Study Notes:

Quantum Computing in Slow Pace

量子計算慢慢來

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Draft Version

尚未校稿・僅供参考

持續更新。歡迎回饋、意見或提問

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What is this?

This document is merely a collection of notes during my course studying Quantum Computing. Most of the introductory texts in Quantum Computing do not include extensive elaborations of the matrix derivations involved in developing a concept perhaps due to the large print spans they would take. My notes started with these exercise works when I built my intuition to understand the subject matter.

Later it expanded to serve to structure the topics of interests as well as notes and thoughts on various fundamental and application topics, and for sharing too. Related works of Python codes are also included.

Chapter 1

Quantum Gates

1.1 Basics from Physics to Math

- For a layperson introduction of Quantum Theory: The Fabric of the Cosmos: Quantum Leap (PBS NOVA, Nov 17, 2011).
- Dr. Shankar at Yale gave a fairly clear narrative on Quantum Mechanics for a term in 2011 ¹
 - Thomas Young's Double Slit Experiment, 2013
 - Fourier Tranform
 - Euler's Equation: $e^{ix} = \cos(x) + i\sin(x)$

Wave-Particle Duality of Matter; Schrödinger Equation (MIT OCW 2017, 光電效應實驗), but as for 40:02:

- Feynman's Derivation of the Schrödinger Equation
- How did Schrödinger end up with his equation? How did he decide that his wave was going to be scalar as opposed to a vector field like E&M wave? Etc.

Schrodinger's Equation

Introduction to Quantum Mechanics: Schrodinger Equation

Nobody knows how the wave function collapses:

- Copenhagen: 由於觀測而發生塌縮 (量子論縱覽, 人人出版2020, Page 79)
- Many World: decoherence of quantum state when interact with the environment which effectively "split" the universe into mutually unobservable alternate histories. (More on Wikipedia)

"Researchers observed that <u>carbon</u> atoms can tunnel. They thus overcome an energetic barrier, although they do not actually possess enough energy to do that. ... At very low temperatures under ten Kelvin, one molecule form is significantly preferred due to the energy difference."

Spin and the shape of electrons

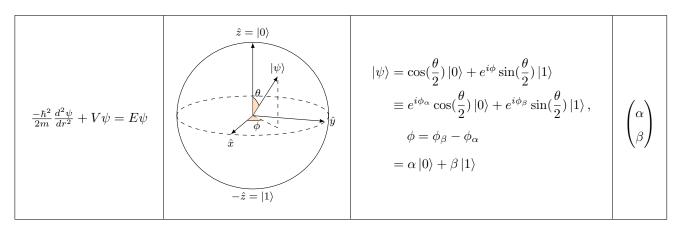
- Electrons DO NOT Spin, 2021
- How do we know if electrons are really spinning? 2018
- Carbon displays quantum effects, Ruhr-Universitaet-Bochum, 2017

¹Compton Effect

- \bullet Electrons Are Perfectly Spherical, New Measurements Confirm, 2018
- \bullet Electron Appears Spherical, Squashing Hopes for New Physics Theories, 2013

1.1.1 Bloch Sphere

"These representations on the Bloch's circle (sphere) are combinations of the two wave functions. ... What is the physical meaning of the circle (sphere)? ... There is no physical meaning. The Bloch's circle (sphere) is a visualization; it's a way thinking about these vectors. ...", Cameron Akkar.



$$\begin{split} |0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} : \ \theta = 0^\circ, \ |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} : \ \theta = 180^\circ. \\ X \, |0\rangle &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \ X \, |1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{split}$$

量測 measure 時 $|\psi\rangle$ 塌縮至 \hat{z} 軸

$$H |0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle = |+\rangle,$$

$$H |+\rangle = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2 \\ 0 \end{pmatrix} = |0\rangle;$$

$$H |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} |0\rangle - \frac{1}{\sqrt{2}} |1\rangle = |-\rangle,$$

$$H |-\rangle = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 \\ -2 \end{pmatrix} = |1\rangle.$$

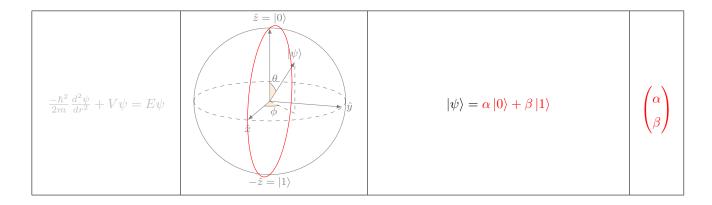
右掌大拇指:軸,四指:|\psi\,,掌面:旋轉方向

$$Z |0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

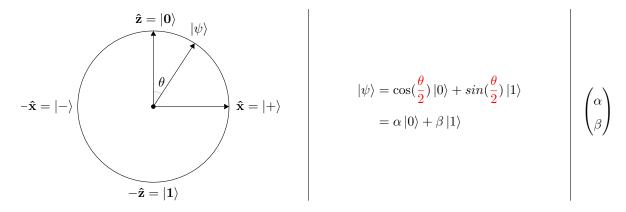
$$Z |1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|1\rangle, \ \theta = -180^{\circ}.$$

$$Y |0\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ i \end{pmatrix} = i |1\rangle,$$

$$Y |1\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 0 \end{pmatrix} = -i |0\rangle.$$

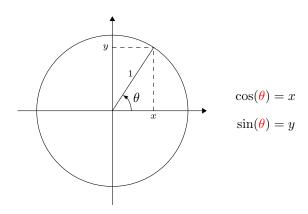


For the sake of simplicity, if we maintain $\phi=0^\circ,\,^2$



§8.5 Limitations of the quantum operations formalism in Quantum Computation and Quantum Information (Nielson and Chuang 2010, Page 394 bottom)

Compare:



 $^{^2{}m Okay}$ up till the Grover's

1.1.2 Products of Matrices

Inner & outer products — Lecture 5 — Matrix Algebra for Engineers Tensor Product

1.1.3 Quantum Annealing

Webinar: Quantum Computing by a Quantum Annealer Quantum annealing with more than one hundred qubits D-Wave

1.2 Part I

1.2.1 Hadamard

$$|0\rangle + |1\rangle + |2\rangle + |3\rangle$$
 — $f(x) = 2x^2 - 5x + 6$ — $|6\rangle + |3\rangle + |4\rangle + |9\rangle$

参考:鍾豪著,零與一之間的威力/量子電腦的原理,科學月刊 2021 (5 月號) 617 期,第 26 頁 Quantum Computing as a High School Module (Perry et al., 2020, Page 71 §9.2 Limitations)

注意:不能只單純理解為 qubit 進入 |0> 和 |1> 機率各半的狀態

$$|0\rangle$$
 H H $|0\rangle$

$$|1\rangle - H - H - |1\rangle$$

還是要知道在 Bloch's Sphere 或是利用(複數)矩陣運算上的定義。

参考 Quantum Computing as a High School Module (Perry et al., 2020, Page 50 top)

1.2.2 CNOT

學習單

先完成 (A), (B), (C), (D): (還沒學過矩陣乘法的同學可以參考連結)

如果
$$q_0 = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
 而 $q_1 = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,

$$(A) q_1 q_0 = |10\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix}, 參考連結$$

也就是 $a_{00} =?, a_{01} =?, a_{10} =?, a_{11} =?$. 若讓 q_1 以 CNOT 控制 q_0 ,

$$CNOT|\mathbf{10}\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix}, 也就是 |??\rangle (如下)$$

同樣地,

(B)
$$|00\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \\ ? \\ ? \times \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix}$$

$$CNOT|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

(C)
$$|01\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \\ ? \\ ? \times \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$$

$$CNOT|01\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

(D)
$$|11\rangle = |?\rangle \otimes |?\rangle = \begin{pmatrix} ? \times \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} \\ ? \times \begin{pmatrix} ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix}$$

$$CNOT|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{pmatrix} = |??\rangle$$

但是請注意: $a_{00}, a_{01}, a_{10}, a_{11}$ 可能是滿足 $a_{00}^2 + a_{01}^2 + a_{10}^2 + a_{11}^2 = 1$ 的任何實數組合 各 qubit 可能處於不同的疊加態。例如,若

$$q_0 = |\alpha\rangle = \frac{\sqrt{3}}{2} |0\rangle + ?|1\rangle = \frac{\sqrt{3}}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + ? \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ ? \end{pmatrix},$$

$$q_1 = |\beta\rangle = \frac{3}{5}|0\rangle + ?|1\rangle = \frac{3}{5}\begin{pmatrix} 1\\0 \end{pmatrix} + ?\begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} ?\\? \end{pmatrix},$$

$$q_1q_0 = |etalpha
angle = |eta
angle\otimes|lpha
angle = egin{pmatrix} ? \times ? \ ? \ ? \ ? \end{pmatrix} = egin{pmatrix} ? \ ? \ ? \ ? \ \end{cases}$$
,(注意這四個數的平方和為1)

$$CNOT |\beta\alpha\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = \begin{pmatrix} ? \\ ? \\ ? \\ ? \end{pmatrix} = ? |00\rangle + ? |01\rangle + ? |10\rangle + ? |11\rangle$$

