Week 9

Lecture 17
Optimization problems, Encoding problems as energies, Quadratic Binary Optimization (QUBO), Problem embedding

Lecture 18
Adiabatic Quantum Computing

Lab 9
Using DWave machines

Quantum Optimization

Physics 90045
Lecture 17

Overview

This lecture we will talk about mapping Optimization Problems to physical systems:

- Cooling as an optimization algorithm
- QUBO problems
- Examples of QUBO problems:
  - Subset sum, Graph Partitioning and Travelling Salesman
- Embedding problems in quantum computing architectures

Kaye 8.5
Rieffel 13.4.2

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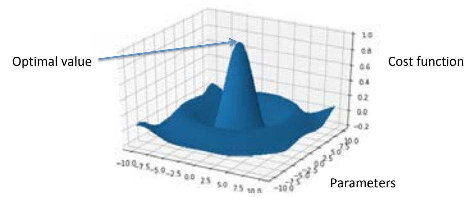
Optimization Problems

Given some cost-function or "objective function" we would like to maximize/minimize. Often the inputs/parameters are constrained.



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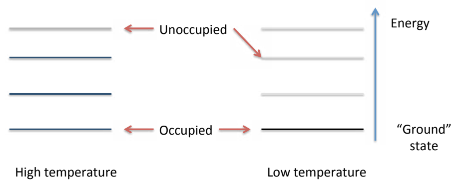
Physics and computation: Cooling

Physical systems naturally perform optimization problems. For example, if you cool a system towards absolute zero, it will populate the the lowest energy level.



At low temperatures, physical systems are naturally finding the lowest energy configuration they can. They're performing computation.

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Reminder: Measuring Observables

IN QM an observable (eg. energy) is represented by a Hermitian matrix. The values measured of when measuring the observable are the **eigenvalues** of the corresponding matrix.

In the simplest case, the matrix is a diagonal matrix and the eigenvalues are listed down the diagonal:

Energy of the $|0\rangle$ state

H stands for "Hamiltonian" The total energy in the system.

$$H = Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Energy of the $|1\rangle$ state

In more complicated cases you may have to *diagonalize* the matrix first, using an eigenvalue decomposition.

Encoding Problems into the Energy

In building a quantum computer, we have built a perfectly controllable quantum system. We can do different algorithms to try to find the state with the lowest energy.

How can we encode an objective function into the energy of a system?

For a single qubit:

Z	+1 energy for 0 -1 energy for 1
EZ	+E energy for 0 -E energy for 1
$-EZ$	+E for the 1 state -E for the 0 state

Measuring Observables (multiple qubits)

Each observable (eg. energy) is represented by a Hermitian matrix. The values measured of when measuring the observable are the **eigenvalues** of the corresponding matrix.

In the simplest case, the matrix is a diagonal matrix and the eigenvalues are listed down the diagonal:

H stands for "Hamiltonian" The total energy in the system.

$$H = Z \otimes Z = \begin{array}{cl} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} & \begin{array}{l} \text{Energy of the } |00\rangle \text{ state} \\ \text{Energy of the } |01\rangle \text{ state} \\ \text{Energy of the } |10\rangle \text{ state} \\ \text{Energy of the } |11\rangle \text{ state} \end{array} \end{array}$$

In more complicated cases you may have to *diagonalize* the matrix first, using an eigenvalue decomposition.

Two Qubit Ising Interactions

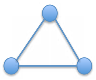
"Ising spin" couplings only involve two qubits, and just Z operators:

$Z_1 Z_2$	+1 for 00 or 11 state -1 for 01 or 10 state	Anti-ferromagnetic
$-Z_1 Z_2$	-1 for 00 or 11 state +1 for 01 or 10 state	Ferromagnetic

Total Energy of the System

Consider a system that has an energy function:

$$E = J_{12}z_1z_2 + J_{23}z_2z_3 + J_{13}z_1z_3 + B_1z_1 + B_2z_2 + B_3z_3$$



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 -> Z_i (where Zi is the Z operator on the ith qubit):

$$\boxed{H = \underbrace{J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3}_{\text{Pairwise interactions between qubits}} + \underbrace{B_1Z_1 + B_2Z_2 + B_3Z_3}_{\text{Bias on individual qubit}}}$$

