A QML application: solving QUBO models with the Variational Quantum Eigensolver

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Combinatorial Optimisation Problems

- The field of Combinatorial Optimisation (CO) is one of the most important areas in the field of optimisation, with a wide variety of real-world applications
  - Optimisation problems are concerned with making decisions in settings where a large number of yes/no must be made
  - Each set of decisions yields a corresponding **objective function value** (e.g. a cost or profit value) that needs to be minimised or maximised
- This kind of problems are NP-complete

- Typical optimisation problems are:
  - Resource allocation problems (e.g. flight-gate assignment)
  - Distance minimisation (e.g. traveller salesman problem)
  - Profit maximisation (e.g. credit scoring)
  - ...

The Quadratic Unconstrained Binary Optimisation Problem

In recent years, we have discovered that a mathematical formulation known as the Quadratic Unconstrained Binary Optimisation problem (QUBO), can cover an extraordinary variety of important CO problems

QUBO formulation

$$\text{minimise/maximise} \quad C(\mathbf{x}) = \mathbf{x}^t Q \mathbf{x} \tag{1}$$

where:

- $\mathbf{x}$ is a vector of binary decision variables
- Q is a square matrix of constants that describes the constraints of the specific problem
- C is called cost function because it expresses the cost of each solution

The Ising Model

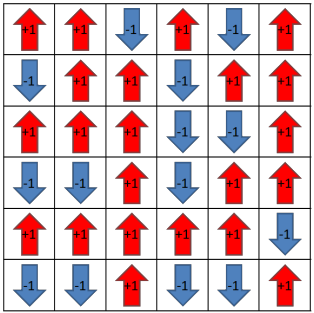
To solve the minimization problem in an efficient way, we use a model coming from the physics world: the Ising model.

The Ising Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j\sigma_j$$

describes a N particle system where

- J_{ij} and h_j are coupling constants related to the interactions between nearest neighbors and to the effect of an external field, respectively
- σ_k is the Pauli (usually Z) operator measuring the k-th spin with possible outcomes $\{-1, +1\}$



From Ising to quantum systems

The cost function $C(\mathbf{x})$ can be easily translated into an Ising Hamiltonian $\mathcal{H}$ for a N-qbit system. Our problem could be written as:

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

Such formulation describes a quantum system:

- The Hamiltonian $\mathcal{H}$ is an operator that measures the energy of the system
- ψ is a generic state of the system

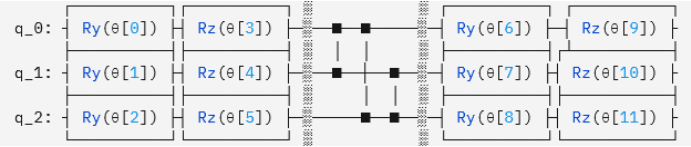
The minimization problem becomes the search for the ground state, or finding the state ψ that minimizes the energy of the system.

Why QUBO with VQE?

- QUBO problems are NP-complete, exact solvers will fail to stop in reasonable time, the best solution is brute force
  - Metaheuristic methods find a high quality solution, not necessarily optimal, in a limited amount of time
- With the Ising Hamiltonian, the solution of the QUBO formulation can be computed in polynomial time using two possible quantum approaches:
  - Quantum annealing
  - Hybrid approach: QAOA or VQE

The Variational Quantum Eigensolver (VQE)

- The Variational Quantum Eigensolver (VQE) is an iterative hybrid classical-quantum algorithm that is used to find the ground state of a system
  - The QPU evolves an input state $|\psi_i\rangle$ to give an output state $|\psi_{i+1}\rangle$ using a quantum circuit defined by:
    - A structure, or **ansatz**, $U(\theta_i)$ which describes the order set of quantum gates
    - A set of parameters θ_i that dictates the behavior of these quantum gates



  - The CPU computes the expectation value $\langle\psi_i|\,\mathcal{H}\,|\psi_i\rangle$ and the classical optimizer (e.g. SPSA) selects the new set of rotation angles θ_{i+1} for the next iteration

Steps of VQE

While the energy estimate is not satisfactory, the iterative scheme is:

1. The state $|\psi_i\rangle$ ($|\psi_0\rangle = |0\rangle$) and the set of angles θ_i (randomly initialized) are fed to the **QPU** which computes the output state $|\psi_{i+1}\rangle = U(\theta_i)\,|\psi_i\rangle$
2. The **CPU** computes the expectation value $\langle\psi_{i+1}|\,\mathcal{H}\,|\psi_{i+1}\rangle$ or the energy of the system when it is in the state ψ_{i+1}
3. On the **CPU** the classical optimizer (e.g. SPSA) selects the new set of rotation angles θ_{i+1} for the next iteration, which starts in the state $|\psi_{i+1}\rangle$, with the goal to minimize the energy of the system

$$\psi_1 = U(\theta_0)\,|0\rangle \qquad \psi_2 = U(\theta_1)\,|\psi_1\rangle \quad \ldots \quad \psi_{i+1} = U(\theta_i)\,|\psi_i\rangle$$

The complexity of the VQE algorithm

- **Step 1: constant** - The bound is the number of shots S needed to get an accurate measurement of the expectation value, $O(10^3)$ is a good approximation.
- **Step 2: polynomial** - Computing the expectation value of a state requires applying the Pauli operator σ_Z $O(N^2)$ times.
- **Step 3: linear** - Classical optimizers find a minimum in $O(N)$.

Conclusion

With the VQE we have found a polynomial scaling, that is better than the one expected for the best known classical algorithm.

Disclaimer: this is true asymptotically, with small graphs and on simulators the classical algorithm still performs better. With larger graphs and quantum hardware we can see the performance improvement.