Solution

If
$$q_0 = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
 and $q_1 = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$,
$$q_1 q_0 = |10\rangle = |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \times \begin{pmatrix} 1 \\ 0 \\ 1 \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

 $a_{00} = 0, a_{01} = 0, a_{10} = 1, a_{11} = 0.$ Let q_1 control q_0 with CNOT,

$$CNOT|\mathbf{10}\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, i.e. |\mathbf{11}\rangle \text{ by below}$$

likewise,
$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \times \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$CNOT|00\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \times \begin{pmatrix} 0 \\ 1 \\ 0 \times \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$CNOT|01\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|11\rangle = |1\rangle \otimes |1\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & \times \begin{pmatrix} 0 \\ 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$CNOT|11\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 & 0 \end{pmatrix}$$

Xref: Quantum Computing for Everyone, Bernhardt 2019, Chapter 4, Page $64{\sim}67$

But please note: a_{00} , a_{01} , a_{10} , a_{11} may be any combination of real numbers that satisfies $a_{00}^2 + a_{01}^2 + a_{10}^2 + a_{11}^2 = 1$. (Each qubit may be in different variance of superposition of states.) For example, if

$$q_0 = |\alpha\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle = \frac{\sqrt{3}}{2}\begin{pmatrix} 1\\0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2}\\\frac{1}{2} \end{pmatrix},$$

$$q_1 = |\beta\rangle = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle = \frac{3}{5}\begin{pmatrix} 1\\0 \end{pmatrix} + \frac{4}{5}\begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} \frac{3}{5}\\\frac{4}{5} \end{pmatrix},$$

$$q_1 q_0 = |\beta \alpha\rangle = |\beta\rangle \otimes |\alpha\rangle = \begin{pmatrix} \frac{3}{5} \times \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \\ \frac{4}{5} \times \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{4\sqrt{3}}{10} \\ \frac{4\sqrt{3}}{10} \\ \frac{4}{10} \end{pmatrix}, \text{ (note that the squares of all elements sum up to 1)}$$

$$CNOT \left| \beta \alpha \right\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4\sqrt{3}}{10} \\ \frac{4}{10} \end{pmatrix} = \begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4}{10} \\ \frac{4\sqrt{3}}{10} \end{pmatrix} = \frac{3\sqrt{3}}{10} \left| 00 \right\rangle + \frac{3}{10} \left| 01 \right\rangle + \frac{4}{10} \left| 10 \right\rangle + \frac{4\sqrt{3}}{10} \left| 11 \right\rangle$$

The 2 qubits are entangled now, so we can't decompose them into 2 separated qubits for distinct wave probabilities for each qubit as

$$\begin{pmatrix} \frac{3\sqrt{3}}{10} \\ \frac{3}{10} \\ \frac{4}{10} \\ \frac{4\sqrt{3}}{10} \end{pmatrix} = |\delta\gamma\rangle, \text{ If } |\gamma\rangle = c_0 |0\rangle + c_1 |1\rangle, \text{ and } |\delta\rangle = d_0 |0\rangle + d_1 |1\rangle,$$

$$|\delta\gamma\rangle = |\delta\rangle \otimes |\gamma\rangle = egin{pmatrix} d_0 imes egin{pmatrix} c_0 \ c_1 \ d_1 imes egin{pmatrix} c_0 \ c_1 \ \end{pmatrix} = egin{pmatrix} d_0c_0 \ d_0c_1 \ d_1c_0 \ d_1c_1 \ \end{pmatrix} = egin{pmatrix} rac{3\sqrt{3}}{10} \ rac{3}{10} \ rac{4}{10} \ rac{4\sqrt{3}}{10} \ \end{pmatrix}$$

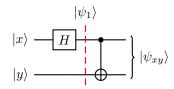
Xref: Quantum Computing as a High School Module (Perry et al., 2020, Page 58 §7.4 second example).

Multiple Qubits are in entanglement \Leftrightarrow

The state of the Multiple Qubits combined can not be expressed as a tensor product of each of the 2 qubits.

The No-Cloning Theorem: you can't treat the qubits in entanglement individually.

1.2.3 Bell States



Let
$$|x\rangle = x_0 |0\rangle + x_1 |1\rangle = \begin{pmatrix} x_0 \\ x_1 \end{pmatrix}, |y\rangle = y_0 |0\rangle + y_1 |1\rangle = \begin{pmatrix} y_0 \\ y_1 \end{pmatrix}$$

$$H|x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} x_0 + x_1 \\ x_0 - x_1 \end{pmatrix}$$

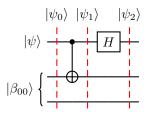
$$|\psi_1\rangle = (H |x\rangle) \otimes |y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_0 \\ (x_0 - x_1)y_1 \end{pmatrix}$$

$$|\psi_{xy}\rangle = CNOT |\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_0 \\ (x_0 - x_1)y_1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} (x_0 + x_1)y_0 \\ (x_0 + x_1)y_1 \\ (x_0 - x_1)y_1 \\ (x_0 - x_1)y_0 \end{pmatrix}$$

/V,	$ y\rangle = 0\rangle$ $y_0 = 1, y_1 = 0$	$ y angle = 1 angle$ $y_0 = 0, y_1 = 1$	
$ x\rangle = 0\rangle$ $x_0 = 1$ $x_1 = 0$	$ \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} + \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}) = \frac{ 00\rangle + 11\rangle}{\sqrt{2}} $	$\frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\1\\0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix} + \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix} = \frac{ 01\rangle + 10\rangle}{\sqrt{2}}$	
$ x\rangle = 1\rangle$ $x_0 = 0$ $x_1 = 1$	$ \begin{vmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\-1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix} - \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}) = \frac{ 00\rangle - 11\rangle}{\sqrt{2}} $	$\begin{bmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\-1\\0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix} - \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}) = \frac{ 01\rangle - 10\rangle}{\sqrt{2}}$	

Xref: Quantum Computation and Quantum Information (Nielson and Chuang 2010, Page 26)

1.2.4 Teleportation



$$Let \ |\psi\rangle = \alpha \, |0\rangle + \beta \, |1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$|\psi_{0}\rangle = |\psi\rangle \otimes |\beta_{00}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ 0 \\ 0 \\ 1 \\ \beta \times \begin{pmatrix} \alpha \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ 0 \\ 0 \\ \alpha \\ \beta \\ 0 \\ 0 \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} (\alpha(|000\rangle + |011\rangle) + \beta(|100\rangle + |111\rangle)), \text{ (exercise: verify)}$$

$$|\psi_1\rangle = (CNOT_{2qb} \otimes I_{1qb}) \, |\psi_0\rangle = (\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}) \, |\psi_0\rangle = \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0 & 0 & 0 \\ 0 & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0 & 0 \\ 0 & 0 & 0 & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & |\psi_0\rangle \\ 0 & 0 & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & 0 \end{pmatrix} |\psi_0\rangle$$

$$|\psi_2\rangle = (H_{1qb} \otimes I_{1qb} \otimes I_{1qb}) |\psi_1\rangle = \left(\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right) |\psi_1\rangle$$

$$= \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}) |\psi_1\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}) |\psi_1\rangle$$

$$=\frac{1}{2}\begin{pmatrix}1&0&0&0&1&0&0&0\\0&1&0&0&0&1&0&0\\0&0&1&0&0&0&1&0\\0&0&0&1&0&0&0&1\\1&0&0&0&-1&0&0&0\\0&1&0&0&0&-1&0&0\\0&0&1&0&0&0&-1&0\\0&0&0&1&0&0&0&-1\end{pmatrix}\begin{pmatrix}\alpha\\0\\0\\\alpha\\0\\\beta\\\beta\\\alpha\\-\beta\\-\beta\\\alpha\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\alpha\\\beta\\\beta\\\alpha\\-\beta\\-\beta\\\alpha\end{pmatrix}$$

$$= \frac{1}{2} (\alpha(|000\rangle + |011\rangle + |100\rangle + |111\rangle) + \beta(|001\rangle + |010\rangle - |101\rangle - |110\rangle))$$

$$=\frac{1}{2}(\left|00\right\rangle \left(\alpha \left|0\right\rangle +\beta \left|1\right\rangle \right)+\left|01\right\rangle \left(\alpha \left|1\right\rangle +\beta \left|0\right\rangle \right)+\left|10\right\rangle \left(\alpha \left|0\right\rangle -\beta \left|1\right\rangle \right)+\left|11\right\rangle \left(\alpha \left|1\right\rangle -\beta \left|0\right\rangle \right)\right)$$

