

# Week 10

## Lecture 19

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

## Lecture 20

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

## Lab 9

Optimization problems

# Hybrid Quantum/Classical Optimization Algorithms

Physics 90045  
Lecture 20

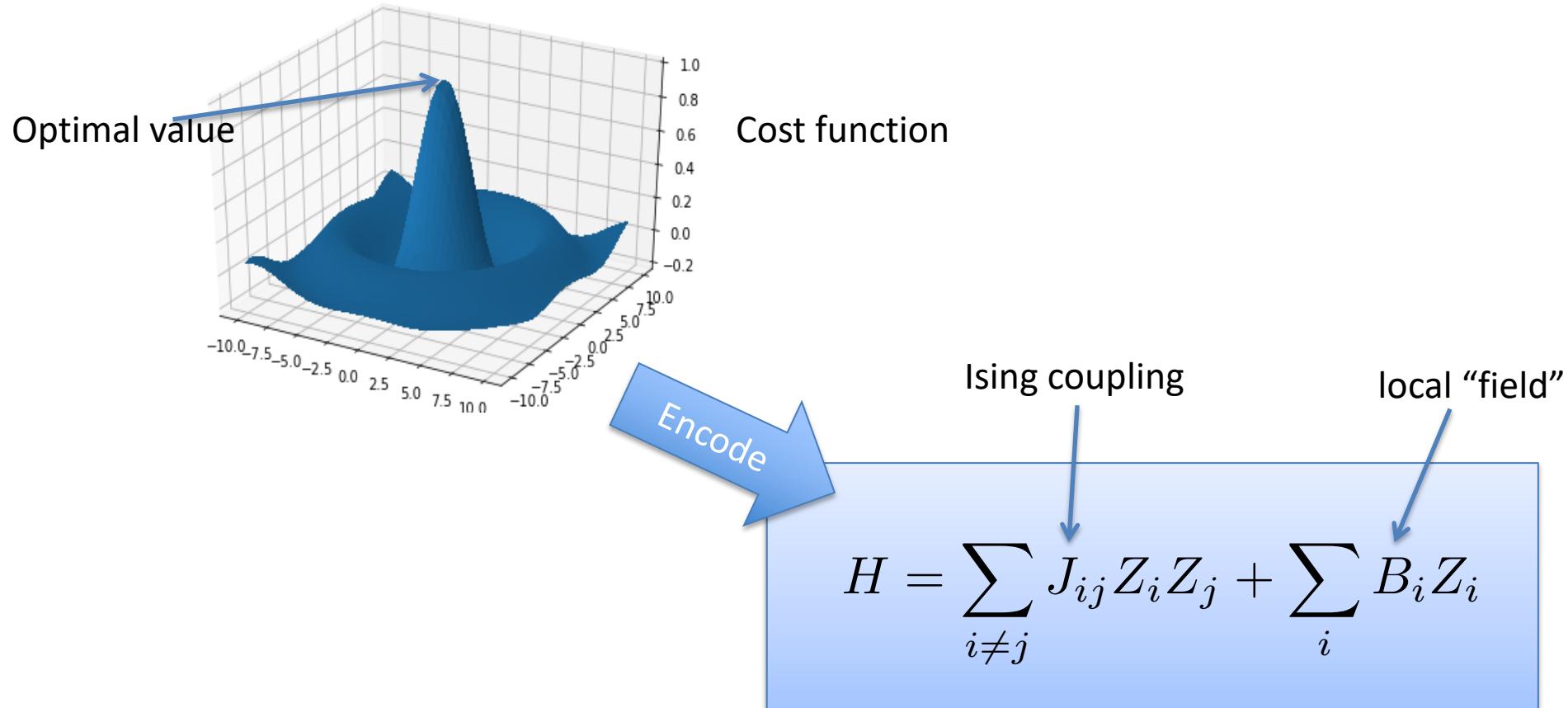
# Overview

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.

# Review of last lecture

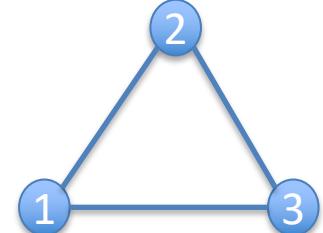


We can encode problems in the energy of the system, but we had no way of minimizing the energy. Today we will see a hybrid technique which allows us to minimize the energy of a quantum system.

# Recall 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  $z_i \rightarrow Z_i$  (where  $Z_i$  is the  $Z$  operator on the  $i$ th qubit):

$$H = J_{12}Z_1Z_2 + J_{23}Z_2Z_3 + J_{13}Z_1Z_3 + B_1Z_1 + B_2Z_2 + B_3Z_3$$



Pairwise interactions between qubits

Bias on individual qubit

# Mapping the Spin Glass form to QC

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

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

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

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

Ising coupling                                  local “field”

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:

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

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

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

Quadratic term

# 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:

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

# Example: Number partitioning

Given a set,  $S$ , of numbers:

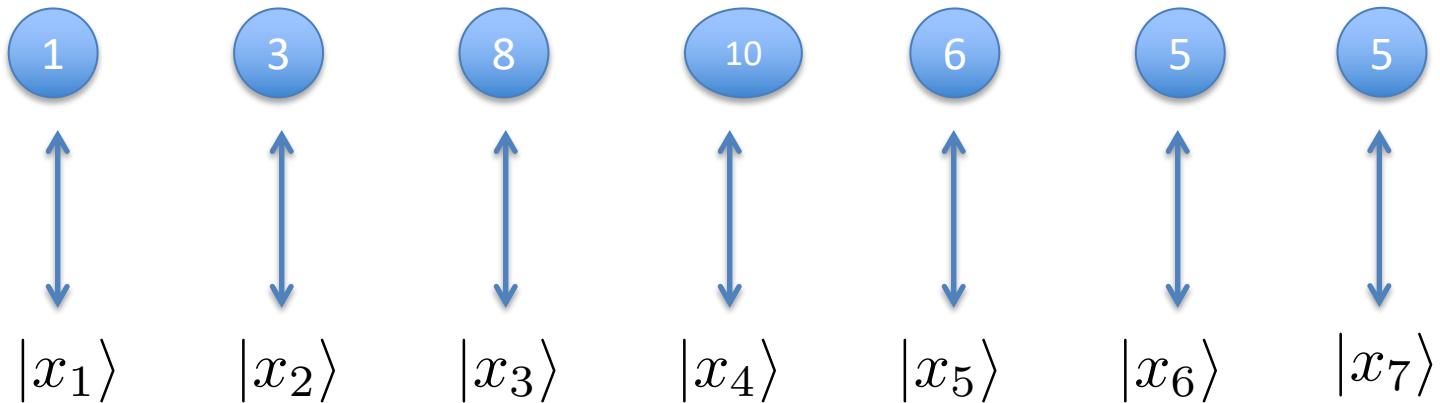
**1, 3, 8, 10, 6, 5, 5**

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}**

# 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

# 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  $i^{\text{th}}$  number

$\pm 1$

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

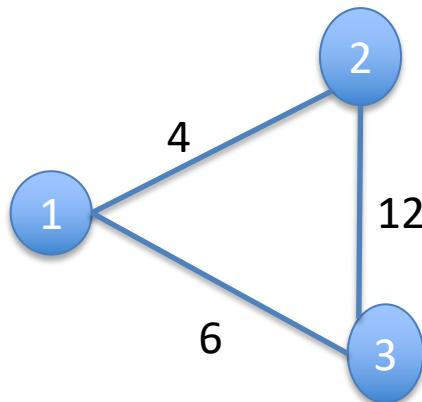
# Number partitioning as a QUBO problem

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):

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

Coupling is the product of numbers

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



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

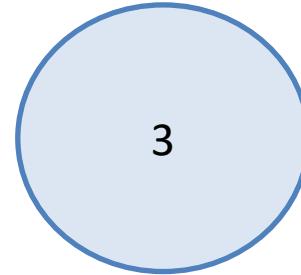
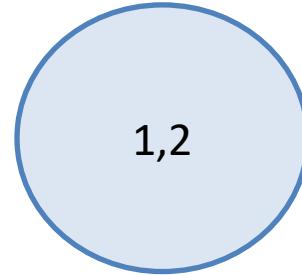
Finding minimum energy state will solve the problem!

# Solution for our Number Partitioning

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

Two degenerate solutions:

$$|110\rangle \quad |001\rangle$$



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

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

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

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

# 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.

# Structure of Algorithm

QAO/Quantum Computer

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

on the quantum computer, where  $\theta$  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  $\theta$ . Original paper found these for a MAX-CUT problem.

# Structure of Algorithm

Q# / Quantum Computer

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

on the quantum computer, where  $\theta$  can be any adjustable gate parameter.

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

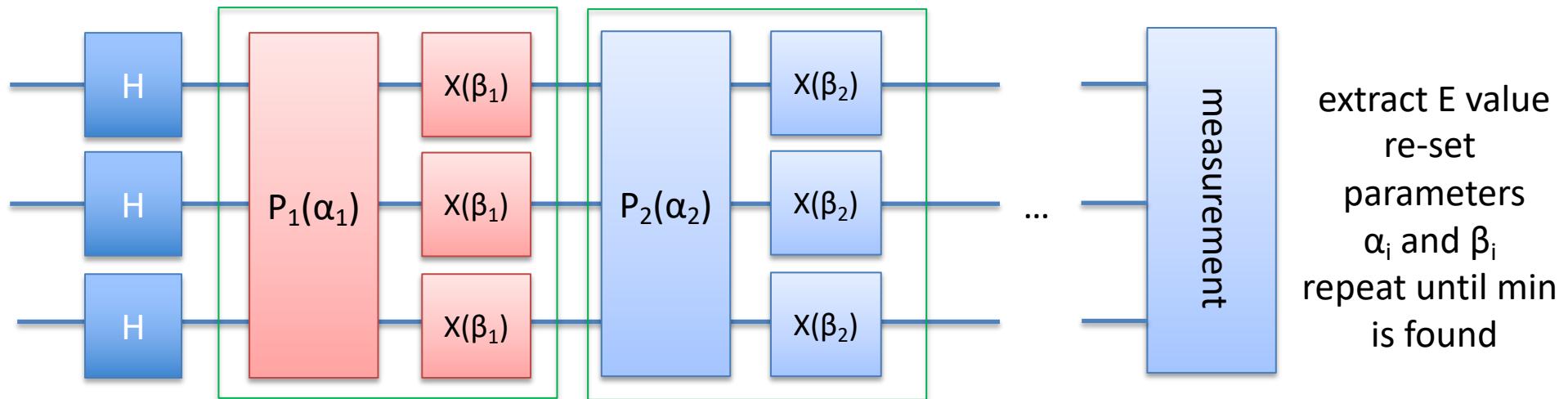
## (3) Use a **classical optimization** technique such as the Nelder–Mead simplex method, determine new values of $\theta$ that decrease $E$ .

