Quantum Circuits
Week 6

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1 Quantum algorithms

Our final topic in this course is a brief overview of the most promising algorithms that demonstrate a quantum advantage. Our treatment is far from complete, since the field of quantum algorithms has matured enough to be considered an independent research discipline.

2 Quantum Fourier transform (QFT)

The classical discrete Fourier transform is an operation that represents complex-valued vectors as a linear sum of the Fourier basis

$$y_m = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n e^{2\pi i m n/N}$$

where $x = (x_0, \ldots, x_{N-1})^\intercal, y = (y_0, \ldots, y_{N-1})^\intercal \in \mathbb{C}$, and $e_m(n) = \frac{1}{\sqrt{N}} e^{2\pi i m n/N},\ n, m = 0, 1, 2, \ldots, N-1$ are the Fourier basis.
Despite its similar mathematical representation, the QFT doesn't compute any complex coefficients as the DFT. Its primary role is to create an n-qubit superposition state via a basis transformation. Without this resource, none of the foretold quantum advantages can be manifested. QFT transforms basis states as

$$\mathcal{F} |n\rangle = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} e^{2\pi i m n/N} |m\rangle$$

While for any arbitrary state $|\Psi\rangle = \sum_{n=0}^{N-1} \alpha_n |n\rangle$

$$\begin{aligned}\mathcal{F}\,|\Psi\rangle &= |\Phi\rangle \\ &= \sum_{m=0}^{N-1} \alpha_m\,|m\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1}\sum_{n=0}^{N-1} \alpha_n e^{2\pi i m n/N}\,|m\rangle\end{aligned}$$

where $\alpha_m = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \alpha_n e^{2\pi i m n/N} = \sum_{n=0}^{N-1} \alpha_n \left(e^{2\pi i/N}\right)^{mn}$, such that $W_N = \frac{1}{\sqrt{N}} e^{2\pi i/N}$.
Then by defining Ω_N as the matrix

$$\Omega_N = \frac{1}{\sqrt{N}} W_N^{mn}, 0 \leq m, n \leq N-1,$$

we can write the matrix representation of the Fourier operator (ex).
By virtue of the Fourier *inverse theorem* , it is straight forward to show that the QFT operator is *unitary* (ex).
Letting $N = 2^k$, we can write the QFT of an n-qubit state as[1]

$$\frac{1}{\sqrt{2^k}} \bigotimes_{l=1}^{k} \left(|0\rangle + e^{i2\pi m/2^l}\,|1\rangle \right)$$

2.1 Example

Suppose that $n = 3$, in binary representation this can be written as a the 2-bit string "11". Quantum mechanically we define this as a two-qubit tensor product state $|1\rangle \otimes |1\rangle \equiv |11\rangle$. The previous state can be transformed to the Fourier domain as

$$\begin{aligned}\mathcal{F} &= \frac{1}{\sqrt{2^2}} \sum_{m=0}^{3} e^{2\pi i (3m)/2^2}\,|m\rangle \\ &= \frac{1}{2}\left[\,|00\rangle + e^{i3\pi/2}\,|01\rangle + e^{i3\pi}\,|10\rangle + e^{i9\pi/2}\,|11\rangle\,\right]\end{aligned}$$

Recalling our discussion in the past week, we can verify that the transformed vector indeed belongs to the 4-dimensional Fourier space.

[1] Full derivation can be found in the Qiskit textbook.

2.2 Quantum phase estimation

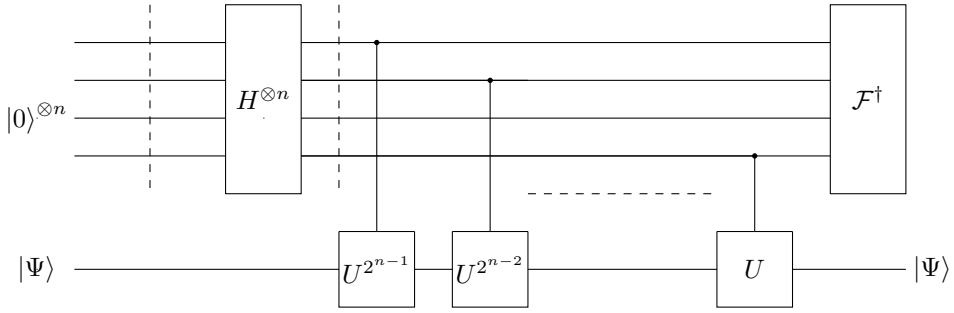

Figure 1: *A sketch of the quantum phase estimation circuit.*

A practical application that relies on the QFT is the problem of estimating the phase of an eigen-state of a unitary operator. A unitary operator U can be implemented as

