Quantum Complexity Theory

Lecture Notes

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Contents

Preamble

These lecture notes derive from a sequence of scribe notes taken from the Fall 2022 iteration of CSE 291 / Math 277A (Quantum Complexity Theory). This document represents a continual and iterative process to bring those notes into a more cohesive whole. Any mistakes can be assumed to have been introduced by me. Please feel free to email me (`dgrier@ucsd.edu`) if you notice any.

These course notes are written for graduate students with a strong mathematical background, but not necessarily any previous experience with quantum computing. Some previous exposure to complexity theory will be extremely useful. I recommend the excellent Arora-Barak textbook for those looking to brush up on that background.

Overview

The goal of these notes is to rigorously compare, using the tools of complexity theory, the power of quantum and classical computers. We will see some settings in which quantum computers outperform their classical counterparts and some settings in which quantum computers are no better than brute force classical approaches. Given the recent explosion of progress in actually building a quantum computer, it is becoming more important than ever that we understand the difference in the quantum and classical worlds and what they allow us to compute. The exploration in these notes will take us to the forefront of quantum computing research, where we'll look at the complexity-theoretic foundations of these recent experiments.

Chapter 1

Foundations of Quantum Mechanics

Before we can reason about the power of quantum computers, we must obviously first understand what kinds of computations they unlock. We will start with the pure foundations: What is a quantum state, and what kinds of operations can you perform on that state?

From there, we will define a computational model (analogous to the classical Turing machine) that captures the essence of a quantum computer.

1.1 The basics of quantum computation

What is the state of a quantum system? Let's start by analogy to one of the simplest classical objects—a biased coin. Since it will be convenient later, let's suppose the coin has two sides, corresponding to a 0-outcome and a 1-outcome (perhaps more traditionally these two outcomes would be called "heads" and "tails").

To be even more concrete, let's suppose the coin is biased so that it lands on the 0-outcome with 30% probability and on the 1-outcome with 70% probability. Suppose we flip the coin in the air, and we want to describe the probability distribution over outcomes when the coin lands. We could represent it by the length-2 vector:

$$\begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix} \begin{matrix} \leftarrow \text{Probability of } 0\text{-outcome} \\ \leftarrow \text{Probability of } 1\text{-outcome} \end{matrix}$$

In some sense, this represents the "state" of the coin if we know the coin has landed on one side or the other, but we have not yet looked at which outcome.

If we *were* to look at the outcome, then the state of the system immediately changes to whichever outcome we saw:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \leftarrow \begin{matrix} 0\text{-outcome} \\ \text{with certainty} \end{matrix} \qquad \text{or} \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \leftarrow \begin{matrix} 1\text{-outcome} \\ \text{with certainty} \end{matrix}$$

since there is no ambiguity in the outcome once we've observed it.

Stepping back a bit, let's look at the full description of states and operations in this classical probability framework. First, notice that instead of a coin with just 2 outcomes, we could have as many outcomes as we like (think of a biased die); but for simplicity, let's assume there are only finitely many. In a system with d outcomes, the state of the system would be described

by a vector of d probabilities. The key property of this vector is that each probability is non-negative and all probabilities sum up to 1.

The set of operations that we could perform on this system are the set of operations that take probability vectors to probability vectors. Specifically (and we will see how this changes in the quantum setting soon), these operations preserve the ℓ_1-norm of the vector, where the ℓ_1-norm of vector $v = (v_1, v_2, \ldots, v_d) \in \mathbb{C}^d$ is defined as

$$\|v\|_1 := \sum_{i=1}^{d} |v_i|$$

Qubits

Let's now complete the analogy of the classical probabilistic bit discussed above with the quantum variant called a *qubit*. Instead of assigning two outcomes (0 and 1) a probability, we instead assign them a complex number called an *amplitude*. We represent a qubit as a column vector in $\mathbb{C}^2$. For example,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{pmatrix} \begin{matrix} \leftarrow \text{Amplitude on } 0\text{-outcome} \\ \leftarrow \text{Amplitude on } 1\text{-outcome} \end{matrix}$$

Let's now discuss what it means to "look" at a quantum state, which is called *measurement* in the quantum setting. The measurement axiom of quantum mechanics, called the *Born rule*, says that you see a particular outcome with the squared magnitude of the amplitude. For the example above, this means we'd see the 0-outcome with probability $|1/\sqrt{2}|^2 = 1/2$ and the outcome will be 1 with probability $|i/\sqrt{2}|^2 = 1/2$. Once again, when you observe this outcome the qubit *collapses* to whichever outcome you observed.

From the Born rule, we can derive a condition on the amplitudes of a qubit. Suppose we have a qubit with amplitudes $\alpha, \beta \in \mathbb{C}$. The Born rule states that we see the outcome with probability $|\alpha|^2$ and $|\beta|^2$, respectively. Since there are only two outcomes, these two probabilities must sum up to 1 (i.e., we must see either the O or 1 outcome when we measure). We arrive at the following condition for the amplitudes of a qubit: $|\alpha|^2 + |\beta|^2 = 1$.

Stepping back again, let's give a complete mathematical description of a quantum state. We can generalize to quantum state with d outcomes (called a *qudit* for $d > 2$), which is represented by a length-d complex vector. The key property of this vector is that the squared magnitudes of the amplitudes sum to 1. In other words, the ℓ_2-norm of the vector is 1. The ℓ_2-norm of any $v = (v_1, v_2, \ldots, v_d) \in \mathbb{C}^d$ is defined as

$$\|v\|_2 := \sqrt{\sum_{i=1}^{d} |v_i|^2}.$$

It is an amazing fact that moving from the classical to the quantum setting is in some sense just moving from the ℓ_1 to the ℓ_2 norm.

Unitary matrices

Because the set of valid quantum states must have unit ℓ_2-norm, the set of viable quantum operations must preserve the ℓ_2-norm of the state. However, not all such operations are valid.

An axiom of quantum mechanics dictates that quantum operations must also be *linear*. We will see a slight generalization of this later, but for now, you can think of this linearity as implying that quantum operations are matrices. Applying a quantum operation to a quantum state simply means multiplying the vector of the state with the matrix of the quantum operation.

Matrices preserving the ℓ_2-norm have a beautiful characterization—namely, they are the *unitary* matrices, i.e., matrices $U \in \mathbb{C}^{d\times d}$ such that $UU^\dagger = I$. Here, "$\dagger$" is the conjugate transpose operation and "I" is the identity matrix.

1.2 Multi-qubit quantum computation

In general, we think of large classical computations as a sequence of operations on some bit string. In this way we can break up some large complex operation into a sequence of simpler operations. The number of operations required to build the more complex operation is a proxy for how complex that operation really is. Similarly, in quantum systems, we want to build up larger more complex operations from simpler ones. To do this, we first need to understand what a quantum systems consisting of multiple qubits, so that we can understand what it means to locally apply some quantum operation.

Tensor product of states

Once again, let's start with a discussion of multiple classical random bits, and see how it generalizes to qubits. Let A, B be two random bits. Each bit has some probability of being in the 0 or 1 outcome. Together, the two bits give rise to a probability distribution over pairs of outcomes (i.e., 00, 01, 10, and 11). We can derive the probability of a particular pair of outcomes by multiplying the probabilities of the individual outcome for each bit. For example, let

$$A = \begin{pmatrix} 0.3 \\ 0.7 \end{pmatrix} \begin{matrix} \leftarrow 0 \\ \leftarrow 1 \end{matrix} \qquad , \qquad B = \begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} \begin{matrix} \leftarrow 0 \\ \leftarrow 1 \end{matrix}$$

Then the product distribution associated to A and B together gives rise to the vector

$$AB = \begin{pmatrix} 0.18 \\ 0.12 \\ 0.42 \\ 0.28 \end{pmatrix} \begin{matrix} \leftarrow 00 \\ \leftarrow 01 \\ \leftarrow 10 \\ \leftarrow 11 \end{matrix}$$

Combining two separate qubits into a single system is exactly the same. Let $v, w \in \mathbb{C}^2$ be vectors representing two qubits. The vector of the joint system is called the *tensor product* $v \otimes w$ of the two vectors v and w. The tensor product operation yields the vector containing all products of amplitudes. The example looks identical to the classical setting:

$$v = \begin{pmatrix} \sqrt{0.3} \\ \sqrt{0.7} \end{pmatrix} \begin{matrix} \leftarrow 0 \\ \leftarrow 1 \end{matrix} \qquad , \qquad w = \begin{pmatrix} \sqrt{0.6} \\ \sqrt{0.4} \end{pmatrix} \begin{matrix} \leftarrow 0 \\ \leftarrow 1 \end{matrix}$$

and

$$v \otimes w = \begin{pmatrix} \sqrt{0.18} \\ \sqrt{0.12} \\ \sqrt{0.42} \\ \sqrt{0.28} \end{pmatrix} \begin{matrix} \leftarrow 00 \\ \leftarrow 01 \\ \leftarrow 10 \\ \leftarrow 11 \end{matrix}$$

Formally, the tensor product operation $\otimes$ is defined over any pair of vectors $v \in \mathbb{C}^a$ and $w \in \mathbb{C}^b$ (not necessarily of the same length) as

$$v \otimes w := \begin{pmatrix} v_1 w \\ \vdots \\ v_a w \end{pmatrix} = \begin{pmatrix} v_1 w_1 \\ \vdots \\ v_1 w_d \\ v_2 w_1 \\ \vdots \\ v_a w_b \end{pmatrix}$$

From this definition, one can derive the following properties of the tensor product, which hold for all complex vectors v, w, z and scalars $\alpha, \beta \in \mathbb{C}$:

Scalar multiplication:	$(\alpha v) \otimes (\beta w) = (\alpha\beta)(v \otimes w)$
Associativity:	$(v \otimes w) \otimes z = v \otimes (w \otimes z)$
Distributivity:	$v \otimes (w + z) = v \otimes w + v \otimes z$

We have that the tensor product of two qubits is represented by a length-4 complex vector, the tensor product of three qubits is represented by a length-8 vector, and so on. One of the key questions we will ask in these notes is: how much of this exponentially is really there? Of course, when it comes to quantum states constructed from tensor products of qubits, the answer is... not much. To describe such a state, we simply need the 2 amplitudes for each individual qubit, a total of $2n$ amplitudes for an n-qubit state, rather than the 2^n amplitudes in the tensor product vector.

Critically, however, not all quantum states over qubits can be described in this way. That is, we can start with tensor product of single-qubit quantum states, apply a sequence of quantum operations, and arrive at a state which cannot be described by any tensor product of single-qubit states. Such states are called *entangled*.

Our first example of an entangled 2-qubit state is the following:

$$\begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{pmatrix}$$

which is known (amongst other names) as the *Bell state*. Before we prove this state is entangled, let's take a moment to consider what would happen if we measured this state. We would see the 00 outcomes with probability $1/2$ and the 11 outcome with probability $1/2$. In other words, if we made the measurement and we saw that the first qubit was 0, we would immediately know the second qubit was also 0. This description gets even stranger when

we consider the possibility that we could dramatically separate the first and second qubits, putting each on either end of the galaxy (hard to do in practice, of course!). Measuring at one end of the galaxy immediately tells us outcome of the qubit at the other end.[1]

To prove the Bell state is entangled, we argue by contradiction. Suppose otherwise, then we would have

$$\begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} \otimes \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} \alpha_0\beta_0 \\ \alpha_0\beta_1 \\ \alpha_1\beta_0 \\ \alpha_1\beta_1 \end{pmatrix}$$

for some complex amplitudes $\alpha_0, \alpha_1, \beta_0, \beta_1$. Comparing the left and right equations, we get the constraints:

$$\frac{1}{\sqrt{2}} = \alpha_0\beta_0, \;\; 0 = \alpha_0\beta_1, \;\; 0 = \alpha_1\beta_0, \;\; \frac{1}{\sqrt{2}} = \alpha_1\beta_1.$$

One can check this system of equations has no feasible solution, and therefore, the Bell state must entangled.

Tensor product of matrices

The tensor product of matrices is the unique operator which respects the tensor product of the underlying states. That is, for unitaries $U \in \mathbb{C}^a$ and $V \in \mathbb{C}^b$, the tensor product unitary $U \otimes V$ is the unique linear operator such that

$$(U \otimes V)(v \otimes w) = (Uv) \otimes (Vw)$$

for all states $v \in \mathbb{C}^a$ and $w \in \mathbb{C}^b$. This definition lines up with our intuition that if we apply a unitary to a specific qubit, then it should not affect any other qubit.

Formally, one can give a (rather more cumbersome) definition of the tensor product of arbitrary matrices $U \in \mathbb{C}^a$ and $V \in \mathbb{C}^b$ as:

$$U \otimes V = \begin{pmatrix} u_{11}V & u_{12}V & \cdots & u_{1a}V \\ u_{21}V & u_{22}V & \cdots & u_{2a}V \\ \vdots & \vdots & \ddots & \vdots \\ u_{a1}V & u_{a2}V & \cdots & u_{aa}V \end{pmatrix}.$$

Written out somewhat more explicitly when $a = b = 2$, we have

$$U \otimes V = \begin{pmatrix} u_{11}\begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} & u_{12}\begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} \\ u_{21}\begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} & u_{22}\begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} u_{11}v_{11} & u_{11}v_{12} & u_{12}v_{11} & u_{12}v_{12} \\ u_{11}v_{21} & u_{11}v_{22} & u_{12}v_{21} & u_{12}v_{22} \\ u_{21}v_{11} & u_{21}v_{12} & u_{22}v_{11} & u_{22}v_{12} \\ u_{21}v_{21} & u_{21}v_{22} & u_{22}v_{21} & u_{22}v_{22} \end{pmatrix}.$$

[1] A significant amount of ink has been spilled on exactly what is happening at a physical layer when a measurement like this is made. Look up the "quantum measurement problem". Thankfully for one of the most cherished pysical laws, this entanglement phenomenon does *not* allow for faster than light communication.

Partial measurement

With the tensor product, we can now talk about unitary matrices applied to a subset of qubits in our computation. As it turns out, it is also makes sense to measure a subset of qubits. Once again, we can appeal to our classical intuition. Suppose we have the following classical distribution over outcomes:

$$\begin{pmatrix} 0.3 \\ 0.1 \\ 0.3 \\ 0.3 \end{pmatrix} \begin{matrix} \leftarrow 00 \\ \leftarrow 01 \\ \leftarrow 10 \\ \leftarrow 11 \end{matrix}$$

Suppose we look at the second coin, but not the first. The probability the see the 0-outcome for the second coin is

$$\Pr[00\text{-outcome}] + \Pr[10\text{-outcome}] = .3 + .3 = .6$$

since both of those outcomes are consistent with seeing 0 for the second coin. By an identical calculation, we see the 1-outcome for the second coin with 40% probability.

Let's suppose we do see the second coin in the 0-outcome. Now we must calculate the distribution on the first coin conditioned on seeing the second coin in the 0-outcome. For either outcome $b \in \{0, 1\}$, we have

$$\Pr[b \text{ for first coin} \mid 0 \text{ for second coin}] = \frac{\Pr[(b \text{ for first coin}) \wedge (0 \text{ for second coin})]}{\Pr[0 \text{ for second coin}]}.$$

In our example, the probability we see the 0-outcome on the first coin conditioned on having seen 0 for the second outcome is just $.3/.6 = .5$. In practice, its often easiest to do these calculations by simply removing the outcomes that are inconsistent with the partial measurement, and then renormalizing the vector. For our example where we've seen the 0-outcome on the second coin, we have

$$\begin{pmatrix} 0.3 \\ 0.1 \\ 0.3 \\ 0.3 \end{pmatrix} \xrightarrow{\text{Remove inconsistent outcomes}} \begin{pmatrix} 0.3 \\ 0 \\ 0.3 \\ 0 \end{pmatrix} \xrightarrow{\text{Renormalize}} \begin{pmatrix} 0.5 \\ 0 \\ 0.5 \\ 0 \end{pmatrix}.$$

Once again, the quantum setting is identical except everything is done with respect to the ℓ_2-norm rather than the ℓ_1-norm. For completeness, let's look at a similar example with a quantum state:

$$\begin{pmatrix} \sqrt{0.3} \\ \sqrt{0.1} \\ \sqrt{0.3} \\ \sqrt{0.3} \end{pmatrix} \begin{matrix} \leftarrow 00 \\ \leftarrow 01 \\ \leftarrow 10 \\ \leftarrow 11 \end{matrix}$$

The probability we see the 0-outcome for second qubit is $|\sqrt{.3}|^2 + |\sqrt{.3}|^2 = .6$, and the distribution on the first qubit conditioned on this outcome is

$$\begin{pmatrix} \sqrt{0.3} \\ \sqrt{0.1} \\ \sqrt{0.3} \\ \sqrt{0.3} \end{pmatrix} \xrightarrow{\text{Remove inconsistent outcomes}} \begin{pmatrix} \sqrt{0.3} \\ 0 \\ \sqrt{0.3} \\ 0 \end{pmatrix} \xrightarrow{\text{Renormalize}} \begin{pmatrix} \sqrt{0.5} \\ 0 \\ \sqrt{0.5} \\ 0 \end{pmatrix}.$$

This procedure will be easier to describe more formally once we've introduced the notation in the following section.

1.3 Dirac notation and inner products

Let's start this section by introducing a method for writing quantum states, called *Dirac notation*. While this notation may at first seem somewhat unnecessary, it turns out to be quite natural. The most basic notational idea is that we will use a "ket", which looks like $|\cdot\rangle$, to describe a vector that is supposed to be a quantum state (i.e., a unit vector with respect to the ℓ_2-norm). Importantly, we reserve certain vectors special states. In particular, the 0-outcome and 1-outcome states, which we have previously been referring to somewhat awkwardly, are now associated with the following vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

So, for example, we can write an arbitrary single-qubit quantum state $|\psi\rangle$ as

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

for amplitudes $\alpha, \beta \in \mathbb{C}$. To write multi-qubit states in this notation, we employ another useful shorthand for bit strings $x \in \{0,1\}^n$:

$$|x\rangle := |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$$

We call such states the *classical basis states*. Now, any n-qubit state $|\psi\rangle$ can be written as linear combination of the classical basis states:

$$|\psi\rangle = \sum_{x \in \{0,1\}^n} \alpha_x\,|x\rangle$$

where $\alpha_x \in \mathbb{C}$ is some complex amplitude for each $x \in \{0,1\}^n$. For example, we can write the Bell state introduced in the previous section as

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}.$$

Inner products

Every quantum state lives in a vector space $\mathbb{C}^d$. We will often use that this vector space is actually a *Hilbert space*, meaning that it is equipped with an inner product: for vectors $v, w \in \mathbb{C}^d$, their *inner product* is defined as

$$v^\dagger w = \sum_{i=1}^{d} \overline{v_i} w_i.$$

In Dirac notation, we write $\langle\psi|$ (pronounced "bra"-ψ) to denote the conjugate transpose of the state $|\psi\rangle$. Therefore, the inner product between two state $|\psi\rangle$ and $|\varphi\rangle$ is written as

$$\langle\psi|\varphi\rangle := \overset{\text{bra}}{\downarrow}\langle\psi| \cdot \overset{\text{ket}}{\downarrow}|\varphi\rangle$$

where the lefthand side shows yet another shorthand. Now we can finally see the reason for the weird names "bra" and "ket". When you put them together to form an inner product, you get the phrase "braket", which looks like "bracket" if you squint.

Why go through all this trouble to create a shorthand for inner products? Perhaps most importantly, the inner product induces a natural distance measure on quantum states. If the inner product of two states is 1, then the states are identical. If the inner product is 0, then the states are perfectly distinguishable.

Outer products

We can also use Dirac notation to denote the outer product between states in the natural way. For states $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^d$, their outer product is

$$|\psi\rangle\langle\varphi| := \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_d \end{pmatrix} \begin{pmatrix} \overline{\varphi_1} & \overline{\varphi_2} & \cdots & \overline{\varphi_d} \end{pmatrix} = \begin{pmatrix} \psi_1\overline{\varphi_1} & \psi_1\overline{\varphi_2} & \cdots & \psi_1\overline{\varphi_d} \\ \psi_2\overline{\varphi_1} & \psi_2\overline{\varphi_2} & \cdots & \psi_2\overline{\varphi_d} \\ \vdots & \vdots & \ddots & \vdots \\ \psi_d\overline{\varphi_1} & \psi_d\overline{\varphi_2} & \cdots & \psi_d\overline{\varphi_d} \end{pmatrix}$$

The outer product is useful for describing quantum operations. For example, an arbitrary n-qubit unitary U can be written as

$$U = \sum_{x,y \in \{0,1\}^n} u_{x,y} |x\rangle\langle y|$$

where $u_{x,y} = \langle x| U |y\rangle \in \mathbb{C}$ is the amplitude the unitary places on the state $|x\rangle$ on input $|y\rangle$. In this case, $|x\rangle\langle y|$ is just matrix which is 1 at entry (x, y) and 0 everywhere else.

Summary – Quantum computation over n qubits

States:	$\|\psi\rangle \in \mathbb{C}^{2^n}$ such that $\sum_{x\in\{0,1\}^n} \|\langle x\|\psi\rangle\|^2 = 1$
Operations:	$U \in \mathbb{C}^{2^n \times 2^n}$ such that $U^\dagger U = U^\dagger U = I$ Applying U to $\|\psi\rangle$ results in the state $U\|\psi\rangle$
Measurement:	State collapses to $\|x\rangle$ with probability $\|\langle x\|\psi\rangle\|^2$

1.4 Mixed states

For many questions in quantum computation, the formalism of states and operations we've previously developed is sufficient. For example, most quantum algorithms start with some classical basis state, apply some unitary operation, and then measure. However, there is actually a more general form of a quantum state that is useful in a variety of contexts, like when you have noise in your quantum computer.

The quantum states $|\psi\rangle$ we have defined previously are called *pure states*. What makes a state "impure", or as it's traditionally called "mixed"? We say that a state is *mixed* when it represents a probability distrubtion of pure states. To see why these two notions are different, it's helpful to look at an example.

On the one hand, let's take the pure state $|+\rangle := \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ which in some sense equal parts $|0\rangle$ and $|1\rangle$. On the other hand, let's take the mixed state which is either $|0\rangle$ or $|1\rangle$ with 50% probability. These states may superficially seem to be the same (after all, they have the same probability over outcomes when measured), but are actually quite different. To see this, let's examine what happens when we apply the following unitary H, which is called the *Hadamard gate*:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Applying H to our pure state $|+\rangle$, we get

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

In other words, if we were to measure our pure state *after* the application of the unitary operation H, then we are guaranteed to see the outcome $|0\rangle$. This will not be true in our mixed state picture. Let's do the calculation. Applying H to the mixed state, we get

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

and

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

each of which happens with 50% probability. What is the probability we measure $|0\rangle$ now? Given the calculation above of what the Hadamard transformation does to each of our starting states, we have

$$\begin{aligned} \Pr[\text{measure } |0\rangle] = &\Pr[\text{Original state was } |0\rangle] \cdot \Pr[\text{measure } |0\rangle \text{ on state } |+\rangle] \\ &+ \Pr[\text{Original state was } |1\rangle] \cdot \Pr[\text{measure } |0\rangle \text{ on state } |-\rangle] \\ = &\frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2} \end{aligned}$$

We can now see that when our state was a statistical mixture of $|0\rangle$ and $|1\rangle$, the Hadamard transformation didn't change our measurement probabilities at all. In fact, this is a general phenomenon. One can show that no matter what unitary transformation you apply to this mixed state, you will always get $|0\rangle$ and $|1\rangle$ with 50% probability. This will be easy to show using the formalism we now introduce.

Density matrices

General quantum systems are fully described by statistical mixtures of quantum states—that is, an ensemble of pure states $\{|\psi_i\rangle\}_i$ each of which is prepared with probability $p_i \in [0,1]$. The *density matrix* corresponding to this ensemble is

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \in \mathbb{C}^{2^n \times 2^n}$$

where $\sum_i p_i = 1$. One can show that if you have a density matrix ρ and apply a unitary U, that the new density matrix is given by $U\rho U^\dagger$. Furthermore, measurement results in outcome $|x\rangle$ with probability $\langle x| \rho |x\rangle$, whereupon ρ collapses to the state $|x\rangle\langle x|$.

Let's revisit our example of an even statistical mixture of the states $|0\rangle$ and $|1\rangle$. The corresponding density matrix is

$$\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} + \frac{1}{2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{I}{2}.$$

As it turns out this stated is called the *maximally mixed state* since it represents that we essentially have no knowledge of what the underlying state is. To see this, imagine applying any unitary U to this state. We would get

$$U\left(\frac{I}{2}\right)U^\dagger = \frac{UU^\dagger}{2} = \frac{I}{2},$$

as the new state, which is the same state we started with. In other words, no unitary operation changes how the state looks. This proves the claim we made earlier that any unitary followed by measurement would result in outcomes $|0\rangle$ and $|1\rangle$ with equal probability.

What matrices correspond to ensembles of pure states? As it turns out, there is a very nice characterization: ρ is a valid density matrix if and only if ρ is a trace-1 positive semidefinite matrix. Trace-1 implies that $\mathrm{Tr}(\rho) = 1$. Positive semidefinite implies that $\langle\psi| \rho |\psi\rangle \geq 0$ for all pure states $|\psi\rangle$.

The forward direction of this claim can be shown by reasoning directly about the types of matrices that an ensemble of states can give rise to. The reverse direction can be shown by taking the spectral decomposition of ρ, which is valid since we have assumed that ρ is positive semidefinite. The eigenvectors of this decomposition will be the pure states in the decomposition, and the eigenvalues will be the associated probabilities.

Quantum channels

As one might have now guessed, unitary transformations are also not the most general transformation on quantum states. Quantum transformations that work on the level of density matrices are called *quantum channels*. That said, it is not true that every channel which preserves density matrices corresponds to a valid quantum operation. Most importantly, as required by the axioms of quantum mechanics, the channel must be linear. Furthermore, for technical reasons having to do with applying the channel to a restricted set of qubits, we must also require that the quantum channel still maps density matrices to density matrices when it is tensored with the identity map. Maps satisfying all the above conditions are called *completely positive trace preserving (CPTP)*.

Measurement

While there is a more general form of quantum measurements, it turns out that these more general measurements can be simulated by the measurements that we have already introduced. So, for simplicity, we will always assume that we measure our qubits the usual way.

Summary – Quantum computation with n-qubit mixed states

States:	$\rho \in \mathbb{C}^{2^n \times 2^n}$ such that $\mathrm{Tr}(\rho) = 1$ and ρ is positive semidefinite
Operations:	Completely positive trace-preserving maps Φ If Φ is a unitary channel, then $\Phi(\rho) = U\rho U^\dagger$ for unitary $U \in \mathbb{C}^{2^n \times 2^n}$
Measurement:	State collapses to $\lvert x\rangle\langle x\rvert$ with probability $\langle x\rvert \rho \lvert x\rangle$

Partial Trace

One of the most important reasons to introduce the density matrix formalism is to be able to talk about parts of a quantum state in isolation. That is, even if we have an n-qubit pure state, it is not necessarily the case that the state restricted to, say, the first $n/2$ qubits is a pure state.