Repeat these steps until the value of the energy converges

Classical

# QAOA overview

Initialisation    1st iteration



Let's say we want to find an optimal solution for the cost function:

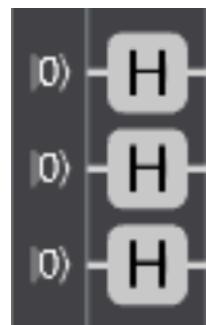
$$H = Z_1 Z_2 + 2Z_2 Z_3 + Z_1$$

# Example QAOA: Phase operations

We want to find an optimal solution (minimum) for the cost function:

$$H = Z_1 Z_2 + 2Z_2 Z_3 + Z_1$$

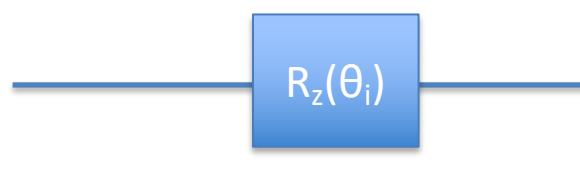
Our first step is to apply Hadamard gates, to produce an equal superposition:



# Phase gates in QAOA circuit: $P(\alpha)$

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

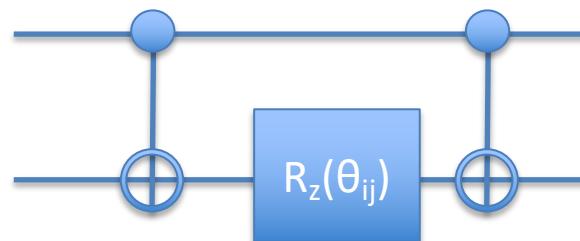
For every Z term in the Hamiltonian:



$$H = \dots + B_i Z_i + \dots$$

$$\theta_i = -\frac{B_i \alpha}{2}$$

For every ZZ term in the Hamiltonian:



$$H = \dots + J_{ij} Z_i Z_j + \dots$$

$$\theta_{ij} = -\frac{J_{ij} \alpha}{2}$$

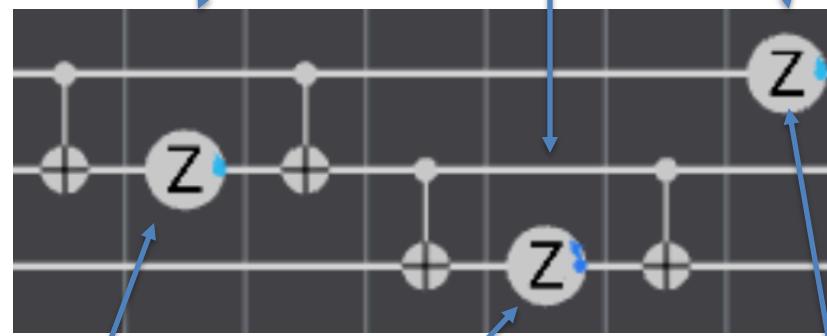
Angles all proportional to their term in the Hamiltonian.

# Phase operation example

Each term's sequence can be placed consecutively. Order of terms does not matter.

$$H = Z_1Z_2 + 2Z_2Z_3 + Z_1$$

Each term in the cost function gets a gate sequence.



Each rotation angle is proportional to the energy term.

