

QCOMPPW101: Simulating a quantum computer

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Based on:

MITx: 8.370.1x Quantum Information Science I, Part I

Practical work Outline: During this practical work we will simulate a quantum computer.

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1 Introduction

The goal of this practical work is to make you program a simulation of a quantum computer. You will have to program it in **Python3**. The only package you have the right to use is **NumPy**, **math** and **Enum**. You will have to program the function:

```
1 quantumComputer (nbQbits: int, quantumGates: list)
```

The input **nbQbits** is the number of qubits in the circuit.

The input **quantumGates** is the list of quantum gates of the circuit.

1.1 Given file

You can download the given file [here](#).

The content of the only given file you have to fill **quantumComputer.py**:

```
import numpy as np
from enum import Enum

#Enumeration for each type of gate our quantum computer handle
class TypeOfQuantumGate(Enum):
    NOT = 1
    HADAMARD = 2
    CNOT = 3

#The class quantum gate
#TypeOfGate is the type of the gate (a value of TypeOfQuantumGate)
#fQbit is the position in the circuit of the first input Qbit of the gate
#sQbit is the position in the circuit of the second input Qbit of the gate ( if the
gate has two input)
class QuantumGate:
    def __init__(self, typeOfGate: TypeOfQuantumGate, fQbit: int, sQbit: int =0 ):
        self.typeOfGate = typeOfGate
        self.fQbit = fQbit
        self.sQbit = sQbit

#The main function, you need to program it without using qiskit
#nbQbits is the number of Qbits of the circuit
#QuantumGates is the list of quantum gates of the circuits
#This function output the state vector of the circuit after executing all the gate
def quantumComputer(nbQbits: int, quantumGates: list):
    pass
```

[number=None] You will have to program in this file.

TypeOfQuantumGate is an **enumeration** for each type of gate our quantum computer handle.

QuantumGate is the class of the quantum gate.

TypeOfGate is the type of the gate (a value of **TypeOfQuantumGate**).

fQbit is the position in the circuit of the first input qubit of the gate.

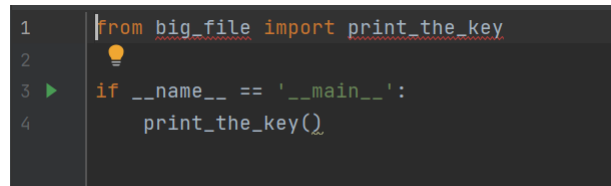
sQbit is the position in the circuit of the second input qubit of the gate (if the gate has two input). You can add functions to **QuantumGate**.

1.2 Submission

Your code will need to be **submitted using github**, on this [assignment](#). The only file that matter to us are the given Python file named quantumComputer.py, and these are the only files that you should 'git add'.

Every practical has a deadline. Today's one is on **Sunday the 5th of december at 23:59**. Only the very last commit is taken into account.

The grade is determined by the script **run_test_suite.py**. To run it through Pycharm, you have to open it and click on the green arrow:



```
1 from big_file import print_the_key
2
3 if __name__ == '__main__':
4     print_the_key()
```

It will output something like this:

```
Your mark is: 0
Your proof of work is: 0,9967204840567662
```

You will have to put the proof of work in this **Excel file**. Your proof of work represent your mark, so update it every time you have a better mark. You also have to push your corresponding work on GitHub.

1.3 Python requirements

The Python requirements are the same of the previous workshop and you can install them with the given requirements.txt

1.4 Reference

You can find an implementation of this practical work at https://drive.google.com/file/d/1iaBw1yT4I48oAII77b8p4_YhF4pGI7Kx/view?usp=sharing.

This implementation uses **Qiskit** but you does not have the right to do so. Nevertheless this can be useful to test your code and disambiguate what you are ask to do. Your practical work has to behave the same way¹.

The reference raise exception for some type of input. Your quantum computer will never be tested for those kinds of inputs.

You do not have to understand how it is coded, only how it works.

1.5 Test

You can find a lot of test in this file : **gigaTest.py**.

1.6 Documentation

The only **Numpy** functions you will need are:

- **zeros**: <https://numpy.org/doc/stable/reference/generated/numpy.zeros.html>
- **matmul**: <https://numpy.org/doc/stable/reference/generated/numpy.matmul.html>
- **transpose**: <https://numpy.org/doc/stable/reference/generated/numpy.transpose.html>
- **kron**: <https://numpy.org/doc/stable/reference/generated/numpy.kron.html>

¹The values will be compared using the NumPy function `isclose`

2 Generate state vector

For validating this section, your quantum computer will have to handle an **empty** list of quantum gate as input. On an empty list your quantum computer should output a vector of 2^{nbQbits} values, with the first value being equal to one and the other values must be equal to zeroes. Your quantum computer must pass this test (no assert must be thrown):

```
arr = np.array([1.+0.j, 0.+0.j, 0.+0.j, 0.+0.j, 0.+0.j, 0.+0.j, 0.+0.j, 0.+0.j])
comparison = np.array_equal(arr, quantumComputer(3,[]))
assert(comparison)
arr = np.array([1.+0.j, 0.+0.j, 0.+0.j, 0.+0.j])
comparison = np.array_equal(arr, quantumComputer(2,[]))
assert(comparison)
```

Tips 1: The code below does not throw any error assert

```
assert(1. == 1. + 0.j)
```

Tips 2: checks the function `numpy.zeros` ;)

3 Handle one gate

The goal of this section is to make your quantum computer handle one gate with one input.