$$U = e^{-i\gamma A} = e^{-i\gamma \sum\limits_{n} a|a\rangle\langle a|}$$

where eigenstates of U have eigenvalues of the form $e^{-i\theta}$, such that $\theta = a\gamma$.
Projective measurements on the eigenstates wipe out the overall global phase of the state, that's why we introduce the phase estimation circuit to retrieve this information[2]

2.3 Procedure

(1) We first prepare a huge superposition resource by applying the n-tensor product Hadamard operator $H^{\otimes n}$ to a stack of auxiliary qubits all prepared in the ground stare $|0\rangle^{\otimes n}$.

(2) When U^{2^n} is applied to $|\Psi\rangle$ it gives $U^{2^n}|\Psi\rangle = e^{i2^n\theta}|\Psi\rangle$

(2) At this stage the overall state of the system is written as

$$\big[\frac{1}{(\sqrt{2})^n}(|0\rangle + |1\rangle)^{\otimes n}\big] \otimes |\Psi\rangle$$

(3) Then applying n controlled-U operations gives

$$\big[\frac{1}{(\sqrt{2})^n}(|0\rangle + e^{i\theta 2^{n-1}}|1\rangle) \otimes (|0\rangle + e^{i\theta 2^{n-2}}|1\rangle) \ldots \otimes (|0\rangle + e^{i\theta}|1\rangle)\big] \otimes |\Psi\rangle$$

(4) It is then straight forward to put the above expression in the QFT form, then applying $\mathcal{F}^{\dagger}$ gives an expression that has a delta-peak at $2^n\theta$, thus the final state is projected to $|2^n\theta\rangle|\Psi\rangle$.

[2]For more details please consult " Quantum Computation and Quantum Information"-*Nielsen & Chuang*.

3 Grover's algorithm

On the average, identifying an element in an unsorted database of N distinct elements requires $N/2$ searches. Classically, the time taken by this operation is of the order of N. However, Grover showed in his protocol that by exploiting quantum parallelism, we can achieve a quadratic speed by performing the same task in $\sqrt{N}$ steps. In our exercise sheet we go through the entire protocol in details and derive this result ourselves. If implemented efficiently, Grover's algorithm would revolutionize the internet industry.

4 The variational quantum eigensolver (VQE)

VQE is a hybrid quantum-classical protocol that utilizes the variational quantum method to find an *optimal* upper bound for the ground state energy level of a quantum system, a molecule for example.

$$\lambda_{\text{min}} \leq \lambda_\theta \equiv \langle \Psi(\theta) | H | \Psi(\theta) \rangle$$

4.1 Procedure

(1) Write down the **Hamiltonian** of the system in terms of its Pauli decomposition. For example, the Hamiltonian of a Hydrogen atom can be represented by two qubits, and hence its Pauli components[3] are

$$H = \gamma_0 I + \gamma_1 Z_0 + \gamma_2 Z_1 + \gamma_3 Z_0 Z_1 + \gamma_4 Y_0 Y_1 + \gamma_5 X_0 X_1$$

(2) Choose a wave-function ansatz $|\Psi\rangle$.

(3) Encode a *parameter* θ into the ansatz via a parameterized quantum circuit described by a unitary transformation $U(\theta)$

$$U(\theta) |\Psi\rangle = |\Psi(\theta)\rangle$$

(4) Calculate the expected value of the **Hamiltonian** in the state $|\Psi(\theta)\rangle$

(5) Optimize θ via classical algorithms till you find the minimum eigenvalue.

[3] "*Scalable Quantum Simulation of Molecular Energies*"