We now introduce a way to "trace out" part of a density matrix of a large system to describe the state on the leftover qubits. To start, let's imagine we start with a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$. For simplicitly, you can at first just assume that $\mathcal{H}_A$ and $\mathcal{H}_B$ are the Hilbert spaces for two different qubits. Formally, the partial trace Tr_B is the unique linear map satisfying

$$\mathrm{Tr}_B(|a_i\rangle\langle a_j| \otimes |b_i\rangle\langle b_j|) = |a_i\rangle\langle a_j| \mathrm{Tr}(|b_i\rangle\langle b_j|),$$

where $a_i, a_j \in \mathcal{H}_A$ and $b_i, b_j \in \mathcal{H}_B$ are basis elements for the two subsystems.

So, if we have some state ρ_{AB} that lives in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, then the density matrix for the subsystem A after ignoring the subsystem B is given by

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}).$$

If we apply the partial trace operator to a product state we get, unsurprisingly,

$$\mathrm{Tr}_B(\rho_A \otimes \rho_B) = \rho_A.$$

What happens when we take the partial trace of the Bell state? The density matrix is given by

$$\rho_{\text{Bell}} := \left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)\left(\frac{\langle 00| + \langle 11|}{\sqrt{2}}\right) = \frac{|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|}{2}$$

so tracing out the second qubit, we get (by linearity of the partial trace)

$$\begin{aligned}
\mathrm{Tr}_2(\rho_{\text{Bell}}) &= \frac{1}{2}\left(\mathrm{Tr}_2(|00\rangle\langle 00|) + \mathrm{Tr}_2(|00\rangle\langle 11|) + \mathrm{Tr}_2(|11\rangle\langle 00|) + \mathrm{Tr}_2(|11\rangle\langle 11|)\right) \\
&= \frac{1}{2}\left(|0\rangle\langle 0| \mathrm{Tr}(|0\rangle\langle 0|) + |0\rangle\langle 1| \mathrm{Tr}(|0\rangle\langle 1|) + |1\rangle\langle 0| \mathrm{Tr}(|1\rangle\langle 0|) + |1\rangle\langle 1| \mathrm{Tr}(|1\rangle\langle 1|)\right) \\
&= \frac{1}{2}\left(|0\rangle\langle 0| \cdot 1 + |0\rangle\langle 1| \cdot 0 + |1\rangle\langle 0| \cdot 0 + |1\rangle\langle 1| \cdot 1\right) \\
&= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2}.
\end{aligned}$$

That is, if we take the Bell state and trace out a qubit, we are left with the maximally mixed state. This may give you some sense of the fragility of quantum computations. If you take an entangled state and lose a single qubit, it may become completely useless.

Reconciling the pure and mixed states

Often it will be easier to reason about pure states rather than mixed ones. As we've seen before, this is in some sense fundamentally impossible—there are mixed states which behave completely differently from pure ones. That said, there is also some sense in which there is an equivalence between the two settings. Namely, for every n-qubit mixed state ρ, there is a $(2n)$-qubit pure state such that tracing out the last n qubits of $|\psi\rangle$ leaves the state ρ. This process is called *purification*.

We will give an explicit purification procedure. First, let ρ be an arbitrary n-qubit mixed state:

$$\rho = \sum_{x\in\{0,1\}^n} p_x \, |\psi_x\rangle\langle\psi_x|$$

The following state will be a purification of ρ:

$$|\psi\rangle \coloneqq \sum_{x\in\{0,1\}^n} \sqrt{p_x} \, |\psi_x\rangle \otimes |x\rangle$$

Let B be the system consisting of the last n qubits. Tracing out B, we get the density matrix:

$$\begin{aligned}
\mathrm{Tr}_B\left(|\psi\rangle\langle\psi|\right) &= \mathrm{Tr}_B\left(\textstyle\sum_{x,y} \sqrt{p_x p_y}\, |\psi_x\rangle\langle\psi_y| \otimes |x\rangle\langle y|\right) \\
&= \textstyle\sum_{x,y} \sqrt{p_x p_y}\, \mathrm{Tr}_B(|\psi_x\rangle\langle\psi_y| \otimes |x\rangle\langle y|) && \text{(Linearity of partial trace)} \\
&= \textstyle\sum_{x,y} \sqrt{p_x p_y}\, |\psi_x\rangle\langle\psi_j| \,\mathrm{Tr}\left(|x\rangle\langle y|\right) && \text{(Definition of partial trace)} \\
&= \textstyle\sum_x p_x \, |\psi_x\rangle\langle\psi_x| && \text{(Trace is 1 iff } x = y\text{)}
\end{aligned}$$

which is precisely the mixed state ρ that we wanted to embed into $|\psi\rangle$.

Are purifications unique? Unfortunately, not. To see this, notice that we can generalize our purification procedure above my multiplying the second register by any n-qubit unitary U:

$$|\psi\rangle \coloneqq \sum_{x\in\{0,1\}^n} \sqrt{p_x} \, |\psi_x\rangle \otimes (U\,|x\rangle).$$

Intuitively, it makes sense that changing the basis of the second register shouldn't affect partial trace since we never used anything special about the classical basis states. Formally, you can check that the computation is agnostic to the choice of unitary U because of the following equalities:

$$\mathrm{Tr}(U\,|x\rangle\langle y|\,U^\dagger) = \mathrm{Tr}(U^\dagger U\,|x\rangle\langle y|) = \mathrm{Tr}(|x\rangle\langle y|)$$

where the first equality uses the cyclic property of the trace and the second using the fact that U is unitary.

1.5 Noteworthy quantum phenomena

Let's start to use the quantum formalism to take note of some interesting phenomena. We start with a classic result which implies that quantum information cannot be copied.

Theorem 1.1 (No-Cloning Theorem)**.** *There is no $(2n)$-qubit unitary U and n-qubit state $|\varphi\rangle$ such that*

$$U(|\psi\rangle \otimes |\varphi\rangle) = |\psi\rangle \otimes |\psi\rangle$$

for all pure states $|\psi\rangle$.

Proof. We argue by constradiction. Suppose such at U and $|\varphi\rangle$ existed, and let $|\psi_1\rangle, |\psi_2\rangle$ be two states we want to copy. In other words, we have

$$U(|\psi_i\rangle \otimes |\varphi\rangle) = |\psi_i\rangle \otimes |\psi_i\rangle$$

for $i \in \{1, 2\}$. Let's now take the inner product of the two states $U(|\psi_1\rangle \otimes |\varphi\rangle)$ and $U(|\psi_2\rangle \otimes |\varphi\rangle)$

$$(|\psi_1\rangle \otimes |\varphi\rangle)U^\dagger U(|\psi_2\rangle \otimes |\varphi\rangle) = \langle\psi_1|\psi_2\rangle \langle\varphi|\varphi\rangle = \langle\psi_1|\psi_2\rangle$$

and compare it to the inner product of $|\psi_1\rangle \otimes |\psi_1\rangle$ and $|\psi_2\rangle \otimes |\psi_2\rangle$:

$$(\langle\psi_1| \otimes \langle\psi_1|)(|\psi_2\rangle \otimes |\psi_2\rangle) = \langle\psi_1|\psi_2\rangle^2.$$

Cloning implies that these two expressions are equal:

$$\langle\psi_1|\psi_2\rangle = \langle\psi_1|\psi_2\rangle^2.$$

However, for any states such that $\langle\psi_1|\psi_2\rangle \notin \{0, 1\}$, the above equation will not hold. That is, cloning breaks for any distinct pair of non-orthogonal states! □

Chapter 2

Computation with Quantum Circuits

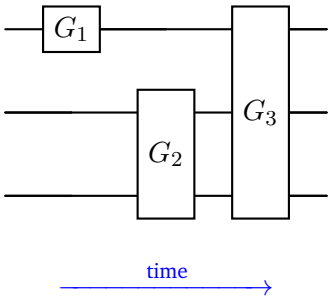
2.1 The quantum circuit model

How do we describe a quantum algorithm? One might think that something like a generalization of the classical Turing machine may be a particularly apt choice, given the centrality of that model to the story of classical theory of computation. While it is possible to define a quantum Turing machine, it turns out to be rather cumbersome to work with.

Instead, we will use a model of computation that more-or-less is the straightforward realization of applying a sequence of unitaries—the *quantum circuit*.

Introduction to quantum circuits

A n-qubit quantum circuit is a collection of unitary operations $G_1, \ldots, G_m$, called *gates*, applied in sequence to a subset of n *wires*. The composition of the gates in the circuit generates a $2^n \times 2^n$ unitary operation. We assume that each gate is in tensor product with the identity operation on each wire that it does not touch. Let's look at a simple example:



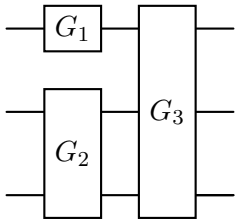
The above diagram is a circut on 3 qubits with 3 gates: the single-qubit gate G_1 is applied first; the 2-qubit gate G_2 is applied next; and finally G_3 is applied as a 3-qubit gate. The unitary matrix representing this circuit is

$$G_3 \left(I \otimes G_2\right) \left(G_1 \otimes I \otimes I\right).$$

Beware: matrix multiplication happens the reverse order of the circuit, which is why G_1 appears last the composition of unitaries. Since G_1 and G_2 act on different wires, we get that

$$\left(I \otimes G_2\right) \left(G_1 \otimes I \otimes I\right) = G_1 \otimes G_2.$$

Therefore, in the diagram, we can put G_1 and G_2 on the same *layer*.



That is, a layer of the circuits consists of a set of gates that can be applied simultaneously since they act on different qubits. The *depth* of a circuit is the number of layers of gates it has. Therefore, the example circuit above has depth 2.

Examples with common gates

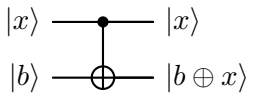
Let's take a look at some of the most common gates used in quantum circuits and the special notation that we use to denote them.

Classical reversible gates

One of the most common two-qubit gates is the *controlled-NOT* or *CNOT* gate. Recall that by linearity, it suffices to define the action of any gate on the computational basis. CNOT has the following action:

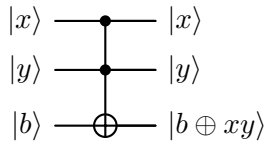
$$|00\rangle \mapsto |00\rangle\,, \quad |01\rangle \mapsto |01\rangle\,, \quad |10\rangle \mapsto |11\rangle\,, \quad |11\rangle \mapsto |10\rangle\,.$$

Notice that CNOT maps any computational basis state to another computational basis state. That is, the CNOT gate is "classical" in the sense that it cannot be used to create superposition of inputs. A CNOT gate in a circuit is depicted as a $\bullet$ symbol (the *control*) connected to a $\oplus$ symbol (the *target*):



Here, we've shown how the CNOT gate acts on general computational basis states, where $x, b \in \{0, 1\}$ are arbitrary bits and $b \oplus x$ denotes their XOR (i.e., addition modulo 2).

Another related gate is the version of the CNOT gate with an extra control, that is, the *controlled-controlled-NOT* gate, most commonly referred to as the *Toffoli* gate. As a circuit, it looks like



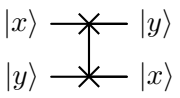
where $x, y, b \in \{0, 1\}$ are arbitrary bits (xy is the product of x and y). Notice that the third bit is flipped exactly when both controls are 1.

The Toffoli gate is in some sense more powerful than the CNOT gate since it can be used to generate the CNOT gate. Notice that if we set the second input qubit above to $|1\rangle$ (i.e., $y = 1$), then the remaining effect on the remaining two qubits is exactly the CNOT gate. We will see later however, that the reverse is not true—we cannot just use the CNOT gate to generate a Toffoli gate.

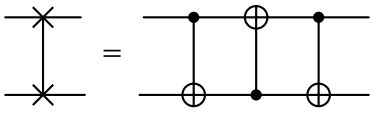
Finally, let's discuss the SWAP gate, another important "classical reversible" gate on 2 qubits. Aplty named, the SWAP gate swaps qubits, i.e., for all $x, y \in \{0, 1\}$ it maps:

$$|xy\rangle \mapsto |yx\rangle .$$

In a circuit diagram, it is depicted as



One can check the following nice identity:



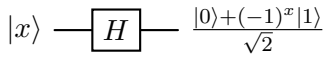
In other words, we can replace every SWAP gate in a circuit with 3 CNOT gates. This is a common theme we will continue to see—we can take some gates as the fundamental ones that will generate the rest.

Change of basis operations

Evidently, we need a gate that can create a superposition of inputs from a classical basis state. The *Hadamard gate* is the canonical choice for such an operation. It has the action

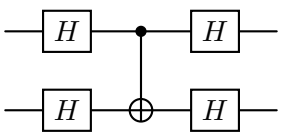
$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} := |+\rangle \qquad\qquad H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} := |-\rangle$$

on the computational basis. Notice that Hadamard gate has given rise to a new basis, the $\{|+\rangle, |-\rangle\}$ basis. In fact, Hadamard switches back and forth between the computational basis and this new basis. That is, the Hadamard gate is its own inverse: $H^2 = I$. As a circuit, it is shown as



for any $x \in \{0, 1\}$.

As another example, let's consider a circuit built from Hadamard and CNOT gates:



One way of understanding this circuit would be to just explicitly compute the unitary matrix $(H \otimes H)\mathrm{CNOT}(H \otimes H)$, but it is often more helpful to instead look at how the system evolves over a basis. Let's see how it acts on the computational basis, considering one gate at a time:

$$|00\rangle \xrightarrow{H\otimes H} |+\rangle \otimes |+\rangle = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) = \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2}$$

That is, after applying $H \otimes H$, we have the uniform superposition over 2-qubit computational basis states. We know that the CNOT gate just permutes the elements of the computational basis, or, in other words, it must do nothing to do the above state:

$$\frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2} \xrightarrow{\mathrm{CNOT}} \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2}.$$

Of course, if we've done nothing to the state, then it must also factorize as

$$|+\rangle \otimes |+\rangle = (H \otimes H)\,|00\rangle\,.$$

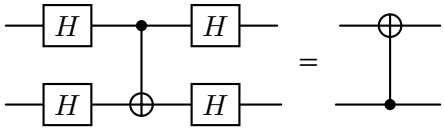
Therefore, the final layer of Hadamard gates returns the state to $|00\rangle$. That is, after all that computation, we see that the circuit acts as the identity on the $|00\rangle$. For completeness, let's see one more case (the input $|01\rangle$) in its entirety:

$$\begin{aligned} |01\rangle &\xrightarrow{H\otimes H} \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \otimes \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = \frac{|00\rangle - |01\rangle + |10\rangle - |11\rangle}{2} \\ &\xrightarrow{\mathrm{CNOT}} \frac{|00\rangle - |01\rangle - |10\rangle + |11\rangle}{2} = |-\rangle \otimes |-\rangle \\ &\xrightarrow{H\otimes H} |11\rangle \end{aligned}$$

If we were to continue with the entire computational basis, we would see

$$|00\rangle \mapsto |00\rangle\,, \quad |01\rangle \mapsto |11\rangle\,, \quad |10\rangle \mapsto |10\rangle\,, \quad |11\rangle \mapsto |01\rangle\,.$$

We've seen this gate before. It's just the CNOT gate with the control on the second qubit instead of the first! That is, we've derived the following circuit identity:



Notice that up until this point, every gate that we've introduced is *real*—the all elements of the unitary matrix representing the gate are real numbers. Let's now introduce some gates that have complex entries.

Phase gates

The gate most commonly referred to as the "phase gate" is the single-qubit diagonal gate S that simply multiplies the $|1\rangle$ state by a phase of i:

$$S\,|0\rangle = |0\rangle \qquad\qquad S\,|1\rangle = i\,|1\rangle$$

Another type of phase gate, most commonly called a T-gate, is the square root of this operation:

$$T|0\rangle = |0\rangle \qquad T|1\rangle = e^{i\frac{\pi}{4}}|1\rangle$$

Unsurprisingly, there are many other common gates that we have yet to define. Thankfully, the gates we have already allow us to do essentially everything we want.

Universality, approximations, and circuit size

A *gate set* is the collections of gates that one can use in the construction of a circuit. Typically, when a gate is included in a gate set, then you're allowed to apply that gate as many times you like on whichever subset of qubits that you like.

Universality captures the notion that a particular gate set can be used to construct any possible quantum operation. There are several different kinds of universality you might want:

- *Exact Universality:* For any n-qubit unitary, there is a circuit that exactly compute the unitary.
- *Approximate Universality:* For any n-qubit unitary, there is a circuit that approximately computes the unitary. One common measure of closeness is the operator norm.
- *Computational Universality:* For any n-qubit unitary, the probability distribution resulting from measuring the first qubit can be approximated by measuring the first qubit of the circuit. For example, it turns out that real quantum gates (without complex entries) are sufficient for computational universality, whereas they clearly fail on the other two notions of universality.

Given that we have a universal gate set, how many gates do we actually need to construct an arbitrary unitary? Let's look at the exact case, where we can get an estimate based on the number of parameters it takes to specify arbitrary unitary matrix. The first claim is that an arbitrary complex $d \times d$ unitary matrix U is specified by d^2 real parameters.

To see this, first note there are d^2 entries in the matrix, each with a complex part and a real part, that is, $2d^2$ real parameters total. However, the unitary constraint $UU^\dagger = I$ imposes d^2 algebraically independent real conditions (d for the fact that the norm of each column should be 1, and $d(d-1)$ conditions for the fact that the complex inner product of each row should be 0).

If our gate set consists of gates that only act on a constant number of qubits (which is often the convention), then each such gate only contributes constantly many real parameters to the construction of the unitary. Therefore, we must have $\Omega(4^n)$ gates to construct an arbitrary n-qubit unitary exactly.

A generalization of this result shows that this lower bound is essentially tight for approximation computation as well—$\Omega(4^n \log(1/\epsilon))$ gates are required to approximately compute any unitary to within ϵ-accuracy with respect to the operator norm [DN06]. That is, a unitary U is ϵ-close to unitary V if

$$\|U - V\|_{\text{op}} = \sup_{\psi} \|(U - V)|\psi\rangle\|_2 \leq \epsilon.$$

Thankfully, there is a matching (up to polylog factors) circuit building algorithm as well.

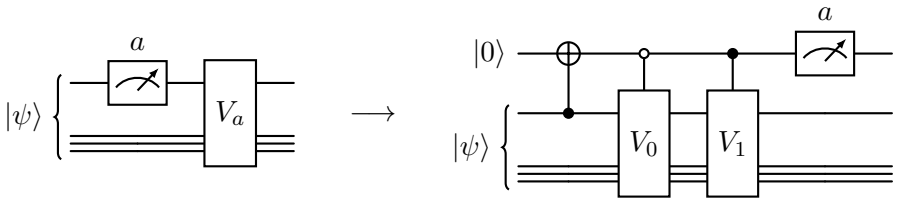
Theorem 2.1 (Solovay-Kitaev [Kit97])**.** *Given an approximately universal gate set, there is a circuit to appoximate any unitary to ϵ-accuracy with $\mathcal{O}(4^n \text{polylog}(\frac{1}{\epsilon}))$ gates.*

The version of the Solovay-Kitaev theorem stated above is actually the result of Bouland and Giurgica-Tiron [BGT21], who show how to work with general gate sets. Unfortunately, their result suffers in the exponent of the log factor. The original and most-efficient Solovay-Kitaev theorems require that if a gate is in the gate set, then its inverse is also in the gate set. The current best result in this setting is by Kuperberg, who shows a bound of $O(4^n \log^{1.441}(1/\epsilon))$ gates [Kup23].

Principle of Deferred Measurement

So far in this section, we've used unitary gates as the only operations in a quantum circuit. That is, we have been implicitly assuming that measurements are performed at the end of the circuit. Measurement is a non-unitary operation, so is it possible that by using intermediate measurements in the "middle" of the circuit, we might be able to more efficiently construct a particular unitary operation?

The *principle of deferred measurement* says that each intermediate measurements can essentially be pushed to the end of circuit by introducing a new ancillary qubit. The resulting probably distribution over all measurments made in the circuit will be the same before and after the transformation. The figure below depicts a general form of this transformation:



The left side shows a quantum circuit where the intermediate measurement has outcome $a \in \{0, 1\}$ and unitary V_a is applied as a result. The right side shows a quantum circuit where this measurement has been deferred to the end of the circuit by pushing it onto an ancilla. (Note: a control gate with an open circle is usually used to denote that the gate is controlled on 0, rather than 1.)

To verify correctness of this procedure, it suffices to check that tracing out the first qubit on the right side circuit results in the same density matrix as you get from the left.

2.2 The complexity class BQP

This section relies on a background in classical complexity theory. For a short review of some of the fundamental classical complexity classes, see Chapter A.

To properly define the quantum complexity class BQP, we need to first discuss how a quantum circuit is encoded. Let us suppose that the circuit is constructed from some reasonable universal gate set (i.e., all the amplitudes used in the gates are efficiently computable). We will use the notation $\langle Q \rangle$ to denote the encoding of a circuit Q as a bit string. We now discuss the requirement for a proper encoding:

1. The encoding is unique: mapping from a circuit to its encoding must be *injective*.

2. The encoding is not too big: if Q has m gates, then $\langle Q \rangle$ has at most $\mathsf{poly}(m)$ bits.

3. The encoding is not too small: if Q has m gates, then $\langle Q \rangle$ has at least m bits.

Equipped with an encoding, we can now talk about Turing machines whose output is (an encoding of) a quantum circuit. A circuit family $\{Q_n\}_{n=1}^{\infty}$ is *poly-time uniform* if there exists a poly-time Turing machine such that on input 1^n outputs $\langle Q_n \rangle$. We are now ready to define the complexity class capturing efficient quantum computation:

Bounded-error Quantum Polynomial Time (BQP):
Languages L such that there exists poly-time uniform class of quantum circuits $\{Q_n\}_{n=1}^{\infty}$ and a polynomial q such that for all $x \in \{0,1\}^n$:

- If $x \in L$, probability of measuring $|1\rangle$ on the first qubit of $Q_n |x\rangle \otimes \left|0^{q(n)}\right\rangle$ is at least $\frac{2}{3}$.
- If $x \notin L$, probability of measuring $|1\rangle$ on the first qubit of $Q_n |x\rangle \otimes \left|0^{q(n)}\right\rangle$ is at most $\frac{1}{3}$.

2.3 How does BQP compare to its classical complexity friends?

In this section, we will see how BQP fits into the zoo of classical complexity classes. To start, let's start with an "obvious" claim—namely, efficient quantum computation is at least as powerful as efficient classical computation. That is, $\mathsf{BPP} \subseteq \mathsf{BQP}$.

To do this, it will be useful to also define BPP in terms of circuits:

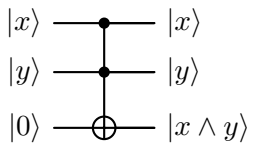
Bounder-error probibalistic polynomial time (BPP)
The class of languages L for which there is a poly-time uniform family of classical circuits $\{C_n\}_{n=1}^{\infty}$ and a polynomial q such that for all $x \in \{0,1\}^n$:

- If $x \in L$, $C(x,r) = 1$ for at least 2/3 of strings $r \in \{0,1\}^{q(n)}$.
- If $x \notin L$, $C(x,r) = 1$ for at most 1/3 of strings $r \in \{0,1\}^{q(n)}$.

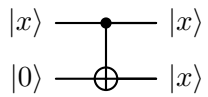
Once again, we assume that the classical circuits are compiled from a reasonable gates like AND and NOT gates.

Theorem 2.2. $\mathsf{BPP} \subseteq \mathsf{BQP}$.

Proof. We will show that quantum circuits can directly simulate AND and NOT gates, which are universal for classical computation. NOT is already unitary operator, so there is nothing to do. To simulate AND, we simply observe that the Toffoli computes AND on the target. That is,



for all $x, y \in \{0,1\}$. Therefore, every gate in a classical circuit can be replaced by a quantum one. Technically, classical circuits can "fan out" the output of a gate to serve as input for several other gates. We can simulate this behavior in a quantum circuit through a simple CNOT gate that acts as a copy gate:



We also need to deal with the random bits in the definition of BPP that are not present in the definition of BQP. This is also straightforward, if we want to simulate a random bit, we simply start the corresponding qubit of the quantum circuit in the $|+\rangle$ state.

Finally, we note that the reduction sketched above can be done efficiently. That is, a poly-time uniform family of classical circuits for a language in BPP implies there is also a poly-time uniform family of quantum circuits for the same language. Therefore, BPP $\subseteq$ BQP. □

What about classical upper bounds on the power of poly-time quantum computation? Let's start with the most basic bound, exponential time:

Theorem 2.3. BQP $\subseteq$ EXP.

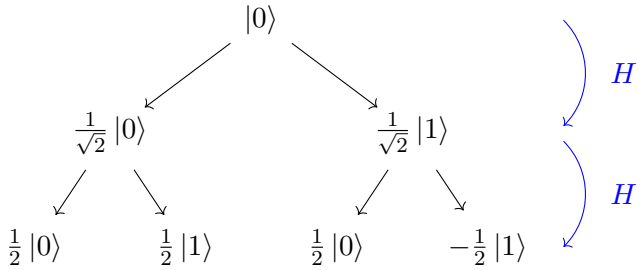
Proof. Any n-qubit state can be represented as a length-2^n complex vector. Every quantum gate on an n-qubit state is unitary matrix of size $2^n \times 2^n$. The state after application of the gate is obtained by simply multiplying the vector by the matrix. Since such matrix-vector products can be computed in $O(4^n)$ time, and simulating the circuit requires at most polynomially many matrix-vector product operations, we then have BQP $\subseteq$ EXP. □

In some sense, the above containment above showcases what many think to be true about quantum computation—to classical simulate a general quantum computer, you fundamentally need some kind of brute-force exponential time computation. However, notice that the exponential-time algorithm is both time inefficient *and* space inefficient. It turns out that a classical simulation is possible with polynomial space, or in other words, BQP $\subseteq$ PSPACE.

The proof of this fact will be to consider a quantum computation as a sum over paths in a tree. Let's explore this idea with an exmaple. Consider the (very simple) circuit H^2. Let's look how the state $|0\rangle$ evolves gate by gate:

$$|0\rangle \xrightarrow{H} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \xrightarrow{H} \frac{\frac{|0\rangle+|1\rangle}{\sqrt{2}} + \frac{|0\rangle-|1\rangle}{\sqrt{2}}}{\sqrt{2}} = \frac{|0\rangle + |1\rangle + |0\rangle - |1\rangle}{2}.$$

We can arrange these same steps in a tree:



Of course, for this simple example, we know the result is simply $|0\rangle$ after simplification. but we don't have to simplify the expression. Instead, we can keep it as a linear combination of $|0\rangle, |1\rangle, |0\rangle, |1\rangle$ with respective coefficients $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$. Why might we want to do this? The

key is that in the tree picture, the final states in the tree are just computational basis states rather than superpositions of computational basis states (as would be the case for a general quantum state). We can keep track of the amplitude and the classical basis state in polynomial space.

To do a generic quantum computation, we will traverse the entire computation tree, summing up the amplitudes when we get to leaves. Let's see how these ideas fit together.

Theorem 2.4. BQP $\subseteq$ PSPACE.

Proof. Let's start by making the simplifying assumption that the quantum circuit is constructed from Toffoli and Hadmard gates since those gates are computationally universal. This means that we can specify any leaf in the tree by a bit string indicating the path taken on all Hadamard gates from the root to the leaf (e.g., a 0 says to take the left branch, and a 1 says taking the right branch). Since the quantum circuit is of polynomial size, these leaf pointers are also of polynomial size.