1.3 Part II

1.3.1 SWAP

$$\begin{split} & \text{Let } |\alpha\rangle = a_0 \, |0\rangle + a_1 \, |1\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}, \, |\beta\rangle = b_0 \, |0\rangle + b_1 \, |1\rangle = \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \\ & \text{SWAP} |\alpha\beta\rangle = |\beta\alpha\rangle \end{split}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_1 b_0 \\ a_0 b_1 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} b_0 a_0 \\ b_0 a_1 \\ b_1 a_0 \\ b_1 a_1 \end{pmatrix}$$

1.3.2 Toffoli (AND/OR/XOR)

Xref: Quantum Computing for Everyone, Bernhardt 2019, Chapter 6, Page 90~91

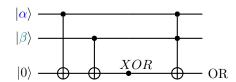
AND

$$\begin{vmatrix} \alpha \rangle & & \\ |\beta \rangle & & \\ |0 \rangle & & & |\gamma \rangle \end{vmatrix} |\psi \rangle$$

$$|\psi\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_0 \beta_0 \\ 0 \\ \alpha_0 \beta_1 \\ 0 \\ 0 \\ \alpha_1 \beta_0 \\ 0 \\ \alpha_1 \beta_1 \\ 0 \end{pmatrix} = \begin{pmatrix} \alpha_0 \beta_0 \\ 0 \\ \alpha_0 \beta_1 \\ 0 \\ 0 \\ \alpha_1 \beta_0 \\ 0 \\ 0 \\ \alpha_1 \beta_1 \end{pmatrix} = \alpha_0 \beta_0 |000\rangle + \alpha_0 \beta_1 |010\rangle + \alpha_1 \beta_0 |100\rangle + \alpha_1 \beta_1 |111\rangle$$

,	$ \beta\rangle = 0\rangle$	$ \beta\rangle = 1\rangle$
12)	$\beta_0 = 1, \beta_1 = 0$	$\beta_0 = 0, \beta_1 = 1$
lpha angle = 0 angle		
$\alpha_0 = 1$	00 <mark>0</mark> >	01 <mark>0</mark> }
$\alpha_1 = 0$		
lpha angle= 1 angle		
$\alpha_0 = 0$	10 <mark>0</mark> }	111
$\alpha_1 = 1$		

OR/XOR



Chapter 2

Quantum Algorithms, Exercises and Advanced Topics

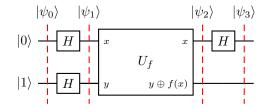
2.1 Deutsch-Jozsa

2.1.1 Deutsch's Algorithm with 1 Qubit

The function f(x) is:

"constant" if regardless the input x, f(x) always produces the same results; i.e. $f(|0\rangle) = f(|1\rangle)$.

"balanced" if for different input x, f(x) produces different results; so $f(|0\rangle) \neq f(|1\rangle)$.



The Deutsch's algorithm:

- 1. Design the oracle U_f according to f(x) so that $U_f | x, y \rangle = | x, y \otimes f(x) \rangle$. It can be one of the four circuits below.
- 2. By looking at the state of 1st qubit of output of the circuit $(H \otimes I)U_f(H \otimes H)(|0\rangle \otimes |1\rangle)$ (i.e. $|\psi_3\rangle$ in the diagram above), can determine whether f(x) is constant or balanced. ¹

$$|\psi_1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} = \frac{|00\rangle - |01\rangle + |10\rangle - |11\rangle}{2} = \frac{1}{2} \begin{pmatrix} 1\\ -1\\ 1\\ -1 \end{pmatrix}$$

 $^{^{1}|\}alpha\beta\rangle = |\alpha\rangle |\beta\rangle = |\alpha\rangle \otimes |\beta\rangle$

For
$$f(x) = |0\rangle$$
,
$$|\psi_0\rangle \quad |\psi_1\rangle \quad U_f \quad |\psi_2\rangle \quad |\psi_3\rangle$$
$$|0\rangle \quad H \quad H$$

$$|\psi_2\rangle = |\psi_1\rangle$$

$$|\psi_{3}\rangle = \frac{1}{2\sqrt{2}} \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 \\ 0 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 0 \\ 0 & 1 \end{pmatrix} & -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix} = \frac{|00\rangle - |01\rangle}{\sqrt{2}} = |\mathbf{0}\rangle \otimes |-\rangle$$

For
$$f(x) = |1\rangle$$
,
$$|\psi_0\rangle \quad |\psi_1\rangle \quad U_f \quad |\psi_2\rangle \quad |\psi_3\rangle$$
$$|0\rangle \quad H \quad H \quad H$$

$$|\psi_2\rangle = (I \otimes X) |\psi_1\rangle = \frac{1}{2} \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0 \\ 0 & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}$$

$$|\psi_3\rangle = -\frac{|00\rangle - |01\rangle}{\sqrt{2}} = |0\rangle \otimes (-|-\rangle)^2$$

For
$$f(x) = x$$
,
$$|\psi_0\rangle \quad |\psi_1\rangle \quad U_f \quad |\psi_2\rangle \quad |\psi_3\rangle$$
$$|0\rangle \quad H \quad H$$

$$|\psi_2\rangle = CNOT |\psi_1\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

$$|\psi_{3}\rangle = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = \frac{|10\rangle - |11\rangle}{\sqrt{2}} = |\mathbf{1}\rangle \otimes |-\rangle$$

 $^{|^2|}q\rangle=\cos{\theta\over2}\,|0\rangle+e^{i\phi}\sin{\theta\over2}\,|1\rangle$: with $-|q\rangle$, $\frac{\theta}{2}$ turns 180°, i.e. θ turns 360°.

For
$$f(x) = x \oplus |1\rangle = \overline{x}$$
, $|\psi_0\rangle \quad |\psi_1\rangle \quad |\psi_f\rangle \quad |\psi_2\rangle \quad |\psi_3\rangle$

$$|0\rangle \quad H \quad H \quad H$$

$$U_f$$

$$|\psi_2\rangle = (I \otimes X) |\psi_f\rangle = \frac{1}{2} \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0 \\ 0 & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix}$$

$$|\psi_3\rangle = |1\rangle \otimes (-|-\rangle)$$

Observation

In order to reflect the balanced nature of the function, the oracle brings the data and target qubits into entanglement whereas the oracles for the constant functions do not, thus with the oracles for constant functions, the second Hadamard gate brings the qubit back to it's original state $|0\rangle$.

The CZ Oracle

$$|\psi_0\rangle \quad |\psi_1\rangle \quad U_f \quad |\psi_2\rangle \quad |\psi_3\rangle$$

$$|0\rangle \quad H \quad H$$

$$|1\rangle \quad H$$

$$|\psi_2\rangle = CZ |\psi_1\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ 1 \end{pmatrix}$$

$$|\psi_3\rangle = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

... Implementation of 1-Qubit Deutsch's Algorithm with Qiskit (Next Page)

djqskt

October 10, 2021

Qiskit 實作: Deutsch-Josza 2021 (CC BY-NC-SA 4.0) Elton Huang

```
[1]: from ezqc import *
     from math import pi
     # 定義 the Deutsch's Algorithm
     def dj1 (uf):
         qc = EzQC (2)
         qc.set_qubits ([(0, 0), (1, 1)], bb = False)
         qc.h (0)
         qc.h (1)
         qc.barrier ()
         uf (qc)
         qc.barrier ()
         qc.h (0)
         qc.measure (0, 0)
         qc.draw("mpl")
         return ('constant' if list (run_real (qc, shots = 1).keys())[0][1] == '0'
      →else 'balanced')
          # 理論上只跑一次就夠了,會回傳: {'0x': 1} (results of lower qubit indices, \square
      →top of circuit plots, on the right)
          # q1 is of value ket-0 due to no measurement (Todo: verify)
    uf1c00: f(x) = |0\rangle, constant
    uf1c01: f(x) = |0\rangle, constant
    uf1c10: f(x) = |1\rangle, constant
    uf1b00: f(x) = x, balanced
    uf1b10: f(x) = x \oplus |1\rangle = \overline{x}, balanced
```

```
[2]: # 定義 1 qubit 的 4 種 Uf (oracles)

def uf1c00 (qc): # constant
    pass

def uf1c01 (qc): # constant
```

```
qc.p (pi, 1)
                  def uf1c10 (qc): # constant
                                qc.x (1)
                  def uf1b00 (qc): # balanced
                                 qc.cnot (0, 1)
                  # def uf1b01 (qc): # balanced?
                  # qc.cz (0, 1)
                  def uf1b10 (qc): # balanced
                                 qc.cnot (0, 1)
                                 qc.x (1)
[4]: from random import shuffle
                  # 將 4 個 Uf 存到一個 list 中,並註記名稱
                  uf1s = [ ('uf1c00', uf1c00), ('uf1c10', uf1c10), ('uf1b00', uf1b00), ('uf1b10', uf1c10', uf
                     ouf1b10),
                                                    ('uf1c01', uf1c01) ] #, ('uf1b01', uf1b01) ]
                  # 4 個 Uf 隨機排序
                  shuffle (uf1s)
                  # 看看 dj1 是否能做出正確判斷
                  for name, orcl in uf1s:
                                 print ()
                                 print (name + ": " + dj1 (orcl))
               The best backend is ibmq_belem 5 qubit(s)
               Job Status: job has successfully run
               uf1c01: constant
               The best backend is ibmq_belem 5 qubit(s)
               Job Status: job has successfully run
               uf1c10: constant
```

