



Christian Boehme

Quantum Computing (for the curious)

Practical Course High-Performance Computing

What is Quantum Computing?	Small Quantum Circuits with Qiskit	Deutsch's algorithm	Implementing Deutsch's algorithm	Outlook and further resources
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Learning goals

- Formulate small Quantum algorithms as Quantum circuits
- Implement small Quantum circuits with Qiskit
- Understand and implement Deutsch's algorithm

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- The smallest unit of information in QC is the Qubit
- Qubits are represented as two-dimensional vectors \vec{q}
- Two states of the Qubit form its **Computational Basis**: $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Computations with these states are similar to classic computing

Gates: Operations on Qubits

- Operations on Qubits are called gates (cf. logic gates in classical computing)
- Gates are linear transformations of the state vector of a Qubit, i.e. matrices

$$\blacksquare \hspace{0.1cm} X \hspace{0.1cm} | \hspace{0.06cm} 0 \rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \times 1 + 1 \times 0 \\ 1 \times 1 + 0 \times 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = | \hspace{0.06cm} 1 \rangle$$

Brief exercise: Check that $X |1\rangle = |0\rangle$

Quantum Circuits and Measurement

Quantum Circuits are one way to represent quantum computations



- Qubits are measured in the computational basis
- **The result is either** $|0\rangle$ or $|1\rangle$ and is stored in a classical bit

Superposition and the Hadamard gate

Say "hello" to the **Hadamard** or **H** gate:

$$\blacksquare H |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right] = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$$

Brief exercise: Check that
$$H \ket{1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \ket{0} - \frac{1}{\sqrt{2}} \ket{1}$$

After the H gate the Qubit's state is a linear combination of basis states

This is called superposition

The H gate is it's own inverse, applying it to $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ yields $|0\rangle$

Applying H to
$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
 yields $|1\rangle$

(Check, if you like!)

Superposition measurement

Let's measure our superposition:



In a superposition $a\ket{0}+b\ket{1}$, $a,b\in\mathbb{C}$

- the probability to measure Qubit state $|0\rangle$ equals a^2
- \blacktriangleright the probability to measure Qubit state |1
 angle equals b^2
- This also means $|a|^2 + |b|^2 = 1$

(This is Schrödinger's cat: We are officially Quantum now!)

Multiple Qubit states

Qubit states are combined by tensor product, i.e. for two Qubits:

$$\begin{aligned} |a\rangle \otimes |b\rangle &= \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix} \\ &= a_0 b_0 |00\rangle + a_0 b_1 |01\rangle + a_1 b_0 |10\rangle + a_1 b_1 |11\rangle \\ &= \text{Measuring 2 Qubits results in probabilities} \\ |a_0 b_0|^2 + |a_0 b_1|^2 + |a_1 b_0|^2 + |a_1 b_1|^2 = 1 \end{aligned}$$
$$\begin{aligned} &= \text{For example: } |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |01\rangle \end{aligned}$$

Can be extended to n Qubits: |q₁⟩ ⊗ |q₂⟩ ⊗ ... ⊗ |q_n⟩
 Grows exponentially, only 30+ Qubits can be simulated classically

Christian Boehme

The CNOT gate

The **CNOT** or **XOR** gate is a 2 Qubit gate:

$$q_0: - q_1: -$$

• (Note Qiskit's Qubit order: $|q_1q_0\rangle$)

Or, as a matrix:

$$egin{pmatrix} a_1 & 0 & 0 & 0 \ 0 & 0 & 0 & 1 \ 0 & 0 & 1 & 0 \ 0 & 1 & 0 & 0 \end{pmatrix} egin{pmatrix} a_{00} \ a_{01} \ a_{10} \ a_{10} \ a_{11} \end{pmatrix} = egin{pmatrix} a_{00} \ a_{11} \ a_{10} \ a_{01} \end{pmatrix}$$

2 Qubit gates have two outputs, as Quantum gates need to be reversible

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Entanglement

Consider the following circuit:



- Each Qubit is equally likely to be measured as |0
 angle and as |1
 angle
- However, both Qubits will always be in the **same** state after measurement

This is called entanglement

- Einstein's spooky action at a distance: More Quantum weirdness!
- What happens: $CNOT(I \otimes H) |00\rangle = CNOT[\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)] = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

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Exercise 1

- Install qiskit with ". qiskit.sh"
- Run exbase.py
 - Is the probability distribution as you expected?
 - \blacktriangleright Can you write the corresponding superposition in terms of basis states $|00\rangle$, ...
- \blacksquare Entangle the two Qubits, but put the control Qubit in $|1\rangle$ state before applying the H gate
 - ► I.e., implement:



Think about the result: Is it what you expected? Why or why not?