Specifically, if the quantum circuit has h Hadamard gates, then we can designate a path as a length-h bit string. If we iterate through all of these leaf pointers, we can traverse the entire computation tree. Since the leaf pointers are of polynomial size and the intermediate states of the computation tree consist of a computational basis state and a single amlitude, we can traverse the entire tree using only polynomial space. To finish, the classical simulation algorithm, we need to specify what information we collect at the leaves of the tree once the traversal processes them.

We will devise a classical algorithm that computes the acceptance probability of the quantum circuit. If the final state of the quantum circuit is

$$|\psi\rangle = \sum_{y\in\{0,1\}^{n-1}} \alpha_{0y}\,|0y\rangle + \alpha_{1y}\,|1y\rangle\,,$$

then our goal is compute the probability of measuring $|1\rangle$ on the first qubit:

$$p_{\text{acc}} = \sum_{y\in\{0,1\}^{n-1}} |\alpha_{1y}|^2.$$

Our plan will now simple—for each $y \in \{0,1\}^{n-1}$, we traverse the entire tree looking for computation paths that end in a $|1y\rangle$ state, adding up the amplitudes as we go. The full pseudocode for the algorithm is below:

$p_{\text{acc}} \leftarrow 0$
for $y \in \{0,1\}^{n-1}$ **do**
  $\alpha_{1y} \leftarrow 0$
  for path $p \in \{0,1\}^h$ in computation tree **do**
    if path p ends in leaf state $|1y\rangle$ with amplitude β **then**
      $\alpha_{1y} \leftarrow \alpha_{1y} + \beta$
  $p_{\text{acc}} \leftarrow p_{\text{acc}} + |\alpha_{1y}|^2$
return p_{acc}

If the calculated the probability of acceptance is greater than 2/3, the classical algorithm accepts; otherwise, it rejects. □

Can this be improved? Somewhat surprisingly, the answer is "yes". Poly-size quantum circuits can be simulated in PP, which captures decision problems solvable by counting the number of satisfying instances of an NP problem. Formally, recall the definition of PP: the class of languages L such that there exists a deterministic poly-time Turing machine M and polynomial q such that for all $x \in \{0,1\}^n$

- If $x \in L$, then $M(x,y)$ accepts for more than $1/2$ of strings $y \in \{0,1\}^{q(n)}$.
- If $x \notin L$, then $M(x,y)$ accepts at most $1/2$ of strings $y \in \{0,1\}^{q(n)}$.

Theorem 2.5. BQP $\subseteq$ PP.

Proof. Once again, let's look at the computation tree of a poly-size quantum circuit built from Toffoli and Hadmard gates. Once again, the number of leaves in the tree is given by 2^h where h is the number of Hadamard gates. The key idea is it that because the magnitude of the amplitude at every leaf is exactly $1/\sqrt{2^h}$, the final amplitude on any given basis state is proportional to the number of leaves that have a positive sign minus the number of leaves that have a negative sign. Let the final state before measurement of the quantum algorithm be

$$|\psi\rangle = \sum_{x \in \{0,1\}^n} \alpha_x |x\rangle .$$

Let a_x be the fraction of all leaf nodes that are in state $|x\rangle$ and have positive weight, and let b_x be the fraction of all leaf nodes that are in state $|x\rangle$ and have positive weight. We can express the amplitude of the state as

$$\alpha_x = \sqrt{2^h}(a_x - b_x)$$

for real numbers $a_x, b_x \geq 0$.

Now consider the following classical algorithm. Randomly and uniformly follow one branch of the tree and record the state $|x\rangle$ at the leaf, then return to the beginning of the tree and randomly follow another branch of the tree and record the state $|y\rangle$ at the leaf. If $x \neq y$, then flip a coin to determine if we accept or reject the input. However, if $x = y$, then we want to determine if the signs of these states are likely to add constructively or destructively. Explicitly, if the first qubit of $x = y$ is a 1, then accept if the coefficients on x and y have the same sign and reject if they have opposite signs, and if the first qubit of $x = y$ is a 0, then accept if the coefficients have opposite signs and reject if they have the same sign.

Let's now see why this combination of accept/reject rules would give you an algorithm which accepts more than 50% of the time only when the quantum algorithm accepts. Notice that when $x \neq y$, our decision rule is simply a coin flip, which succeeds with probability 50% regardless of the truth. It suffices to show our decision rule succeeds with probability strictly more than $1/2$ when $x = y$. Notice that the probability of seeing the state $|x\rangle$ twice with constructive weights is given by

$$\Pr[\text{seeing } |x\rangle \text{ twice with constructive weights}] = a_x^2 + b_x^2.$$

The probability of seeing the state $|x\rangle$ twice with destructive weights is given by

$$\Pr[\text{seeing } |x\rangle \text{ twice with destructive weights}] = 2a_x b_x$$

Suppose the quantum algorithm accepts (i.e., measures "1" on the first qubit) with probability p_{acc}. We get

$$p_{\text{acc}} = \sum_{y\in\{0,1\}^{n-1}} \alpha_{1y}^2 = 2^h \sum_{y\in\{0,1\}^{n-1}} (a_{1y} - b_{1y})^2 . \tag{2.1}$$

On the other hand, this implies that the algorithm rejects with probability

$$1 - p_{\text{acc}} = \sum_{y\in\{0,1\}^{n-1}} \alpha_{0y}^2 = 2^h \sum_{y\in\{0,1\}^{n-1}} (a_{0y} - b_{0y})^2 \tag{2.2}$$

Dividing by 2^h and subtracting Equation (2.2) from (2.1), we get

$$\begin{aligned}\frac{2p_{\text{acc}} - 1}{2^h} &= \sum_y (a_{1y} - b_{1y})^2 - \sum_y (a_{0y} - b_{0y})^2 \\ &= \sum_y (a_{1y}^2 + b_{1y}^2 + 2a_{0y}b_{0y}) - \sum_y (a_{0y}^2 + b_{0y}^2 + 2a_{1y}b_{1y})\end{aligned}$$

Notice that the first sum on the right hand side corresponds exactly to the probability of seeing either (i) two states starting with 1 and with constructive weights, or (ii) two states starting with 0 and with destructive weights. Ignoring the 50-50 coin tosses from the classical simulation procedure that don't end in the same state, this is exactly the probability that the procedure outputs YES. Similarly, the second sum is the probability that our classic simulation procedure outputs NO. This then gives

$$\frac{2p_{\text{acc}} - 1}{2^h} = \Pr[\text{simulation outputs YES}] - \Pr[\text{simulation outputs NO}],$$

Hence, when $p_{\text{acc}} \geq 2/3$ left hand side is positive. Since the classic simulation is more likely to output YES, and so the PP machine accepts. When $p_{\text{acc}} \leq 1/3$, the left hand side is negative, so the classical simulation is more likely to output NO, and therefore the PP machine rejects. This concludes the proof. □

Looking at all of these complexity classes and inclusions, we can start to get some intuition for why it is hard to definitively prove that efficient quantum computation (i.e., BQP) is more powerful than efficient classical computation (i.e., P). First, using Theorem 2.2, we have that P ⊆ BPP ⊆ BQP. Second, using Theorem 2.4, we have that BQP ⊆ PSPACE. Chaining these two results together, we can sandwhich BQP in between P and PSPACE:

$$\mathsf{P} \subseteq \mathsf{BQP} \subseteq \mathsf{PSPACE}.$$

So, now suppose we could definitively prove that quantum computation is strictly more powerful than classical computation, i.e., that P ⊊ BQP. Then, by transitivity, we would simultaneously have shown that P ⊊ PSPACE. However, the P vs. PSPACE question is one of the many notoriously difficult questions in classical complexity, commensurate in some sense to the famous P vs. NP question. That is, we can't hope to prove quantum advantage without also solving some decades old and famously difficult problems in classical complexity.

Part of the goal in these lecture notes will be to find ways to make progress anyways. In some settings, we will only be able to show theoretical evidence (rather than definitive proof) of quantum advantage. In other settings, we will be able to show definitive quantum advantage, but only by changing the question slightly.

Chapter 3

Query Complexity

In this chapter, we explore one of our first tools for comparing the power of quantum and classical computation—*query complexity*. In the query complexity setting, we imagine there is some property of a function that we are trying to compute. The catch is that we can only learn things about the function by "querying" its value on a single input at a time. The number of times we need to query the function to learn the property is new measure of complexity (rather than something like the gate count in the quantum circuit).

The benefit of this approach is that the blackbox nature of the function greatly restricts the kinds of algorithms (both quantum and classical) that you could use to solve the problem. This will allow us to prove tight bounds on the query complexity for both the quantum and classical computers. When the quantum computation requires significantly fewer queries, we have evidence of a quantum advantage. In fact, many of the efficient query algorithms we will discuss in this chapter are also efficient in the more traditional sense (i.e., in BQP), and therefore, form the basis for some of the most promising quantum algorithms.

For some intuition for the power of this setting, imagine a kind of satisfiability problem captured by a function $f\colon \{0,1\}^n \to \{0,1\}$. That is, we'd like to know if there is some input $x \in \{0,1\}$ such that $f(x) = 1$. Now imagine the function is instantiated by polynomially many constraints, e.g., an NP-complete problem like 3-SAT. It is a famously open problem if NP-hard problem like this can be solved in polynomial time. However, when we look at the query version of this problem—that is, we can only query f on inputs $x \in \{0,1\}^n$ one at a time—the problem is obviously hopelessly difficult for a classical polynomial-time machine. If there is at most one possible input x such that $f(x) = 1$, we have to make exponentially many queries to determine if such an x exists.

Despite the restricted access model for query algorithms, we will see that there can still be nontrivial algorithms for a variety of different problems. The purpose of this section is to showcase how quantum algorithms fare in this setting in comparison to their classical counterparts.

3.1 Defining a quantum oracle

Querying a function $f\colon \{0,1\}^n \to \{0,1\}^m$ is pretty straightforward in the classical circuit setting—the queries consist of n-input m-output gates, and the query complexity is the number of these query gates that are required to solve the problem.

Let's now discuss what exactly it means to query the function quantumly. We will use two oracle models. First, we define the *standard oracle* B_f which acts on two registers, an input register and a output register:

$$B_f |x\rangle |b\rangle = |x\rangle |b \oplus f(x)\rangle$$

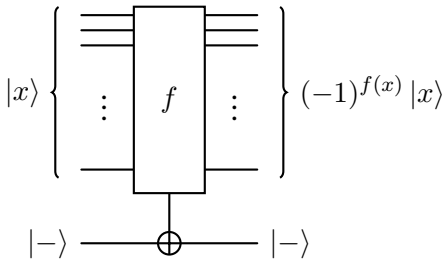
for all $x \in \{0,1\}^n$ and $b \in \{0,1\}^m$. That is, the standard oracle just computes the value of the function on the input and dumps it (reversibly) into the output register.

Is this a reasonable model? In other words, how can we justify that we are not cheating by giving the quantum algorithm a query model which is fundamentally more powerful than the query model in the classical setting (in a way which it unrelated to the power of quantum computation)? One way to see this is to imagine what it would look like to instantiate the function f for a practical problem. For any setting where there is a classical circuit for f (e.g., in our example where f was a 3-SAT formula), then the quantum circle can implement the oracle B_f by straightforwardly implenting the classical circuit in superposition. On the other hand, if there's no classical circuit for f, then the classical oracle also doesn't make any sense!

As it turns out, it's often useful to have another query model where the output of f is computed in the phase of the input. For every function $f\colon \{0,1\}^n \to \{0,1\}$, the *phase oracle* O_f is defined so that

$$O_f |x\rangle = (-1)^{f(x)} |x\rangle$$

for all $x \in \{0,1\}^n$. The phase oracle is only marginally different from the standard oracle. In fact, the standard oracle can simulate the phase oracle with a single ancilla qubit:



The circuit diagram shows the B_f oracle where the function f is computed on the $|x\rangle$ register and XOR'd into the $|-\rangle$ register. We have

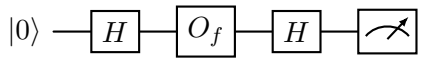
$$|x\rangle |-\rangle \xrightarrow{B_f} |x\rangle \left(\frac{|f(x)\rangle - |1 \oplus f(x)\rangle}{\sqrt{2}} \right) = (-1)^{f(x)} |x\rangle |-\rangle = (O_f |x\rangle) |-\rangle .$$

An almost-identical construction shows that the B_f oracle can be simulated by a single query to a controlled-O_f oracle.

3.2 Fourier sampling problems

Let's start with one of the simplest examples of a quantum-classical query separation. Our goal will be determine if a function $f\colon \{0,1\} \to \{0,1\}$ is constant or not, i.e., if $f(0) = f(1)$ or not. Classically, it is clear that we need two queries. We must check both $f(0)$ and $f(1)$ to know if they are equal.

We claim there is a simple 1-query quantum circuit (Deutsch's algorithm) for this task:



Tracing through the circuit, we get

$$|0\rangle \xrightarrow{H} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \xrightarrow{O_f} \frac{(-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle}{\sqrt{2}} = (-1)^{f(0)}\left(\frac{|0\rangle + (-1)^{f(0)\oplus f(1)}|1\rangle}{\sqrt{2}}\right)$$
$$\xrightarrow{H} (-1)^{f(0)}|f(0)\oplus f(1)\rangle$$

Therefore, if $f(0) = f(1)$, we will measure $|0\rangle$ with 100%, and if $f(0) \neq f(1)$, we will measure $|1\rangle$ with 100% probability. That is, we have a quantum algorithm that distinguishes between constant and non-constant functions with 100% probability.

A 1 vs. 2-query separation may not seem like a big deal, but essentially the exact same algorithm can lead to a much more impressive separation. To get these impressive separations, however, we will have to make a sacrifice. Namely, we will need to look at *promise problems*, that is, problems where the input function f has some specific property, called the "promise". Importantly, we will never judge our algorithm's correctness on functions f that don't satisfy the promise. This will allow us to devise algorithms that exploit some very specific structure for a query advantage.

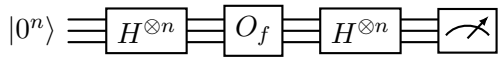
Let's begin with a problem that's the n-qubit generalization of Deutsch's problem:

Deutsch-Jozsa problem

Function:	$f\colon \{0,1\}^n \to \{0,1\}$
Promise:	f is either
	Constant: All outputs of f are equal. $\forall x, y \in \{0,1\}^n$, $f(x) = f(y)$; or
	Balanced: f has equal number of 0 and 1 outputs. $\lvert\{x \lvert f(x) = 1\}\rvert = 2^{n-1}$.
Goal:	Determine if f is constant or balanced.

Notice that a classical deterministic machine requires $2^{n-1}+1$ queries to f. In the worst case, the first 2^{n-1} queries to f yield the same output. It could be that all other unqueried inputs yield the same value (i.e., the function is constant) or all unqueried values yield the other value (i.e., the function is balanced). Therefore, we need 1 more query to solve the problem.

Miraculously, the quantum algorithm still only needs 1 query, and in fact, the quantum circuit is nearly identical to the one we saw previously:



Let's step through the circuit, one layer of gates at a time:

1. Apply a layer of Hadamard gates:

$$|0^n\rangle \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle$$

2. Apply the phase oracle:

$$\frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \xrightarrow{O_f} \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle$$

3. Apply final layer of Hadamard gates:

$$\frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle \xrightarrow{H^{\otimes n}} \frac{1}{2^n} \sum_{x,y \in \{0,1\}^n} (-1)^{f(x)+x \cdot y} |y\rangle$$

   Here, we are using "$\cdot$" to denote the inner product between x and y as binary vectors (i.e., $x \cdot y = \sum_{i=1}^n x_i y_i$). To see why this is true, we remark that the result of applying an n-fold Hadamard gate on an arbitrary classical state $|x\rangle$ can be written as

$$\begin{aligned} H^{\otimes n} |x\rangle &= \bigotimes_{i=1}^n \left(|0\rangle + (-1)^{x_i} |1\rangle \right) = \bigotimes_{i=1}^n \left((-1)^{x_i \cdot 0} |0\rangle + (-1)^{x_i \cdot 1} |1\rangle \right) \\ &= \bigotimes_{i=1}^n \left(\sum_{y_i \in \{0,1\}} (-1)^{x_i \cdot y_i} |y_i\rangle \right) = \sum_{y \in \{0,1\}^n} (-1)^{\sum_{i=1}^n x_i y_i} |y\rangle . \end{aligned}$$

What happens when we measure the state in Step 3? Let's look specifically at the probability we measure the all-zeros state (i.e., $y = 0^n$). Since $x \cdot 0^n = 0$ for all $x \in \{0,1\}^n$, the amplitude on $|0^n\rangle$ is

$$\frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)}.$$

If the function f is constant, then $f(x) = f(0^n)$ for all $x \in \{0,1\}^n$, so

$$\frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(0^n)} = \frac{(-1)^{f(0^n)}}{2^n} \left(\sum_{x \in \{0,1\}^n} 1 \right) = (-1)^{f(0^n)}$$

In other words, if we were to measure the state, then we would observe the all-zeros state with 100% probability.

If f is balanced, instead of all the amplitudes on the all-zeros state adding up constructively, they all cancel each other out:

$$\frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} = \frac{|\{x \mid f(x) = 0\}| - |\{x \mid f(x) = 1\}|}{2^n} = 0.$$

That is, if f is balanced, then we measure a state which is *not* the all-zeros state with 100% probability. Combining the two cases above, we can see that whether or not we measure the all-zeros state immediately solves the Deutsch-Jozsa problem.

At first glance, this 1 vs. $\Theta(2^n)$ quantum-classical query separation seems quite amazing, and possibly the best we could hope for. However, recall that the classical lower bound was for *deterministic* classical computation. If we were to allow for classical randomness, the problem becomes dramatically simpler. The classical algorithm would simply query f

on a few uniformly random inputs. If the function is balanced, then you are likely to see two different outputs using only constantly many queries (to formalize this argument, use the Chernov bound). That is, quantum algorithms are at best only marginally better than classical randomized algorithms for the Deutsch-Jozsa problem.

Let's now consider a similar problem where the classical algorithm will struggle a bit more:

Berstein-Vazirani problem

Function:	$f\colon \{0,1\}^n \to \{0,1\}$
Promise:	f is linear. For all $x \in \{0,1\}^n$, $f(x) = x \cdot s$ for some secret string $s \in \{0,1\}^n$
Goal:	Find s.

Once again, let's start by discussing the best classical query algorithm. Unlike the Deutsch-Jozsa problem, there is a fairly efficient algorithm—only n queries are needed. To see this, consider the algorithm that the queries f on the inputs $e_1 := 10\cdots0$, $e_2 := 010\cdots0$, and so on up to $e_n := 0\cdots01$. Notice that $f(e_i) = e_i \cdot s = s_i$, so each query reveals one of the n bits of s.

Can we do better? perhaps by using randomness? Unfortunately, not. To see this, consider that each query $x \cdot s = f(x)$ gives us a linear equation (over $\mathbb{F}_2$) where there are n unknown variables (i.e., the n bits of s). A linear system of equations with n-variables can only have a unique solution if there are at least n equations. Therefore, we require at least n queries.

As it turns out, the quantum algorithm is identical to the one for the Deutsch-Josza problem—a layer of Hadamards, followed by the phase oracle, followed by another layer of Hadamards. The only thing that changes is what we conclude from the measurement. Therefore, let's start from the state we constructed in Step 3 in our algorithm for the Deutsch-Josza problem:

$$\frac{1}{2^n}\sum_{x,y\in\{0,1\}^n}(-1)^{f(x)+x\cdot y}\,|y\rangle\,.$$

Using the fact that $f(x) = x \cdot s$, we get

$$\frac{1}{2^n}\sum_{x,y\in\{0,1\}^n}(-1)^{x\cdot s+x\cdot y}\,|y\rangle = \frac{1}{2^n}\sum_{x,y\in\{0,1\}^n}(-1)^{x(s\oplus y)}\,|y\rangle$$

Looking at the amplitude on state $|s\rangle$, we see that the term $(-1)^{x(s\oplus y)} = 1$ for all x since $s \oplus s = 0$. Since there are 2^n values for x, we immediately get that amplidude on $|s\rangle$ is 1. In other words, we measure $|s\rangle$ with 100% probability, but s was exactly what we were looking for!

Therefore, the Berstein-Vazirani problem gives us a 1 vs. n quantum-classical query separation. While this is less impressive than the initial separation we obtained for the Deutsch-Jozsa problem, it's worth emphasizing that this separation even holds against randomized classical algorithms.

As a final remark, we note that both the Deutsch-Josza and Berstein-Vazirani algorithms are instances of *Fourier sampling*. To see this, let's quickly introduce the Fourier basis. First, for all $y \in \{0,1\}^n$, we define the basis functions

$$\chi_y(s) := y \cdot s \pmod 2$$

for all $y \in \{0,1\}^n$. These functions are orthonormal with respect to following inner product on real-valued functions $f, g \colon \{0,1\}^n \to \mathbb{R}$:

$$\langle f, g \rangle := \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)+g(x)}.$$

To see orthonormality of these basis vectors, we compute

$$\langle \chi_y, \chi_z \rangle = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{x \cdot y + x \cdot y} = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{x \cdot (y \oplus z)} = \begin{cases} 1 & \text{if } y = z \\ 0 & \text{if } y \neq z \end{cases}.$$

Since we've defined a basis of 2^n independent functions, every Boolean function $f \colon \{0,1\}^n \to \{0,1\}$ can be written uniquely as

$$f(x) = \sum_{y \in \{0,1\}^n} \hat{f}(y) \chi_y(x)$$

for coefficients $\hat{f}(y) \in \mathbb{R}$. Using the inner product, we can explicitly compute the Fourier coefficients as

$$\hat{f}(y) = \langle f, \chi_y \rangle = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)+\chi_y(x)}.$$

Let's now consider what the Deutsch-Josza/Berstein-Vazirani algorithm does when we expand f in the Fourier basis. Once again, explicitly computing $H^{\otimes n} O_f H^{\otimes n} |0^n\rangle$, we get

$$\frac{1}{2^n} \sum_{x,y \in \{0,1\}^n} (-1)^{f(x)+x \cdot y} |y\rangle = \sum_{y \in \{0,1\}^n} \left(\frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)+\chi_y(x)} \right) |y\rangle = \sum_{y \in \{0,1\}^n} \hat{f}(y) |y\rangle .$$

In other words, what our quantum algorithm is actually doing for the Deutsch-Josza and Berstein-Vazirani problems is sampling a $y \in \{0,1\}^n$ with probability equal to $|\hat{f}(y)|^2$. Therefore, any function f that has simple Fourier expansion is immediately a promising candidate for an efficient quantum query algorithm.

3.3 Hidden subgroup problems

Let's now deviate slightly from our Fourier sampling framework to obtain a problem on which the classical algorithm will really struggle:

Simon's problem

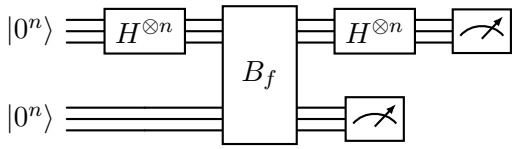
Function:	$f \colon \{0,1\}^n \to \{0,1\}^n$
Promise:	Outputs of f are paired by secret $s \in \{0,1\}^n$. That is, $f(x) = f(y)$ iff $x = y \oplus s$.
Goal:	Find s.

Notice that to solve Simon's problem it suffices to find a collision, a pair of strings $x \neq y$ such that $f(x) = f(y)$. If we find such an input pair, we can deduce s by taking their difference:

$$f(x) = f(y) \implies x = y \oplus s \implies s = x \oplus y.$$

Notice that if we query random inputs, we can expect to find a collision after only $O(\sqrt{2^n})$ queries via the birthday paradox bound. In fact, this algorithm can be derandomized so that $O(\sqrt{2^n})$ queries are sufficient for a classical determistic algorithm [CQ18]. Intuitively, after k queries, we've looked at $\binom{k}{2} \approx k^2$ pairs of inputs, so we need $k \approx 2^{n/2}$ queries to find one of the 2^{n-1} pairs. This same argument also suffices to give a lower bound of $\Omega(\sqrt{2^n})$ queries.

The quantum algorithm proceeds by running the following circuit $O(n)$ times:



Let's once again analyze this circuit layer by layer:

1. Apply a layer of Hadamard gates:

$$|0^n\rangle\,|0^n\rangle \xrightarrow{H^{\otimes n}\otimes I^{\otimes n}} \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle\,|0^n\rangle\,.$$

2. Apply the standard oracle:

$$\frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle\,|0^n\rangle \xrightarrow{B_f} \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle\,|f(x)\rangle$$

3. Measure the second register, getting outcome $f(x)$:

$$\frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle\,|f(x)\rangle \xrightarrow{\text{measure}} \frac{|x\rangle + |x\oplus s\rangle}{\sqrt{2}}\,|f(x)\rangle$$

   The idea is that there are only two inputs that are consistent with a measurement of $f(x)$ in the second register, both x and $x \oplus s$. Therefore, the first register is a superposition over those inputs. We can now drop the second register since it is unentangled with the first.

4. Apply another layer of Hadamard gates:

$$\frac{|x\rangle + |x\oplus s\rangle}{\sqrt{2}} \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2^{n+1}}} \sum_{y\in\{0,1\}^n} \left((-1)^{x\cdot y} + (-1)^{y\cdot(x\oplus s)}\right)|y\rangle$$

5. Measure first register to obtain uniformly random $y \in \{0,1\}^n$ such that $y \cdot s = 0$:

$$\frac{1}{\sqrt{2^{n+1}}} \sum_{y\in\{0,1\}^n} \left((-1)^{x\cdot y} + (-1)^{y\cdot(x\oplus s)}\right)|y\rangle = \frac{1}{\sqrt{2^{n+1}}} \sum_{y\in\{0,1\}^n} (-1)^{x\cdot y}\left(1 + (-1)^{y\cdot s}\right)|y\rangle$$

   From the right hand side, we can see that if $y \cdot s = 1$, the amplitude on state $|y\rangle$ is 0. On the other hand, if $y \cdot s = 0$, then the amplitude is $(-1)^{x\cdot y}/\sqrt{2^{n-1}}$. Taken together, this implies that the measurement returns a uniformly random $y \in \{0,1\}^n$ such that $y \cdot s = 0$.

To complete the quantum algorithm for Simon's problem, we note that the measurement result y gives us a random linear equation (over $\mathbb{F}_2$), $y \cdot s = 0$. If we could collect the $n-1$ linearly independent equations that span the subspace orthogonal to s, we could solve for the bits of s. Since our measurement results are uniformly random within this space, we will collect $n-1$ linearly independent equations with only $O(n)$ measurements with high probability.

To conclude, we finally have a problem in which quantum computers are getting an *exponential* advantage over classical computers—$O(n)$ vs. $O(\sqrt{2^n})$ queries. In fact, Simon's problem is special case of a wider class of problems which (sometimes) admit fast quantum algorithms.

Hidden Subgroup Problem (HSP)

Function:	$f : G \to \{0,1\}^*$ where G is a group
Promise:	f is constant on a hidden subgroup $H \leq G$. That is, $f(x) = f(y)$ iff $xH = yH$.
Goal:	Find H.

Notice that Simon's problem is HSP for the group $G = \mathbb{Z}_2^n$ and the subgroup $H = \{0^n, s\}$. In fact, the discrete log problem in $\mathbb{Z}_N^\times$ (a crucial step in Shor's integer factorization algorithm) can be cast as an instance of HSP for the additive abelian group $G = \mathbb{Z}_N \times \mathbb{Z}_N$. Both of these algorithms fall within a wide class of efficiently solvable HSP instances:

Theorem 3.1 (Kitaev [Kit95]). *HSP for finite abelian groups is in quantum polynomial time.*

What about non-abelian groups? The story is surprisingly subtle. While we don't know of any efficient quantum algorithms for such groups, there are efficient algorithms as measured by the query complexity:

Theorem 3.2 (Ettinger, Høyer, Knill [EHK04]). *The query complexity of HSP for any finite group G is polynomial in* $\log |G|$.