2

The best backend is ibmq_belem 5 qubit(s) Job Status: job has successfully run

The best backend is ibmq_belem 5 qubit(s) Job Status: job has successfully run

The best backend is ibmq_belem 5 qubit(s)

uf1c00: constant

uf1b00: balanced

Job Status: job has successfully run

uf1b10: balanced











0.0.1 Study CZ Orcale

[2]:

$$|\psi_0\rangle = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}$$

 $q_1 \otimes q_0$, swap the middle to match $q_0 \otimes q_1$

```
[3]: qc.h (0)
qc.h (1)
qc.barrier ()
Statevector.from_instruction(qc).draw("latex", prefix="|\psi_1\\rangle = ")
```

[3]:

$$|\psi_1
angle = egin{bmatrix} rac{1}{2} & rac{1}{2} & -rac{1}{2} & -rac{1}{2} \end{bmatrix}$$

[4]: qc.cz (0, 1)
qc.barrier ()
Statevector.from_instruction(qc).draw("latex", prefix="|\psi_2\\rangle = ")

[4]:

$$|\psi_2
angle = egin{bmatrix} rac{1}{2} & rac{1}{2} & -rac{1}{2} & rac{1}{2} \end{bmatrix}$$

[5]: qc.h (0)
Statevector.from_instruction(qc).draw("latex", prefix="|\psi_3\\rangle = ")

[5]:

$$|\psi_3\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

[7]: qc.draw("mpl");



2.1.2 Deutsch-Josza Algorithm with 2 Qubits

1. bring all qubits to superpositions

$$|\psi_1\rangle = (H \otimes H \otimes H) |001\rangle = \frac{1}{\sqrt{2}} (+|000\rangle - |001\rangle + |010\rangle - |011\rangle + |100\rangle - |101\rangle + |110\rangle - |111\rangle)$$

Constant

For $f(x^{\otimes 2}) = |0\rangle$,

2. apply oracle

$$|\psi_2\rangle = |\psi_1\rangle$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = (H \otimes H \otimes I) |\psi_2\rangle = \frac{1}{\sqrt{2}^1} (+|000\rangle - |001\rangle)$$

For $f(x^{\otimes 2}) = |1\rangle$,

2. apply oracle

$$|\psi_2\rangle = (I \otimes I \otimes X) |\psi_1\rangle = \frac{1}{\sqrt{2}^3} (-|000\rangle + |001\rangle - |010\rangle + |011\rangle - |100\rangle + |101\rangle - |110\rangle + |111\rangle)$$

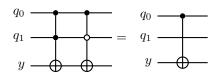
3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(-|000\rangle + |001\rangle)$$

Balanced

For $f(|11\rangle) = f(|10\rangle) = |1\rangle$

Note: $y \oplus |1\rangle = \overline{y}$, so the oracle is



(Note this is just the oracle, it needs to be plugged into the circuit with the Hadamard gates before and after according to the Deutsch-Josza algorithm)

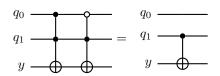
2. apply oracle

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3} (+|000\rangle - |001\rangle + |010\rangle - |011\rangle - |100\rangle + |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1} (+|100\rangle - |101\rangle)$$

For
$$f(|11\rangle) = f(|01\rangle) = |1\rangle$$



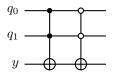
2. apply oracle

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle - |010\rangle + |011\rangle + |100\rangle - |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(+|010\rangle - |011\rangle)$$

For $f(|11\rangle) = f(|00\rangle) = |1\rangle$



2. apply oracle

$$\begin{split} |\psi_2\rangle &= \tfrac{1}{\sqrt{2}^3}(-|000\rangle + |001\rangle + |010\rangle - |011\rangle + |100\rangle - |101\rangle - |110\rangle + |111\rangle)\\ \text{3. apply } H^{\otimes 2} \text{ to the data qubits} \end{split}$$

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(-|110\rangle + |111\rangle)$$

Next Page: Matrix Works

dj2

October 10, 2021

0.1 Two-Qubit Deutsch-Josza

2021 (CC BY-NC-SA 4.0) Elton Huang

```
[1]: from importlib import reload
  import numpy as np
  from IPython.display import display, Math
  import qmtx as qm
  import ezqc
  reload (qm)
  reload (ezqc)
```

[1]: <module 'ezqc' from '/Volumes/extra0/elton4k12/spqc/ezqc.py'>

0.2 Constant

- **0.2.1** For $f(x^{\otimes 2}) = |0\rangle$,
 - 1. bring all qubits to superpositions

$$|\psi_1\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle + |010\rangle - |011\rangle + |100\rangle - |101\rangle + |110\rangle - |111\rangle)$$

2. apply orcale

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle + |010\rangle - |011\rangle + |100\rangle - |101\rangle + |110\rangle - |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(+|000\rangle - |001\rangle)$$

0.2.2 For $f(x^{\otimes 2}) = |1\rangle$

2. apply oracle

[5]: psi2 = np.dot (qm.kron3 (qm.i1, qm.i1, qm.x1), psi1) qm.ket3 (psi2, "\\psi_2")

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(-|000\rangle + |001\rangle - |010\rangle + |011\rangle - |100\rangle + |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

[6]: psi3 = np.dot (qm.kron3 (qm.h1, qm.h1, qm.i1), psi2) qm.ket3 (psi3, "\\psi_3")

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(-|000\rangle + |001\rangle)$$

0.3 Balanced

0.3.1 For
$$f(|11\rangle) = f(|10\rangle) = |1\rangle$$

note: $y \oplus |1\rangle = \overline{y}$

2. apply oracle

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle + |010\rangle - |011\rangle - |100\rangle + |101\rangle - |110\rangle + |111\rangle)$$

[8]: # simplified
 psi2s = np.dot (qm.cix, psi1)
 qm.ket3 (psi2s, "\\psi_{2s}\", raw=False)

$$|\psi_{2s}\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle + |010\rangle - |011\rangle - |100\rangle + |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

[9]: psi3 = np.dot (qm.kron3 (qm.h1, qm.h1, qm.i1), psi2)
qm.ket3 (psi3, "\\psi_3", raw=False)

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(+|100\rangle - |101\rangle)$$

```
0.3.2 For f(|11\rangle) = f(|01\rangle) = |1\rangle
```

2. apply oracle

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(+|000\rangle - |001\rangle - |010\rangle + |011\rangle + |100\rangle - |101\rangle - |110\rangle + |111\rangle)$$

[11]: qm.ket3 (np.dot (qm.icx, psi1), "\\psi_{2s}\", raw=False)
simplified

$$|\psi_{2s}\rangle = \frac{1}{\sqrt{2}^3} (+|000\rangle - |001\rangle - |010\rangle + |011\rangle + |100\rangle - |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(+|010\rangle - |011\rangle)$$

0.3.3 For
$$f(|11\rangle) = f(|00\rangle) = |1\rangle$$

2. apply oracle

$$|\psi_2\rangle = \frac{1}{\sqrt{2}^3}(-|000\rangle + |001\rangle + |010\rangle - |011\rangle + |100\rangle - |101\rangle - |110\rangle + |111\rangle)$$

3. apply $H^{\otimes 2}$ to the data qubits

$$|\psi_3\rangle = \frac{1}{\sqrt{2}^1}(-|110\rangle + |111\rangle)$$

... 3-Qubit Matrix Work (Next Page)

3qbgates

October 10, 2021

0.1 3-Qubit Gate Matrix Works

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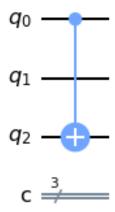
```
[1]: from importlib import reload
  import numpy as np
  from IPython.display import display, Math
  import qmtx as qm
  import ezqc
  reload (qm)
  reload (ezqc)
```