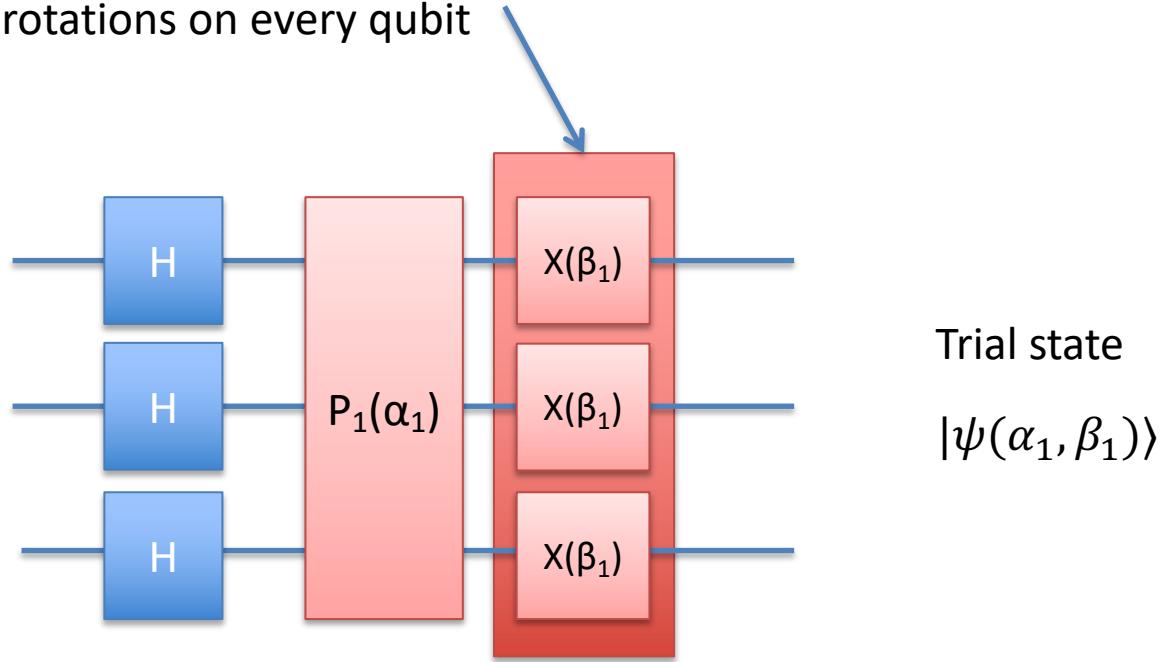
$$\theta_{12} = -\frac{\alpha}{2}$$

$$\theta_{23} = -\frac{2\alpha}{2} = -\alpha$$

$$\theta_1 = -\frac{\alpha}{2}$$

# X-rotations

X-rotations on every qubit



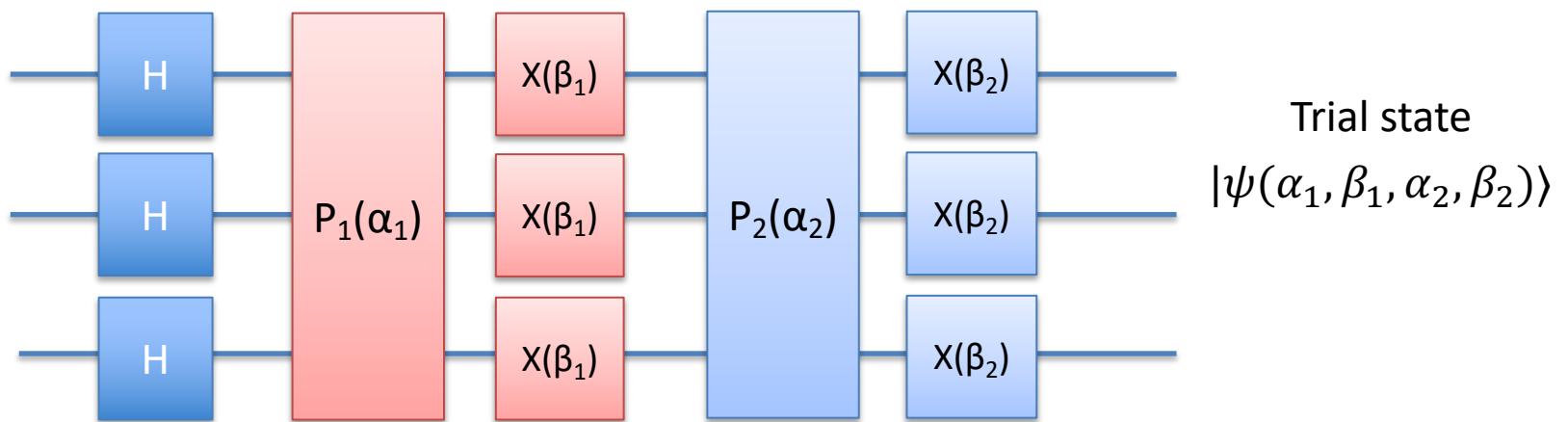
Preparation of a trial state, for k=1 iterations

# X rotation

After the phase operation, we add x-rotations (again with an angle,  $\beta$ , which we optimize):



# Two iterations



Preparation of a trial state, for  $k=2$  iterations

# Measuring the energy

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

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

Ising coupling                                  local “field”

For example:

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

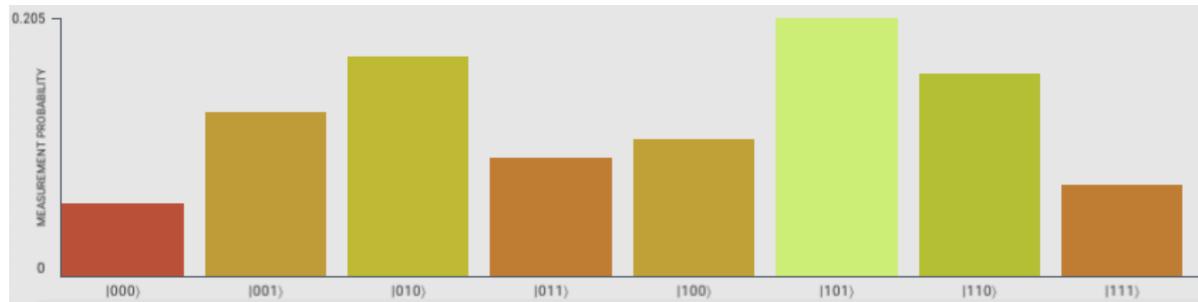
A better approximation to the ground state (depending on the number of steps, k, and the choice of angles) will have a higher probability of measuring the minimum energy, and the lowest energy state.

