, as a matrix
3) Convert your matrix a linear combination of Pauli matrices
4) Parameterize an "Ansatz" wavefunction candidate solution to problem
5) Use hybrid classical/quantum optimization to find the lowest energy and lowest energy state.

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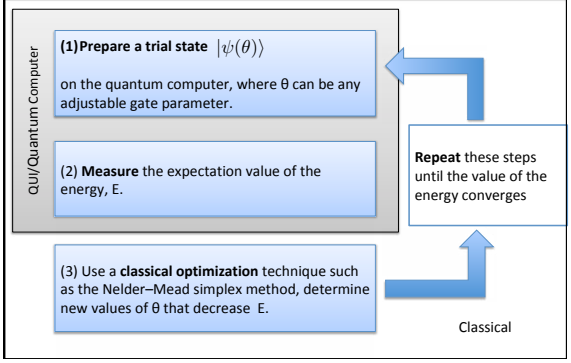
Structure of Algorithm



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Hamiltonian as linear combination of Pauli operators

Always possible decompose a matrix as a sum of Paulis. If you have a matrix only:

$$E_i = \frac{\mathrm{Tr}\left[\sigma_i H\right]}{d}$$

Where d is the dimension of the system, H is the Hamiltonian and σ_i is the Pauli. If the matrix is Hermitian, the co-efficients you find, E_i, should be real.

Express the Hamiltonian as a sum of Paulis:

$$H = \sum_i E_i \sigma_i$$

For example:

$$H = B_1 X_1 + B_2 X_2 + J_{12} Z_1 Z_2$$

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Find the expectation value of H

We can express the expectation value of the energy as a sum of expectation values of the Paulis:

$$\langle H \rangle = \sum_i E_i \langle \sigma_i \rangle$$

For our example:

$$\langle H \rangle = B_1\langle X_1 \rangle + B_2\langle X_2 \rangle + J_{12}\langle Z_1 Z_2 \rangle$$

For a given trial state, these can be found directly from experiment (or through the QUI)

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Reminder: How to measure Paulis

Measure X:

Measure Y:

Measure Z:

In the QUI you record probabilities rather than measure and building statistics!

Unlike for QEC codes, you don't need to add an extra qubit to measure correlations. Eg. For ZZ you can just multiply yourself given the state which is measured!

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VQE: Jordan Wigner Transformation

A classic of physics from 1928, by Jordan and Wigner. You've got a system of qubits. You want to use it to simulate fermions (eg. someone's given you a chemistry problem involving electrons). Electrons do not behave the same as qubits.

How do we do this?

Tempting solution:

$$\sigma_j^+ \rightarrow \frac{X_j + iY_j}{2} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}_j = f_j^+$$ Create a fermion at the j[th] site?

$$\sigma_j^- \rightarrow \frac{X_j - iY_j}{2} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}_j = f_j^-$$ Destroy a fermion at the j[th] site?

This is close but **WRONG!** The commutation relations between different sites are wrong (fermions anti-commute).

$$[f_j, f_k] = 0$$

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Jordan Wigner Transformation

Correct solution:

$$\sigma_j^+ \rightarrow Z_1 Z_2 \ldots Z_{j-1} \frac{X_j + iY_j}{2}$$

$$\sigma_j^- \rightarrow Z_1 Z_2 \ldots Z_{j-1} \frac{X_j - iY_j}{2}$$

Jordan and Wigner: Images from Wikipedia

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Picking a VQE Ansatz

QAOA State

Use a combination of X rotations and phase rotations.

Adiabatic Methods

Slowly vary the Hamiltonian, in a parameterized way, to obtain an approximation to the ground state.

Coupled Cluster Methods

First start in a (often unentangled) reference state, which can be calculated classically, eg. with mean field methods.

Consider successively more complicated perturbations away from this reference state: First we consider just (parameterized) single qubit rotations away from the reference state. Then we consider unitaries with both single qubit rotations and two body interactions, then one, two and three body interactions. As with QAOA we can consider several rounds of interaction.

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Nelder-Mead Classical Optimization

A classical method of optimization.

- Classical optimization technique
- Requires only the calculation of few points at each step

Based on simplex:

A *simplex* S in n dimension is defined as the convex hull of n+1 vertices: $x_0,\ldots,x_n$

Eg. Triangle in 2D

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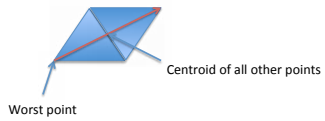
Nelder-Mead operations

Start with an initial simplex
Repeat until the convergence is reached:
Test if we've reached convergence
If not then transform the working simplex

Four types of transformation to test:

1) Reflection



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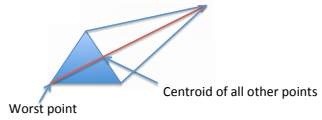
Nelder-Mead operations

2) Expand



3) Contract

4) Shrink

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Visualization

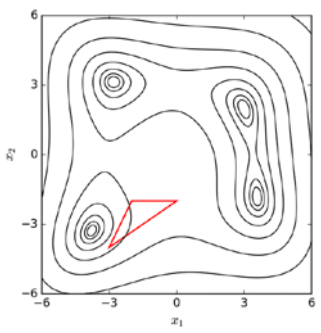

Image: Nicoguaro, Wikipedia

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Classical

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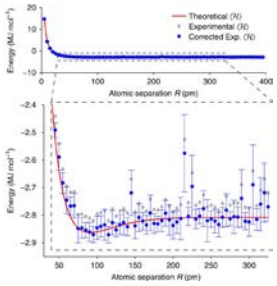
Example: Inter-molecular distance



He-H$^+$

Peruzzo, Aspuru-Guzik, O'Brien et al, *Nature Communications,* **5**, 4213 (2014)

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