As some small taste for the power of such HSP instances, if the Ettinger-Høyer-Knill algorithm could be made time-efficient, then there would be an efficient quantum algorithm for the graph isomorphism problem, which has long evaded fast classical techniques.

3.4 Grover's algorithm and the unstructured search problem

So far, we've seen some huge quantum speedup for various query problems. Importantly, however, these exponential speedups have been for promise problems where the input instance comes from some restricted class. Let's now move on to consider *total problems*, where the problem must be well-defined over all possible instances.

One might wonder why we cannot just take any promise problem for which a quantum computer had some kind of advantage and extend it to inputs for which it wasn't previously defined. Unfortunately, the issue is that we cannot easily detect the inputs for which the original promise held. Since we *must* be able to detect those inputs to answer consistently on all inputs, it's unclear how to make such a strategy work. If fact, such a strategy provably cannot work:

Theorem 3.3 (Aaronson, Ben-David, Kothari, and Tal [ABDKT20])**.** *The deterministic query complexity of a total function is at most the quantum query complexity of that function to the fourth power.*

In other words, total functions can only yield polynomial query speedups. That said, the bound in the theorem is tight up to log factors [ABB+17]—there is a total problem on which determinstic algorithms require quartically many more queries than the best quantum algorithm. Instead of looking at total problems in general, let's look at a specific total problem that has shaped a lot of the discussion around quantum computers.

Unstructured search
Function: $f\colon \{0,1\}^n \to \{0,1\}$
Goal: Find $x \in \{0,1\}^n$ such that $f(x) = 1$ (or report none exists)

It's worth taking a moment to appreciate how monumental a fast quantum algorithm for unstructured search would be. Since problems in NP can be phrased as unstructured search problems (e.g., given a SAT formula, find a satisfying assignment), a poly-time quantum algorithm for unstructured search would immediately imply that NP $\subseteq$ BQP. Of course, by Theorem 3.3, we already know such a simple strategy for solving NP problems won't work. That is, since classical computers require expoentially many queries to solve unstructured search, so must quantum computers.

To see that exponentially many classical queries are required, consider the case where there is at most one input which evaluates to 1. Any classical deterministic algorithm will need to make 2^n queries since it might get unlucky and query $2^n - 1$ zeroes. Randomness doesn't help—even if you query half of the inputs, you only have a $1/2$ chance at choosing the input that evaluates to 1.

BBBV lower bound for search

While Theorem 3.3 leaves open the possibility that unstructured search can be solved with $O(2^{n/4})$ queries, this is unfortunately still too optimistic.

Theorem 3.4 (Bennett, Bernstein, Brassard, Vazirani [BBBV97])**.** *The quantum query complexity of unstructured search is* $\Omega(\sqrt{2^n})$.

As we will see later, there are actually many possible ways to prove this lower bound, but the BBBV lower bound was the first and perhaps most intuitive lower bound technique, so let's start with that. First, notice that a generic quantum query algorithm alternates between applying some unitary and applying the oracle. In other words, after t queries, the state of our system looks like

$$U_t O_f U_{t-1} \cdots O_f U_1 O_f U_0 \left|0^n\right\rangle .$$

To be fully rigorous here, we would also need to specify a set of ancillary workspace qubits, but this will not change the analysis and only make the notation more cumbersome, so we will drop these extra qubits.

A key point about this decomposition is that the unitaries $U_0, U_1, \ldots, U_t$ are fixed and are independent of what the oracle does. When there are few oracle queries, our goal will be to show that for every choice of unitaries, there is some state $|y\rangle$ that always has small

amplitude when queried by the oracle. Because of this, it will be very difficult for the algorithm to "see" whether or not this item is marked. Therefore, we can fool the algorithm into accepting/rejecting when it shouldn't.

Let's first consider what our algorithm does on the constant-zero function. In this case, the oracle is just the identity, and the algorithm should reject. The state of the algorithm after t queries is

$$|\psi_t\rangle := U_t U_{t-1} \cdots U_1 U_0 |0^n\rangle = \sum_{x \in \{0,1\}^n} \alpha_{x,t} |x\rangle .$$

Supposing there are T total queries, define the quantity

$$m_x := \sum_{t=0}^{T-1} |\alpha_{x,t}|^2.$$

to be the sum of the squares of the magnitudes on x over all states $|\psi_t\rangle$ we have right before the tth oracle call. We have that

$$\sum_{x \in \{0,1\}^n} m_x = \sum_{x \in \{0,1\}^n} \sum_{t=0}^{T-1} |\alpha_{x,t}|^2 = \sum_{t=0}^{T-1} \left(\sum_{x \in \{0,1\}^n} |\alpha_{x,t}|^2 \right) = \sum_{t=0}^{T-1} 1 = T.$$

Since m_x is non-negative, this implies that there must exist some $y \in \{0,1\}^n$ such that $m_y \leq T/2^n$ (otherwise, the sum is greater than T). This y will be the element that the algorithm fails to properly consider if T is too small. The above argument gives us a bound on the sum of the squares of the magnitudes for the input y, but it will turn out that we will actually need a bound on the sum of the magnitudes themselves. Fortunately, by Cauchy-Schwarz, we have

$$\sum_{t=0}^{T} |\alpha_{y,t}| \leq \sqrt{\sum_{t=1}^{T} |\alpha_{y,t}|^2 \cdot T} = \sqrt{m_y T} \leq \frac{T}{\sqrt{2^n}}.$$

Since we can refer to the all-zeros function as the identity, let f be the function which is 1 on y and 0 elsewhere. Our goal is to distinguish the oracle for f from the oracle for the identity, but for the purposes of analysis, let's consider a set of rather strange oracles $\{O^{(t)}\}_{t=0}^{T}$. Here, $O^{(t)}$ is defined to be the identity for the first t queries and f on the remaining $T - t$ queries. In other words, the oracle is interpolates between our two function instances. Let's define the set of states arising from the application of these oracles as

$$|\varphi^{(t)}\rangle := U_T O^{(t)} U_{T-1} \cdots O^{(t)} U_1 O^{(t)} U_0 |0^n\rangle = U_T O_f U_{T-1} \cdots O_f U_{t+1} O_f |\psi_t\rangle$$

So, for example, we have that $|\varphi^{(T)}\rangle = |\psi_T\rangle$ is the state for the complete execution of the quantum algorithm for the constant-zero function, and $|\varphi^{(0)}\rangle$ is the state for the execution of the quantum algorithm for f.

If we can show that $|\varphi^{(t+1)}\rangle$ is close to $|\varphi^{(t)}\rangle$ for all t, then by the triangle inequality, we will be able to conclude that the states from the two different problem instances are also close to each other. We have the following:

$$\begin{aligned}
\| |\varphi^{(t+1)}\rangle - |\varphi^{(t)}\rangle \| &= \| U_T O_f U_{T-1} \cdots O_f U_{t+2} O_f |\psi_{t+1}\rangle - U_T O_f U_{T-1} \cdots O_f U_{t+1} O_f |\psi_t\rangle \| \\
&= \| (U_T O_f U_{T-1} \cdots O_f U_{t+2} O_f U_{t+1}) |\psi_t\rangle - (U_T O_f U_{T-1} \cdots O_f U_{t+1}) O_f |\psi_t\rangle \| \\
&= \| |\psi_t\rangle - O_f |\psi_t\rangle \| \\
&= 2|\alpha_{y,t}|
\end{aligned}$$

where we have used the fact that unitaries preserves the 2-norm and the fact that $O_f |\psi_t\rangle = |\psi_t\rangle - 2\alpha_{y,t} |y\rangle$. Combining everything together, we get

$$\||\varphi^{(T)}\rangle - |\varphi^{(0)}\rangle\| \leq \sum_{t=0}^{T-1} \||\varphi^{(t+1)}\rangle - |\varphi^{(t)}\rangle\| \leq 2 \sum_{t=0}^{T-1} |\alpha_{y,t}| \leq \frac{2T}{\sqrt{2^n}}.$$

Hence, we see that for $T \ll \sqrt{2^n}$, the two states are close under ℓ_2 norm. We want to show that if the states are close, then all measurement procedures fail to distinguish them with high probability. To formalize this, let us define the *total variation distance* between two discrete probability distributions p, q:

$$\mathrm{TV}(p, q) = \frac{1}{2}\|p - q\|_1 = \frac{1}{2} \sum_i |p_i - q_i|.$$

The total variation distance is important because it determines the maximum probability with which we can distinguish two probability distributions. That is, suppose with 50% probability we sample from p and with 50% probability we sample from q, the maximum probability with which we can guess which distribution was sampled from is $1/2 + \mathrm{TV}(p, q)/2$.

Lemma 3.5. *If $\||\phi\rangle - |\psi\rangle\|_2 < \epsilon$, then the total variation distance from measuring $|\phi\rangle$ and $|\psi\rangle$ is at most 2ϵ.*

Proof. Suppose $|\phi\rangle = \sum \alpha_x |x\rangle$, $|\psi\rangle = \sum \beta_x |x\rangle$. For ease of notation, assume α_x, β_x are all real numbers, though the proof still works if we allow them to be complex. Let $\gamma_x = \beta_x - \alpha_x$. Now we write

$$\||\phi\rangle - |\psi\rangle\|_2 = \sqrt{\sum_x \gamma_x^2} \leq \epsilon.$$

Let p, q be the distributions of measuring $|\phi\rangle$, $|\psi\rangle$ respectively. Then, we have that (twice) their total variation distance is

$$\begin{aligned}
\sum_x |\alpha_x^2 - \beta_x^2| &= \sum_x (\beta_x - \alpha_x)(\beta_x + \alpha_x) \\
&= \sum_x \gamma_x(\gamma_x + 2\alpha_x) \\
&\leq \sum_x \gamma_x^2 + 2|\gamma_x \alpha_x| && \text{(triangle inequality)} \\
&\leq \|\gamma\|_2^2 + 2\|\gamma\|_2 \|\alpha\|_2 && \text{(Cauchy–Schwarz)} \\
&\leq \epsilon^2 + 2\epsilon\,,
\end{aligned}$$

which is at most 4ϵ since $\epsilon \leq 2$ by the triangle inequality ($\||\phi\rangle - |\psi\rangle\|_2 \leq \||\phi\rangle\|_2 + \||\psi\rangle\|_2 = 2$). Hence the TV distance is at most 2ϵ. □

Putting everything together, we have shown that for any quantum algorithm with T queries, there is a state we should accept and one we should reject which we can distinguish with probability at most $\frac{1}{2} + \frac{2T}{\sqrt{2^n}}$. To correctly answer at least $2/3$ of the time, this must be at least a constant larger than $1/2$, which requires $T = \Omega(2^{n/2})$.

Grover's algorithm

While a $\Omega(\sqrt{2^n})$ query lower bound for search is an unpleasant reality, notice that the situation is not as bad as it could be—after all, the classical algorithm requires $\Omega(2^n)$ queries. Can we devise a devise a quantum algorithm that gets this quadratic improvement over the classical algorithm? We can!

Theorem 3.6 (Grover's algorithm)**.** *There is a $O(\sqrt{2^n})$ time quantum algorithm for unstructured search.*

It will turn out that the simplest version of Grover's algorithm depends on the number of marked items, that is, inputs x such that $f(x) = 1$. Therefore, let's assume for now that there is only a single marked item. We will see in the analysis that this is the "hard" case.

The entirety of Grover's algorithm is simply alternating between the phase oracle (i.e., O_f) and the "Grover diffusion operator" defined as

$$D := 2\left|u\right\rangle\!\left\langle u\right| - I$$

where $\left|u\right\rangle := H^{\otimes n}\left|0^n\right\rangle$ is the uniform superposition.

Claim 3.7. *The diffusion operator $D := 2\left|u\right\rangle\!\left\langle u\right| - I$ is a unitary operation that reflects[1] about $\left|u\right\rangle$. Furthermore, D can be constructed with linearly-many gates in log depth.*

Proof. To verify that D is unitary, we can simply compute

$$DD^\dagger = (2\left|u\right\rangle\!\left\langle u\right| - I)\cdot(2\left|u\right\rangle\!\left\langle u\right| - I)^\dagger = 4\left|u\right\rangle\!\left\langle u\right| - 2\left|u\right\rangle\!\left\langle u\right| - 2\left|u\right\rangle\!\left\langle u\right| + I = I.$$

To see why D is a reflection about $\left|u\right\rangle$, first notice that we can decompose an arbitrary state $\left|\psi\right\rangle$ as its component aligned with $\left|u\right\rangle$ and its component orthogonal to $\left|u\right\rangle$.

$$\left|\psi\right\rangle = \alpha\left|u\right\rangle + \beta\left|v\right\rangle\ ,$$

where $\langle u|v\rangle = 0$ and $|\alpha|^2 + |\beta|^2 = 1$. Then, we can verify

$$D\left|\psi\right\rangle = \alpha\left(2\left(\left|u\right\rangle\!\left\langle u\right|\right) - I\right)\left|u\right\rangle + \beta\left(2\left(\left|u\right\rangle\!\left\langle u\right|\right) - I\right)\left|v\right\rangle = \alpha\left|u\right\rangle - \beta\left|v\right\rangle\ ,$$

where we use the fact that $\langle u|u\rangle = 1$ and $\langle u|v\rangle = 0$.

To see that D can be constructed with linearly-many gates in log depth, notice that if we conjugate D by Hadamard, we get the reflection about the all-zeros state: $D_0 = 2\left|0^n\right\rangle\!\left\langle 0^n\right| - I$. Therefore, we just need a circuit for D_0. On the computational basis states, we have $D_0\left|x\right\rangle = (-1)^{x_1\vee\cdots\vee x_n}\left|x\right\rangle$ so we just need to be able to detect if any of the qubits are 1 (which can be done with a linear-size, log-depth reversible circuit) and apply a phase gate depending on the answer. □

[1] By "reflect" about $\left|u\right\rangle$, we mean that D flips the sign of every vector in the subspace orthogonal to $\left|u\right\rangle$.

Algorithm 1 Grover's algorithm

Input: 2^n unknown input bits accessed through the oracle O_f.
Output: $s \in \{0,1\}^n$ such that $f(s) = 1$, or `null` if none exists.

1: $|\psi_0\rangle = H^{\otimes n} |0^n\rangle$
2: **for** $i \in \{1, \ldots, T\}$ **do**
3: $\quad |\psi_i\rangle \leftarrow DO_f |\psi\rangle_{i-1}$
4: $s^* \leftarrow$ measurement of $|\psi_T\rangle$
5: **return** s^* if $f(s^*) = 1$; otherwise, `null`

Examining Grover's algorithm, we see that the final state before we measure is given by

$$DO_f \cdots DO_f DO_f |u\rangle$$

To understand why this algorithm works, it will be extremely useful to take a geometric perspective. To start, notice that our initial state $|u\rangle$ lies in a particular 2-dimensional subspace that is spanned by $|s\rangle$ (our marked item) and $|\Psi\rangle = \frac{1}{\sqrt{2^n - 1}} \sum_{x \neq s} |x\rangle$ (the uniform superposition over all unmarked states):

$$|u\rangle = \frac{1}{\sqrt{2^n}} \sum_x |x\rangle = \frac{1}{\sqrt{2^n}} |s\rangle + \frac{1}{\sqrt{2^n}} \sum_{x \neq s} |x\rangle = \frac{1}{\sqrt{2^n}} |s\rangle + \sqrt{1 - \frac{1}{2^n}} |\Psi\rangle .$$

First, we make the following intriguing observation:

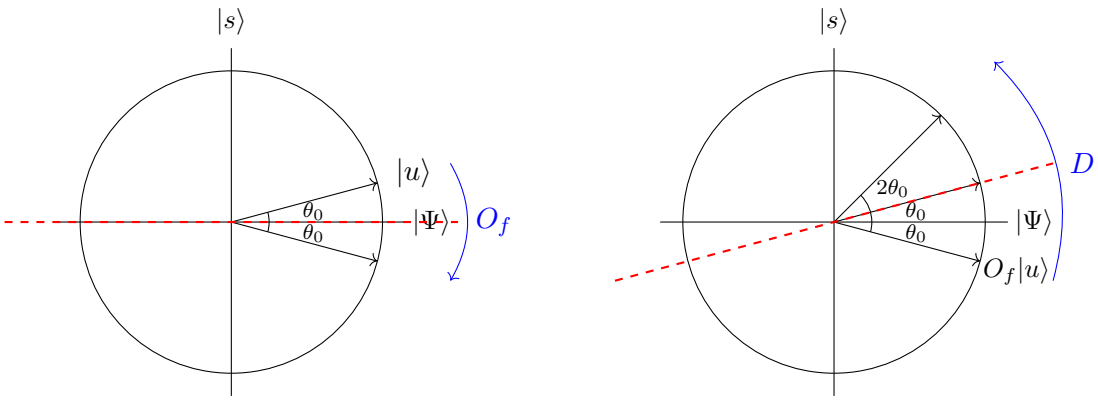
Observation 3.8. *Each Grover iteration keeps the state in the span of $|s\rangle$ and $|\Psi\rangle$.*

Proof. This is easy to see for the phase oracle: $\alpha |s\rangle + \beta |\Psi\rangle \xrightarrow{O_f} -\alpha |s\rangle + \beta |\Psi\rangle$. For the diffusion operator, we have

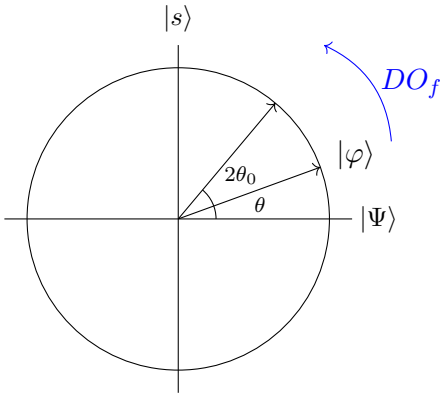
$$\alpha |s\rangle + \beta |\Psi\rangle \xrightarrow{D} (2 |u\rangle\langle u| - I)(\alpha |s\rangle + \beta |\Psi\rangle) = 2(\alpha \langle u|s\rangle + \beta \langle u|\Psi\rangle) |u\rangle - \alpha |s\rangle - \beta |\Psi\rangle$$

but we've already seen above that $|u\rangle$ can be expressed a linear combination of $|s\rangle$ and $|\Psi\rangle$. □

In other words, each Grover operation is a rotation in the plane spanned by $|s\rangle$ and $|\Psi\rangle$. We have that O_f reflects about $|\Psi\rangle$, and the diffusion operation reflects about $|u\rangle$:



If we compose the two operations (i.e., DO_f) and apply them to any arbitray state $|\varphi\rangle$, we simply get a rotation in this space of $2\theta_0$, where θ_0 is the initial angle between $|u\rangle$ and $|\Psi\rangle$:



That is, the evolution of the angle is given by $\theta_0, 3\theta_0, 5\theta_0, \ldots, (2T+1)\theta_0$. Notice that we want to reach the angle $\pi/2$, so we get that we need $T \approx \pi/(4\theta_0)$ steps. In other words, performance our the entire algorithm hinges on the angle θ_0 between our initial state $|u\rangle$ and the unmarked state $|\Psi\rangle$. We have

$$\sin(\theta_0) = \langle u|s\rangle = \frac{1}{\sqrt{2^n}} \implies \theta_0 \approx \frac{1}{\sqrt{2^n}}$$

where we have used that $\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots$ is approximately x for small x. Therefore, to rotate our initial state to the $|s\rangle$ state we need $T = O(\sqrt{2^n})$. After that many queries, we simply measure to obtain the marked state s with high probability.

Of course, this analysis only holds if there was indeed a marked element. However, after we've done this procedure, we measure to obtain to some candidate marked item s^*. We can use one more query to our oracle to check that $f(s^*) = 1$. This completes the analysis of Grover's algorithm for a single marked element.

What happens if there are more than 1 marked items? In this case, let $|s\rangle$ be the uniform superposition over all marked items. If we have m marked elements, then initial angle is $\langle s|u\rangle \approx \sqrt{m/2^n}$ at least when there aren't too many marked items (if there are so many marked items, we can just randomly sample until we find one). Therefore, with the same analysis, the number of queries required to rotate our state to $|s\rangle$ is $O(\sqrt{2^n/m})$. When we measure, we get a uniformly random marked item. This speedup follows our intuition that if there are more marked elements, it should be easier to find one of them.

There is one final question to address. Namely, the above analysis only works when we know the number marked elements. Indeed, if we continue to do more Grover iterations, then our state continues to rotate around the unit circle. If the number of marked items is unknown, how do we know when to stop and measure? The trick is something called "exponential search." We make the following sequence of guesses for m: $2^n, 2^{n-1}, 2^{n-2}, \ldots, 4, 2$. Notice that if we make all n possible guesses, then we are at most a factor of 2 off from the true answer. One can check that this does not dramatically affect the analysis. The reason that the we search in decreasing order is because we want to obtain a speedup in the case that there are actually many marked items. If at any point we find a marked item, then we stop.

Consequences of Grover's algorithm

Consider a variant of Simon's problem:

Collision
Function: $f\colon \{0,1\}^n \to \{0,1\}^n$
Promise: f is 1-to-1 or 2-to-1
Goal: Decide which

Fact 3.9. *Suppose f is 2-to-1. Then for randomly chosen $A, B \subseteq \{0,1\}^n$ with $|A||B| = 2^n$ there is a constant probability that there exists $a \in A$ and $b \in B$ such that $f(a) = f(b)$.*

Theorem 3.10 (Brassard, Høyer, and Tapp [BHT97])**.** *The quantum query complexity of the Collision problem is $O(2^{n/3})$.*

Proof. Pick a random A of size $2^{n/3}$ and B of size $2^{2n/3}$. First query each element of A, which takes $2^{n/3}$ queries. With this, construct the (single query) function $g(x)$ which returns true if there is $a \in A$ with $f(x) = f(a)$. Now run Grover's algorithm on B, to see if g is ever true. This takes $O(\sqrt{2^{2n/3}}) = O(2^{n/3})$ queries. □

3.5 Polynomial method

Let's now look a generic technique for proving quantum query lower bounds known as the polynomial method. To start, it will be convenient to reinterpret the meaning of a quantum query. Namely, instead of using the oracle to apply a function, we use it to reveal a bit of a hidden string. To be clear, these models are identical, only the language we use is different. That is, for a function $f\colon \{0,1\}^n \to \{0,1\}$, we consider the (exponentially long) bit string defined by all its outputs: $x = x_1 x_2 \dots x_{2^n}$ where x_i is the ith output of f when the inputs are ordered in binary. The input to the oracle is now an index into this string of length $N := 2^n$.

Using this language, we will show that the acceptance probability of every quantum query algorithm can be viewed as a polynomial in the x_i variables. To start, recall the generic form of a quantum query algorithm:

$$U_t O_x U_{t-1} \cdots O_x U_1 O_x U_0 \left|0^n\right\rangle .$$

which alternates between unitary operations and the phase oracle for the hidden bitstring x (once again, we've hidden the ancilla register for clarity). Let's start by looking at the affect of the first unitary and oracle call:

$$|0\rangle \xrightarrow{U_0} \sum_{i=1}^{N} \alpha_i |i\rangle \xrightarrow{O_x} \sum_{i=1}^{N} (-1)^{x_i} \alpha_i |i\rangle .$$

Our first observation is that for $x_i \in \{0,1\}$ we can rewrite $(-1)^{x_i}$ as $1 - 2x_i$, so the state becomes

$$\sum_{i=1}^{N} (1 - 2x_i)\alpha_i |i\rangle .$$

Repeating this argument for each query, we arrive at one of the central ideas for the polynomial method:

Claim 3.11. *After t oracle calls, the amplitude of each classical basis state is a polynomial of degree t in the variables $x_1, \ldots, x_N$.*

Proof. The proof follows immediately from the following ideas we saw before: 1) applying a phase oracle increases the degree of the polynomial by at most 1; and 2) applying any unitary does not increase the degree. □

Concretely, after t oracle calls, let's write the state of our system as

$$\sum_{i=1}^{N} \alpha_i(x) |i\rangle ,$$

where each $\alpha_i(x)$ is a degree t polynomial in $x_1, \ldots, x_N$. Let's imagine that we use the quantum algorithm to solve some decision problem where we accept if we measurement outcome falls within some set S. The acceptance probability in that case, would be

$$p(x) := \sum_{i \in S} |\alpha_i(x)|^2.$$

Notice that each $|\alpha_i(x)|^2$ is a polynomial of degree $2t$, so $p(x)$ must also be a polynomial of degree $2t$.

The central idea behind the polynomial method is that low-degree polynomials are "well-behaved" in many respects. If we're trying to devise a quantum algorithm that is solving a complex problem, but the acceptance probability of the algorithm is given by a low-degree polynomial, the polynomial might not be expressive enough to capture the complexity of the problem.

Grover lower bound via the polynomial method

Let's use the polynomial method to tackle the unstructured search problem. We'll focus on the decision variant where we'd like to know if our hidden bitstring $x_1 \cdots x_N$ contains a 1. This variant is sometimes called "OR" since we're trying to determine if $x_1 \vee x_2 \vee \cdots \vee x_N$ is satisfied.

Our first key observation will be that the OR problem is symmetric: no matter what permutation we apply to the string x, the answer to "does there exist a 1 in the string?" should not change. This will allow us to create a *symmetric* polynomial that captures the acceptance probability of the quantum algorithm.

Specifically, let $p(x)$ be the degree $2t$ polynomial for the acceptance probability of a t-query quantum algorithm for the OR problem. Define $q(x)$ to be the polynomial which averages the $p(x)$ polynomials after applying a permutation:

$$q(x) := \frac{1}{N!} \sum_{\pi \in S_N} p(\pi \cdot x)$$

where we denote by $\pi \cdot x$ as the result of applying the permutation to the bit string x, i.e., $\pi \cdot (x_1 \cdots x_N) = x_{\pi^{-1}(1)} \cdots x_{\pi^{-1}(N)}$. By our previous observation (the problem's answer is invariant under permutation of the input string), $q(x)$ should also be at least the acceptance probability of the algorithm. Furthermore, $q(x)$ is now symmetric.

To be clear, $q(x)$ is a multivariate polynomial in $x_1, \ldots, x_N$. However, we now claim that because $q(x)$ is symmetric it can be written as a univariate polynomial $r(z)$ of the same degree where $z = \sum_{i=1}^{N} x_i$.

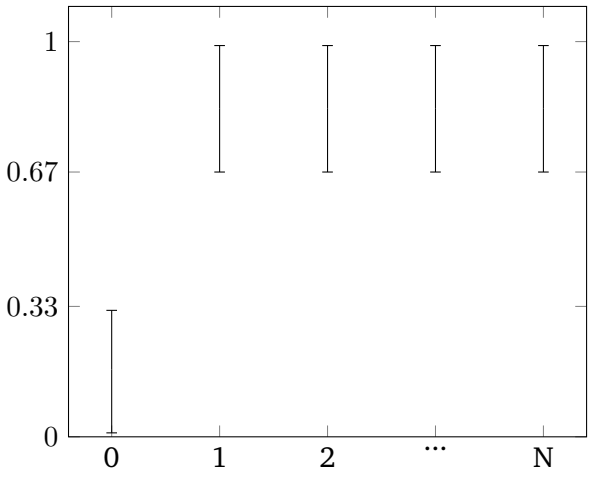
To show this, we will use the following fact: for every symmetric polynomial over Boolean variables, the coefficients of all terms of the same degree are equal. To prove this, simply take the smallest degree for which this is not true and consider the two terms with different coefficients. Setting the variables to be all 1's in one term and the rest 0's gives a different result from setting the variables to be all 1's in the other term and the rest 0's. Since both terms have the same number of variables, this is a contradiction because the function was supposed to be symmetric.

