High-Level Quantum Programming

Miguel Sozinho Ramalho

November, 2018

Table of contents

Meta-Introduction

By now, you should have a good grasp of the *magic underneath the hood* of Quantum Computing. Meaning that quantum circuitry and quantum programming are now within your grasp.

Introduction

This week a different approach will be taken. We will see how quantum computing can be used for the benefit of many other scientific and industry areas. Hopefully, some of the topics you will learn will have a direct application on your life and work.

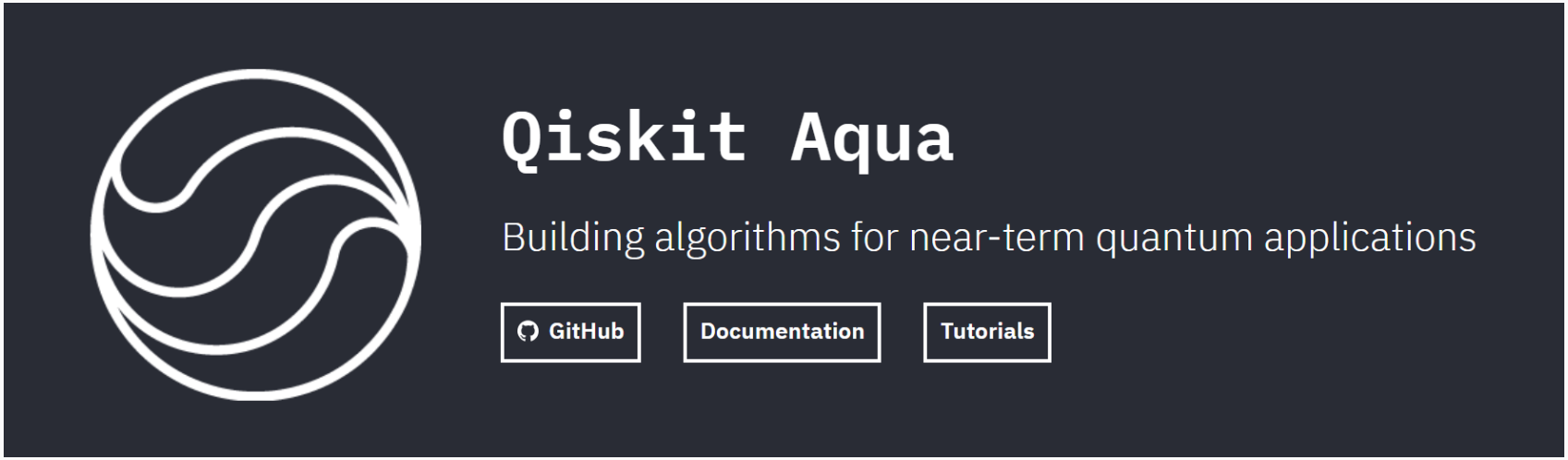
We will do some Qiskit Aqua troubleshooting and then go through the latest examples on qiskit-tutorial on how to use for solving real world problems. This example set is not fully explored and is expected to grow quite a lot in the short term (so keep your eyes open).
*If you are an autodidact, feel free to skip examples on areas that do not interest you.

Motivation

"The better people understand that quantum computing is within their grasp and can be leveraged towards personal gain, the sooner a day will come when running quantum algorithms is but a triviality."

– Miguel Ramalho

Qiskit Aqua



As we saw in Week 1 - Quantum Tools, Qiskit Aqua is the top-level block on the Qiskit full-stack infrastructure. This means it works on a higher level then what we have seen so far, abstracting a quantum compiler and providing an interface much similar to that of classical computing.

The Premise of Qiskit Aqua

Qiskit Aqua contains "a library of cross-domain quantum algorithms upon which applications for near-term quantum computing can be built". **Near-term** means this is the time to look into this, as these algorithms and applications will become feasible in a short time.

Quantum Supremacy

The term **Quantum Supremacy** (not to be mistaken for a mix between *Quantum of Solace* and *The Bourne Supremacy*) stands for the moment in time in which quantum computers can do better than the most powerful computer in simulating a quantum system.
This may seem strange, but the fact is that classical computers are so developed they they are still able to simulate better quantum computers than those in existence, but this classical "quantum simulation" fits into the **NP** family and so there will come a time, in the not so far away future, when they are no longer able to do better than *the real thing*.