[1]: <module 'ezqc' from '/Volumes/extra0/elton4k12/spqc/ezqc.py'>

What are the matrices for the following 3-qubit gate $(q_i = \alpha_i | 0 \rangle + \beta_i | 1 \rangle)$

0.1.1 Gate 1

```
[2]: cix = ezqc.EzQC (3)
  cix.cx (0, 2)
  cix.draw (output="mpl"); # semicolon to workaround draw twice bug
```



For the circuit below,

```
[3]: icx = ezqc.EzQC (3)
icx.cx (1, 2)
icx.draw ("mpl");
```



the corresponding matrix follows ...

```
\alpha_0 \alpha_1 \alpha_2
       +1 0
                         0
                                 0
                                          0
                                                  0
                                                          0
                                                                     \alpha_0\alpha_1\beta_2
                                                          0
             0 + 1 0 0
                                                                     \alpha_0 \beta_1 \alpha_2
0
             +1 \quad 0 \quad 0 \quad 0
                                                                     \alpha_0\beta_1\beta_2
0
               0
                               +1 	 0
                        0
                                               0
                                                          0
                                                                      \beta_0 \alpha_1 \alpha_2
0
                                       +1
                                                0
                                                          0
                                                                      \beta_0 \alpha_1 \beta_2
                                          0
                                                  0
                                                                      \beta_0\beta_1\alpha_2
                                                                      \beta_0\beta_1\beta_2
```

Switching q_0 and q_1 :

```
000)
          (000)
001
           001
010
          100
          101
011
100
          010
101
          011
110
          110
\langle 111 \rangle
          111/
```

Effectively rows 3 and 5 switch and rows 4 and 6 switch respectively.

So the matrix for qc is qc0 with rows columns and 3 and 5 switch and row columns 4 and 6 switch respectively. (striked after verified with Qiskit)

So the matrix for cix is ...

```
[6]: cixm = icxm.copy()
cixm [[2, 4], :] = cixm [[4, 2], :]
cixm [[3, 5], :] = cixm [[5, 3], :]
qm.dumpgates ([cixm])
```

```
0
                              0
                                      0
                                              0
       0
               0
                                                      0
                                                               (\alpha_0\alpha_1\alpha_2)
      +1
               0
                       0
                              0
                                      0
                                              0
                                                     0
                                                               \alpha_0 \alpha_1 \beta_2
0
       0
               0
                       0
                             +1
                                    0
                                              0
                                                     0
                                                               \alpha_0\beta_1\alpha_2
0
      0
               0
                      0
                                                     0
                              0
                                    +1
                                             0
                                                               \alpha_0 \beta_1 \beta_2
0
       0
               0
                     +1
                                    0
                                              0
                                                     0
                            0
                                                                \beta_0 \alpha_1 \alpha_2
0
       0
                      0
                                      0
                                             0
                                                     0
              +1
                              0
                                                               \beta_0 \alpha_1 \beta_2
0
       0
               0
                                              0
                       0
                              0
                                      0
                                                    +1
                                                                \beta_0\beta_1\alpha_2
0
        0
               0
                       0
                                            +1
                                                     0 ,
                              0
                                                                \beta_0\beta_1\beta_2
```

0.1.2 Gate 2: cox

```
[7]: cox = ezqc.EzQC (3)
cox.x (1)
cox.ccx (0, 1, 2)
cox.x (1)
cox.draw ("mpl");
```



```
[8]: ixim = qm.kron3 (qm.i1, qm.x1, qm.i1) qm.dumpgates ([ixim, qm.ccx, ixim])
```

[9]: front2m = np.dot (ixim, qm.ccx)
qm.dumpgates ([front2m, ixim])

cox

[10]: coxm = np.dot (front2m, ixim)
qm.dumpgates ([coxm])

```
0
                                                                   \alpha_0 \alpha_1 \alpha_2
                0
                        0
                                0
                                        0
                                                0
                                                        0
                                                                   \alpha_0 \alpha_1 \beta_2
              +1 	 0
                                        0
                                                        0
                                                                   \alpha_0\beta_1\alpha_2
               0
                     +1
                                                                   \alpha_0 \beta_1 \beta_2
                               0
                                                0
                                                        0
     0
               0
                       0
                             0 + 1
                                             0
                                                        0
                                                                   \beta_0 \alpha_1 \alpha_2
0
                0
                       0
                                     0
                              +1
                                               0
                                                        0
                                                                   \beta_0 \alpha_1 \beta_2
                                0
                                        0
                                                        0
                                               +1
                                                                   \beta_0\beta_1\alpha_2
                0
                                0
                                        0
                                                0
                                                       +1
                                                                   \beta_0\beta_1\beta_2
```

compare ccx

[11]: qm.dumpgates ([qm.ccx])

```
(\alpha_0\alpha_1\alpha_2)
                0
                                                                   \alpha_0 \alpha_1 \beta_2
                        0
                                0
                                                0
                                                        0
                                        0
             +1 	 0
                                0
                                        0
                                                0
                                                        0
                                                                   \alpha_0 \beta_1 \alpha_2
             0
                      +1
                                     0
                                                        0
                                                                   \alpha_0 \beta_1 \beta_2
0
               0
                       0
                              +1
                                     0
                                                0
                                                        0
                                                                   \beta_0 \alpha_1 \alpha_2
0
        0
                0
                       0
                               0
                                      +1
                                              0
                                                        0
                                                                   \beta_0 \alpha_1 \beta_2
                0
                        0
                                0
                                       0
                                                0
                                                       +1
                                                                   \beta_0\beta_1\alpha_2
                        0
                                0
                                        0
                                               +1
                                                        0 ,
                                                                   \beta_0\beta_1\beta_2
```

0.1.3 Gate 3: ocx



```
[13]: xiim = qm.kron3 (qm.x1, qm.i1, qm.i1)
front2m = np.dot (xiim, qm.ccx)
qm.dumpgates ([np.dot (front2m, xiim)])
```

```
0
                                                                    \alpha_0 \alpha_1 \alpha_2
                        0
                                                 0
                                                         0
                                                                    \alpha_0 \alpha_1 \beta_2
      0 \quad 0 \quad +1 \quad 0
                                                                    \alpha_0\beta_1\alpha_2
    \alpha_0 \beta_1 \beta_2
0
                                              0
                                                         0
                                                                    \beta_0 \alpha_1 \alpha_2
               0
                       0
                                0
                                      +1
                                              0
                                                         0
                                                                    \beta_0 \alpha_1 \beta_2
                                                +1
                                                                    \beta_0\beta_1\alpha_2
                                         0
                                                0
                                                        +1/
                                                                    \beta_0\beta_1\beta_2
```

0.1.4 Gate 4: oox

```
[14]: cox = ezqc.EzQC (3)
    cox.x (0)
    cox.x (1)
    cox.ccx (0, 1, 2)
    cox.x (0)
    cox.x (1)
    cox.x (1)
```



```
[15]: xxim = qm.kron3 (qm.x1, qm.x1, qm.i1)
front2m = np.dot (xxim, qm.ccx)
qm.dumpgates ([np.dot (front2m, xxim)])
```

$$\begin{pmatrix} 0 & +1 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & +1 \end{pmatrix} \begin{pmatrix} \alpha_0 \alpha_1 \alpha_2 \\ \alpha_0 \alpha_1 \beta_2 \\ \alpha_0 \beta_1 \alpha_2 \\ \alpha_0 \beta_1 \beta_2 \\ \beta_0 \alpha_1 \alpha_2 \\ \beta_0 \alpha_1 \beta_2 \\ \beta_0 \beta_1 \alpha_2 \\ \beta_0 \beta_1 \beta_2 \end{pmatrix}$$