Let β_i be the coefficient of any term in $q(x)$ which has degree i. Notice that our new variable $z = \sum_{i=1}^{N} x_i$ counts the number of variables which are 1. Therefore, using the above argument, we can write

$$q(x) = \sum_{i=0}^{\deg q} \beta_i \binom{z}{i} = \sum_{i=0}^{\deg q} \beta_i \frac{z(z-1)\cdots(z-i+1)}{i!} = r(z)$$

as the expression that counts how many terms in the original expansion of $q(x)$ had the same degree.

Let's return to our specific problem. To summarize, we have a polynomial $r(z)$ of degree $2t$ which captures the acceptance probability of the quantum algorithm after t queries. If the quantum algorithm were perfect (i.e., had no error), then $r(0) = 0$ and $r(z) = 1$ for all $z \neq 0$. Since the quantum algorithm can err with probability at most $1/3$, the acceptance probabilities must have values in the following ranges:



To be clear, the polynomial $r(z)$ can do whatever it likes on non-integer points, but on the values $0, 1, \ldots, N$, it must fall within the specified ranges. We now want to show that any polynomial which has that behavior must necessarily have relatively high degree. Specifically, we can apply the Markov brothers' inequality:

Theorem 3.12 (Markov brothers' inequality)**.** *If $p(x)$ is a polynomial, then*

$$\max |p'(x)| \leq \left| \frac{\max p(x) - \min p(x)}{N} \right| (\deg p)^2,$$

where the max and min values are for $0 \leq x \leq N$ and $p'(x)$ denotes the first derivative.

Theorem 3.13. *If $r(z)$ as above has the desired properties, then $t = \Omega(\sqrt{N})$.*

Proof. Plugging in r to the Markov brothers' inequality and rearranging and weakening slightly gives us

$$\frac{N}{4t^2}\left(\max_{0\leq z\leq N}|r'(z)|\right) \leq \max_{0\leq z\leq N} r(z)$$

Let $M = \max_{0\leq z\leq N} r(z)$, and pick z_0 with $r(z_0) = M$ (we can do so since $[0, N]$ is compact). Let's analyze two possible cases:

$M < 2$: Note this is the "most likely" case, since we don't expect our function to go skyrocketing. In order to have $r(0) \leq 1/3$ and $r(1) \geq 2/3$, by the mean value theorem there must be some $z \in [0, 1]$ with $r'(z) \geq 1/3$. Plugging this into the brothers' inequality, we get

$$\frac{N}{12t^2} \leq \frac{N}{4t^2}\max|r'(z)| \leq \max r(z) < 2$$

so in this case we know that $t = \Omega(\sqrt{N})$.

$M \geq 2$: In this case, the mean value theorem implies that $|r'(c)| \geq 2(M-1)$ for some $c \in [\lfloor z_0 \rfloor, \lceil z_0 \rceil]$, since r must return down to at most 1 for each integer, and the closest integer is at most $1/2$ away. We get $2N(M-1) \leq M(2t)^2$, so

$$\frac{N}{2t^2} \leq \frac{M}{M-1} \leq 2$$

and hence again we know that $t = \Omega(\sqrt{N})$. □

Combining everything together, we get a new proof of Theorem 3.4 using the polynomial method:

Proof of Theorem 3.4: Any quantum query algorithm that approximates OR with t queries gives rise to a polynomial r of degree $2t$. By Theorem 3.13, any such polynomial must have degree $\Omega(\sqrt{N})$. Hence, the total number of queries must be $\Omega(\sqrt{N})$. □

Observation 3.14. *Suppose we want to construct a quantum algorithm for OR that has perfect accuracy. That is, $r(z) = 1$ for $z = 1, 2, \ldots N$. The fundamental theorem of algebra requires a polynomial of $\deg r \geq N$, so we need at least $N/2$ queries.*

Complexity of Parity

Considering the following simple problem:

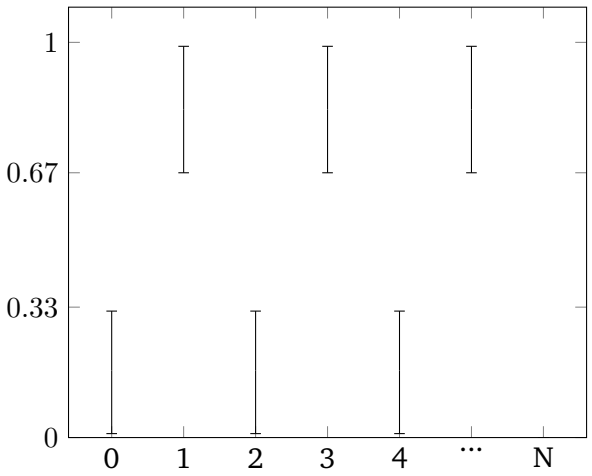
Parity
Hidden string: $x_1 \cdots x_N \in \{0,1\}^N$
Goal: Compute $x_1 \oplus \cdots \oplus x_N$

First, notice that we can use Deutsch's algorithm to compute parity with $N/2$ queries. To see this, first notice Deutsch algorithm can compute $x_j \oplus x_j$ for any pair of bits—in the

"constant" case, $x_i = x_j$ which implies $x_i \oplus x_j = 0$; in the "balanced" case, $x_i \neq x_j$ which implies $x_i \oplus x_j = 1$. Pairing up all the bits, we get an $N/2$ query bound. Somewhat surprisingly, this is exaclty tight:

Theorem 3.15. *The quantum query complexity of the parity function is precisely $N/2$.*

Proof. The parity function is symmetric, so running the polynomial method as above again gives us $r(z)$ which must now have values in these ranges:



In particular, $r(z) = 1/2$ at N distinct values, one each between i and $i+1$ for $0 \leq i < N$. Thus by the fundamental theorem of algebra, $\deg r \geq N$. Since the degree of r is at most twice the number of queries, we must have made at least $N/2$ queries. □

3.6 Adversary method

Perhaps the simplest way to prove query lower bounds is through a powerful technique called the "adversary method". It is a general technique that can apply to all decision problems $\mathcal{P}\colon \{0,1\}^N \to \{0,1\}$, where $\mathcal{P}(x)$ indicates whether or not the hidden bitstring x is part of the language.

For example, for the OR language, $\mathcal{P}(x) = 1$ iff x contains a 1.

Theorem 3.16 (Ambainis Adversary Method [Amb00])**.** *Suppose $\mathcal{P}\colon \{0,1\}^N \to \{0,1\}$. Let $X \subseteq \{0,1\}^N$ be a subset of 0-inputs and let $Y \subseteq \{0,1\}^N$ be a set of 1-inputs—that is, $\mathcal{P}(x) = 0$ for all $x \in X$; and $\mathcal{P}(y) = 1$ for all $y \in Y$. Let $R \subseteq X \times Y$ be any relation over the sets X and Y satisfying the following conditions:*

1. *For every $x \in X$, there are at least m_0 inputs $y \in Y$ such that $(x,y) \in R$.*
2. *For every $y \in Y$, there are at least m_1 inputs $x \in X$ such that $(x,y) \in R$.*
3. *For every $x \in X$ and $i \in \{1,\ldots,N\}$, there are at most s_0 inputs $y \in Y$ with $(x,y) \in R$ and $x_i \neq y_i$.*
4. *For every $y \in Y$ and $i \in \{1,\ldots,N\}$, there are at most s_1 inputs $x \in X$ with $(x,y) \in R$ and $x_i \neq y_i$.*

The quantum query complexity of $\mathcal{P}$ is $\Omega\left(\sqrt{\frac{m_0 m_1}{s_0 s_1}}\right)$.

Once again, let's use this to prove a lower bound for OR.

Proof of Theorem 3.4: Let $X = \{0^N\}$ be the set that only contains the all-zeros string and $Y = \{x : |x| = 1\}$ be the set containing those strings with exactly one 1. We also let $R = X \times Y$ be all pairs of strings in X and Y. We have that, $m_0 = N$, $m_1 = 1$, $s_0 = 1$, $s_1 = 1$, so the query complexity is $\Omega(\sqrt{N})$. □

Query lower bounds via reduction

Let's define a promise-free variant of the Collision problem:

Element Distinctness
Function: $f\colon \{0,1\}^n \to \{0,1\}^n$
Goal: Determine if there are distinct inputs $x, y \in \{0,1\}^n$ such that $f(x) = f(y)$

Recall that for the Collision problem, the goal was to find a collision when we were promised that f was either 2-to-1 or 1-to-1. For Element Distinctness, we no longer have that promise. Indeed, f could very close to a 1-to-1 function, and yet there could still be inputs which collide. Element Distinctness is clearly a harder problem than Collision, but... how much harder?

It turns out that proving a quantum query lower bound from scratch for Element Distinctness is quite challenging, but suppose we knew the following lower bound for the Collision problem:

Theorem 3.17 ([Shi02])**.** *The quantum query complexity of Collision is* $\Omega(2^{n/3})$.

Our goal will be to reduce the Collision problem to the Element Distinctness problem, so that an efficient query algorithm for Element Distinctness implies an efficient query algorithm for Collision.

Theorem 3.18. *The quantum query complexity of Element Distinctness is* $\Omega(2^{2n/3})$.

Proof. Suppose there is a quantum query algorithm for Element Distinctness with $o(2^{2n/3})$ queries. We claim that this implies a quantum query algorithm for Collision with $o(2^{n/3})$ queries, contradicting the lower bound of Theorem 3.17.

Therefore, suppose we have some instance f of Collison. Sample a random subset $R \subset \{0,1\}^n$ of size $|R| = 2^{n/2}$. By the Birthday Paradox (see Fact 3.9), with high probability, there exists $x, y \in R$ such that $f(x) = f(y)$ if f is 2-to-1. Now run the Element Distinctness algorithm with f restricted to the subset R to determine whether a collision exists. The query complexity of the algorithm is then $o((2^{n/2})^{2/3}) = o(2^{n/3})$. We conclude that any quantum query algorithm for Element Distinctness must make $\Omega(2^{\frac{2n}{3}})$ oracle queries. □

Chapter 4

Complexity of Clifford circuits

Clifford operations are just those unitaries constructed from circuits of CNOT, Hadamard, and Phase gates. As we've seen throughout these notes, the Clifford gates have appeared in many quantum algorithms. As we will soon see, this is not just a coincidence. The Clifford gates have some extremely nice properties. Perhaps too nice! In fact, Clifford circuits can be efficiently simulated on a classical computer. Nevertheless, we will eventually see that this is not the end of the story. Clifford circuits show a surprising advantage over classical circuits when the comparison point is the depth of the circuit.

4.1 Clifford circuits, the gate definition

Let's start by defining Clifford circuits in the simplest possible way, by the list of gates that comprise them—controlled-not (CNOT), Hadamard (H), and Phase (S). The set of all unitaries that arise from Clifford circuits is called the *Clifford group*. A *Clifford state* or a *stabilizer state* is obtained by applying a Clifford circuit to the all-zeros state.

To recap, the fundamental Clifford gates are

$$\mathrm{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}.$$

One way to start to understand the power and limitations of Clifford circuits is just to play around with them, applying variations to see what kinds of states you can create. One thing you will notice is that you get a discrete set of gates, and with a bit more mathematics, you can give an exact characterization of what these states look like. This will be our first approach to proving the famous Gottesman-Knill theorem:

Theorem 4.1 (Gottesman–Knill [Got98])**.** *There is a classical polynomial-time algorithm to sample from the output distribution of any Clifford circuit.*

As previously mentioned, our plan to prove this theorem will be keep track of the state vector of the quantum state as we apply each Clifford gate in the circuit. Of course, we can't write out the entire state vector, as this would require exponential space. It turns out, however, that Clifford states have the following special form:

Lemma 4.2. *[DM03, VDN10] Every n-qubit Clifford state can be written as*

$$|\psi\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{x \in \mathcal{A}} (-1)^{q(x)} i^{\ell(x)} |x\rangle$$

where

- *$\mathcal{A}$ is an affine space: $\mathcal{A} = \{My + b \pmod 2 \mid y \in \{0,1\}^r\}$ for $M \in \{0,1\}^{n \times r}$ and $b \in \{0,1\}^n$.*
- *$q(x)$ is a quadratic form: $q(x) = \sum_{i<j} q_{ij} x_i x_j$ with $q_{ij} \in \{0,1\}$.*
- *$\ell(x)$ is a linear form: $\ell(x) = \sum_i \ell_i x_i$ with $\ell_i \in \{0,1,2,3\}$.*

The natural proof of this statement also gives a classical simulation algorithm. That is, starting with the all-zeroes state (which is trivially of the above form), show how it evolves under the application of each one of the fundamental Clifford operations. Since each update to the state takes polynomial time, the entire computation will take polynomial time. By induction, we need to understand the following cases:

- **Apply S on qubit i:**

$$S|\psi\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{x \in \mathcal{A}} (-1)^{q(x)} i^{\ell(x)} S|x\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{x \in \mathcal{A}} (-1)^{q(x)} i^{\ell(x)} i^{x_i} |x\rangle$$

  In other words, if we let $\ell'(x) = l(x) + x_i \pmod 4$, then we have an updated representation of the state with Affine space $\mathcal{A}$, quadratic form $q(x)$, and linear form $\ell'(x)$.

- **Apply CNOT from qubit i to qubit j:**

$$\mathrm{CNOT}|\psi\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{x \in \mathcal{A}} (-1)^{q(x)} i^{\ell(x)} \mathrm{CNOT}|x\rangle = \frac{1}{\sqrt{|\mathcal{A}|}} \sum_{x \in \mathcal{A}} (-1)^{q(x)} i^{\ell(x)} |\mathrm{CNOT}x\rangle$$

  where the last equation reflects the fact that CNOT can be identified with an $n \times n$ Boolean matrix which XOR's the ith bit into the jth bit of the n-bit vector x. Therefore, we now have

  - *Affine space:* $\mathcal{A}' = \{M'y + b' \mid \forall y \in \{0,1\}^n$ for $M' = \mathrm{CNOT}M$ and $b' = \mathrm{CNOT}b$.
  - *Quadratic form:* Notice that we can write $q(x) = x^T Q x$ for some upper triangular matrix Q. Therefore, the updated quadratic form can be written as $q'(x) = q(\mathrm{CNOT}x) = x^T Q' x$ with $Q' = \mathrm{CNOT}^T \cdot Q \cdot \mathrm{CNOT}$.
  - *Linear form:* Similar to above, we can write $\ell(x) = \ell^T x$ for the vector $\ell = (\ell_1, \ldots, \ell_n)$. Therefore, the updated linear form can be written as $\ell'(x) = \ell(\mathrm{CNOT}x) = (\ell')^T x$ where $(\ell')^T = \ell^T \mathrm{CNOT}$.

- **Apply H:** The proof for applying H is nontrivial, so we leave it for now. See proof in [VDN10].

In conclusion every Clifford state $|\psi\rangle$ can be written of the form in Lemma 4.2. Furthermore, the inductive proof reveals a polynomial-time algorithm to compute $\mathcal{A}, \ell, q$ of a state given the sequence of Clifford gates that construct the state.

4.2 Clifford circuits, the stabilizer picture

In the stabilizer picture of simulation [Got98], we do not represent a quantum state by its state vector, but rather as a list of "stabilizers" of the state, i.e., unitary matrices for which the original state vector is an eigenvector. It will turn out that this is a particularly useful representation for states generated by a Clifford circuits. Before we do this, however, let us describe a important subgroup of the Clifford group called the Pauli group that will be the basis of this representation.

Pauli Group

The single-qubit Pauli group is generated by Pauli matrices, which are:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The Pauli matrices also have a bunch of nice properties (I is the 2×2 identity matrix):

- Hermitian: $X = X^\dagger$, $Y = Y^\dagger$, $Z = Z^\dagger$
- Square to the identity: $X^2 = Y^2 = Z^2 = I$
- Traceless: $\mathrm{Tr}(X) = \mathrm{Tr}(Y) = \mathrm{Tr}(Z) = 0$
- Same determinant: $\det(X) = \det(Y) = \det(Z) = -1$
- Anticommutation: $XY = -YX$, $XZ = -ZX$, $YZ = -ZY$
- Cyclic structure: $\begin{array}{lll} XY = iZ & YZ = iX & ZX = iY \\ YX = -iZ & ZY = -iX & XZ = -iY \end{array}$

These Pauli matrices form a group $\mathcal{P}_1$ of order 16 under matrix multiplication, where each element is of the form αP with $\alpha \in \{\pm 1, \pm i\}$ and $P \in \{I, X, Y, Z\}$. More generally, each element of the n-qubit Pauli group $\mathcal{P}_n$ is of the form $\alpha P_1 \otimes P_2 \otimes \cdots \otimes P_n$ where $\alpha \in \{\pm 1, \pm i\}$ and $P_i \in \{I, X, Y, Z\}$.

Although $|\mathcal{P}_n| = 4 \cdot 4^n$, $\mathcal{P}_n$ is generated by just $2n$ elements: Pauli elements with a single Z and Pauli elements with a single X. For example, on 3-qubits, the generators are

Z-elements	X-elements
$Z \otimes I \otimes I$	$X \otimes I \otimes I$
$I \otimes Z \otimes I$	$I \otimes X \otimes I$
$I \otimes I \otimes Z$	$I \otimes I \otimes X$

and using the multiplication properties of the Pauli matrices, one can check that these do indeed generate the entire group.

We will often refer to the Pauli elements without the phase as the n-qubit Pauli matrices. In fact, the n-qubit Pauli matrices are particularly nice because they form a basis for all complex matrices:

Fact 4.3. *The n-qubit Pauli matrices form a basis for all complex $2^n \times 2^n$ matrices.*

Proof. Treat each $2^n \times 2^n$ matrix A as a vector of length 4^n denoted by $\mathrm{vec}(A)$. Then, we can express inner products between matrices A and B as $\mathrm{vec}(A) \cdot \mathrm{vec}(B) = \mathrm{Tr}(AB^\dagger)$.

We now claim that all 4^n Pauli matrices are linearly independent. To see this, let $P = P_1 \otimes \cdots \otimes P_n$ and $Q = Q_1 \otimes \cdots \otimes Q_n$ be two distinct n-qubit Pauli matrices. We have that

$$\mathrm{Tr}(PQ) = \mathrm{Tr}(P_1Q_1 \otimes \cdots \otimes P_nQ_n) = \mathrm{Tr}(P_1Q_1) \cdots \mathrm{Tr}(P_nQ_n) = 0$$

since there must exist at least some index i for which $P_i \neq Q_i$. In more detail, notice that when $P_i \neq Q_i$ for $P_i, Q_i \in \{I, X, Y, Z\}$ that $P_iQ_i = \alpha R$ for $\alpha \in \{\pm 1, \pm i\}$ and $R \in \{X, Y, Z\}$. Therefore, $\mathrm{Tr}(P_iQ_i) = \alpha \,\mathrm{Tr}(R) = 0$ since the Pauli matrices are traceless.

Since we have a space of dimension 4^n and all 4^n Pauli matrices are linearly independent, we must have that the span of the Pauli matrices is the entire space. □

As a special case, we can look at the Pauli decomposition for density matrices of pure states.

Fact 4.4. *Let $|\psi\rangle$ be an n-qubit pure state. The density matrix $|\psi\rangle\langle\psi| = \sum_{P \in \{I,X,Y,Z\}^{\otimes n}} \alpha_P P$ with $\alpha_P \in \mathbb{R}$ and $\sum_P \alpha_P^2 = 2^{-n}$.*

Proof. By Fact 4.3, we can write $|\psi\rangle\langle\psi| = \sum_P \alpha_P P$ where $P \in \{I, X, Y, Z\}^{\otimes n}$ and $\alpha_P \in \mathbb{C}$. Since the Pauli matrices are Hermitian, we have

$$|\psi\rangle\langle\psi| = \sum_P \alpha_P P = \sum_P \alpha_P^* P.$$

This implies that $\alpha_P = \alpha_P^*$ since the P are linearly independent, which in turn implies that the α_P coefficients are real. Furthermore, using the purity of $|\psi\rangle$ we have

$$1 = \mathrm{Tr}(|\psi\rangle\langle\psi|) = \mathrm{Tr}(|\psi\rangle\langle\psi| \cdot |\psi\rangle\langle\psi|) = \sum_{P,Q} \alpha_P \alpha_Q \,\mathrm{Tr}(PQ) = \sum_P \alpha_P^2 \,\mathrm{Tr}(I^{\otimes n}) = 2^n \sum_P \alpha_P^2$$

where we've used that $\mathrm{Tr}(PQ) = 0$ for $P \neq Q$, $P^2 = I^{\otimes n}$, and $\mathrm{Tr}(I^{\otimes n}) = 2^n$. □

Pauli matrices and stabilizer groups

Now that we have defined the Pauli group, let's use it to help us represent a quantum state.

Definition 4.5. *For n-qubit state $|\psi\rangle$, we say unitary U stabilizes $|\psi\rangle$ iff $U|\psi\rangle = |\psi\rangle$. Let the stabilizer group $\mathrm{Stab}(|\psi\rangle) \subseteq \mathcal{P}_n$ be the set of all Pauli elements that stabilize $|\psi\rangle$.*

Fact 4.6. *$\mathrm{Stab}(|\psi\rangle)$ is an Abelian group under matrix multiplication.*

Proof. If Pauli elements P and Q both stabilize $|\psi\rangle$, then so do PQ and $P^\dagger$.

To argue that this group must be Abelian, notice that any two Pauli's P and Q either commute ($PQ = QP$) or anti-commute ($PQ = -QP$). Suppose that P and Q anti-commute. We get the following contradiction:

$$|\psi\rangle = PQ\,|\psi\rangle = -QP\,|\psi\rangle = -\,|\psi\rangle\,.$$

Therefore, P and Q must commute, and the stabilizer group is Abelian. □

Does the stabilizer group constitute a reasonable representation state? By a counting argument, one can see that there exist many quantum states whose stabilizer groups are empty, so this stabilizer representation won't be very good for them. On the other hand, if the stabilizer group is large enough, then it is a unique representation of the state:

Fact 4.7. *For any stabilizer group of size 2^n, there is only one state (up to global phase) with that stabilizer group. Additionally, for any stabilizer state $|\psi\rangle$, we have*

$$|\psi\rangle\langle\psi| = \frac{1}{2^n} \sum_{P \in \mathrm{Stab}(|\psi\rangle)} P.$$

Proof. Let $|\psi\rangle$ be an n-qubit state with $|\mathrm{Stab}(|\psi\rangle)| = 2^n$. Let $|\varphi\rangle\langle\varphi|$ be the density matrix of any state stabilized by every element in $\mathrm{Stab}(|\psi\rangle)$. We claim that this density matrix is unique. To see this, first expand $|\varphi\rangle\langle\varphi|$ in the Pauli basis using Fact 4.4: $|\varphi\rangle\langle\varphi| = \sum_P \alpha_P P$. Now take any $Q \in \mathrm{Stab}(|\psi\rangle)$. We have

$$1 = \mathrm{Tr}(|\varphi\rangle\langle\varphi|) = \mathrm{Tr}(Q\,|\varphi\rangle\langle\varphi|) = \sum_P \alpha_P \,\mathrm{Tr}(QP) = \alpha_Q \,\mathrm{Tr}(I^{\otimes n}) = \frac{\alpha_Q}{2^n}$$

where we have used (in order) that Q stabilizes $|\varphi\rangle$, that $\mathrm{Tr}(QP) = 0$ for $Q \neq P$, and that $Q^2 = I^{\otimes n}$ for any Pauli. In other words, for each of the 2^n stabilizers in $\mathrm{Stab}(|\psi\rangle)$, the corresponding coefficient in the Pauli expansion is 2^{-n}. Notice that this implies all other Pauli coefficients must be zero since by Fact 4.4 we have

$$2^{-n} = \sum_P \alpha_P^2 = \sum_{Q \in \mathrm{Stab}(|\psi\rangle)} \alpha_Q^2 + \sum_{P \notin \mathrm{Stab}(|\psi\rangle)} \alpha_P^2 = 2^{-n} + \sum_{P \notin \mathrm{Stab}(|\psi\rangle)} \alpha_P^2.$$

Since the α_P coefficients are real, their squares must be non-negative. On the other hand, the above equation implies that $\sum_{P \notin \mathrm{Stab}(|\psi\rangle)} \alpha_P^2 = 0$, so they must all be zero. □

Because of this, let's focus our attention on states that have stabilizer groups of size 2^n. This raises the obvious question: which states have these large stabilizer groups? Well, to start, notice that the all-zeroes state is stabilized by every Pauli matrix which is a tensor product of identity matrices (I) and Pauli-Z matrices. There are 2^n such matrices, so they comprise the entire stabilizer group.

We now have a stabilizer representation of our initial state. A reasonable requirement is that we can determine how the stabilizer group changes when we apply a unitary to the state:

Fact 4.8. *U stabilizes $|\psi\rangle$ iff $VUV^\dagger$ stabilizes $V\,|\psi\rangle$.*

Proof. $|\psi\rangle = U\,|\psi\rangle \iff V\,|\psi\rangle = VU\,|\psi\rangle = (VUV^\dagger)V\,|\psi\rangle$ □

In other words, if we apply a gate to our state, then we can update the stabilizer group representation by conjugating every stabilizer by the gate. In general, we don't have any guarantee on the form of $VUV^\dagger$. That is, even if U is a Pauli matrix, it's conjugation under an arbitrary unitary might not be Pauli.

We are now ready to reveal the key feature of Clifford circuits:

Theorem 4.9. *The Clifford group is the* normalizer *of the Pauli group. That is, a unitary U is Clifford iff $UPU^\dagger$ is in the Pauli group for all Pauli matrices P.*

For now, we just describe the direction which is important Clifford circuit simulation: if U is Clifford, then $UPU^\dagger$ is in the Pauli group. To make our lives easier, we will simplify down to just a few special cases that we have to check:

- *Only have to check* CNOT*, H, and S:* Since U is Clifford, we can write $U = g_1 \cdots g_m$ as a product of CNOT, H, and S gates. Therefore, if each gate g_i maps Pauli elements to Pauli elements under conjugation, then we have

  $$UPU^\dagger = g_1 \cdots g_{m-1}(g_m P g_m^\dagger) g_{m-1}^\dagger \cdots g_1 = g_1 \cdots g_{m-2}(g_{m-1} P' g_{m-1}^\dagger) g_{m-2}^\dagger \cdots g_1 = \cdots$$

  is another Pauli matrix.

- *Only have to check generators of the Pauli group:* Recall that every n-qubit Pauli P can be expressed as the product of $2n$ different generators, which consist of the Pauli elements with a single Z term and a single X term. Therefore, if we specify how a unitary affects each such generator under conjugation, then we can determine its more general behavior. Namely, if $P = P_1 P_2 \cdots P_k$ for Pauli generators P_i, then

  $$UPU^\dagger = UP_1P_2 \cdots P_k U^\dagger = (UP_1U^\dagger)(UP_2U^\dagger)U \cdots U^\dagger(UP_kU^\dagger)$$

  for any unitary U.