ALBERT R. BROCCOLI'S EON PRODUCTIONS PRESENTS DANIEL CRAIG
AS IAN FLEMING'S JAMES BOND 007 IN
QUANTUM SUPREMACY
12A
007.COM

Running algorithms in Qiskit Aqua

First and foremost: `pip install qiskit-aqua`

Then, we need to understand which algorithms have already been implemented in Qiskit Aqua. A comprehensive list can be found in the docs, some that you may recognize are:

- Grover Search
- Quantum Dynamics (Simulating Universal Quantum Systems)
- Support Vector Machine Quantum Kernel (Machine Learning)
- CPLEX (Constraint Solver)

Running algorithms in Qiskit Aqua

Qiskit Aqua is very declarative, in fact, running an algorithm can be thought of as defining a description of your problem, for instance in a JSON file or in a Python Dictionary. It is a composition of the following settings (For more information, check the docs.):

Problem The type of experiment
(`"energy" | "excited_states" | "ising" | "search" ...`)

Input/Oracle The way to specify the input to the problem, depends on the type (SAT configuration, dataset, oracle, ...)

Algorithm Optional specification of the algorithm to use (each problem has default algorithms) and its configurations

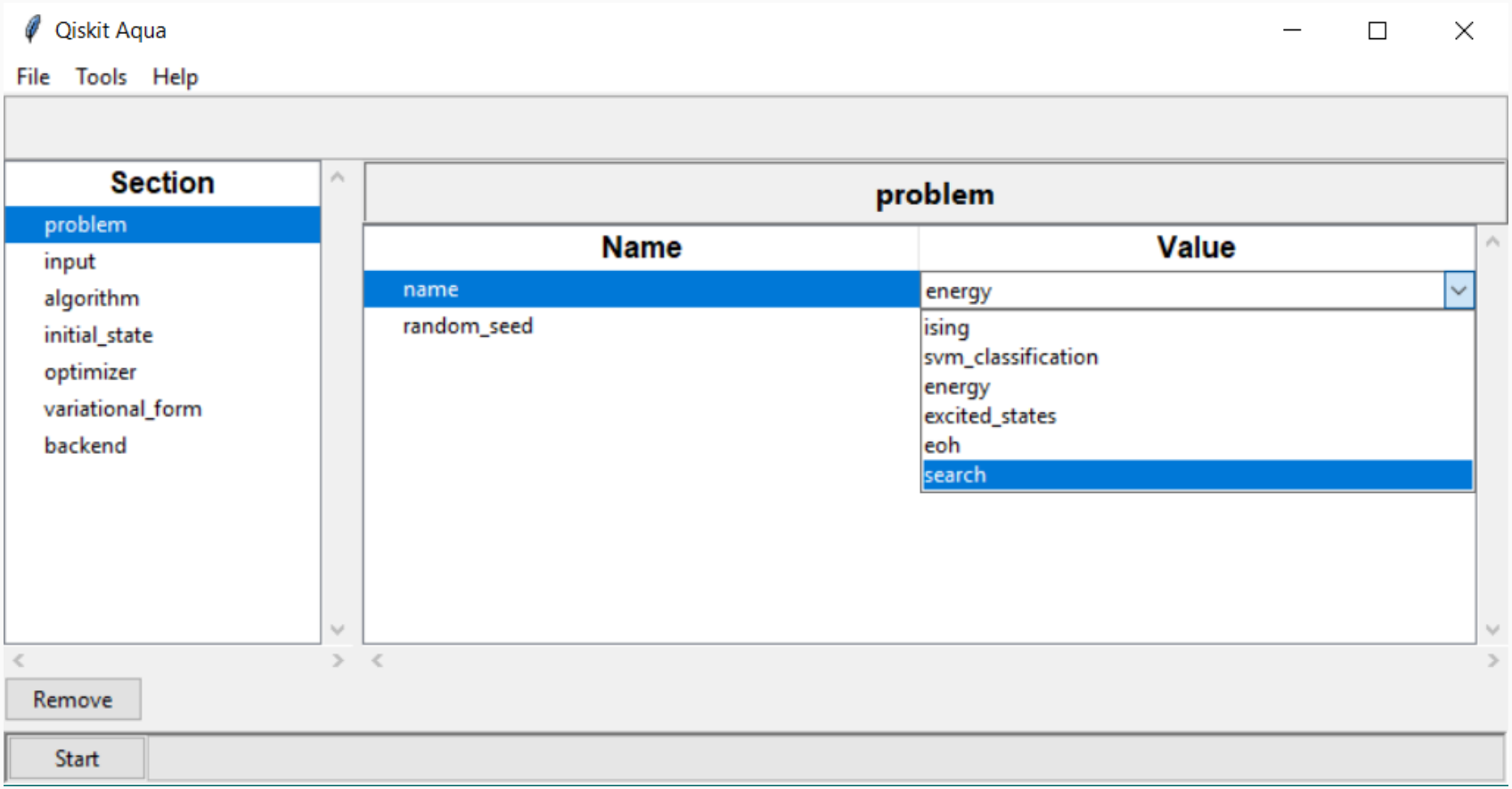
Backend Which device to use (simulator, real device), highly customizable with number of shots (how many times should an experiment be repeated), activate compiler optimization, specify device noise parameters, ...