3.1 Iterative kronecker product

The solution of this part is given below and in the file: [computeMatrix.py](#)

To do so, you will have to program the function **computeMatrix**. This function takes into input a matrix :2x2 **baseMatrix**, an integers : **nbQbit**, and an integer **fQbit**. This function output:

$$I_2^{\otimes(\text{nbQbit}-fQbit-1)} \otimes \text{matrix} \otimes I_2^{\otimes fQbit}$$

. Let's consider

$$I^{\otimes 3} = I \otimes I \otimes I$$

and

$$I^{\otimes 0} = [1]$$

The function must pass this test:

```
m = [[5]]
arr = [[5]]
assert (np.array_equal(computeMatrix(m, 1, 0), arr))

m = [[5]]
arr = [[5.0,0],
[0,5.0]]
assert (np.array_equal(computeMatrix(m, 2, 0), arr))

m = [[0,1],
[1,0]]
arr = [[0., 1., 0., 0.],
[1., 0., 0., 0.],
[0., 0., 0., 1.],
[0., 0., 1., 0.]]
assert(np.array_equal(computeMatrix(m,2,0), arr))
m = [[1,2],[3,4]]
arr = [[1., 0., 2., 0.],
[0., 1., 0., 2.],
[3., 0., 4., 0.],
[0., 3., 0., 4.]]
assert(np.array_equal(computeMatrix(m,2,1), arr))
```

```
m = [[1,2],[3,4]]
arr = np.kron(np.kron(np.identity(2),m), np.identity(2))
assert(np.array_equal(computeMatrix(m,3,1), arr))
```

Here is the solution of the exercise:

```
def computeMatrix(baseMatrix, nbQbit, fQbit):
    res = np.identity(1)
    for j in range(nbQbit):
        i = nbQbit - 1 - j
        if(i == fQbit):
            res = np.kron(res, baseMatrix)
        else:
            res = np.kron(res, np.array([[1,0],[0,1]]))
    return res
```

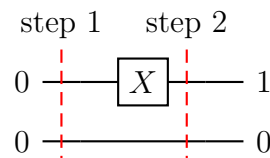
3.2 Handle one NOT gate

Now you have all the key in hand to handle one **NOT** gate.

To do so, if there is a **NOT** gate in the circuit you will have to:

1. compute your state vector (for example for 2 qubits you compute [1. 0. 0. 0.])
2. compute the **NOT** gate corresponding matrix using the function **computeMatrix**. Do this accordingly to the number of qubits in the circuit and its position in the circuit. Here is the matrix you have to give in input to **computeMatrix** in this case: $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
3. multiply the transposition of your state vector with the matrix you have just computed.

Here is the evolution of the state vector during the computation:



At step 1 the state vector is equal to:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$$

At step 2 the state vector is equal to:

$$\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \times \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}$$

Here what it does in pseudo-code:

```
def quantumComputer(nbQubits, quantumGates):
    stateVector = generate the state vector
    (for example for 2 qubits you compute [1. 0. 0. 0.])
    CorrespondingMat = computeMatrix([[0,1],[1,0]], nbQubits,
        quantumGates[0].fqubit)
    return CorrespondingMat * transpos(stateVector)
```

Your quantum computer must pass this test:

```
arr = quantumComputer(2,[QuantumGate(TypeOfQuantumGate.NOT,0)])
assert(np.array_equal(arr,[0., 1., 0., 0.]))
```

3.3 Handle one Hadamard gate

Now you will have to handle one Hadamard gate. To compute the corresponding matrix of an Hadamard gate you just have to act like for the **NOT** gate, except that you use the Hadamard matrix as a 2x2 matrix:

$$\frac{1}{\sqrt{2}} \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Your quantum computer must pass this test:

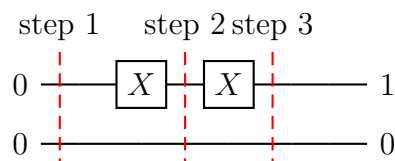
```
arr = quantumComputer(1,[QuantumGate(TypeOfQuantumGate.HADAMARD,0)])
assert(np.isclose(arr,[1/math.sqrt(2), 1/math.sqrt(2) ])).all())
```

4 Handle many gates

For validating this section, your quantum computer must handle many gate.

To do so, first you have to compute the corresponding matrix of every gate and then multiply them in the reverse order.