 \dots Implementation of 2-Qubit Deutsch-Josza with Qiskit (Next Page)

dj2qskt

October 10, 2021

Qiskit 實作: Deutsch-Josza 2021 (CC BY-NC-SA 4.0) Elton Huang

```
[1]: from ezqc import *
     # 定義 the Deutsch's Algorithm
     def dj2b (uf, shots = 1): # returns True if balanced
         qc = EzQC (3)
         qc.set\_qubits ([(0, 0), (1, 0), (2, 1)], bb = False)
         for i in range (3):
             qc.h (i)
         qc.barrier ()
         uf (qc)
         qc.barrier ()
         qc.h (0)
         qc.h (1)
         qc.measure (0, 0)
         qc.measure (1, 1)
         if shots == 1:
             runres = sorted (run_sim (qc, shots = shots).items(), key=lambda item:
      \rightarrowitem[1])
         else:
             runres = sorted (run_real (qc, shots = shots).items(), key=lambda item:
      \rightarrowitem[1])
             # 跑數次取多數決,因為會有雜訊所造成的誤差了
             # 會回傳: {'Oxx': 1} (results of lower qubit indices, top of circuit_
      \rightarrowplots, on the right)
             # q2 is of value ket-0 due to no measurement (Todo: verify, done -\Box
      \rightarrowmeasure 1)
             print (runres, "\n")
         return (False if runres [-1][0] == '000' else True)
```

```
name 名稱
                 function 函數
                                                    prpperty 性質
                 f(x^{\otimes 2}) = |0\rangle
uf2c0
                                                    constant
uf2c1
                 f(x^{\otimes 2}) = |1\rangle
                                                    constnat
uf2b101
                 f(|11\rangle) = f(|10\rangle) = |1\rangle
                                                    balanced
                 f(|11\rangle) = f(|10\rangle) = |1\rangle
uf2b101s
                                                    balanced
                 f(|11\rangle) = f(|01\rangle) = |1\rangle
uf2b011
                                                    balanced
                 f(|11\rangle) = f(|01\rangle) = |1\rangle
                                                    balanced
uf2b011s
                 f(|11\rangle) = f(|00\rangle) = |1\rangle
uf2b001
                                                    balanced
                 f(|11\rangle) = f(|10\rangle) = |0\rangle
uf2b100
                                                    balanced
                 f(|11\rangle) = f(|10\rangle) = |0\rangle
                                                    balanced
uf2b100s
uf2b010
                 f(|11\rangle) = f(|01\rangle) = |0\rangle
                                                    balanced
                 f(|11\rangle) = f(|01\rangle) = |0\rangle
                                                    balanced
uf2b010s
                 f(|11\rangle) = f(|00\rangle) = |0\rangle
uf2b000
                                                    balanced
```

```
[2]: # 定義 1 qubit 的 4 種 Uf (oracles)
     def uf2c0 (qc): # constant
         pass
     def uf2c1 (qc): # constant
         qc.x (2)
     def uf2b101 (qc): # balanced
         qc.ccx (0, 1, 2)
         qc.x (1)
         qc.ccx (0, 1, 2)
         qc.x (1)
     def uf2b100 (qc): # balanced
         uf2b101 (qc)
         qc.x (2)
     def uf2b011 (qc): # balanced
         qc.ccx (0, 1, 2)
         qc.x (0)
         qc.ccx (0, 1, 2)
         qc.x(0)
     def uf2b010 (qc): # balanced
         uf2b011 (qc)
         qc.x (2)
     def uf2b101s (qc): # balanced
         qc.cx (0, 2)
     def uf2b100s (qc): # balanced
```

```
uf2b101 (qc)
    qc.x (2)
def uf2b011s (qc): # balanced
   qc.cx (1, 2)
def uf2b010s (qc): # balanced
   uf2b011 (qc)
   qc.x (2)
def uf2b000 (qc): # balanced
   qc.ccx (0, 1, 2)
   qc.x (0)
   qc.x (1)
   qc.ccx (0, 1, 2)
   qc.x (0)
   qc.x (1)
def uf2b001 (qc): # balanced
   uf2b000 (qc)
   qc.x (2)
```

uf2c0: Correct
uf2c1: Correct
uf2b101: Correct
uf2b100: Correct
uf2b011: Correct
uf2b010: Correct
uf2b101s: Correct
uf2b100s: Correct
uf2b101s: Correct
uf2b011s: Correct
uf2b011s: Correct
uf2b010s: Correct
uf2b010s: Correct
uf2b010s: Correct

```
[4]: import sympy as sp
     # 8 個 Uf 隨機排序
     shuffle (uf2s)
     # 看看今天跑到幾個 shots 才能全對
     sh = 3
     while True:
        print ("shots: " + str (sh) + "\n")
        incorrect = 0
        for name, orcl, expb in uf2s:
            print (name)
            if dj2b (orcl, shots = sh) != expb:
                 incorrect += 1
                 break
         # print (sh, "shots: 錯", incorrect, "個")
         if incorrect == 0:
            print (sh, "shots 完成")
            break
         else:
            sh = sp.nextprime (sh)
    shots: 3
    uf2b100s
    The best backend is ibmq_belem 5 qubit(s)
    Job Status: job has successfully run
    [('000', 1), ('001', 2)]
    uf2b000
    The best backend is ibmq_belem 5 qubit(s)
    Job Status: job has successfully run
    [('011', 3)]
    uf2b011s
    The best backend is ibmq_belem 5 qubit(s)
    Job Status: job has successfully run
    [('010', 3)]
    uf2b011
    The best backend is ibmq_belem 5 qubit(s)
    Job Status: job has successfully run
    [('001', 1), ('010', 1), ('011', 1)]
```

uf2c1

[('000', 3)]

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run

uf2b010s

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 1), ('010', 2)]

uf2b001

The best backend is ibmq_lima 5 qubit(s)
Job Status: job has successfully run
[('011', 3)]

uf2c0

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 3)]

uf2b100

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('010', 1), ('000', 2)]

shots: 5

uf2b100s

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 1), ('001', 4)]

uf2b000

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 1), ('001', 1), ('011', 3)]

uf2b011s

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('010', 5)]

uf2b011

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('011', 1), ('001', 2), ('010', 2)]

uf2c1

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 5)]

```
uf2b010s
```

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('001', 1), ('010', 2), ('011', 2)]

uf2b001

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 1), ('010', 2), ('011', 2)]

uf2c0

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 5)]

uf2b100

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('011', 2), ('001', 3)]

uf2b101

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('000', 1), ('010', 1), ('011', 1), ('001', 2)]

uf2b010

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('010', 2), ('011', 3)]

uf2b101s

The best backend is ibmq_belem 5 qubit(s)
Job Status: job has successfully run
[('001', 5)]

5 shots 完成

2.2 More Oracle-Based

2.2.1 Berstein-Vazirani

2.2.2 Simon

2.3 Grover's

- Why is it phase?
- How does it work?

 $Quantum\ Computing\ for\ Everyone\ {\it Page}\ 179:$

- flips about the mean
- \bullet CZ, the matrix reversable operations: controlling and controlled no-differently entangled

2.4 Exercise: Superposition

$$|1\rangle + |2\rangle + |3\rangle + |7\rangle \longrightarrow \boxed{f(x) = 2x} \longrightarrow |2\rangle + |4\rangle + |6\rangle + |14\rangle$$

$$\frac{1}{2}(|0001\rangle + |0010\rangle + |0011\rangle + |0111\rangle) \longrightarrow \boxed{f(x) = 2x} \longrightarrow \frac{1}{2}(|0010\rangle + |0100\rangle + |0110\rangle + |1110\rangle)$$

Lee et. al, $\mathit{Quantum~Shift~Register},\,2001$

2.5 Quantum Circuit Synthesis

Shende et. al, Synthesis of Quantum Logic Circuits

Page 2 bottom

Page 5 top §2.1 end: $2^3 = 8 \gg 2^1 + 2^2 = 5$

"Much interest in quantum computing is driven by this exponential scaling of the state space, and the loss of independence between different subsystems is called $quantum\ entanglement$."

 ${\bf Matteo},\ Parallelizing\ quantum\ circuit\ synthesis,\ 2015$

Chapter 3

Applications¹

IBM Quantum Challenge Africa 2021 IBM Quantum Challenge 2021

3.1 Optimization

- 3.1.1 Quadratic Problems with Qiskit
- 3.1.2 Knapsack with Ocean

3.2 Monte Carlo Method

Monte Carlo Method

¹... to appreciate the values

3.3 Machine Learning

Quantum's advantage solves black box bit riddle

Demonstration of quantum advantage in machine learning

3.3.1 Qiskit ML

IBM Quantum Challenge Fall 2021 Challenge $3\mathrm{c}$

 \bullet Multi-class classifiers with binary classifiers

One-vs-Rest: one classifier for each class: N classifiers (vs. binary tree: N-1 classifiers)

One-vs-One: $\frac{N(N-1)}{2}$ pairs

3.3.2 TensorFlow Quantum

3.4 Chemical Simulation

"every finitely realizable physical system can be perfectly simulated by a universal model computingmachine operating by finite means'. Classical physics and the universal Turing machine, because the former is continuous and the latter discrete, do not obey the principle, at least in the strong form above." - D. Deutsch 1985

Exploring greener approaches to nitrogen fixation: 103 electrons in 71 orbitals

Protein crystallization

- sequence \rightarrow predict shapes
- shape analysis
- hybrid: e.g. 高能物理的方式預測 interactions

3.4.1 Molecular Dynamics with Qiskit

3.4.2 Published Works

On the construction of model Hamiltonians for adiabatic quantum computation and its application to finding low energy conformations of lattice protein models, 2008

Finding low-energy conformations of lattice protein models by quantum annealing, 2012

 $Quantum\ annealing\ versus\ classical\ machine\ learning\ applied\ to\ a\ simplified\ computational\ biology\ problem,\ 2018$

Quantum Molecular Unfolding, Mente AI, 2021

- shape, reactivity: shape \rightarrow reactivity \rightarrow energy cost
- approach assumption: pocket rigid, ligand flexible
- fixed length chemical bonds with a subset *rotatable* (torsionals) which split the molecule in two nonempty disjointed fragments, when virtually removed
- 3 phases in Molecular Docking: (1) Ligand expansion, (2) Initial Placement and (3) Shape Refinement inside the pocket

Molecular Unfolding find the unfolded shape of the ligand (torsion configuration) that maximizes the total sum of internal distances between pairs of atoms in the ligand (molecular volume).

