Variational Quantum Eigensolvers

Simon Martiel

TP 2 – Quantum Computing
7/1/2022

What you should already know

Quantum Phase Estimation

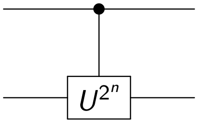
Input: Unitary operator $U = e^{-iHt}$, and eigenvector $U|\psi\rangle = e^{\theta i}|\psi_i\rangle$

Output: The first k bits of θ

Runtime: $O(2^k)$ (for an arbitrary U)

This algorithm is:

- a core algorithm in Quantum Computing (Shor, Quantum Chemistry)
- quite costly, because we need to implement:



and a Quantum Fourier Transform

Poor man's QPE: Variational Quantum Eigensolver (VQE)

Variational Quantum Eigensolver

Input: Some Hamiltonian $H = \sum_i \alpha_i h_i$ (with a small number of terms)
Output: An approximation of the lowest eigenvalue E_0 of H

- Pick a family of quantum states $|\psi(\theta)\rangle$
- Using a quantum computer and a classical optimizer find:

$$\theta^* = argmin_\theta \langle\psi(\theta)|H|\psi(\theta)\rangle$$

- Return $\langle\psi(\theta^*)|H|\psi(\theta^*)\rangle$

We will only consider $H = \sum_i \alpha_i P_i$ where P_i are Pauli operators

$$\langle\psi|H|\psi\rangle = \sum_i \alpha_i \langle\psi|P_i|\psi\rangle$$

In myQLM:

- $H = \sum_i \alpha_i P_i$ can be described using

```
from qat.core import Observable, Term

my_hamiltonian = Observable(
    10,     # Number of qubits
    pauli_terms=[
        Term(2., "XZY", [0, 2, 4])
    ]
)
```

[See tp_vqe_bits.ipynb, first cell]

Ingredients for a VQE

Evaluating $\langle\psi|H|\psi\rangle$

In myQLM:

- Given a circuit C and H, one can construct a Job
- Sending the Job to a simulator will return $\langle 0|C^\dagger HC|0\rangle$

```
from qat.qpus import get_default_qpu

job = circuit.to_job(observable=my_hamiltonian)
result = get_default_qpu().submit(job)
print('Energy:', result.value)
```

[See tp_vqe_bits.ipynb, second cell]

Ingredients for a VQE

Finding θ^* (classical optimization)

We will need to find θ^* that minimize the energy $\langle\psi(\theta)|H|\psi(\theta)\rangle$

- We will describe $|\psi(\theta)\rangle = C(\theta)|0\rangle$ using a parametrized circuit $C(\theta)$
  [See tp_vqe_bits.ipynb, third cell]
- The energy $\langle\psi(\theta)|H|\psi(\theta)\rangle$ is evaluated using a quantum processor (in our case, a simulator called PyLinalg)
- We will find $\theta^\star$ using a variational optimizer
  (a wrapper around scipy.optimize.minimize)
  [See tp_vqe_bits.ipynb, fourth cell]

Ingredients for a VQE

Choosing the family $|\psi(\theta)\rangle$

The choice of $|\psi(\theta)\rangle = C(\theta)|0\rangle$ is crucial:

- it should be rather simple (cheap)
- but capture some symmetries of H
  In particular it should have good chances of approximating the ground state of H

This is what we will focus on in this TP!

This TP

https://github.com/smartiel/tp_vqe_centrale

We will study Ising Hamiltonian of the form:

$$H = \sum_{i<j} a_{i,j}\sigma_z^i\sigma_z^j$$

We will incrementally complicated circuits $C(\theta)$:

- Family 1: simple linear circuits
- Family 2: circuit with the same interactions as H
- Family 3: circuit with the same interaction strengths as H

For each family we will:

- test it on some Hamiltonians, and evaluate their quality
- exhibit quality deficits for some instances

This TP

https://github.com/smartiel/tp_vqe_centrale

The TP can be found in [tp_vqe.ipynb]

- questions are inside the notebook
- some questions don't require code, just some text answer (you can write the answer in the notebook, in french if you want)
- some questions have a "test" cell to check that your code works on some simple cases

It will be graded.

Deadline in one week: 14/01/2021 23:59:59!

Refer to [tp_vqe_bits.ipynb] for myQLM related stuff.

MyQLM documentation (use the search tool, top left)