Troubleshooting Qiskit Aqua

After installing head to a command line and run `qiskit_aqua_ui`. If nothing happens, you should make sure you add your python `bin` folder to the system variable path, it should be something like: `"C:\Program Files\Python 36\Library \bin "`.
The same solution goes for the cvxopt error when running python scripts.

Troubleshooting Qiskit Aqua

When everything is properly installed you should see something like (The Qiskit Aqua GUI for editing experimental settings):



Grover's algorithm in Qiskit Aqua

Go ahead and run the following code, while trying to understand it:

```
from qiskit_aqua import run_algorithm
# problem in DIMACS CNF format:
sat_cnf = """
p cnf 3 5
-1 -2 -3 0
1 -2 3 0
1 2 -3 0
1 -2 -3 0
-1 2 3 0
"""
params = {
    'problem': {'name': 'search'},
    'oracle': {'name': 'SAT', 'cnf': sat_cnf},
    'algorithm': {'name': 'Grover'},
    'backend': {'name': 'qasm_simulator'}
}
print(run_algorithm(params)['result']) # [1, -2, 3] or another
```

Artificial Intelligence

If you work in Machine Learning, you probably know how the Support Vector Machine(SVM) works. It is simply an algorithm for supervised learning.
Qiskit Aqua comes with more than one implementation of SVM Kernels. We will have a complete exercise on it this week (optional).

More Artificial Intelligence related algorithms are expected to be implemented on Qiskit Aqua in the future, and you may even implement your own!

Artificial Intelligence (SVM)

Here's an example of a configuration for an SVM classification model:

```
params = {
    'problem': {
        'name': 'svm_classification',
        'random_seed': 1219 # same seed ensures reproducibility
    },
    'algorithm': {
        'name': 'QSVM.Kernel'
    },
    'backend': {
        'name': 'qasm_simulator',
        'shots': 1024
    },
    'feature_map': {
        'name': 'SecondOrderExpansion',
        'depth': 2,
        'entanglement': 'linear'
    }
}
```

Optimization

Still related to AI, there is another very important topic nowadays in both research and industry settings: **optimization**.

In this week's exercises you will have 2 examples of optimization problems: maximum cut and the iconic traveling salesman problem. These can both be reduced to a traditional model called ising model that has been studied from a quantum point of view. Thus, by using the ising solver in Qiskit Aqua we are able to solve many different problems, literally the only limitation is our ability to map problem formulations into know and solved problems.

Chemistry in Qiskit Aqua

Lastly, and especially directed at chemistry related research, there are also examples of extrapolation of quantum mechanical properties that allow to make simulation on the behaviour of atoms, electrons and on the evolution of molecule configurations.
If you think about it, what better to simulate an atomic process than quantum?

As a matter of fact, there is a complete repository form the Qiskit team dedicated to chemistry algorithms for research on the field.

Chemistry in Qiskit Aqua

We will not go much deeper into explaining the typical approaches, as this should be done by those students that truly benefit from it. However, here is an example of how such problems may be configured (the input comes from HDF5 files):

```
# Input dictionary to configure Qiskit aqua Chemistry
# for the chemistry problem.
aqua_chemistry_dict = {
    'driver': {'name': 'HDF5'},
    'HDF5': {'hdf5_input': 'H2/0.7_sto-3g.hdf5'},
    'operator': {'name': 'hamiltonian'},
    'algorithm': {'name': 'VQE'},
    'optimizer': {'name': 'COBYLA'},
    'variational_form': {'name': 'UCCSD'},
    'initial_state': {'name': 'HartreeFock'},
    'backend': {'name': 'statevector_simulator'}
}
```

Hands-on

This week there will be quite a few exercise tutorials available, each student is expected to select and study at least one of them. Here are the topics covered in each:

1. Grover algorithm with Qiskit Aqua (search)
2. SVM for Breast Cancer classification (Artificial Intelligence)
3. Maximum Cut problem (optimization)
4. Traveling Salesman problem (optimization)
5. Computing the ground state energy of an H_2 molecule (Chemistry)

Where to learn more?

- Qiskit Aqua documentation seriously a good point to start
- Qiskit Aqua official tutorials
- Qiskit Aqua community tutorials
- A comprehensive analysis of Quantum Programming SDKs and languages including, of course, Qiskit