Quantum Computation and Simulation

Exercise set 1

Exercise 1

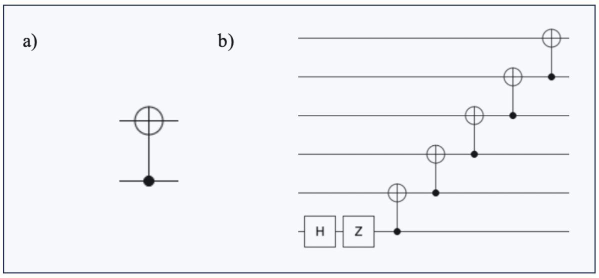
On circuit theory.

a) Write down the unitary that represents the upside-down CNOT gate in Fig. a)

b) What is the state resulting from the circuit shown in Fig. b) to $|0\rangle^{\otimes 6}$?

c) What is the result of measuring the X operator on the first qubit of that state?

d) How would you perform the $X^{\otimes n}$ measurement in practice? (i.e. assuming your quantum computer can only measure in the computational basis)



Exercise 2

Bernstein–Vazirani's algorithm. Consider a vector $\mathbf{a} = (a_1, \ldots, a_n) \in \{0,1\}^n$ and the function $f : \{0,1\}^n \to \{0,1\}$ defined by

$$f(x) = \mathbf{a} \cdot x \pmod 2 = a_1 x_1 + \cdots + a_n x_n \pmod 2 = a_1 x_1 \oplus \cdots \oplus a_n x_n, \quad x \in \{0,1\}^n.$$

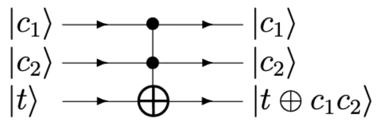
Classically, n evaluations of f are needed to discover $\mathbf{a}$.

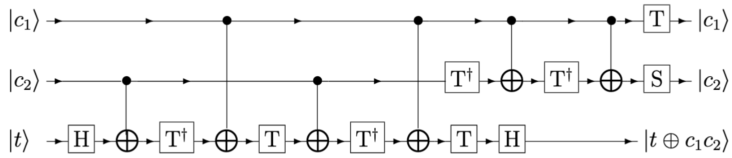
a) Show that, assuming a quantum oracle U_f with $n+1$ input and output qubits (as in Deutsch–Jozsa), one can discover $\mathbf{a}$ with probability 1 using a single call to U_f.

b) Now let $f(x) = b \oplus (\mathbf{a} \cdot x)$ with unknown $b \in \{0,1\}$. *(i)* With the same circuit, can you still determine $\mathbf{a}$ with probability 1 in one query to U_f? *(ii)* What about b?

Exercise 3

Construction of the Toffoli gate with CNOT**,** H**,** T**, and** S**.** Verify that the controlled-controlled-NOT (Toffoli) gate, mapping $|c_1, c_2, t\rangle \mapsto |c_1, c_2, t \oplus c_1 c_2\rangle$, is equivalent to the following circuit built from CNOT, H, T, and S gates



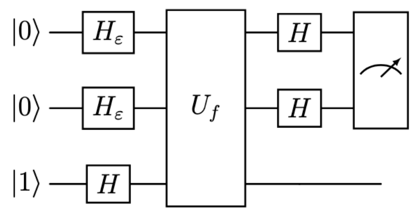


Exercise 4

Deutsch–Jozsa with imperfect Hadamards. Recall that the goal of the DJ algorithm is to decide if $f : \{0, \}^n \mapsto \{0, 1\}$ is balanced or constant. Here we analyze a variation of this problem with imperfect Hadamard gates. For simplicity we take $n = 2$. The imperfect Hadamard gates H_ε are defined as

$$H_\varepsilon|0\rangle = \sqrt{\tfrac{1+\varepsilon}{2}}|0\rangle + \sqrt{\tfrac{1-\varepsilon}{2}}|1\rangle, \quad H_\varepsilon|1\rangle = \sqrt{\tfrac{1-\varepsilon}{2}}|0\rangle - \sqrt{\tfrac{1+\varepsilon}{2}}|1\rangle.$$

and consider the Deutsch-Josza circuit: Verify that H_ϵ is unitary. Then analyze this circuit and



compute the success probability of the algorithm.

Exercise 5

An algorithm involving the Quantum Fourier Transform. Let $M = 2^m$. For $x \in \{0, \dots, M-1\}$ an integer, recall that the quantum Fourier transform (QFT) is defined as

$$\text{QFT}\,|x\rangle = \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} e^{2\pi i x y/M}\,|y\rangle\,.$$

Let $f : \{0, \dots, M-1\} \to \{0, \dots, M-1\}$ be an arithmetic function, and let V_f be the $M \times M$ matrix defined by

$$V_f\,|x\rangle = e^{-2\pi i f(x)/M}\,|x\rangle\,.$$

a) What are the matrix elements of both QFT and V_f in the basis $\{|x\rangle\,,\, x = 0, \dots, M-1\}$? Prove that these two matrices are unitary.

b) Let

$$|\Psi\rangle = (\text{QFT})\, V_f\, H^{\otimes m}\,|0\rangle\,,$$

where $|0\rangle$ is the state corresponding to the integer $0 \in \{0, \dots, M-1\}$. Explain how to represent this identity by a quantum circuit, specifically, how to represent the various states with qubits and how many qubits are needed, and then draw the circuit.

c) Compute the state at each stage in the circuit, and in particular the output state $|\Psi\rangle$.

d) Let $A, B \in \{0, \ldots, M-1\}$ and define $f(x) = Ax + B \bmod M$. After measuring the state in the computational basis:

   (i) What is the minimum number of measurements needed to determine the value of A?

   (ii) Can we also determine B by this process?

Exercise 6

Simulating quantum dynamics of a spin system. Consider the following Hamiltonian defined on two qubits:

$$\hat{\mathcal{H}} = \hat{\sigma}_1^x \hat{\sigma}_2^x + \hat{\sigma}_1^y \hat{\sigma}_2^y,$$

where we use the standard definition for the Pauli matrices:

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

a) Write $\hat{\mathcal{H}}$ as a 4x4 matrix in the standard basis $|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$, $|1,1\rangle$. Find the smallest eigenvalue and the corresponding eigenstate.

b) Consider the problem of simulating quantum dynamics starting from the initial state $|0,0\rangle$ using a quantum computer. Show that the FSIM(θ,ϕ) gate (as implemented on Google hardware, for example) can be used to obtain $|\psi(t)\rangle = \exp\left(-it\hat{\mathcal{H}}\right)|0,0\rangle$. Determine what values of θ and ϕ are necessary. Recall that the FSIM gate is defined as

$$\mathrm{FSIM}(\theta,\phi) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & -i\sin(\theta) & 0 \\ 0 & -i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

c) Now consider the problem of approximating the ground state of $\hat{\mathcal{H}}$ using a variational ansatz. We will consider the ansatz

$$|\Psi(\gamma_1,\gamma_2)\rangle = \mathrm{CNOT} \times \mathrm{RY}_1(\gamma_1) \times \mathrm{RY}_2(\gamma_2)|0,0\rangle$$

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

and

$$\mathrm{RY}(\gamma) = \exp(-i\hat{\sigma}^y\gamma/2) = \begin{bmatrix} \cos(\gamma/2) & -\sin(\gamma/2) \\ \sin(\gamma/2) & \cos(\gamma/2) \end{bmatrix}$$

Find the expression of the energy as a function of the parameters γ_1 and γ_2. For what values of the parameters do you recover the exact ground-state energy computed at point 1?