Designing Peptides on a Quantum Computer, 2019

Förster resonance energy transfer: Role of diffusion of fluorophore orientation and separation in observed shifts of FRET efficiency, 2017

Efficient quantum simulation of photosynthetic light harvesting, 2018

3.4.3 OpenFermion

Chapter 4

Explore and Exercise

4.1 IBM Quantum Errors

Noise is one of the utmost problems with Quantum Computer hardware technology presently.

This exercise demonstrates how to check the map of error rates for each qubits in an IBM Qunatum computer with Qiskit and a brief example to verify it.

Further indepth exercise may involve Qiskit-Pulse, the pulse-level programming kit.

(Next page)

errors

October 7, 2021

Explore and Exercise: *Errors* 2021 (CC BY-NC-SA 4.0) Elton Huang

```
[1]: from qiskit import *
  from qiskit.visualization import plot_error_map
  IBMQ.load_account() # ezqc.SetCloud()
  backend = IBMQ.get_provider('ibm-q').get_backend('ibmq_lima')
  plot_error_map(backend)
```

[1]:

ibmq_lima Error Map



qiskit.compiler.transpile: initial_layout qiskit.result.Result.get_counts: measured states of the vector of qubits

```
[2]: from qiskit.tools.monitor import job_monitor
     def runiton (qc, res, phqb):
         global backend
         qc_trans = transpile(qc, backend, initial_layout=[phqb],__
      →optimization_level=3)
         job = backend.run(qc_trans, shots=8192)
         # print(job.job_id())
         job_monitor(job)
         output = job.result().get_counts()
         print('Run with qubit #' + str (phqb))
         print('Probability of correct answer : {:.2f}'.format(output[res]/8192))
[3]: qc0 = QuantumCircuit(1, 1)
     qc0.reset(0)
     qc0.measure(0, 0)
     qcx = QuantumCircuit(1, 1)
     qcx.reset(0)
     qcx.x(0)
     qcx.measure(0, 0)
[3]: <qiskit.circuit.instructionset.InstructionSet at 0x7f1760070d00>
[4]: for qc, res in [ (qc0, '0'), (qcx, '1') ]:
         display (qc.draw())
         for i in range (backend.configuration().n_qubits):
```



Job Status: job has successfully run Run with qubit #0
Probability of correct answer : 0.99
Job Status: job has successfully run Run with qubit #1
Probability of correct answer : 1.00

runiton (qc, res, i)

Job Status: job has successfully run

Run with qubit #2

Probability of correct answer : 1.00 Job Status: job has successfully run

Run with qubit #3

Probability of correct answer: 0.99 Job Status: job has successfully run

Run with qubit #4

Probability of correct answer: 0.99



Job Status: job has successfully run

Run with qubit #0

Probability of correct answer : 0.96 Job Status: job has successfully run

Run with qubit #1

Probability of correct answer : 0.97 Job Status: job has successfully run

Run with qubit #2

Probability of correct answer : 0.97 Job Status: job has successfully run

Run with qubit #3

Probability of correct answer : 0.95 Job Status: job has successfully run

Run with qubit #4

Probability of correct answer : 0.82

4.2 Virtual Quantum Optics Laboratory

The Virtual Quantum Optics Laboratory

Appendices

Appendix A

ezqc.py

```
# EzQC Library
    # 2021 (CC BY-NC-SA 4.0) Elton Huang
    import numpy as np
    from qiskit import * # QuantumCircuit, transpile, IBMQ
    from qiskit.providers.aer import QasmSimulator
    # from qiskit.visualization import plot_histogram
    import matplotlib.pyplot as plt
    from qiskit.providers.ibmq import least_busy
10
    from qiskit.tools.monitor import job_monitor
12
13
    bCloudYet2Set = True
14
    def SetCloud ():
15
        global provider, bCloudYet2Set
16
        while True:
17
            try:
18
                 # print ("loading IBMQ account ...")
19
                provider = IBMQ.load_account()
20
                break
21
            except:
22
                 IBMQ.save_account (input ("IBMQ Token:"))
23
        bCloudYet2Set = False
24
25
    def run_sim (circuit, shots = 1024):
26
        simulator = QasmSimulator()
27
        compiled_circuit = transpile (circuit, simulator)
28
        counts = simulator.run (compiled_circuit, shots = shots).result().get_counts (compiled_circuit)
29
        # print("\nResults:",counts)
30
31
        return (counts)
32
    def run_real (circuit, shots = 1024): # real hw?
33
        global bCloudYet2Set
34
        if 'google.colab' in sys.modules:
35
            print ("You are on Google Colab. Switching to simulation ...")
36
            return (run_sim (circuit))
37
38
            if bCloudYet2Set:
39
40
            devices = provider.backends (filters = lambda x: x.configuration().n_qubits > circuit.num_qubits
41
                                                          and not x.configuration().simulator
42
                                                          and x.name() not in ['ibmq_bogota'], simulator = False)
43
             # bogota: borken
44
             if len (devices) == 0: # not necessary, bm: sim_stab 200s, colab/min 2mins
45
                 devices = provider.backends (filters = lambda x: x.configuration().n_qubits > circuit.num_qubits
46
```

```
and x.name() not in ['ibmq_bogota'], simulator = False)
             # print (devices)
48
             backend = least_busy (devices)
49
             print ("The best backend is", backend, backend.configuration().n_qubits, "qubit(s)")
50
             job = execute (circuit, backend = backend, shots = shots)
51
             job_monitor (job, interval = 5)
52
             result = job.result()
53
             counts = result.get_counts(circuit)
54
             # print("\nResults:",counts)
55
             return (counts)
56
57
     def plot (counts):
58
         fig = plt.figure(figsize = (10, 5)) # default 6.4x4.8 inches
59
         ax = fig.add_axes([0,0,1,1])
60
         x = sorted (counts.keys(), key=lambda x: int(x, 2))
61
         y = list (counts [i] for i in x)
62
63
         ax.bar (x, y, width = 0.5, color = 'cornflowerblue')
64
         ax.set_ylabel('Frequency')
65
         ax.set_xlabel('Measurement Output')
66
         for i, v in enumerate (y):
             ax.text(i - .25, v + 3, str (v) + " / " + str (round (100 * v / sum (y))) + "%", color='blue', fontweight='bold')
67
68
         plt.show()
69
     class EzQC (QuantumCircuit):
70
71
         def __init__ (self, qbn):
72
             super().__init__ (qbn, qbn)
73
74
         # fb = True to add front barrier
75
         def __fb (self, **kwargs):
76
             if 'fb' in kwargs.keys() and kwargs.get ('fb') == True:
77
                 self.barrier ()
78
79
         # bb = False to omit back barrier
80
         def __bb (self, **kwargs):
81
             if 'bb' not in kwargs.keys() or kwargs.get ('bb') != False:
82
83
                 self.barrier ()
84
         def set_qubits (self, qubit_ketv_pair_list, **kwargs):
85
             self.__fb (**kwargs)
86
             for qb, kv in qubit_ketv_pair_list:
                 self.reset (qb)
                 if kv == 1:
89
                     self.x (qb)
90
             self.__bb (**kwargs)
91
92
         # reset = False for no reset to ket-0
93
         def ghz (self, list3qbs, **kwargs):
94
             self.__fb (**kwargs)
95
             if 'reset' not in kwargs.keys() or kwargs.get ('reset') != False:
96
                 for i in list3qbs:
97
                      self.reset (i)
98
             self.h (list3qbs [0])
99
             self.cx (list3qbs [0], list3qbs [1])
100
             self.cx (list3qbs [0], list3qbs [2])
101
             self.__bb (**kwargs)
102
103
104
         def cox (self, q0, q1, q2, **kargs):
             self.__fb (**kwargs)
105
             self.x (q1)
106
             self.ccx (q0, q1, q2)
             self.x (q1)
             self.__bb (**kwargs)
```