Mapping the Spin Glass form to QC

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

$$E = \sum_{i \neq j} J_{ij}z_iz_j + \sum_i B_iz_i$$

This is convert to a convenient form to map onto a quantum computer:

Ising coupling

local "field"

$$H = \sum_{i \neq j} J_{ij}Z_iZ_j + \sum_i B_iZ_i$$

In QM, energy is represented as a matrix!

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

QUBO Problems

QUBO stands for "Quadratic Unconstrained Binary Optimization"

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

$$E(x_1, \ldots, x_n) = \sum_i c_ix_i + \sum_{i,j} Q_{ij}x_ix_j$$

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 the numbers:

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

Is there a way to partition these numbers into two disjoint partitions, such that the sum of the elements in both partitions is the same?

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

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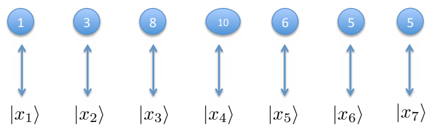
Graph Partitioning to QUBO

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



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

Qubits are $|0\rangle$ if they're in partition 0, $|1\rangle$ if they're in partition 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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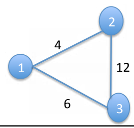
Number partitioning as a QUBO problem

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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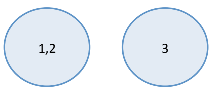
Solution for our Number Partitioning

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

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



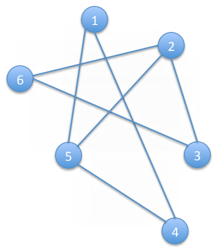
$$E = 4 - 6 - 12 + 14 = 0$$

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

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

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

Example: Graph Partitioning



What is a partition of the set of vertices, V, into two subsets *of equal size* such that the number of edges connecting the two partitions is minimized?

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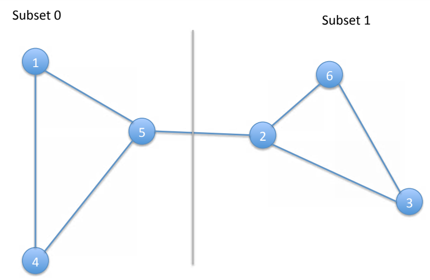
Example: Graph Partitioning



What is a partition of the set of vertices, V, into two subsets *of equal size* such that the number of edges connecting the two partitions is minimized?

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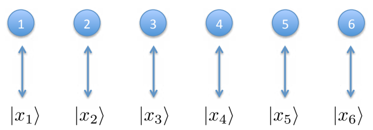
Graph Partitioning to QUBO



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

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Even numbers in each subset

$$H_A = \left(\sum_i Z_i\right)^2$$

As before, having an equal number of terms in each partition will evaluate to zero. Unequal numbers result in a positive value.

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Number of edges joining the subsets

$$H_B = \sum_{i,j \in E} \frac{I - Z_i Z_j}{2}$$

Evaluates to 0 if the edge is in the same partition, but +1 if the edge goes between partitions. In total H_B counts the number of edges between the two partitions.

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Total Hamiltonian

$$H_A = \left(\sum_i Z_i\right)^2$$

Same number of vertices in each partition.

$$H_B = \sum_{i,j \in E} \frac{I - Z_i Z_j}{2}$$

Number of edges between partitions.

In total then, with A>>B:

$$H = AH_A + BH_B$$

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Travelling Salesman Problem (TSP)

Given several (n) cities and the distances between them, find the shortest path (Hamiltonian cycle) which visits all of them once and returns to the original city.

- TSP is an example of an NP-Complete problem (Karp, 1972) and best known classical algorithms require exponential time.
- Has many direct practical applications including planning, logistics, DNA sequencing, and astronomy.
- Largest solved tour is approximately 85,000 sites with heuristic methods able to find solutions (for million site tours) within 2-3% of the optimal tour.