Here is the evolution of the state vector if there is two not gate on the first qubit:



At step 1 the state vector is equal to:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$$

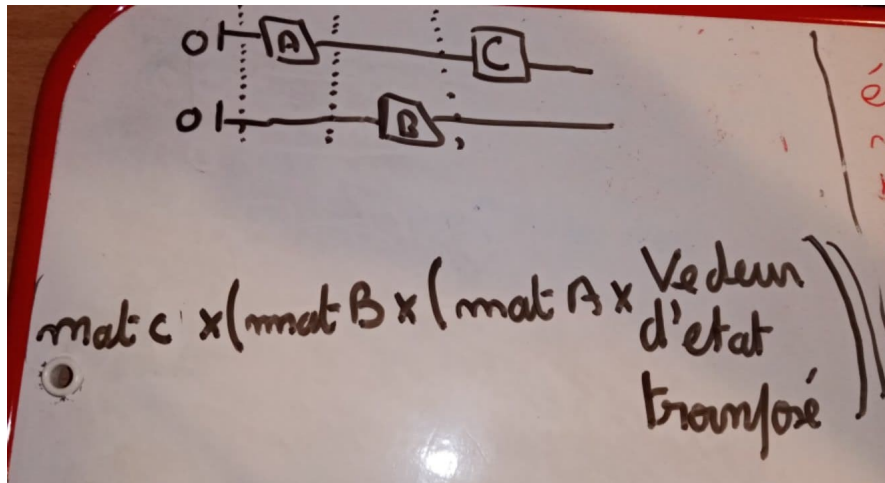
At step 2 the state vector is equal to:

$$\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \times \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}$$

At step 3 the state vector is equal to:

$$\left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \times \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \times \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^t = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$$

Here a drawing that will help you:



Your quantum computer must pass this test:

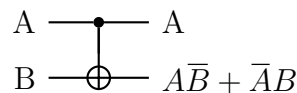
```
arr = quantumComputer(1, [QuantumGate(TypeOfQuantumGate.NOT, 0),
QuantumGate(TypeOfQuantumGate.HADAMARD, 0)])
assert(np.isclose(arr, [1/math.sqrt(2), -1/math.sqrt(2)]).all())
```

5 Bonus: Handle CNOT gate

5.1 Compute CNOT matrix

Program the function **computeCNOT**. This function takes in input an integers: **nbQbit**, an integers: **fQbit** and an integer: **sQbit**. Consedering **fQbit** as the control qubit². This function outputs the corresponding **CNOT** matrix. To compute this matrix there is an elegant way you can find here: [click here](#). Yet this way is complicated, so we will explain a simpler, less elegant way.

For two bit in the classical computing world the **CNOT** gate act this way:



And has this truth table:

fQbit	sQbit	fQbit output	sQbit output
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

So in our quantum computing world, for 2 qubits, using the IBM convention, we have a such "truth table":

²fQbit and sQbit must be different. Yet your work will never be tested with fQbit = sQbit

Input	Output
$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$
$\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$
$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$
$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

So we have a such corresponding matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Here a pseudo-code algorithm that computes the corresponding matrix for the general case:

```

getTheBit(i,j): return the jth bit of i

notTheBit(i,j): negate jth bit of i and return the number

computeCNOT(nQubits, fQubit,sQubit):
create a (2**nbQubits) * (2**nbQubits) matrix m, filled with 0.
for i in 0, 2**nbQubits :
    if(getTheBit(i,fQubit) == 1):
        j = notTheBit(i,sqbit)
        m[i,j] =1
    else:
        m[i,i] =1
return m

```

Your function computeCNOT must pass this test:

```

arr = [[1., 0., 0., 0.],
[0., 0., 0., 1.],
[0., 0., 1., 0.],
[0., 1., 0., 0.]]
assert(np.array_equal(computeCNOT(2,0,1) , arr))

```

5.2 Back to our quantum computer

Now you have all you need to handle **CNOT** gate in our quantum computer. Just to do it! Your quantum computer must pass this test now:

```
arr =quantumComputer(2,[QuantumGate(.TypeOfQuantumGate.NOT,1),
    QuantumGate(.TypeOfQuantumGate.CNOT,1,0)])
assert(np.array_equal(arr , [0,0,0,1]))
```

6 Compute Probability

Program the function **computeProbability**. This function takes in inputs an array of complex numbers: **tab**. This function output an array of the same dimension. Every coefficient of the output is computed this way:

$\forall i \in [0, \text{length}(\text{tab})[$

$$\text{output}[i] = \frac{|\text{tab}[i]|^2}{\sum_{k=0}^{\text{tab.length}()-1} |\text{tab}[k]|^2}$$

This function must pass this test:

```
arr =quantumComputer(1,[QuantumGate(.TypeOfQuantumGate.NOT,0),
    QuantumGate(.TypeOfQuantumGate.HADAMARD,0)])
assert(np.isclose(computeProbability(arr),[0.5,0.5]).all())
```

This function computes the probability of each combination to comes out when you mesure every qubit.