To complete the proof, we can simply show how each of CNOT, H, and S affects the Pauli generators:

P	$HPH^\dagger$
X	Z
Z	X

P	$SPS^\dagger$
X	Y
Z	Z

P	$\mathrm{CNOT}P\mathrm{CNOT}^\dagger$
$X \otimes I$	$X \otimes X$
$I \otimes X$	$I \otimes X$
$Z \otimes I$	$Z \otimes I$
$I \otimes Z$	$Z \otimes Z$

As a direct consequence, we can simulate Clifford circuits by keeping track of the stabilizer group and how it changes under the application of each gate in the circuit.

There are two remaining issues to address in order to obtain an efficient classical simulation of Clifford circuits using stabilizer groups. The first is a question of efficiency: if we need to keep track of all 2^n stabilizer elements, then our algorithm would take exponential time. However, once again, we only need to keep track of the *generators* of the stabilizer group:

Fact 4.10. *Let $|\psi\rangle$ be an n-qubit Clifford state. There exists n Pauli generators $g_1, \ldots g_n \in \mathcal{P}_n$ such that every $P \in \mathrm{Stab}(|\psi\rangle)$ can be expressed as the product of generator elements. Furthermore, the generators are independent in the sense that no generator can be expressed as the product of the other generators.*

Proof. Recall that the stabilizer group of the all-zeroes state consists of all the Z-type Pauli elements. One can check that this group is generated by the Pauli matrices with a single Z term: $Z \otimes I \otimes \cdots \otimes I$, $I \otimes Z \otimes \cdots \otimes I$, …, $I \otimes I \otimes \cdots \otimes Z$. There are n such generators, and it is of minimal size.

Since every Clifford state is of the form $U|0^n\rangle$ for Clifford unitary U, we have that the stabilizer group is generated by $UZ_iU^\dagger$ where Z_i is the Pauli matrix with a single Z in the ith register. □

It's worth noting that although every stabilizer group can be represented by n generators $g_1, \ldots, g_n$, this representation is far from unique. In particular, one can check that multiplying the first generator into the second yields a new set of generators $g_1, g_1g_2, \ldots, g_n$. In some cases, this idea will allow us to simplify our set of stabilizer generators using a multiplicative version of Gaussian elimination.

Let's turn our attention to the final issue: how do we deal with measurements? Without loss of generality, let's just focus on a computational basis measurement on the first qubit. There are two cases:

Deterministic Measurement: This occurs when the state is either $|0\rangle \otimes |\psi'\rangle$ or $|1\rangle \otimes |\psi'\rangle$. In other words, measuring the state results in $|0\rangle$ or $|1\rangle$ with probability 1, and it doesn't change the state. Even though we don't need to update our stabilizer group representation, there are still two potential issues: how do we determine if the measurement will be deterministic? and how can we determine the outcome of the measurement?

For the first problem, notice that there cannot be any Pauli stabilizers of the form $X \otimes P$ or $Y \otimes P$ for $P \in \mathcal{P}_{n-1}$ because both stabilizers would flip the first qubit. We claim that if these stabilizers are not present, then the measurement will be deterministic. To see this, notice that a computational basis measurement projects the first qubit onto $|0\rangle$ or $|1\rangle$. We can express this projection as $|0\rangle\langle 0| = (I + Z)/2$ and $|1\rangle\langle 1| = (I - Z)/2$, respectively. Notice, however that if g stabilizes $|\psi\rangle$ and it is of the form $I \otimes P$ or $Z \otimes P$, then it still stabilizes the state after projection:

$$g\left(\frac{I \pm Z}{2} \otimes I \otimes \cdots \otimes I\right)|\psi\rangle = \left(\frac{I \pm Z}{2} \otimes I \otimes \cdots \otimes I\right) g\,|\psi\rangle = \left(\frac{I \pm Z}{2} \otimes I \otimes \cdots \otimes I\right)|\psi\rangle\,.$$

Since the stabilizer group has not changed and the stabilizer group is unique (Fact 4.7), the measurement must have been deterministic.

In summary, we can now easily detect whether or not the measurement will be deterministic by checking if all of the stabilizer generators start with either an I or a Z. To determine the result of the measurement, we must now learn whether or not the state is of the form $|0\rangle \otimes |\psi'\rangle$ or $|1\rangle \otimes |\psi'\rangle$. Notice that the first state is stabilized by $Z \otimes I \otimes \cdots \otimes I$, while the second state is stabilized by $-Z \otimes I \otimes \cdots \otimes I$. We simply need to decide which. We can find it using Gaussian elimination in time $O(n^3)$.

Random Measurement: Since the measurement is not deterministic, there must exist some stabilizer generator that starts with either an X or a Y. Using Lemma 4.2, one can check that the measurement result is either $|0\rangle$ or $|1\rangle$ with 50% probability. Therefore, it is easy to output the result of the measurement. The difficulty is in updating the stabilizer representation.

Once again, the stabilizers that start with I or Z remain in the stabilizer group because they still stabilize the state after projection. On the other hand, we do need to remove the stabilizers which start with X or Y because they anti-commute with the projection. There is a fairly nice way of doing this: take one of the stabilizer generators that starts with an X or Y and multiply it into all of the remaining stabilizer generators that start with an X or

Y. One can check that now all the stabilizer generators start with either an I or Z except for one. Now, remove the remaining stabilizer generator that starts with an X or Y. What's left are $n-1$ stabilizer generators, so we only need to add one more. If the measurement outcome was $|0\rangle$, add the stabilizer generator $Z \otimes I \otimes \cdots \otimes I$ and if it was $|1\rangle$ add the stabilizer generator $-Z \otimes I \otimes \cdots \otimes I$. This completes the measurement protocol. It takes time $O(n^2)$.

4.3 Clifford circuits in $\oplus$L

The Gottesman-Knill Theorem (Theorem 4.1) says that Clifford circuits can be simulated in polynomial time. As it turns out, however, this is not the tightest classical characterization of the computational power of Clifford circuits. That is, one might hope that even smaller classical classes contain the languages computable by Clifford circuits, perhaps ones with low space or shallow circuits. The true answer is that Clifford circuits are captured by a rather strange class called $\oplus$L (pronounced "parity L").

Let's start with perhaps the most straightforward definition that makes explicit reference to the "parity" in $\oplus$L.

$\oplus$L: Languages K such that there exists a deterministic log-space Turing machine M and polynomial q such that for all $x \in \{0,1\}^n$

- If $x \in K$, then $M(x,y) = 1$ for an odd number of $y \in \{0,1\}^{q(n)}$.
- If $x \notin K$, then $M(x,y) = 1$ for an even number of $y \in \{0,1\}^{q(n)}$.

There is, however, a more useful characterization. Namely, $\oplus$L contains those languages that are log-space reducible to solving polynomize-size CNOT circuits. What kinds of problems can be solved by CNOT circuits of polynomial size? It turns out that most linear algebra problems over $\mathbb{F}_2$ fall into this category. For example, computing the determinant or inverse of a matrix over $\mathbb{F}_2$ are $\oplus$L-complete problems [Dam90].

We will show that Clifford circuits fall into this same category of $\oplus$L-complete problems. Or, in other words, the Hadamard and Phase gates in the definition of a Clifford circuit don't confer any additional computational powers to Clifford circuits. The CNOT gates alone are sufficient. To do this, let's first fix what we mean by a Clifford circuit problem: given a Clifford circuit (say, as an explicit list of gates), decide if measuring the first qubit will be $|1\rangle$ with 100% probability.

Before we show that this Clifford circuit problem is $\oplus$L-complete, let's first get some intuition about where the linear alegbra over $\mathbb{F}_2$ is hidden in Clifford circuits. The first idea is that we can associate every Pauli operator with two bits:

$$I \leftrightarrow 00 \qquad X \leftrightarrow 10 \qquad Y \leftrightarrow 11 \qquad Z \leftrightarrow 01$$

If we were to ignore the issue of signs, we can see that multiplying two Pauli operators corresponds to adding the two bit strings over $\mathbb{F}_2$. For example, the fact that $P^2 = I$ for all Pauli operators P corresponds to the fact that $x \oplus x = 0$ for all bit strings $x \in \{0,1\}^2$. Similarly, multiplying any Pauli P by the identity yields P in the same way that $x \oplus 00 = x$. Finally, we have that multiplying any two non-identity Paulis yields the third Pauli (up to sign), and indeed we see the same behavior for the bit strings.

What we have essentially just shown is that every Pauli P can be written as $\alpha X^x Z^z$ where $\alpha \in \mathbb{C}$ is some phase and $xz \in \{0,1\}^2$ is the bit representation of the Pauli. Of course, this idea readily generalizes to Pauli strings $P = P_1 \otimes \cdots \otimes P_n$ where we can write $P = \alpha X^x Z^z$ for some bit strings $x \in \{0,1\}^n$ and $z \in \{0,1\}^n$. Here, we have used X^x as a shorthand for $X^{x_1} \otimes \cdots \otimes X^{x_n}$, and similarly for Z^z. Once again, the important fact is that multiplying any two Pauli operators simply corresponds to adding their respective x and z bitstrings over $\mathbb{F}_2$.

We've arrived at a nice fact: since the stabilizers of a Clifford state form a group (under multiplication), the bit string representations of the stabilizers form a linear subspace (under addition mod 2) of $\{0,1\}^{2n}$. This bit representation of the stabilizer group is so nice that it's often given its own named data structure called a *tableau*. Specifically, let $|\psi\rangle$ be a stabilizer state with generators $P_1 \propto X^{x_1} Z^{z_1}, \ldots, P_n \propto X^{x_n} Z^{z_n}$ (once again, let's drop the phases). The tableau is written so that each row of the tableau corresponds to a generator:

$$\left(\begin{array}{c|c} \overset{X\text{-part}}{\begin{matrix} x_1 \\ \vdots \\ x_n \end{matrix}} & \overset{Z\text{-part}}{\begin{matrix} z_1 \\ \vdots \\ z_n \end{matrix}} \end{array}\right) = \left(\begin{array}{ccc|ccc} x_{11} & \cdots & x_{1n} & z_{1n} & \cdots & z_{1n} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nn} & z_{nn} & \cdots & z_{nn} \end{array}\right) \in \{0,1\}^{n \times 2n}$$

Many operations that you might want to peform on a stabilizer state now correspond to linear algebraic operations over the tableau. As one example, recall that the Hadamard operations flips the X and Z stabilizers under conjugation. So, applying a Hadamard gate to your stabilizer state corresponds to swapping with ith column of the X matrix with the ith column of the Z matrix.

We're now ready to show how to efficiently solve Clifford problems.

Theorem 4.11. *The Clifford circuit problem is* $\oplus$L*-complete.*

Proof. Since Clifford circuits are a generalization of CNOT circuits, the Clifford circuit problem is certainly $\oplus$L-hard. So, our focus will be on showing that the Clifford circuit problem is in $\oplus$L. We will use the fact that it suffices to show that the Clifford circuit problem can be solved by log-space (i.e., L) machines with access to a $\oplus$L oracle [HRV00]. That is, the goal will be to simulate a Clifford circuit using a logspace machine with access to an oracle that can solve linear algebra problems over $\mathbb{F}_2$.

To start, note that we can compute any bit of the tableau by essentially running the entire Clifford simulation algorithm. That is, for any specific bit of the tableau, ask the oracle "What is this bit of the tableau after applying the sequence of linear algebraic manipulations corresponding to each of the gates in the input". Since we can enumerate over all gates in the input with logarithmic memory, this takes at most logarithmic memory.

Notice that we have ignored the sign bits of the Pauli operators. To keep track of the sign bit, the claim is that we can simply re-run the entire simulation algorithm computing 1 bit of the tableau at a time. Whenever we update the tableau with a gate that would have flipped the sign of the Pauli, we keep track of this change. Since we're only ever storing a pointer to where we are in the computation and a single bit about the sign, this can be done in log space.

Let's suppose the tableau after measurement is $\left(\begin{array}{c|c} A & B \end{array}\right)$ for matrices $A, B \in \{0,1\}^{n \times n}$. The measurement will be deterministic if there exists a solution $s \in \{0,1\}^n$ such that $sA = 0^n$ and $sB = 10^{n-1}$. However, this is once again a linear alebra question we can ask the oracle.

That is, the bits of s that are equal to 1 indicate which stabilizer generators we should multiply together to get the Pauli $\pm Z \otimes I \otimes \cdots \otimes I$. Once we have the solution, all that remains is to check what *sign* the stabilizer generator has. Notice however that we can compute the sign of a product of generators in log space by first computing the sign of the first Pauli in each product, then the second Pauli and so on. □

4.4 Constant-depth circuits

Let's step back a bit and consider where Clifford circuits sit in the hiearchy of complexity classes. It is widely considered that $\oplus\mathsf{L}$ is strictly contained in P. That is, Clifford circuits seem like a really poor example to showcase the power of quantum computation. They aren't even universal for *classical* computation.

However, this is not quite the end of story. There are certainly weaker complexity classes than $\oplus\mathsf{L}$, and it is upon these smaller classes that our quantum advantage claims will rest. Let's take a moment to introduce these shallow circuit classes, in both the classical and quantum settings.

Nick's class (NC^0)
The class of languages L such that there exists a uniform family of constant-depth, polynomial-size classical circuits $C_n \colon \{0,1\}^n \to \{0,1\}$ built from AND, OR, and NOT gates with bounded fanin where $x \in L$ if and only if $C_n(x) = 1$.

Quantum NC^0 (QNC^0)
The class of languages L such that there exists a uniform family of constant-depth, polynomial-size quantum circuits $\{Q_n\}_{n=1}^{\infty}$ built from 1- and 2-qubit gates such that for all $x \in \{0,1\}$

- If $x \in L$, probability of measuring $|1\rangle$ on the first qubit of $Q_n |x\rangle |0 \cdots 0\rangle$ is at least $2/3$
- If $x \notin L$, probability of measuring $|1\rangle$ on the first qubit of $Q_n |x\rangle |0 \cdots 0\rangle$ is at most $1/3$

Looking at these two classes, we're left with an intriguing question: Can we prove quantum advantage with shallow circutis? That is, can we show that there is some constant-depth quantum circuit (i.e., in QNC^0) that can solve a decision problem that cannot be solved by constant-depth classical circuit (i.e., NC^0)? We could even hope to get greedier, and show that even shallow Clifford circuits can't be simulated by any constant-depth classical circuit. Unfortunately, and perhaps a bit surprisingly, the answer is no!

The following theorem says that as long as we're considering decision problems, we'll never get quantum advantage with constant-depth circuits of this kind.

Theorem 4.12. $\mathsf{QNC}^0 = \mathsf{NC}^0$.

Proof. We use a light-cone argument. Suppose we have a quantum circuit Q with depth at most a constant d, and we only measure the first qubit at the end. There is a light cone of input qubits that could possibly affect the first output qubit, and this light cone also has depth at most d. Then at most 2^d input qubits can affect our final measurement—where 2^d is another constant. (Note that the base 2 is coming from the definition of QNC^0 being based on 1- and 2-qubit gates only.) Now we can simply classically simulate the constant-size computation over these 2^d qubits. □

Therefore, if we want to have any hope of achieving quantum advantage in constant depth, we will need to modify our question. One might at first assume that we need to add some new types of operations to our class of quantum circuits in order to get them to be more powerful than their classical counterpats. However, as it turns out, all that is required is a change in perspective. When we inspect the proof of Theorem 4.12, we see that the fact that we were only measuring a single-qubit was critical. If we were to measure all of the qubits of the quantum circuit, there might be some correlations between the output bits that would be hard to simulate classically. Indeed, we will see that it is exactly these kinds of multi-output "relation" problems that are provably hard for shallow classical circuits to simulate.

To start, let's give the formal definitions of the relation variants of NC^0 and QNC^0:

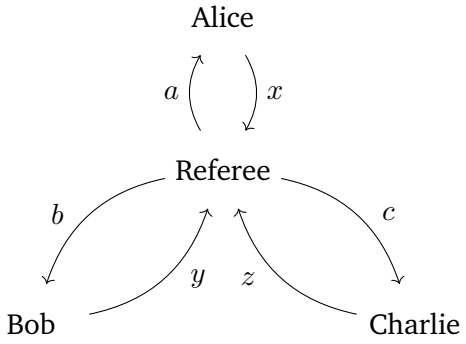
Relational NC^0 (FNC^0)
The class of relations $R \subseteq \{0,1\}^* \times \{0,1\}^*$ such that there exists a uniform family of constant-depth, polynomial-size classical circuits $C_n \colon \{0,1\}^n \to \{0,1\}^*$ built from AND, OR, and NOT gates with bounded fanin where $C_n(x) \in R(x)$ for all $x \in \{0,1\}^n$.

Relational QNC^0 (FQNC^0)
The class of relations $R \subseteq \{0,1\}^* \times \{0,1\}^*$ such that there exists a uniform family of constant-depth, polynomial-size quantum circuits $\{Q_n\}_{n=1}^{\infty}$ built from 1- and 2-qubit gates such that on input $x \in \{0,1\}^n$, measuring polynomially many qubits of $Q_n |x\rangle |0 \cdots 0\rangle$ results in outcome $|y\rangle$ with $y \in R(x)$ with probability at least 2/3.

To be concrete, our new question is whether or not we can find a relation in FQNC^0 that is not in FNC^0. The key to finding such a relation will be to show that classical constant-depth circuits are hopelessly bad at simulating correlations between qubits that are "far apart" in the quantum circuit. To formalize this story, we will use the language of quantum nonlocal games.

4.5 Quantum nonlocal games - GHZ and Parity Halving

A nonlocal game is a game in which several noncommunicating player tried to collectively solve some problem posed to them by a referee. Such games are easiest to get a sense of through an example. We start with the GHZ game, which is nonlocal game with a referee and three players. The referee sends bit $a \in \{0,1\}$ to Alice, $b \in \{0,1\}$ to Bob, and $c \in \{0,1\}$ to Charlie. Alice sends back bit $x \in \{0,1\}$, Bob sends back $y \in \{0,1\}$, and Charlie sends back $z \in \{0,1\}$. Alice, Bob, and Charlie can agree on a strategy ahead of time but cannot communicate during the game.



The players receive a uniformly random input with even Hamming weight (i.e., $a \oplus b \oplus c = 0$). The players win the game if the XOR of their outputs is equal to the OR of their inputs (i.e., $x \oplus y \oplus z = a \vee b \vee c$). Let's first consider the highest probability the players win the game using a classical strategy.

Theorem 4.13. *The best classical strategy for the GHZ game wins with 75% probability.*

Proof. To win with 75% probability, each player can ignore their input and always just output 1. Note that the promise $a \oplus b \oplus c = 0$ means there are only four possible scenarios for the game:

a	b	c	$a \vee b \vee c$
0	0	0	0
1	1	0	1
0	1	1	1
1	0	1	1

Since the players receive a uniformly random row, the OR of the outputs is 1 with 75% probability. Since the XOR of their outputs will always be 1, the players win with 75% probability.

To see that the players cannot win with higher probability, let's first consider the players have deterministic strategies. In other words, there is some explicit function that each player applies to their input to determine what they will output. We can write Alice's function as $A\colon \{0,1\} \to \{0,1\}$ and similarly for Bob (B) and Charlie (C). If the players are correct for all four questions, then we have

$$\begin{aligned} A(0) \oplus B(0) \oplus C(0) &= 0 \\ A(1) \oplus B(1) \oplus C(0) &= 1 \\ A(0) \oplus B(1) \oplus C(1) &= 1 \\ A(1) \oplus B(0) \oplus C(1) &= 1. \end{aligned}$$

However, if we add them all these equations, we can see that all terms on the lefthand side cancel and the sum on the righthand side is 1. Therefore, we get that $0 = 1$, a contradiction. Since it is impossible to correctly answer all four questions, they can at most get three questions correct, i.e., 75% chance of winning.

If Alice, Bob, and Charlie run classical randomized algorithms, their strategy will only be a convex combination of deterministic strategies. Concretely, suppose there are n deterministic strategies $D_1, \ldots, D_n$ for Alice, Bob, and Charlie. If they are randomized, they execute

strategy D_i with probability p_i, where $\sum_i p_i = 1$. We have already shown that for any fixed D_i, the probability of winning is at most 75%. In the randomized setting, the probability of winning is now $\sum_i p_i \Pr[\text{win on } D_i] \leq \sum_i p_i(0.75) \leq 0.75$. Thus for all classical strategies, deterministic or randomized, the best possible win probability is 75%. □

Theorem 4.14 (Greenberger-Horne-Zeilinger [GHZ89])**.** *There exists a quantum strategy for the GHZ game, such that the three players win with probability 1.*

Proof. The three players Alice, Bob and Charles share a three-qubit entangled state:

$$|\text{GHZ}\rangle = \frac{|0_A 0_B 0_C\rangle + |1_A 1_B 1_C\rangle}{\sqrt{2}}.$$

Here, we have shown the subscript on each qubit to indicate which player holds it. That is, Alice has the first qubit, Bob has the second, and Charlie has the third. All three players use the following strategy when they receive a bit $s \in \{0, 1\}$ from the referee:

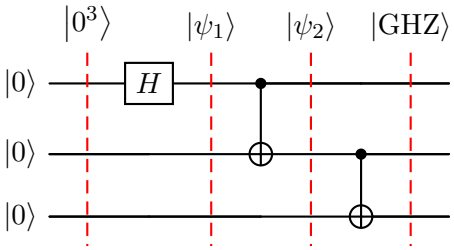
If $s = 0$: apply a Hadamard gate and measure (equivalently, measure in the X basis), and return the outcome to the referee.

If $s = 1$: apply a phase gate followed by a Hadamard gate and measure (equivalently, measure in the Y basis) and return the outcome to the referee.

Notice that both the starting state and all measurement operators used in this game are Clifford. Therefore, we can use the stabilizer group representation to analyze the strategy.

Lemma 4.15. *The stabilizer group of the GHZ state is generated by* $\{XXX, ZZI, IZZ\}$.

Proof. The GHZ state is generated by the following circuit:



By tracing the evolution of the stabilizer group generators we get,

$$\begin{matrix} ZII \\ IZI \\ IIZ \\ \text{Stab}(|0^3\rangle) \end{matrix} \xrightarrow{H\otimes I\otimes I} \begin{matrix} XII \\ IZI \\ IIZ \\ \text{Stab}(|\psi_1\rangle) \end{matrix} \xrightarrow{\text{CNOT}\otimes I} \begin{matrix} XXI \\ ZZI \\ IIZ \\ \text{Stab}(|\psi_2\rangle) \end{matrix} \xrightarrow{I\otimes\text{CNOT}} \begin{matrix} XXX \\ ZZI \\ IZZ \\ \text{Stab}(|\text{GHZ}\rangle) \end{matrix}$$

□

Lemma 4.16. *Let $|\psi\rangle$ be any Clifford state whose stabilizer group contains a Pauli element that is a tensor product of Z and I elements. That is, $|\psi\rangle$ is stabilized by $P = \alpha P_1 \otimes \cdots \otimes P_n$ such that $P_i \in \{Z, I\}$ and $\alpha = \{\pm 1\}$. Measure $|\psi\rangle$ in the computational basis, but consider only the measurements on qubits i such that $P_i = Z$. If $\alpha = 1$, then the parity of the measurement results is even; otherwise ($\alpha = -1$), the parity is odd.*

Proof. Let a be a bit string $a \in \{0,1\}^n$ and P be a Pauli matrix $P \in \{X, Y, Z, I\}$. We will use the notation P^a to denote the n-qubit Pauli operator

$$P^a := P^{a_1} \otimes \cdots \otimes P^{a_n}$$

where $P^0 = I$. Using this notation and the assumption of the lemma, $|\psi\rangle$ has a stabilizer of the form $(-1)^b Z^z$ where $z \in \{0,1\}^n$ is a bit string and $b \in \{0,1\}$ is the sign (i.e., $(-1)^b Z^z |\psi\rangle = |\psi\rangle$). Notice also that for any $x \in \{0,1\}^n$, we have $|x\rangle = X^x |0\rangle$. This is because applying the Pauli string X^x corresponds to applying the Pauli X operator to qubit i if $x_i = 1$ and the identity operator if $x_i = 0$. Therefore, we have

$$\langle x|\psi\rangle = (-1)^b \langle 0| X^x Z^z |\psi\rangle$$

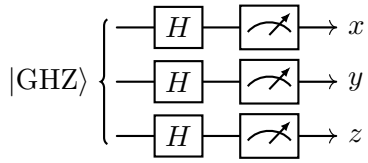
By (anti-)commutativity property of Pauli strings, we have $X^x Z^z = (-1)^{x \cdot z} \cdot Z^z X^x$, which then gives

$$\langle x|\psi\rangle = (-1)^{x \cdot z \oplus b} \langle 0| Z^z X^x |\psi\rangle = (-1)^{x \cdot z \oplus b} \langle 0| X^x |\psi\rangle = (-1)^{x \cdot z \oplus b} \langle x|\psi\rangle$$

where we've used that Z^a is a stabilizer of the all zeros state: $\langle 0| Z^a = \langle 0|$. Notice that if we want $\langle x|\psi\rangle$ to be nonzero (i.e., there is some chance to output measurement result $|x\rangle$), we need that $x \cdot z \oplus b = 0$; otherwise, we get that $\alpha = -\alpha$ for some non-zero complex number α. In other words, if $b = 0$, the parity of the measurement results on the non-identity elements of the stabilizer must be even; and similarly, if $b = 1$, the parity must be odd. □

Now we will perform a case analysis on the values of the inputs (a, b, c) to show that our strategy always succeeds. We only need to consider the cases $(a, b, c) \equiv (0, 0, 0)$ and $(a, b, c) \equiv (1, 1, 0)$. The cases $(a, b, c) \equiv (0, 1, 1)$ and $(a, b, c) \equiv (1, 0, 1)$ follow from symmetry. In each case, we would keep track of the evolution of the stabilizer group generators and then apply Lemma 4.16.

- $(a, b, c) \equiv (0, 0, 0)$: All three players measure in the X basis:

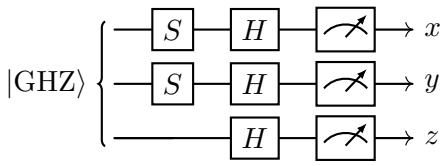


  Using Lemma 4.15 to obtain the generators of our starting state, their evolution is given by

$$\begin{matrix} XXX \\ ZZI \\ IZZ \end{matrix} \xrightarrow{H^{\otimes 3}} \begin{matrix} ZZZ \\ XXI \\ IXX \end{matrix}$$

  As the stabilizer group of the state being measured contains the Pauli string ZZZ, Lemma 4.16 states that the output must have even parity, i.e., $x \oplus y \oplus z = 0$

- $(a, b, c) \equiv (1, 1, 0)$: Alice and Bob (who received bit a and b) measure their qubits in the Y basis. Charlie measures in the X basis. The circuit representation in this case is



We get

$$\begin{matrix} XXX \\ ZZI \\ IZZ \end{matrix} \xrightarrow{S\otimes S\otimes I} \begin{matrix} YYX \\ ZZI \\ IZZ \end{matrix} \xrightarrow{H\otimes H\otimes H} \begin{matrix} YYZ \\ XXI \\ IXX \end{matrix}$$

Using group closure properties, $-ZZZ = (YYZ)(XXI)$ is in the stabilizer group of the state being measured. Therefore, by Lemma 4.16 the measurement output must have odd parity, ie. $x \oplus y \oplus z \oplus = 1$.