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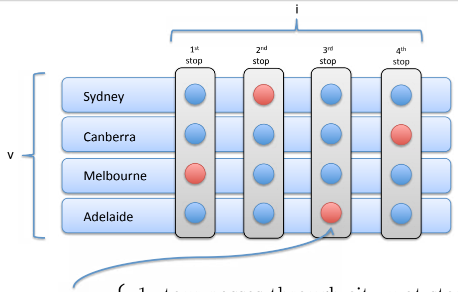
Mapping TSP to QUBO problem



$$x_{i,v} = \begin{cases} 1, & \text{tour passes through city } v \text{ at step } i \\ 0, & \text{otherwise} \end{cases}$$

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Energy Penalties

Each city appears exactly once in the cycle:

$$H_{city} = \sum_v \left(1 - \sum_i x_{v,i}\right)^2$$

Each step has exactly one city:

$$H_{step} = \sum_i \left(1 - \sum_v x_{v,i}\right)^2$$

Only paths between cities with edges between them are taken:

$$H_{cycle} = \sum_i \sum_{u \to v \notin E} x_{u,i} x_{v,i+1}$$

Any path making a cycle will have energy, E=0, with all other combinations having higher energy.

Shortest cycle

To find the shortest cycle, add an energy penalty of the length of the cycle:

$$H_{length} = \sum_i \sum_{u \to v \in E} W_{uv} x_{u,i} x_{v,i+1}$$

Finding the lowest energy arrangement of $x_{v,i}$ of

$$H_{TSP} = A(H_{city} + H_{site} + H_{cycle}) + BH_{length}$$

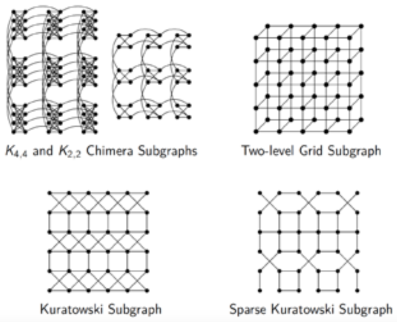
will solve the corresponding TSP problem (A>>B).

We can make the problem quantum mechanical by mapping classical variables $x_{v,i}$ to qubits (and operators):

$$x_{v,i} \to \frac{I + Z_{v,i}}{2}$$

The problem is now to find the ground state of a quantum mechanical Hamiltonian
-> several ways to do this by coding the problem onto a QC
i.e. digital (e.g. QAOA/VQE next lecture) or analogue (e.g. AQC, later on)

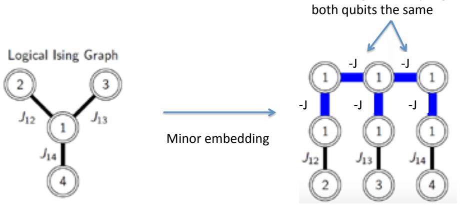
Quantum Computer Layouts



From:
S. Tonetto
MSc thesis

Embedding computational problems

Ferromagnetic couplings,
both qubits the same



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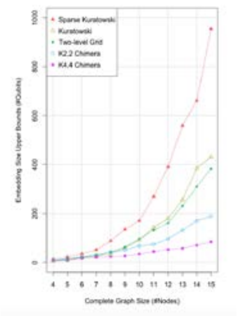
Embedding complete graph



Graph from:
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Speed up of optimization algorithms

It is proven (Aharononv, Kempe, et al) that you can map any circuit onto an equivalent optimization problem, with only a polynomial difference in resources (including time required to solve).

Their cost functions involve more than just "Z" – carefully worked out "gadgets".

Just because we can find an encoding of a problem in a way which a quantum computer could solve it, doesn't say anything about the speed up.

Typically, we when considering hard problems such as NP-Complete problems (e.g. TSP) we expect to achieve a quadratic speedup in accordance with quantum search on unstructured problems.

Given the power of classical heuristics to attack such problems, the development and power of "quantum heuristics" is an open question.

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