# One round QAOA

The whole circuit (using just one round,  $p=1$ ) is therefore:



Using values of  $\alpha = 0.2\pi$  and  $\beta = -0.1\pi$ , we get:



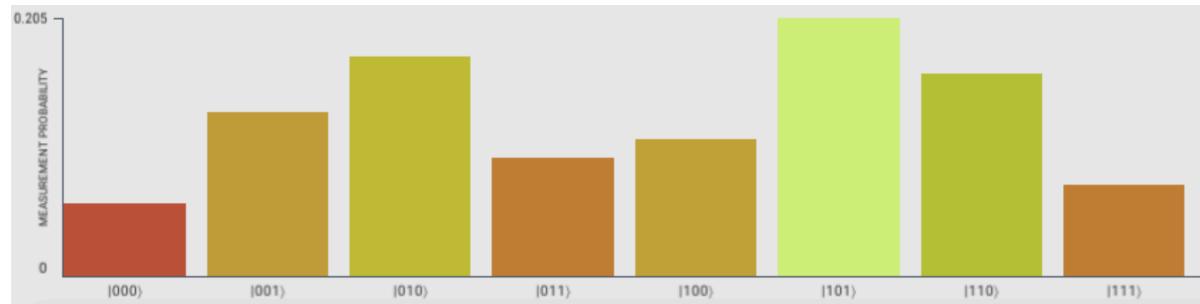
Here 101 is the solution. We have not optimized the angles at all, but already you can see (even on our first try) that its amplitude has increased. Optimising the angles would increase it further.

# One round QAOA

The whole circuit (using just one round,  $p=1$ ) is therefore:



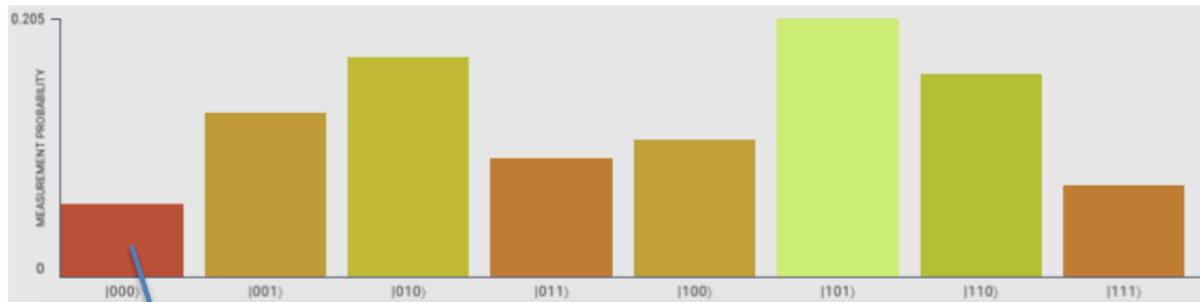
Using values of  $\alpha = 0.2\pi$  and  $\beta = -0.1\pi$ , we get:



Work out the average energy, adjust the angles and rerun the experiment, until we come to a minimum energy.

# Calculating the average energy

$$E = \langle Z_1 Z_2 \rangle + 2\langle Z_2 Z_3 \rangle + \langle Z_1 \rangle$$



$$E = p_{000}E_{000} + p_{001}E_{001} + \dots + p_{111}E_{111}$$

For the  $|000\rangle$  state

$$\begin{cases} Z_1 = 1 \\ Z_2 = 1 \\ Z_3 = 1 \end{cases} \longrightarrow E_{000} = 1 + 2 + 1$$

Adjust the circuit parameters (according to classical optimization algorithm) and repeat to minimize the expectation of energy!

# Calculating the energy

$$H = Z_1 Z_2 + 2Z_2 Z_3 + Z_1$$

State, i	$Z_1$	$Z_2$	$Z_3$	$Z_1 Z_2$	$Z_2 Z_3$	$Z_1$	$E_i$
$ 000\rangle$	1	1	1	1	1	1	4
$ 001\rangle$	1	1	-1	1	-1	1	0
$ 010\rangle$	1	-1	1	-1	-1	1	-2
$ 011\rangle$	1	-1	-1	-1	1	1	2
$ 100\rangle$	-1	1	1	-1	1	-1	0
$ 101\rangle$	-1	1	-1	-1	-1	-1	-4
$ 110\rangle$	-1	-1	1	1	-1	-1	-2
$ 111\rangle$	-1	-1	-1	1	1	-1	2

# Calculating the average energy

Obtained from running quantum computer

State, $i$	$E_i$	Probability, $p_i$	$p_i E_i$
$ 000\rangle$	4	0%	0
$ 001\rangle$	0	20%	0
$ 010\rangle$	-2	20%	-0.4
$ 011\rangle$	2	0%	0
$ 100\rangle$	0	10%	0
$ 101\rangle$	-4	40%	-1.6
$ 110\rangle$	-2	0%	0
$ 111\rangle$	2	10%	0.2

\*Made up  
probabilities for  
demonstration!