Optional exercise 1.a

There exists an entangled state where 2 Qubits are always in different states after measurement:



- Implement the Quantum circuit producing that state
- Hint: You need one additional gate

Optional exercise 1.b

Consider this maximally entangled state of 4 Qubits:



- Implement the Quantum circuit producing that state
- For this you need to extend the Quantum circuit to 4 Qubits: circuit = QuantumCircuit(4)
- Hint 1: Start with entangling 2 Qubits
- Hint 2: The first three Qubits are now in state $\frac{1}{\sqrt{2}}|000\rangle + \frac{1}{\sqrt{2}}|011\rangle$
- Hint 3: Switch $|011\rangle$ to $|111\rangle$ but **not** $|000\rangle$ to $|100\rangle$. What gate does this?

Deutsch's problem

- Consider an unknown function of a one bit input x
- The output f(x) could either be **constant** 0 or 1 or depend on x (**balanced**)
- Two tests required classically to determine balanced vs. constant
- Quantum circuit for the problem:



Remember: Quantum gates must be reversible

Quantum solution part 1: Phase kickback

- Our U(f) gate transforms $|x\rangle |y\rangle$ to $|x\rangle |y \oplus f(x)\rangle$ (\oplus : plus, then modulo 2)
- Let's "cheat": Instead of using $|0\rangle$ for $|y\rangle$ we use $\frac{1}{\sqrt{2}}(|0\rangle |1\rangle)$
- Then, if we apply our gate U(f): $U(f) |x\rangle \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$ $= |x\rangle \frac{1}{\sqrt{2}} (|f(x)\rangle - |1 \oplus f(x)\rangle)$ $= (-1)^{f(x)} |x\rangle \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$

Now we have encoded information in the sign (or **phase**) of the input Qubit!

This is called **phase kickback** and is used in many Quantum algorithms

Quantum solution part 2: Input superposition

- We will now use the function information encoded in the phase
- We initialize $|x\rangle$ as superposition of both possible values: $|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
- We can ignore the output Qubit and get, after applying U(f): $(-1)^{f(x)} |x\rangle = \frac{1}{\sqrt{2}} ((-1)^{f(|0\rangle)} |0\rangle + (-1)^{f(|1\rangle)} |1\rangle)$
- That means constant functions result in $|q_0
 angle = \pm \frac{1}{\sqrt{2}}(|0
 angle + |1
 angle)$
- **B**alanced functions result in $|q_0
 angle=\pmrac{1}{\sqrt{2}}(|0
 angle-|1
 angle)$
- (Note that multiplying a Qubit state globally by -1 does not change it)
- \blacksquare Use the H gate and measure to get $|0\rangle$ for constant and $|1\rangle$ for balanced
- We have solved Deutsch's problem in one try!
- Deutsch-Josza extends this to input length n: One try vs. worst case $2^{n-1} + 1$

Exercise: Implementing Deutsch's algorithm

Deutsch's algorithm:

- Prepare the input (0) Qubit in $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ state
- Prepare the output (1) Qubit in $\frac{1}{\sqrt{2}}(|0\rangle |1\rangle)$ state
- Apply the oracle
- Apply the Hadamard gate to Qubit 0 and 1 each
- Measure: If $|10\rangle$, the function is constant, else it is balanced
- Please implement this in debase.py
- Implement pre- and postprocessing as described
- Implement at least one constant and one balanced oracle
- \blacksquare Constant oracles are constant $|0\rangle$ and constant $|1\rangle$
- Balanced oracles are identity and negate

Optional exercise: Extend Deutsch to Deutsch-Josza

- We will not cover the math here (but it's very similar to Deutsch)
- Tasks:
 - Use 3 instead of 1 input Qubits (4 Qubits in total)
 - Prepare the input and output Qubit states as before
 - > You can reuse your constant oracle
 - Implement at least one balanced oracle
 - \blacktriangleright This should output $|0\rangle$ for half of the possible inputs, $|1\rangle$ for the other half
 - > Extension (harder): Can you implement a random set of balanced oracles?
 - Implement postprocessing and measuring as before
 - > You should measure $|1000\rangle$ for constant (and something else for balanced)

State of Quantum Computing

- Noisy, intermediate-size Quantum era (NISQ)
- Quantum Computers with dozens (in development: hundreds) of Qubits
- High error rate (noise) due to external influences and imperfect control
- Full error tolerance in NISQ era unachievable due to overhead
- Quantum advantage in real world applications requires thousands or millions of Qubits
- Great time to do basic research if interested in algorithms and/or Quantum mechanics
- Promising fields are Quantum Chemistry, Combinatorial Optimization, Machine Learning

Further reading

- Recap linear algebra: Essence of linear algebra on YouTube
- Deutsch's algorithm explained using a state machine: Quantum Computing for Computer Scientists on YouTube
- Introduction for self study:

Quantum computing for the very curious

- Everything on Qiskit, lots of tutorials: https://qiskit.org/
- Good textbooks:
 - Quantum Computing: An Applied Approach by Jack D. Hidary
 - Quantum Computing verstehen von Matthias Homeister
- Brief overview of the field (link to arxiv.org):

Quantum Computing in the NISQ era and beyond, John Preskill

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Questions?



Credit: IBM