Thus, we conclude that whenever the parity of the input is even (i.e., $a \oplus b \oplus c = 0$), the three players return bits x, y, z such that $x \oplus y \oplus z = a \vee b \vee c$. In other words, they always answer correctly to the referee. □

We now have a nonlocal game where the quantum strategy does provably better than the classical strategy. However, if we think about turning the GHZ game into a quantum-classical circuit separation, we are confronted with the fact that the game only involves a constant number of input/output bits. Any relation with three input bits and three output bits can trivially be solved by even a constant-depth classical circuit (i.e., in FNC^0).

Our first goal will be to generalize the GHZ game so that it involves n players. We will use the Parity Halving Game introduced in [WKST19]:

Parity Halving Game

Input:	$x_1, \ldots, x_n \in \{0,1\}$
Promise:	$x_1 \oplus \cdots \oplus x_n = 0$
Goal:	Output $y \in \{0,1\}^n$ such that $\lvert y\rvert \equiv \lvert x\rvert/2 \pmod 2$

Notice that we can think of the Parity Halving Game as follows: if the Hamming weight of the input is $0 \bmod 4$, then output a string of Hamming weight $0 \bmod 2$; if the Hamming weight of the input is $2 \bmod 4$, then output a string of Hamming weight $1 \bmod 2$.

When $n = 3$, the Parity Halving Game is exactly the GHZ game. In fact, the quantum strategy is identical. Each player starts with 1 qubit of the n-qubit cat state:

$$|😺_n\rangle := \frac{|0^n\rangle + |1^n\rangle}{\sqrt{2}}.$$

Then, each player applies an phase gate if their input bit was 1. Finally, all players apply a Hadamard gate and measure. Let's now show that this strategy wins with 100% probability. This will give an alternative proof of the quantum strategy for the original GHZ game.

Theorem 4.17. *For $m = n$, there is a quantum strategy to win the Parity Halving Game with probability 1.*

Proof. Following the quantum strategy, each player applies a phase gate to their cat qubit when their input bit is 1. We get

$$\frac{|0^n\rangle + |1^n\rangle}{\sqrt{2}} \xrightarrow{S^{x_1}\otimes\cdots\otimes S^{x_n}} \frac{|0^n\rangle + i^{|x|}\,|1^n\rangle}{\sqrt{2}} = \frac{|0^n\rangle + (-1)^{|x|/2}\,|1^n\rangle}{\sqrt{2}}$$

where the last equality uses the fact that the Hamming weight of the input is even. If the Hamming weight of the input is $0 \bmod 4$, then $|x|/2$ is even, so we get the cat state again. However, if the Hamming weight of the input is $2 \bmod 4$, then $|x|/2$ is odd, so we get the cat state with a -1 phase on the $|1^n\rangle$ part. We now simply need to analyze the affect of applying a layer of Hadamard gates to such states. For bit $b \in \{0,1\}$, we get

$$\begin{aligned}\frac{|0^n\rangle + (-1)^b\,|1^n\rangle}{\sqrt{2}} \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2^n}}\sum_{y\in\{0,1\}^n}|y\rangle + \frac{1}{\sqrt{2^n}}\sum_{y\in\{0,1\}^n}(-1)^{|y|\oplus b}\,|y\rangle\right)\\ = \frac{1}{\sqrt{2^{n+1}}}\sum_{y\in\{0,1\}^n}(1+(-1)^{|y|\oplus b})\,|y\rangle\end{aligned}$$

If $b = 0$, then we can see that all the odd strings will have 0 amplitude since $1 + (-1)^{|y|} = 0$. Similarly, if $b = 1$, then all the even strings will have 0 amplitude.

Putting everything together, we see that when $|x|/2$ is even (i.e., the $b = 0$ case), we sample a uniformly random bit string with even parity, and when $|x|/2$ is odd, we sample a uniformly random bit string with odd parity. This exactly solves the Parity Halving game. □

We now turn to the classical lower bound. We will see that as we increase the number of players, the maximum winning probability decreases exponentially:

Theorem 4.18. *Any classical strategy for the Parity Halving Game wins with probability at most* $\frac{1}{2} + 2^{-\lceil n/2\rceil}$.

Proof. As in the proof of Theorem 4.13 it suffices to analyze classical deterministic strategies. Notice that on input $x_i \in \{0,1\}$, the ith player can has exactly 4 functions that determine the output: 0, 1, x_i, or $x_i \oplus 1$. In other words, if we collect the responses from all players, their joint answer is some linear function

$$(a_1, a_2, \ldots, a_n) \oplus (b_1x_1, b_2x_2, \ldots, b_nx_n)$$

for some fixed bits $a_1, \ldots, a_n, b_1, \ldots b_n \in \{0,1\}$. Therefore, the parity of their output is given by $a \oplus b \cdot x$ for $a = a_1 \oplus \cdots \oplus a_n$ and b the n-bit string for the b_i. Our goal is to determine how well such a linear strategy can correlate with the correct strategy of the Parity Halving Game.

To capture the correct strategy, let $f(x) = \mathrm{Re}(i^{|x|})$ be the real part of $i^{|x|}$. Notice that

$$f(x) = \begin{cases} 1 & \text{if } x \equiv 0 \pmod 4 \\ -1 & \text{if } x \equiv 2 \pmod 4 \\ 0 & \text{if } x \text{ outside promise} \end{cases}$$

which indeed lines up with the intended behavior. The correlation between the correct strategy and the linear strategy is given by

$$\chi = \frac{1}{2^{n-1}} \left| \sum_{\substack{x \in \{0,1\}^n \\ \text{s.t. } |x| \equiv 0 \pmod 2}} (-1)^{a+b\cdot x} f(x) \right|$$

That is, χ is the fraction of inputs where the linear strategy is correct minus the fraction of inputs where it is incorrect. One can then check that the probability of being correct is given by $(1+\chi)/2$.

The first key observation is that $f(x) = 0$ on those inputs x falling outside the promise. This allows us to drop the condition on the sum (that the Hamming on $x \in \{0,1\}$ is $0 \bmod 2$) and factorize the sum into a product:

$$\begin{aligned}
2^{n-1}\chi &= \left| \sum_{x\in\{0,1\}^n} (-1)^{a+b\cdot x} \mathrm{Re}(i^x) \right| \\
&\leq \left| \mathrm{Re}\left(\sum_{x\in\{0,1\}^n} (-1)^{a+b\cdot x} i^{|x|} \right) \right| \\
&= \left| \mathrm{Re}\left(\sum_{x\in\{0,1\}^n} (-1)^{b_1 x_1 + \cdots b_n x_n} i^{x_1+\cdots+x_n} \right) \right| \\
&= \left| \mathrm{Re}\left(\sum_{x_1\in\{0,1\}} (-1)^{b_1 x_1} i^{x_1} \right) \cdots \left(\sum_{x_n\in\{0,1\}} (-1)^{b_n x_n} i^{x_n} \right) \right| \\
&= \left| \mathrm{Re}(1 + i^{2b_1+1}) \cdots (1 + i^{2b_n+1}) \right|
\end{aligned}$$

In other words, the correlation will depend on the real part of the product of n complex numbers of the form $(1 \pm i)$. If we were to take out a factor of $\sqrt{2}$, each of these would be an 8th root of unity. Multiplying any two, we get

$$\frac{1+i(-1)^\alpha}{\sqrt{2}} \cdot \frac{1+i(-1)^\beta}{\sqrt{2}} = \frac{1-(-1)^{\alpha+\beta}+((-1)^\alpha+(-1)^\beta)i}{2} = \begin{cases} \pm i & \text{if } \alpha = \beta \\ 1 & \text{if } \alpha \neq \beta \end{cases}$$

for any bits $\alpha, \beta \in \{0,1\}$. Therefore, if n is even, then we can pair up the elements of the product, so the product is in the set $\{\pm 1, \pm i\}$ and the real part is in the set $\{0, \pm 1\}$. Clearly, χ is maximized in this setting when the product is non-zero. If n is odd, then we have one leftover root of unity, so the product is in the set $\{\frac{\pm 1 \pm i}{\sqrt{2}}\}$ and the real part is in the set $\{\pm\frac{1}{\sqrt{2}}\}$. We get that

$$\chi \leq \frac{\sqrt{2^n}}{2^{n-1}} \cdot \begin{cases} 1 & \text{if } n \text{ is even} \\ \frac{1}{\sqrt{2}} & \text{if } n \text{ is odd} \end{cases} = \frac{1}{2^{\lceil n/2 \rceil - 1}}.$$

The theorem follows immediately since the probabilty of winning over a random input is given by $(1+\chi)/2$. □

While this would conclude the analysis of the standard Parity Halving Game, it turns out we will need a slightly stronger result when we try to convert this nonlocal game separation to a circuit separation. Namely, we will consider a version of the game where k of the inputs are fixed to some values known by all players. One can very slightly modify proof of Theorem 4.18 to see that the maximum classical winning probability is given by $\frac{1}{2} + 2^{\lceil (n-k)/2 \rceil}$.

4.6 Circuit separations from quantum nonlocal games

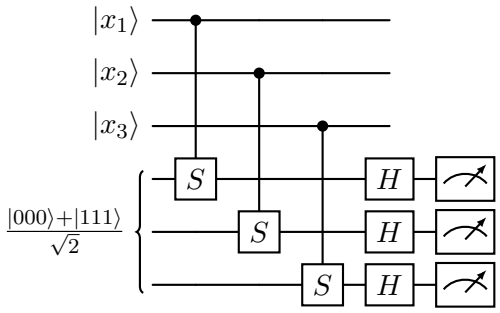
Notice that there is a somewhat natural correspondence between a quantum nonlocal game with n players and a circuit with n input wires and n output wires. If each output was only allowed to depend on a unique input, then this correspondence would be exact. Of course, for general circuits this will not be true. For constant-depth circuits, however, we will show that such a condition is approximately true.

Recall our goal: we want to show that there is some relation in FQNC^0 that is not in FNC^0. One idea is to show that the relation coming from the Parity Halving Game suffices. Let's restate a slight generalization of that problem:

Parity Halving Problem ($\mathrm{PHP}_{n,m}$)
Input: $x \in \{0,1\}^n$ such that $|x| \equiv 0 \pmod 2$
Output: $y \in \{0,1\}^m$ such that $|y| \equiv |x|/2 \pmod 2$

Notice in particular that we've generalized to allow for outputs of a size m, which is not necessarily equal to n (as would be the case for the nonlocal game). Clearly, if you can solve the Parity Halving Problem for $m = n$, then you can solve it for $m > n$ by just outputting some extra zero bits.

Unfortunately, it is still not clear why the Parity Halving Problem should be in FQNC^0. To see this, consider the straightforward implementation of the quantum strategy for the Parity Halving Game as a quantum circuit shown below for the $n = 3$ case:



Since the controlled-phase gates can be applied in parallel, this seems like a constant-depth circuit. However, the problem is that the quantum circuit is allowed to start with the cat state in an ancilla register. Unfortunately, one can show that the cat state *cannot* be constructed by a constant-depth circuit. To circumvent this issue, we will have to modify our definition of the Parity Halving Problem. However, for now, let's put this issue aside.

Let $\mathsf{FQNC}^0/$😸 be the complexity class of function problems solvable using an ancillary cat state. By the above construction, we have that $\mathrm{PHP}_{n,n} \in \mathsf{FQNC}^0/$😸. Let's show that it is not in FNC^0.

Theorem 4.19. *The Parity Halving Problem* $\mathrm{PHP}_{n,m}$ *is not in* FNC^0 *for* $m = o(n^2)$.

Proof. Suppose there is some classical NC^0 circuit solving the Parity Halving Problem with n input bits and m output bits. While it will likely be true that the circuit has outputs that depend on multiple input bits (i.e., not satisfying the condition of a nonlocal game), the proof idea will be to find a collection of output bits for which the input/output behavior does look like a nonlocal game.

The starting point will be to understand which input bits affect which output bits. Recall that NC^0 circuits have bounded fanin, so every output bit is affected by at most constantly many input bits. This is the standard "lightcone" argument we saw in Theorem 4.12. In fact, we will use two kinds of lightcones in this proof. The lightcone of an input bit is the set of outputs that the input bit affects, and the lightcone of an output bit is the set of input bits that affect it. Because NC^0 circuits have unbounded fanout, the size of any individual input bit lightcone can also be unbounded. Because NC^0 circuits have bounded fanin, the the size of any output bit lightcone is bounded by a constant, say $\ell = O(1)$.

Notice that if we have a bound on the number of input bits that can affect an output, this immediately gives a bound on the number of output bits that can be affected by an average input bit. To formalize this argument, consider a bipartite graph on $n + m$ vertices, with the input bits on the left side and the output bits on the right side. Connect an input bit with an output bit if that output bit depends on the input. By the lightcone argument, the degree of each output bit is at most ℓ. Since there are m output bits and the sum of the degrees in each bipartition must agree, the average degree of the input bits must be also be $\ell m/n$.

Let's now consider yet another graph that will indicate the if the lightcone of an input bit intersects with the lightcone of another input bit. That is, two input bits are connected in the graph if there is an output bit which is affected by both of them. Notice that we are looking for a large independent set in this graph. Notice that an input that has degree k in the original graph has degree at most $k\ell$ in the intersection graph since each output bit in the lightcone of an input bit can itself be affected by at most ℓ inputs. Therefore, the average degree in the intersection graph is $\ell^2 m/n$. By Turán's Theorem, any graph with n vertices and average degree $\ell^2 m/n$ must have an independent set of size at least $s := \lceil n^2/(n + \ell^2 m)\rceil$.

To complete the proof, it suffices to "isolate" the input bits in the independent set by fixing the remaining input bits to some constant values. Notice that if the original circuit suceeded on a random input with probability p, then by an averaging argument, there must be a setting of the other input bits so that the circuit is still correct with probability at least p on the remaining input bits. We can now apply Theorem 4.18 and the discussion afterwards to see that the circuit correctly computes the relation on at most a $1/2 + 2^{-\lceil s/2\rceil}$ fraction of inputs. That is, if $m = o(n^2)$, the classical circuit only has an exponentially small advantage over guessing randomly. □

Separating FQNC^0 from FNC^0

Let's now return to the issue of the cat state not being constructible by QNC^0 circuits. We start with a weakened definition of the cat state called the "poor man's cat state", that is, any state of the form:

$$\frac{|z\rangle + |\overline{z}\rangle}{\sqrt{2}}$$

where $z \in \{0,1\}^n$ and $\overline{z} = (z_1 \oplus 1, \ldots, z_n \oplus 1)$ is the complement. Of course, if we could construct the poor man's cat state for a particular z, then this is just as good as constructing the cat state itself since we could apply a layer of Pauli-X gates to map it to the cat state. What will show instead is that there is a constant-depth quantum circuit to construct a *random* poor man's cat state.

The key to understanding this construction the following nice property of any bit string and its complement: for any $z \in \{0,1\}^n$, $\overline{z}$ is the unique bitstring (other than z itself) such that the parity of any two bits of $\overline{z}$ is the same as the parity of the corresponding bits in z. That is, for any $i, j \in [n]$, we have $z_i \oplus z_j = \overline{z}_i \oplus \overline{z}_j$.

Let's see why this is true. Let $a, b \in \{0,1\}^n$ be different bit strings satisfying the parity condition. Since a and b must be different, let's assume without loss of generality that a starts with a 0 and b starts with a 1. We have

$$\begin{aligned} a &= 0\ a_2\ a_3\ \cdots\ a_n \\ b &= 1\ b_2\ b_3\ \cdots\ b_n \end{aligned}$$

By assumption, the parity of the first two bits of a is equal to the parity of the first two bits of b, so we get

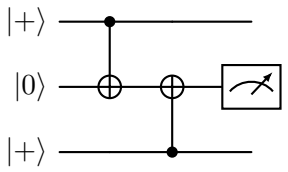
$$a_1 \oplus a_2 = b_1 \oplus b_2 \quad \Longrightarrow \quad 0 \oplus a_2 = 1 \oplus b_2 \quad \Longrightarrow \quad b_2 = a_2 \oplus 1$$

In other words, b_2 is the complement of a_2. Repeating the exact same argument for bits 2 and 3, we get

$$a_2 \oplus a_3 = b_2 \oplus b_3 \quad \Longrightarrow \quad a_2 \oplus a_3 = (a_2 \oplus 1) \oplus b_3. \quad \Longrightarrow \quad b_3 = a_3 \oplus 1$$

and so b_3 is the complement of a_3. Repeating the argument for all n bits completes the claim. In fact, we've shown something a little bit stronger. Inspecting the argument, we only need to constrain the parity of bits that are adjacent (i.e, bits i and $i+1$).

This immediately gives rise to an idea for constructing a poor man's cat state: prepare the superposition over all bit strings, and then constrain the parity of all adjacent bits. Quantumly, we can constrain the parity by first computing the parity (with a couple of CNOT gates) and the measuring it:



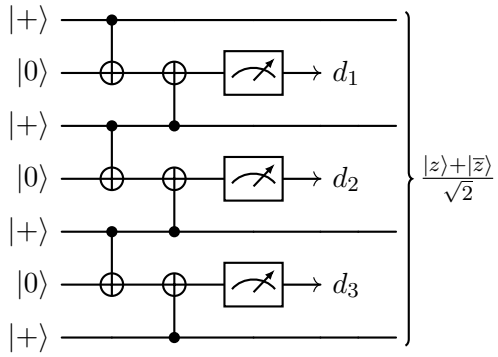
Here, the first and third qubits are a superposition over all basis states, and the middle qubit is the parity. Before measurement, we have

$$\frac{1}{2}\sum_{x,y\in\{0,1\}} |x\rangle\,|0\rangle\,|y\rangle \xrightarrow{\text{CNOT gates}} \frac{1}{2}\sum_{x,y\in\{0,1\}} |x\rangle\,|x\oplus y\rangle\,|y\rangle = \left(\frac{|000\rangle + |101\rangle}{2}\right) + \left(\frac{|011\rangle + |110\rangle}{2}\right)$$

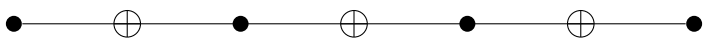
where we have grouped the final expressions by their parity. You can see that after measurement, the state remaining on the first and third qubits is

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}} \quad \text{or} \quad \frac{|01\rangle + |10\rangle}{\sqrt{2}}.$$

Generalizing this construction immediately gives a poor man's cat state. To construct an n-qubit poor man's cat state, start in the uniform superposition of n-qubits and use $n-1$ of the parity gadgets above to constrain the parity of adjacent qubits. For $n = 4$, we get



where $z_i \oplus z_{i+1} = d_i$ for $i \in \{1, 2, 3\}$. We can visualize this construction as a line of qubits, interspersed with parity qubits:

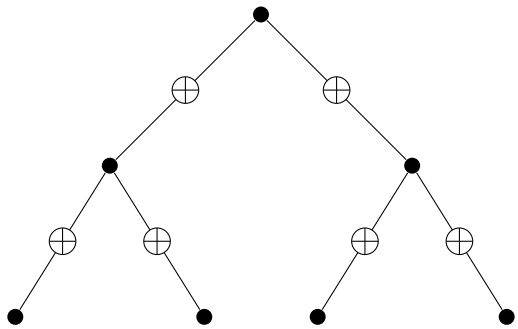


Here the solid black dots ($\bullet$) represent the poor man's cat state qubits and the white dots ($\oplus$) represent the parity qubits which are to be measured. As previously discussed, such a construction (where the qubits are arranged in a 1-dimensional line) is perfectly reasonable for constructing a poor man's cat state. However, it will not be the version we want to use for our separation.

What we will ultimately want is that it is easy to compute any bit of z by knowing the first bit z_1 and a few of the parity measurements. For the line construction, we can determine the ith bit of z by a telescoping sum:

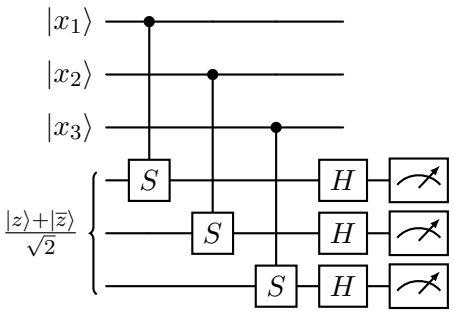
$$d_{i-1} \oplus d_{i-2} \oplus \cdots \oplus d_1 \oplus z_1 = (z_i \oplus z_{i-1}) \oplus (z_{i-1} \oplus z_{i-2}) \oplus \cdots \oplus (z_2 \oplus z_1) \oplus z_1 = z_i.$$

This has the somewhat unfortunate consequence that z_n requires a sum of $n-1$ parities. In turns out that we can do better by arranging our qubits into a binary tree. We can think of placing the cat qubits at the vertices of the tree and the parity qubits on the edges:



By an identical argument to the line case, the above construction still yields a poor man's cat state. However, now notice that to compute z_i starting from z_1, we only need to sum up the parities along the path from z_1 to z_i in the tree. Since a binary tree has diameter $O(\log n)$, we only need to sum up $O(\log n)$ parity bits.

We finally have our complete construction of our poor man's cat state. It's reasonable to now ask... what is it good for? Let's simply use the same construction as before, but replace the cat state with the poor man's version:



After we apply the phase gates on the cat state qubits, we get

$$\frac{i^{z\cdot x}|z\rangle + i^{\overline{z}\cdot x}|\overline{z}\rangle}{\sqrt{2}} = i^{z\cdot x}\frac{|z\rangle + (-i)^{z\cdot x}i^{\overline{z}\cdot x}|\overline{z}\rangle}{\sqrt{2}} = i^{z\cdot x}\frac{|z\rangle + (-1)^{z\cdot x}i^{|x|}|\overline{z}\rangle}{\sqrt{2}}.$$

The gobal phase of $i^{z\cdot x}$ doesn't matter for measurement, so once again, the state before the Hadamards is either the original poor man's cat state or the cat state with a minus sign on the $|\overline{z}\rangle$ term. Let $b := (z\cdot x) + |x|/2$ be this phase. We get

$$\begin{aligned}\frac{|z\rangle + (-1)^b|\overline{z}\rangle}{\sqrt{2}} \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2^n}}\sum_{y\in\{0,1\}^n}(-1)^{z\cdot y}|y\rangle + \frac{1}{\sqrt{2^n}}\sum_{y\in\{0,1\}^n}(-1)^{\overline{(z\cdot y)}\oplus b}|y\rangle\right)\\ = \frac{1}{\sqrt{2^{n+1}}}\sum_{y\in\{0,1\}^n}(-1)^{z\oplus y}(1+(-1)^{|y|\oplus b})|y\rangle\end{aligned}$$

In other words, once again, when $b \equiv 0 \pmod 2$, the measured string must have even Hamming weight, and when $b \equiv 1 \pmod 2$, the measured string must have odd Hamming weight. That is, the measurement results in a $y \in \{0,1\}^n$ such that

$$|y| \equiv |x|/2 + (z\cdot x) \pmod 2.$$

This almost exactly the original Parity Halving condition except there is an extra $z\cdot x$ term. Since this is what the quantum circuit gives us, let's just define the a new version of the Parity Halving Problem, which is exactly that.

Relaxed Parity Halving Problem (RPHP_n)

Implicit Graph:	Connected tree $T=(V,E)$ with $\|V\|=n$ and diameter $O(\log n)$
Input:	$x \in \{0,1\}^{\|V\|}$ such that $\|x\| \equiv 0 \pmod 2$
Output:	$y \in \{0,1\}^{\|V\|}$ and $d \in \{0,1\}^{\|E\|}$ such that there exists a $z \in \{0,1\}^{\|V\|}$ satisfying • $\|y\| \equiv \|x\|/2 + (z\cdot x) \pmod 2$; and • $z_u \oplus z_v = d_{(u,v)}$ for all $(u,v) \in E$.

Notice that in the Relaxed Parity Halving Problem, we not only ask for the output of the quantum circuit on the poor man's cat state (i.e., the $y \in \{0,1\}^{|V|}$), but also the list of parities

(i.e., the $d \in \{0,1\}^{|E|}$) that were used to construct the poor man's cat state. The idea will be that a classical circuit solving the relaxed Parity Halving Problem RPHP_n can use these extra parity bits to solve the original Parity Halving Problem $\mathrm{PHP}_{n,m}$ for some $m = o(n^2)$, violating Theorem 4.19.

Let's put everything together.

Theorem 4.20. *The Relaxed Parity Halving Problem* RPHP_n *is in* FQNC^0 *but not* FNC^0.

Proof. We've constructed the Relaxed Parity Halving Problem exactly so that constant-depth quantum circuits can solve it, so let's move onto the classical lower bound. Let's suppose by contradiction that there is a classical NC^0 circuit that solves the RPHP_n problem. That is, it can output a $y \in \{0,1\}^n$ such that $|y| \equiv |x|/2 + (z \cdot x) \pmod 2$.

Our plan will be to construct a constant-depth classical circuit that appends $O(n \log n)$ bits to y that have total parity $(z \cdot x)$. If we can do this, the parity of y plus these new bits will be exactly $|x|/2$. In other words, this new circuit will have solved the original Parity Halving Problem for $m = O(n \log n)$, violating Theorem 4.19.

The challenge is that the classical circuit does not know z. By assumption, it only knows the list of parities d. That said, recall that the parity bits are sufficient to reconstruct every bit of z. That is, each z_t bit for some $t \in V$ can be written as a sum of z_s plus the parity bits on the path from z_s to z_t in the graph (where $s \in V$ is chosen as some arbitrary first vertex). Furthermore, we can assume that $z_s = 0$ since it must be zero for one of z or $\overline{z}$ and we can always swap what we think of as z and $\overline{z}$. For every vertex $t \in V$, let $\mathrm{Path}_{s \to t}$ be the set of edges on the path from s to t. Now, we can write

$$z \cdot x = \sum_{t \in V} z_t x_t = \sum_{t \in V} \left(\sum_{(u,v) \in \mathrm{Path}_{s \to t}} d_{(u,v)} \right) x_t$$

If we were to expand the sum above, we would see that it is the sum of at most $O(n \log n)$ terms of the form $d_{(u,v)} x_t \in \{0,1\}$ since there are n many vertices and the path from any vertex to any other vertex is of size at most $O(\log n)$. Furtheremore, each $d_{(u,v)} x_t$ term is trivial to compute—it's just the product of two bits. An NC^0 circuit can just compute all these bits in parallel.

Thefore, combining the circuit computing these $O(n \log n)$ bits with our original circuit computing y for the Relaxed Parity Halving Problem yields a NC^0 circuit for $\mathrm{PHP}_{n,O(n \log n)}$, contradicting Theorem 4.19. □

We finally have a complete separation of a problem that is solved by a constant-depth quantum circuit, but not a constant-depth classical one. It's worth emphasizing that the quantum circuit was constructed by a sequence of classically-controlled Clifford operations. That is, the input to the Parity Halving Problem specifies a specific quantum circuit built from Clifford gates to run. Recalled that in Theorem 4.11 we showed that Clifford decision problems can be solved in the classical complexity class $\oplus\mathsf{L}$. A slight modification of that result shows that the relation versions of these Clifford problems can also be solved in the function variant of $\oplus\mathsf{L}$. That is, not only do we have a separation between low-depth quantum circuits and low-depth classical circuit, but the quantum circuit is a particularly simple variety.