Calculate the average energy:  $E = \sum_i p_i E_i = -1.8$

# 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!

# Multiple measurements

Original function we would like to minimize:

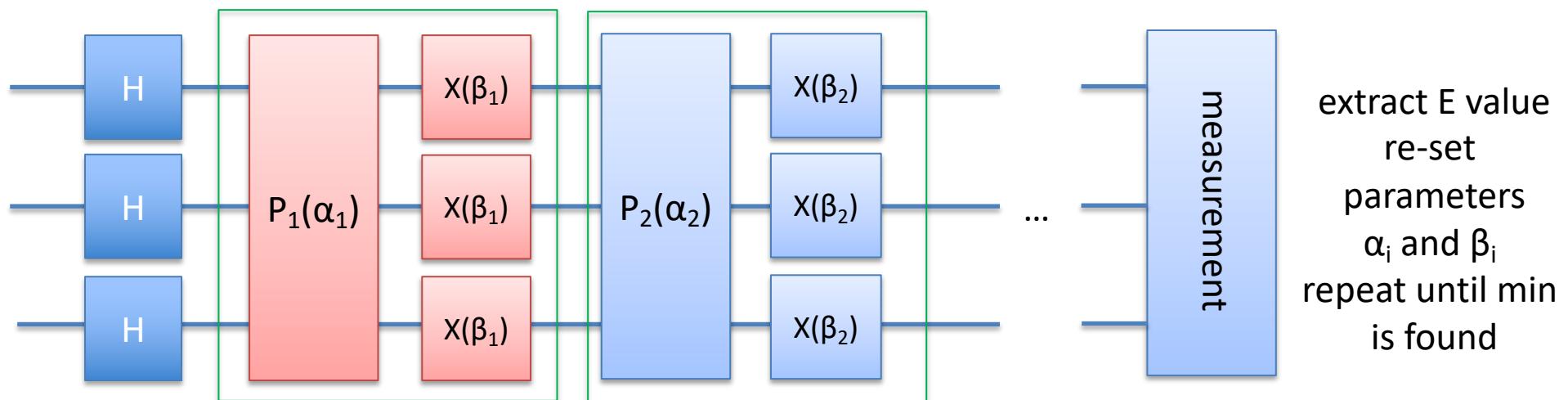
$$H = B_1 Z_1 + B_2 Z_2 + J_{12} Z_1 Z_2$$

Take many samples, to determine:

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

# QAOA overview

Initialisation    1st iteration



# Structure of Algorithm

Q# / Quantum Computer

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

on the quantum computer, where  $\theta$  can be any adjustable gate parameter.

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

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

Repeat these steps until the value of the energy converges

Classical

# 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.

# Structure of Algorithm

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Classical

# Hamiltonian as linear combination of Pauli operators

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

$$E_i = \frac{\text{Tr} [\sigma_i H]}{d}$$

Where  $d$  is the dimension of the system,  $H$  is the Hamiltonian and  $\sigma_i$  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:

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

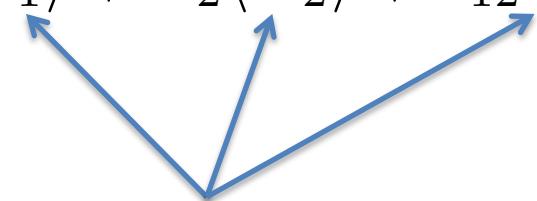
# Find the expectation value of H

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:

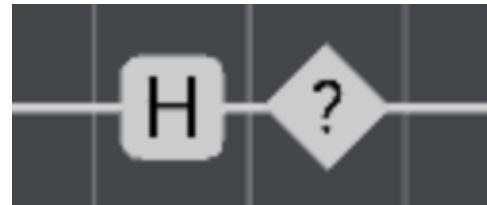
$$\langle H \rangle = B_1 \langle X_1 \rangle + B_2 \langle X_2 \rangle + J_{12} \langle Z_1 Z_2 \rangle$$



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

# 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!

# 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:

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

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

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

$$[f_j, f_k] = 0$$

# Jordan Wigner Transformation

Correct solution:

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

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



Jordan and Wigner: Images from Wikipedia

# 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.

# Nelder-Mead Classical Optimization

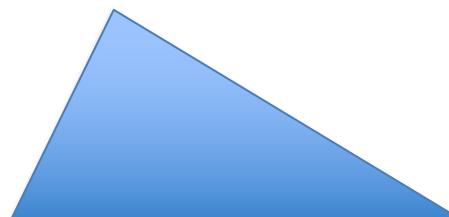
A classical method of optimization.

- 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:  $x_0, \dots, x_n$

Eg. Triangle in 2D



# Nelder-Mead operations

Start with an initial simplex

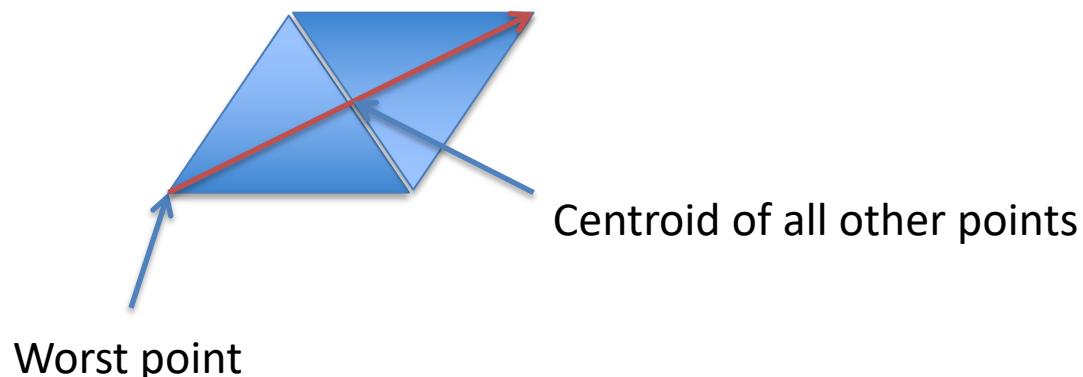
Repeat until the convergence is reached:

Test if we've reached convergence

If not then transform the working simplex

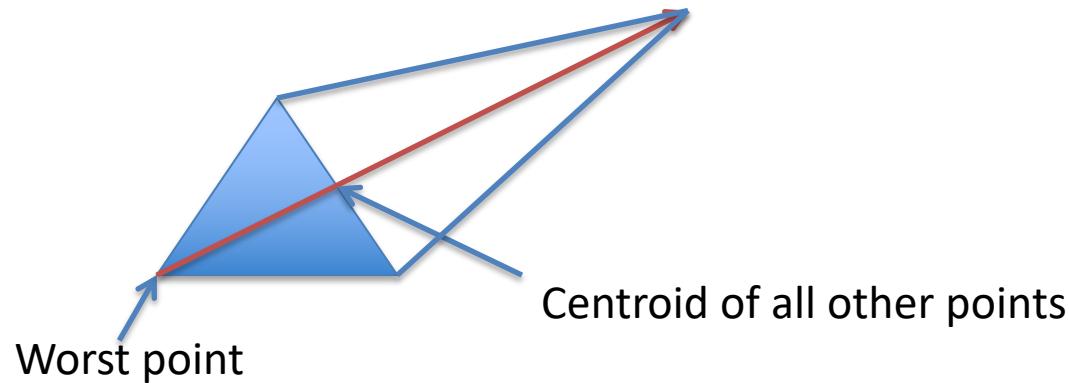
Four types of transformation to test:

## 1) Reflection

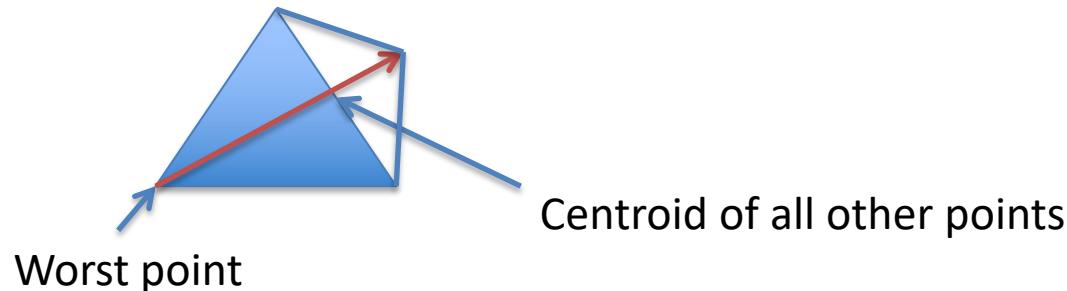


# Nelder-Mead operations

## 2) Expand



## 3) Contract



## 4) Shrink



# Visualization

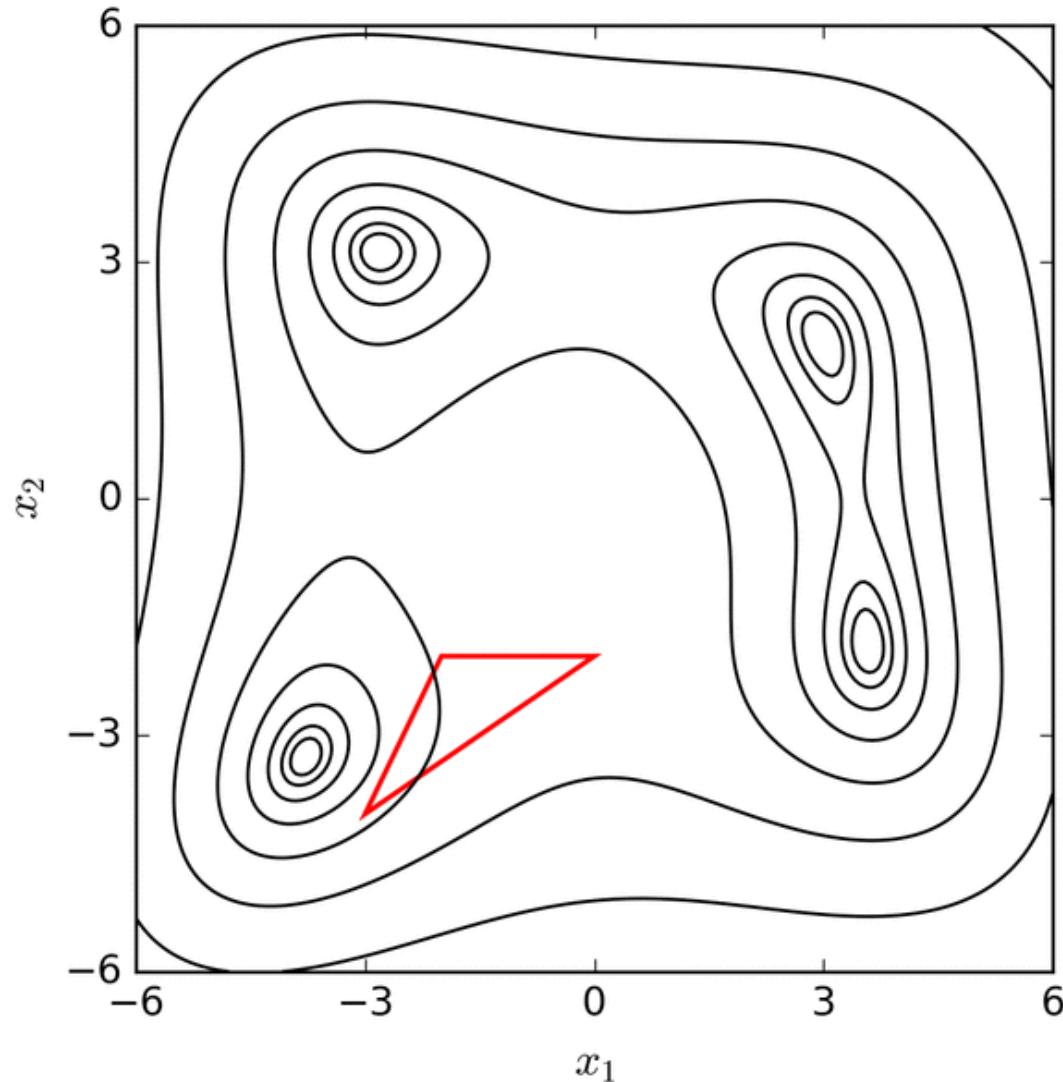


Image:  
Nicoguaro,  
Wikipedia

# Structure of Algorithm

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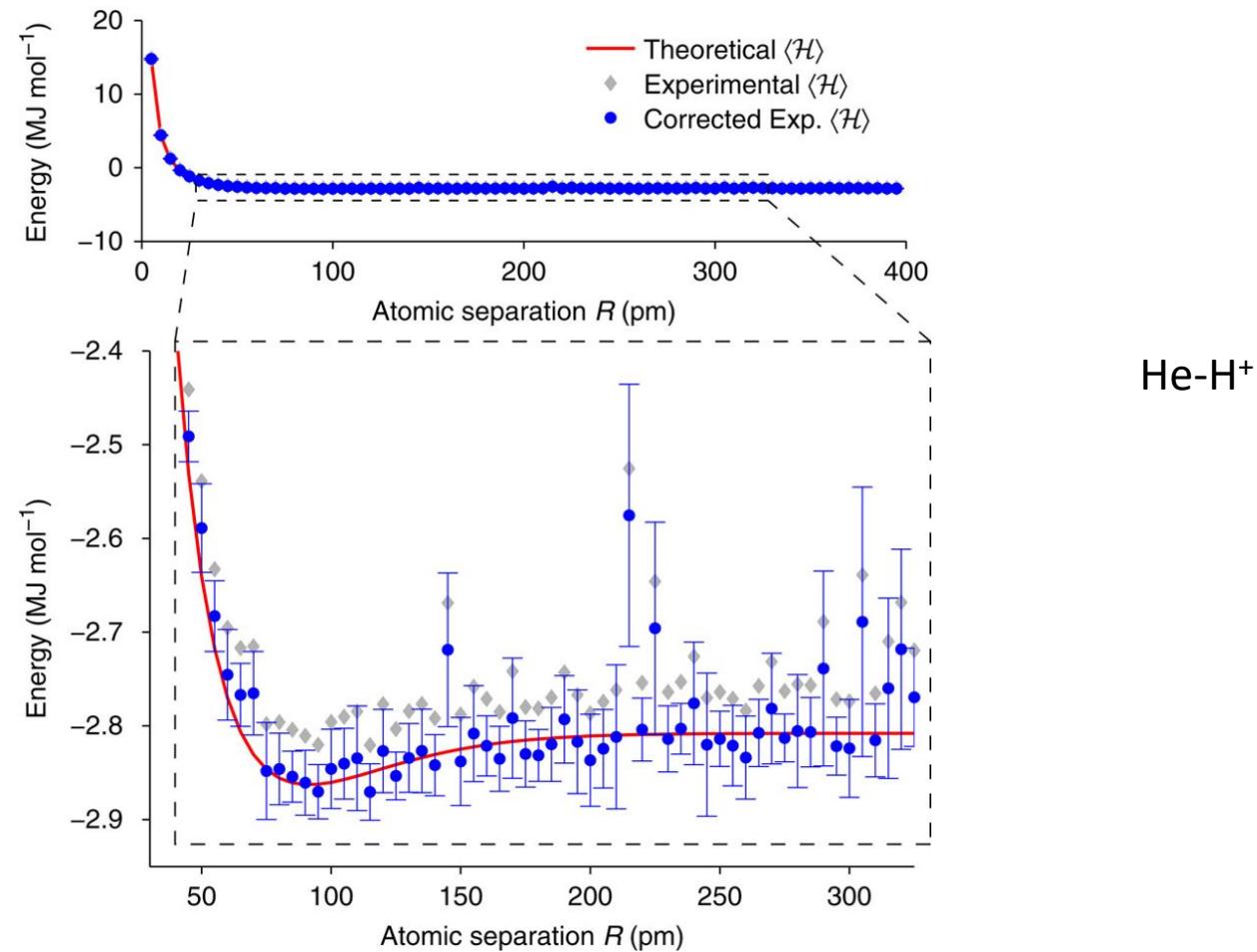
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## (3) Use a **classical optimization** technique such as the Nelder–Mead simplex method, determine new values of $\theta$ that decrease E.

Repeat these steps until the value of the energy converges

Classical

# Example: Inter-molecular distance



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Optimization problems