110

```
def measure_all (self, **kwargs):
self.__fb (**kwargs)
self.measure (list (range (self.num_qubits)), list (range (self.num_qubits)))
```

Appendix B

qmtx.py

```
# qmtx Library
    # 2021 (CC BY-NC-SA 4.0) Elton Huang
    import numpy as np
    # from itertools import product
    from IPython.display import display, Math
    import math
    b3string = ['|000\\rangle', '|001\\rangle', '|010\\rangle', '|011\\rangle',
9
                '|100\\rangle', '|101\\rangle', '|110\\rangle', '|111\\rangle']
10
11
    b3kets = ['\\ket{000}', '\\ket{001}', '\\ket{010}', '\\ket{011}',
12
              '\\ket{100}', '\\ket{101}', '\\ket{110}', '\\ket{111}']
13
14
    opr3 = "\begin{pmatrix} \\alpha_0\\alpha_1\\beta_2 \\\ \ \\
15
                             \alpha_0\beta_1 \alpha_2 \\ \alpha_0\beta_1 \\ \
16
                             \\beta_0 \\alpha_1\\alpha_2 \\\\ \\beta_0 \\alpha_1\\beta_2 \\\\ \
17
                             \\beta_0 \\beta_1 \\alpha_2 \\\\ \\beta_0 \\beta_1 \\deta_2 \\end{pmatrix}"
18
19
    ket0 = np.array ( [[1],
20
                       [0]])
21
22
    ket1 = np.array ( [[0],
23
                       [1]])
24
25
    h1 = 1/np.sqrt(2)*np.array([[1, 1],
26
                                [1,-1]])
27
28
    i1 = np.array([[1, 0],
29
                    [0, 1]])
30
    x1 = np.array([[0, 1],
33
                    [1, 0]])
34
    cx = np.array([[1, 0, 0, 0],
35
                    [0, 1, 0, 0],
36
                    [0, 0, 0, 1],
37
                    [0, 0, 1, 0]])
38
39
    ccx = np.array([[1, 0, 0, 0, 0, 0, 0, 0],
40
                     [0, 1, 0, 0, 0, 0, 0, 0],
41
                     [0, 0, 1, 0, 0, 0, 0, 0],
42
                     [0, 0, 0, 1, 0, 0, 0, 0],
43
                     [0, 0, 0, 0, 1, 0, 0, 0],
44
                     [0, 0, 0, 0, 0, 1, 0, 0],
45
                     [0, 0, 0, 0, 0, 0, 0, 1],
46
```

```
[0, 0, 0, 0, 0, 0, 1, 0]])
48
     cox = np.array ([[1, 0, 0, 0, 0, 0, 0, 0],
49
                       [0, 1, 0, 0, 0, 0, 0, 0],
50
                       [0, 0, 1, 0, 0, 0, 0, 0],
51
                       [0, 0, 0, 1, 0, 0, 0, 0],
52
                       [0, 0, 0, 0, 0, 1, 0, 0],
53
                       [0, 0, 0, 0, 1, 0, 0, 0],
54
                       [0, 0, 0, 0, 0, 0, 1, 0],
55
                       [0, 0, 0, 0, 0, 0, 0, 1]])
56
57
     ocx = np.array ([[1, 0, 0, 0, 0, 0, 0, 0],
58
                       [0, 1, 0, 0, 0, 0, 0, 0],
59
                       [0, 0, 0, 1, 0, 0, 0, 0],
60
                       [0, 0, 1, 0, 0, 0, 0, 0],
61
                       [0, 0, 0, 0, 1, 0, 0, 0],
62
                       [0, 0, 0, 0, 0, 1, 0, 0],
63
64
                       [0, 0, 0, 0, 0, 0, 1, 0],
65
                       [0, 0, 0, 0, 0, 0, 1]])
66
67
     oox = np.array ([[0, 1, 0, 0, 0, 0, 0, 0],
68
                       [1, 0, 0, 0, 0, 0, 0, 0],
69
                       [0, 0, 1, 0, 0, 0, 0, 0],
                       [0, 0, 0, 1, 0, 0, 0, 0],
70
                       [0, 0, 0, 0, 1, 0, 0, 0],
71
                       [0, 0, 0, 0, 0, 1, 0, 0],
72
                       [0, 0, 0, 0, 0, 0, 1, 0],
73
                       [0, 0, 0, 0, 0, 0, 0, 1]])
74
75
     icx = np.array([[1, 0, 0, 0, 0, 0, 0, 0],
76
                       [0, 1, 0, 0, 0, 0, 0, 0],
77
                       [0, 0, 0, 1, 0, 0, 0, 0],
78
                       [0, 0, 1, 0, 0, 0, 0, 0],
79
                       [0, 0, 0, 0, 1, 0, 0, 0],
80
                       [0, 0, 0, 0, 0, 1, 0, 0],
81
                       [0, 0, 0, 0, 0, 0, 0, 1],
82
83
                       [0, 0, 0, 0, 0, 0, 1, 0]])
84
     cix = np.array ([[1, 0, 0, 0, 0, 0, 0, 0],
85
                       [0, 1, 0, 0, 0, 0, 0, 0],
86
                       [0, 0, 0, 0, 1, 0, 0, 0],
87
                       [0, 0, 0, 0, 0, 1, 0, 0],
88
                       [0, 0, 0, 1, 0, 0, 0, 0],
89
                       [0, 0, 1, 0, 0, 0, 0, 0],
90
                       [0, 0, 0, 0, 0, 0, 0, 1],
91
                       [0, 0, 0, 0, 0, 0, 1, 0]])
92
93
     def kron3 (q0, q1, q2): # 3 qubits tensor product
94
         return np.kron (np.kron (q0, q1), q2)
95
96
     def ket3 (psi, var, raw=False): # Todo: ket-n
97
         lnn = 0
98
         out = ""
99
         for r in range (psi.shape[0]):
100
              if abs (psi [r][0]) > 1e-10: # Todo: complex numbers
101
                  lnn += 1
102
                  out += ('-' if psi [r][0] < 0 else '+') + (b3kets [r] if raw else b3string [r]) # Todo: non-uniform coeffecients
103
104
         if raw:
             print (("\ket{" + var.replace('\\\', '\\') + "} = ") +
105
                     (("" if lnn == 1 else
106
                       ("\\frac{1}{\\sqrt{2}^\" + str (int (math.log (lnn, 2))) + \"\") + out +
                      ("" if lnn == 1 else ")")).replace('\\\', '\\'))
108
109
         else:
              display (Math(("|" + var + "\\rangle = ") +
110
```

```
("" if lnn == 1 else
                             ("\\frac{1}{\\sqrt{2}^\" + str (int (math.log (lnn, 2))) + \"\"\") + out +
112
                            ("" if lnn == 1 else ")")))
113
114
     def dump (mtx):
115
         lnn = 0
116
         out = "\\begin{pmatrix} "
117
         for i in range (mtx.shape[0]):
118
             for j in range (mtx.shape[1]):
119
                  if abs (mtx [i][j]) > 1e-10: # Todo: complex numbers
120
                      lnn += 1
121
                      out += '-1 ' if mtx [i][j] < 0 else '+1 ' # Todo: non-uniform coeffecients</pre>
122
                  else:
123
                      out += ' 0 '
124
                  if j + 1 < mtx.shape[1]:
125
                      out += '& '
126
             out += "\\\\"
127
         out += "\\end{pmatrix}"
128
         display(Math(("" if lnn == 1 else
129
                        ("\\frac{1}{\\sqrt{2}^" + str (int (math.log (lnn, 2))) + "}")) + out))
130
131
132
     def dumpgates (mtxs):
133
         sq2n = 0
         out = ""
134
         for mtx in mtxs:
135
             lnn = 0
136
             out += "\\begin{pmatrix} "
137
             for i in range (mtx.shape[0]):
138
                 for j in range (mtx.shape[1]):
139
                      if abs (mtx [i][j]) > 1e-10: # Todo: complex numbers
140
                          lnn += 1
141
                          out += '-1' if mtx [i][j] < 0 else '+1' # Todo: non-uniform coeffecients
142
                      else:
143
                          out += ' 0 '
144
                      if j + 1 < mtx.shape[1]:
145
                          out += '& '
146
                  out += "\\\"
147
148
             out += "\\end{pmatrix}"
             sq2n += lnn // mtx.shape[0] - 1
149
150
         display(Math(("" if sq2n == 0 else
                        ("\\frac{1}{\\sqrt{2}^" + str (sq2n) + "}")) + out + opr3))
151
     # https://jarrodmcclean.com/basic-quantum-circuit-simulation-in-python/
```