How far can we hope to extend these kinds of separations? Can we show that increasingly strong models of classical circuits can't simulate these simple constant-depth quantum circuits? In fact, we can. We start with the classical complexity class AC^0:

Alernating circuits (AC^0)
The class of languages L such that there exists a uniform family of constant-depth, polynomial-size classical circuits $C_n\colon \{0,1\}^n \to \{0,1\}$ built from NOT gates and AND/OR gates with unbounded fanin where $x \in L$ if and only if $C_n(x) = 1$.

That is, AC^0 is the generalization of NC^0 where the gates are allowed to depend on an arbitrary number of input bits. Noticed that our standard lightcone arguments no longer work for AC^0—an output bit could be affected by every input bit. Nevertheless, there is a technique called the "switching lemma" that says that AC^0 circuits are essentially NC^0 circuits after some of the input bits have been randomly restricted to fixed values [Ajt83, FSS84, Has86]. The idea is that large AND and OR gates are very sensitive. If even one input bit of a large AND gate is set to 0, then the entire gate is nullified.

However, as we've seen before with the Parity Halving Game, restricted some of the inputs to the problem doesn't really change it's difficulty. Stringing these ideas together, we get the following:

Theorem 4.21 (Bene Watts, Kothari, Schaeffer, Tal [WKST19])**.** *The Relaxed Parity Halving Problem* RPHP_n *is in* FQNC^0 *but not* FAC^0.

At least for now, this is where we are stuck. We don't know how to show any better separation results (i.e., against a class of circuits larger than FAC^0) in the standard circuit setting. We *will* be able to show a better separation, but it will require us to work in a slightly different circuit model that allows for some interactivity. Before we describe that result, however, we will need to introduce some new tools.

4.7 Measurement-Based Quantum Computation

In some sense, our circuit separation results later will be based on the premise that simulating a constant-depth Clifford is just as hard as simulating a Clifford circuit with arbitrary depth. One of the key tools we will use is a technique called *measurement-based quantum computation*, which is a protocol for collapsing a general quantum circuit into a sequence of single-qubit measurements on some highly-entangled resource state that can be prepared in constant depth.

It should be quite surprising that such a protocol exists. Indeed, it should not be the case that every quantum circuit can be replaced by a constant-depth quantum circuit. Nevertheless, what measurement-based quantum computation shows is that all your entangling quantum operations *can* be applied in constant depth. The price you have to pay is that the measurement choices must be made sequentially—in order to know which measurement to make, you need to know the outcome of the previous measurement. These "adaptive" measurement choices are what restore the non-parallelizability to the circuit.

We will see how this manifests once we see the specifics of the protocol. First, we must introduce the family of resource states we will be using.

Graph states

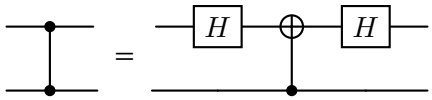
A *graph state* is a particular stabilizer state associated with an undirected graph and built from Hadamard and controlled-Z gates.

Since we haven't encountered the CZ gate before, let's take a moment to define it. A controlled-Z gate (or CZ gate) is defined similarly to the familiar controlled-X (or CNOT) gate—if the first qubit is $|1\rangle$, then apply a Pauli-Z operation to the second qubit. That is, for any bits $x, y \in \{0, 1\}$, we have

$$\mathrm{CZ}\,|x, y\rangle = (-1)^{xy}\,|x, y\rangle\,.$$

Notice that CZ is symmetric in the sense that we can think of either bit as the control. Because of this, it is depicted in quantum circuit diagrams as a control gate with no obvious orientation:

One can see that it is a Clifford operation by the following identity:



To verify this identity, notice that if the bottom qubit is $|0\rangle$, the two Hadamard gates cancel; and if the bottom gate is $|1\rangle$, we apply $HXH = Z$ to the topic qubit.

Let's now return to our construction of graph states. Specifically, the graph state $|G\rangle$ associated with graph $G = (V, E)$ is constructed as follows:

- For every vertex $v \in V$, create a new qubit in the $|+\rangle$ state.
- For every edge $e = (u, v) \in E$, apply a CZ gate on qubits associated to vertices u and v.

For example, the triangle graph (shown below left) corresponds to graph state (shown below right) with CZ gates between all pairs of qubits:

Graph states will be the entangled resource states we use for measurement-based quantum computation. Recall that we want our resource states to be preparable in constant depth, and it is certainly not true that all graph states can be prepared in constant depth. Consider, for some intuition, a graph that has a vertex with high degree. In that case, we would need to apply all CZ gates touching that vertex sequentially. Thankfully, the reverse is also true—if all vertices have low degree, then the corresponding graph state can be prepared in low depth:

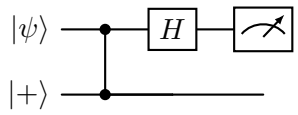
Lemma 4.22. *Let G be any graph with maximum degree Δ. The graph state $|G\rangle$ can be prepared in depth $\Delta + 1$.*

Proof. The proof follows also immediately from Vizing's theorem, which states that any graph with maximum degree D can be "edge colored" with $\Delta + 1$ colors. That is, we can color the edges of the graph with $\Delta + 1$ different colors such that no two edges of the same color are adjacent. To finish the proof, it suffices to see that all edges of the same color can be implemented in the graph state in the same layer, resulting in a graph state with $\Delta + 1$ layers of CZ gates. □

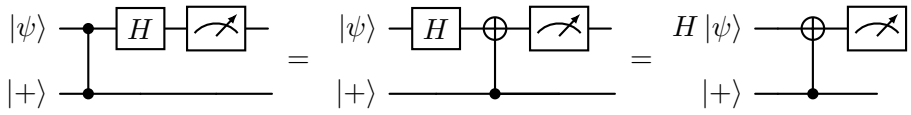
As we will see later, all the graph states we need for measurement-based quantum computation correspond to graphs with constant degree, and therefore can be constructed in constant depth.

The Hadamard Gadget

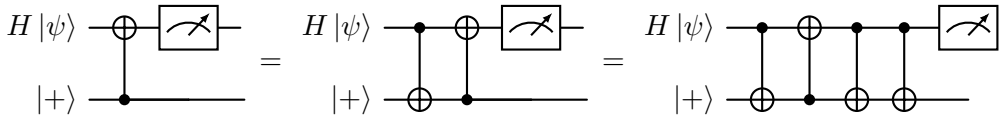
Somewhat surprisingly, the entire MBQC procedure boils down to the analysis of a single gadget:



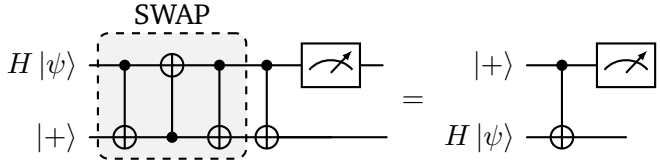
Here, $|\psi\rangle$ is an arbitrary 1-qubit state. We would like to know what is left over on the unmeasured wire. We show this through a sequence of circuit identities. We start by pushing the Hadamard gate across the CZ gate. As a result, the CZ is conjugated by H, becoming CNOT:



In the last step above, we simply pushed the Hadamard into the state. Next, we add 3 CNOT gates to our circuit that also leave it unchanged. First, we add a CNOT gate to the beginning of the circuit, which we can do because the $|+\rangle$ is not affected by the CNOT gate, no matter what $|\psi\rangle$ is. Second, we add two CNOT gates to the end of the circuit since CNOT multiplied by itself is the identity:



The key observation is that the first three CNOT gates multiply out to a SWAP gate. This implies that we can simplify the circuit further by just swapping the two inputs to the circuit:



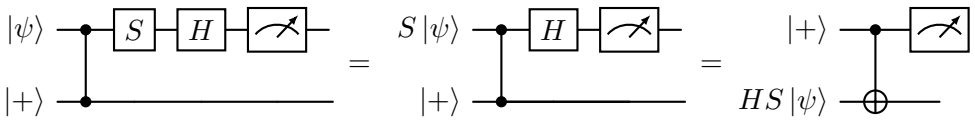
Therefore, the state of the circuit right before the measurement is

$$\mathrm{CNOT}(|+\rangle \otimes H|\psi\rangle) = \mathrm{CNOT}\left(\frac{|0\rangle \otimes H|\psi\rangle + |1\rangle \otimes H|\psi\rangle}{\sqrt{2}}\right) = \left(\frac{|0\rangle \otimes H|\psi\rangle + |1\rangle \otimes XH|\psi\rangle}{\sqrt{2}}\right),$$

In other words, if we measure $|0\rangle$, then the second state is $H|\psi\rangle$, whereas if we measure $|1\rangle$ it is $XH|\psi\rangle$.

Let's recap what we just saw with the Hadamard gadget: we applied a CZ gate between a $|+\rangle$ state and an arbitrary 1-qubit state $|\psi\rangle$; we measured the $|\psi\rangle$ register in the X basis; the state on the remaining register was $X^a H|\psi\rangle$ where $a \in \{0,1\}$ was the outcome of the measurement result. That is, simply by measuring the entangled $|\psi\rangle$ and $|+\rangle$ states, we were able to apply a single-qubit Hadamard gate to our state $|\psi\rangle$ (modulo a random Pauli X term coming from the measurement).

The above analysis shows what happens when we measure in the X-basis. What would happen if we were to measure in the Y-basis (i.e., apply a phase gate, followed by Hadamard, followed by a computational basis measurement)? Surprisingly, we don't have to repeat any of the analysis because we can easily reduce to the X-basis measurement case by pushing the S gate across the CZ gate (we are allowed to do so because the phase gate is a rotation in the Z basis, so $SZS^\dagger = Z$):



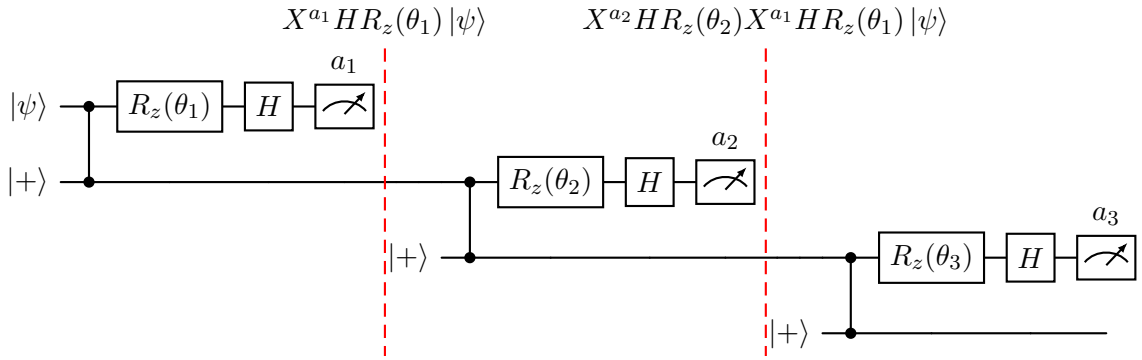
As a result, the second qubit will end up with the state $X^a HS|\psi\rangle$ depending on the outcome $a \in \{0,1\}$ of the measurement. In fact, notice that there's nothing special about the S gate in the analysis above other than the fact that it commutes with CZ gate. So, for example, we can replace the Clifford S gate with any rotation about the Z-axis:

$$R_z(\theta) := \cos(\theta/2)I - i\sin(\theta/2)Z.$$

For example, $R_z(\pi/2) \propto S$ is the familiar Clifford S gate, and $R_z(\pi/4) \propto T$ is the T-gate.

MBQC on a line

The Hadamard gadget allows us to apply a single gate, but by stringing gadgets together, we can affect a larger sequence of single-qubit gates:



Therefore, the state of the final unmeasured qubit is

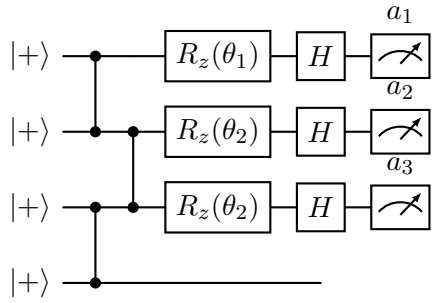
$$X^{a_3} H R_z(\theta_3) X^{a_2} H R_z(\theta_2) X^{a_1} H R_z(\theta_1) |\psi\rangle$$

Let's imagine for a moment that each measurement results in the 0 outcome. We claim that by adjusting the angles which determine the measurement basis, you can affect *any* single-qubit gate:

Fact 4.23 (Euler decomposition)**.** *Every single-qubit unitary can be expressed (up to global phase) as the product $R_z(\theta_3)R_x(\theta_2)R_z(\theta_1)$.*

Using the fact that $R_x(\theta) := \cos(\theta/2)I - i\sin(\theta/2)X = HR_z(\theta)H$, the final state in the example above can be written as $HR_z(\theta_3)R_x(\theta_2)R_z(\theta_1)|\psi\rangle$. Therefore, by Fact 4.23, we can apply any gate to $|\psi\rangle$ just by making the right sequence of measurements (assuming that we always measure 0).

To be clear, we can analyze the above example as a sequence of Hadamard gadgets, but the actual measurements and operations can all happen in parallel. That is, we can flatten the circuit diagram above (and replace $|\psi\rangle$ with $|+\rangle$ for the purposes of symmetry) to obtain:



Putting everything together, we can finally state the main theorem for this section:

Theorem 4.24 (MBQC on a line)**.** *Suppose you want to apply a sequence of arbitrary single-qubit gates $g_1, \ldots, g_n$ to the $|+\rangle$ state. There is a set of single-qubit measurements you can make on the graph state corresponding to a line of $\Theta(n)$ qubits that—assuming all measurement results are 0—results in the state $g_n \cdots g_1 |+\rangle$ on the last unmeasured qubit.*

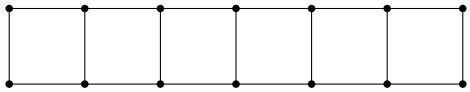
The proof follows from the above discussion. Notice that we start with the graph state on the line (which can be prepared in depth 2) and make single-qubit measurements on it. Therefore, the entire MBQC procedure only requires constant depth, and yet the state we produced seems to require high depth in the standard circuit model. The catch, of course, is that we also require all of the measurement results to be 0.

In reality, if you were to try to run such a procedure in a practical setting, then it would be extraordinarily unlikely that every such measurement would be 0 (though, we circumvent this limitation in both of the complexity consequences that we discuss in this class). There is a way to circumvent this limitation practically as well, which is to *adaptively* measure your qubits. That is, if you know the previous measurement introduced a Pauli-X error, then simply correct for that error when you make the measurement in the next step. However, this once again introduces depth into your quantum circuit since we need to know the result of the measurement on the ith qubit to make the measurement on the $(i+1)$st qubit. Because of this, we will not explore this adaptive protocol in more detail.

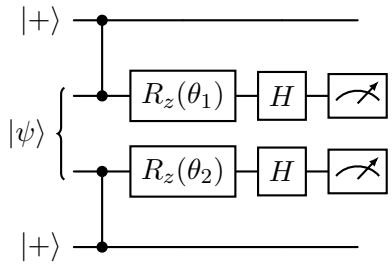
MBQC on the grid

Theorem 4.24 shows that we can induce arbitrary single-qubit computation by making measurements on the graph state corresponding to the line:

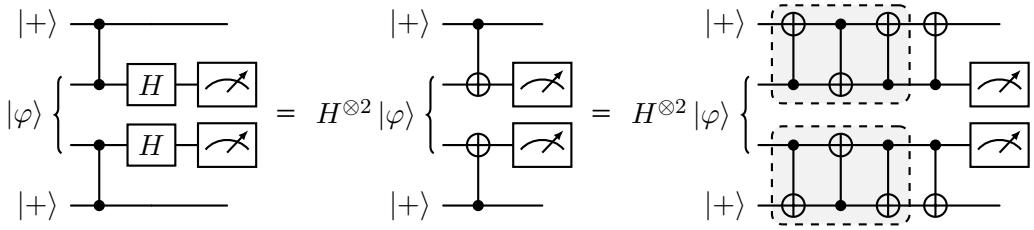
To reiterate, in this picture, we think of each vertex in the graph as a qubit initialized in the $|+\rangle$ state and each line as a CZ gate between those qubits. In this section, we would like to generalize this theorem to describe what happens when you make measurements on the graph state corresponding to the *grid*:



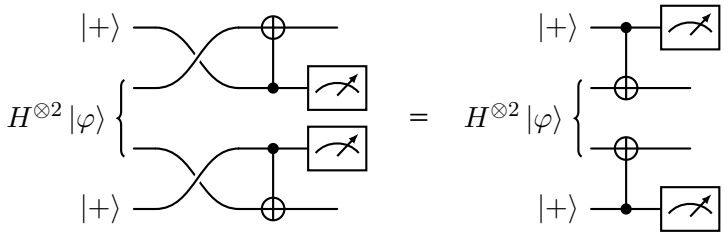
We will start with a $2 \times n$ grid like the one above, and then sketch how to generalize to grids with more rows. Somewhat remarkably, we will essentially need no further tools than what was used for the case of the line—the same gadget will suffice. To start, let's look at what happens when we apply two Hadamard gadgets to a two-qubit state:



One way to analyze these two gadgets is to just carry out the same circuit manipulations we've already seen. Letting $|\varphi\rangle := (R_z(\theta_1) \otimes R_z(\theta_2))\,|\psi\rangle$, we can start again by pushing the R_z gates to the input:



Once again, the CNOT gates in the gray boxes are swaps that can be pushed towards the outputs (last time we pushed towards the input, but that's harder to draw now):



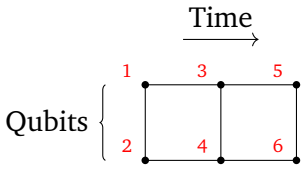
Supposing the measurements are $a_1, a_2 \in \{0, 1\}$, the final state on the remaining qubits is

$$(X^{a_1} H R_z(\theta_1) \otimes X^{a_2} H R_z(\theta_2)) \left|\psi\right\rangle$$

or, in other words, exactly the result of two Hadamard gadgets applied separately. In fact, the reason this works out nicely is precisely because the Hadamard gate is a linear operation (think of it as a unitary followed by a projection). That is, if we decompose $|\psi\rangle$ into the computational basis, we can apply the Hadamard gadget to each term of the sum, yielding the same result.

Let's now return to the 2D grid layout. Recall that for the 1D grid, we could think about the measurement-based quantum computation process as a sequence of gadgets, passing the qubit from one qubit to the next. However, that was in some sense just a trick of the analysis. We saw that all the CZ gates could be commuted to the beginning of the circuit, so that the final measurement-based quantum computation process just looked like a sequence of measurements on a graph state.

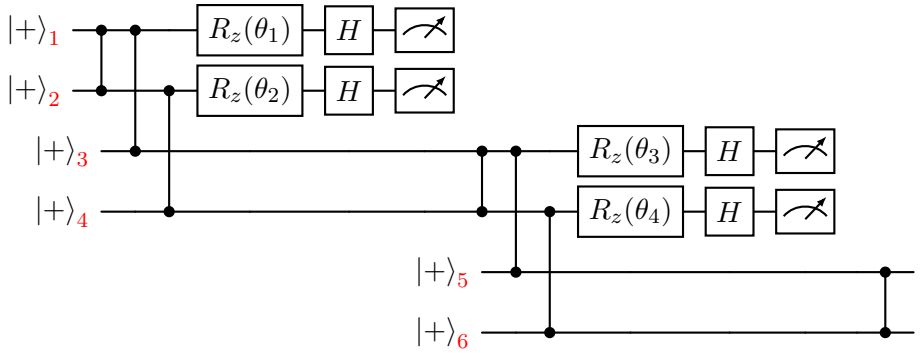
We'll do the same thing for the 2D grid layout, except applying two Hadamard gadgets at a time:



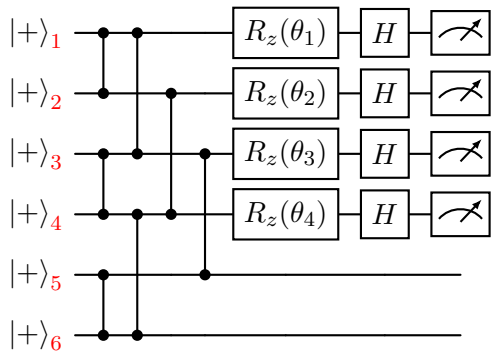
Let's step through the measurement process for the simple 2×3 example above, where we've labeled the 6 qubits we'll be using. The leftmost two qubits (1 and 2) start in the state $|{+}{+}\rangle$ and we immediately apply a CZ gate between them. Then, we create the middle two qubits (3 and 4), each in the state $|+\rangle$. Apply the Hadamard gadget on qubits 1 and 3, and then on 3 and 4. By our previous analysis of the Hadamard gadget on multi-qubit states, the state of the system is now

$$(X^{a_1} H R_z(\theta_1) \otimes X^{a_2} H R_z(\theta_2))\mathrm{CZ} \left|{+}{+}\right\rangle .$$

We can continue by applying a CZ gate between the middle qubits (3 and 4), and then once again applying the Hadamard gadget between the middles qubits and the rightmost qubits. The key observation throughout all of this analysis is that the CZ gates we apply in this construction can all be pushed to the beginning of the circuit since they commute with all other operations that have previously been made. This is readily apparent from the circuit below for this process:



Commuting all the CZ gates to the beginning, we get:



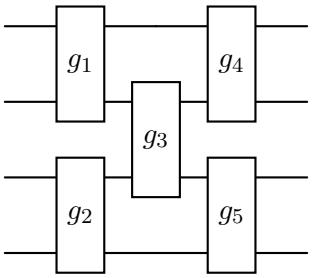
From this, we can clearly see the measurement-based quantum computation process as a sequence of measurements on the graph state corresponding to the grid.

To complete the MBQC protocol, it suffices to show that every 2-qubit gate can be decomposed as a sequence of gates of the form $(H \otimes H)(R_z(\theta_1) \otimes R_z(\theta_2))\mathrm{CZ}$. This is a bit trickier to show, but amounts to essentially a brute force calculation. Therefore, putting everything together, we get

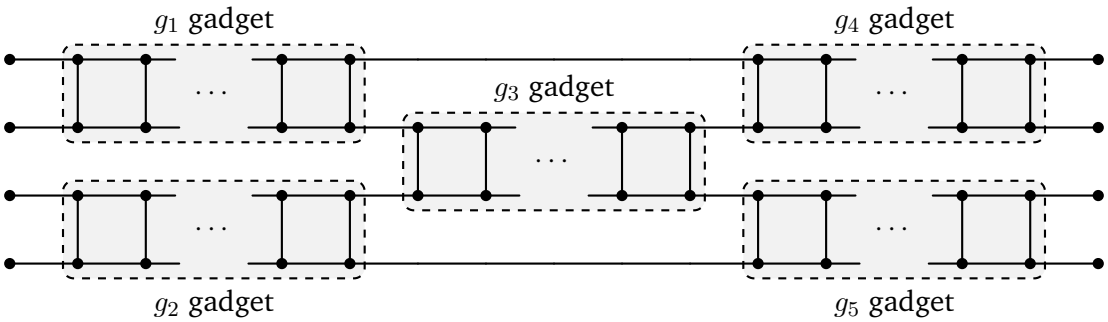
Theorem 4.25 (MBQC on the width-2 grid)**.** *Suppose you want to apply a sequence of arbitrary two-qubit gates $g_1, \ldots, g_n$ to the $|{+}{+}\rangle$ state. There is a set of single-qubit measurements you can make on the graph state corresponding to a $2 \times \Theta(n)$ grid of qubits that—assuming all measurement results are 0—results in the state $g_n \cdots g_1 |{+}{+}\rangle$ on the last two unmeasured qubit.*

Suppose now we wanted to simulate an n-qubit quantum circuit with a measurement-based quantum computation protocol. The idea is essentially the same—each row of the quantum circuit will represent a qubit and each column represents the state of the quantum circuit at a particular time slice. Using the MBQC procedure on grids with two rows (Theorem 4.25), we can simulate a two-qubit gate on any pairs of qubits.

This general construction is perhaps most easily understood through an example. Consider the following 4-qubit quantum circuit built from arbitrary 2-qubit gates $g_1, \ldots, g_5$:



We could simulate this circuit by making measurements on the graph state:



Notice that this is just the usual width-4 grid with some of the connections removed, so the corresponding graph state can still be constructed in constant depth. Each 2-qubit gate requires a gadget of some constant size, so the overall number of qubits in your graph state is bounded above by some constant times

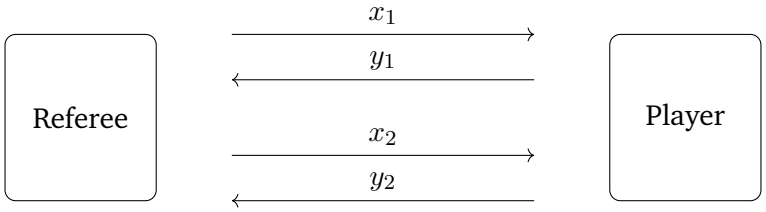
$$(\text{number of qubits in the circuit}) \times (\text{depth of the circuit}).$$

Importantly, since the gate gadgets in the measurement-based quantum computation protocol only act on adjacent rows of the grid, the depth of the circuit must be measured in terms of the depth when gates in the circuit are only allowed to act on adjacent qubits.

4.8 Simulating constant-depth Clifford circuits requires $\oplus$L

Recall our goal: we want to show that simulating constant-depth Clifford circuits requires classical circuits of much higher depth. Since general Clifford circuits can be simulated in the complexity class $\oplus$L, we can at most hope that classical circuits must be at least as powerful as $\oplus$L. We will show that this is indeed the case!

Unfortunately, as discussed earlier, we will no longer be able to use the Parity Halving Problem or, in fact, any relation problem. We will need to move to an entirely new paradigm of computation. The new model will be one that involves interaction—the input is given in two distinct rounds, and the output for the first round must be given before the second round input is known. We can think of this as an interactive protocol between a referee and a player:



The referee asks a question $x_1 \in \{0,1\}^{n_1}$ in the first round, and then the player immediately responds with an answer $y_1 \in \{0,1\}^{m_1}$. The referee then asks a second question $x_2 \in \{0,1\}^{n_2}$, and the player responds accordingly with $y_2 \in \{0,1\}^{m_2}$. The game is governed by a relation

$$R \subseteq \{0,1\}^{n_1} \times \{0,1\}^{n_2} \times \{0,1\}^{m_1} \times \{0,1\}^{m_2},$$

and the player wins if $(x_1, x_2, y_1, y_2) \in R$.

The relation we will use will once again come from measurements on a graph state. For every input length, there will be some understood graph state for which the referee will ask questions. In the first round, the referee will ask the player to measure some subset of qubits of the graph in a specified basis, and the player will respond with some measurement result which is consistent with those questions. In the second round, the referee will specify bases for the remaining qubits of the graph state, and the player must return a measurement result on those qubits consistent with the measurement results given in the first round.

This may seem somewhat odd. From the perspective of the quantum circuit, this interactive protocol is just as easy as the non-interactive protocol—just measure the qubits. However, the interactive problem is very different for a classical device trying to simulate the measurements.

To see why this might be the case, let's consider a classical device which can win the interactive graph state measurement problem. After the classical device has answered the first question, the classical device has a classical description of the graph state after the first round measurements have been made. This gives the classical device a power that a quantum circuit faithfully executing the measurements doesn't have. Namely, the classical device can copy, or perhaps stated more scarily, *clone* its copy of the intermediate state between rounds 1 and 2. Since the classical device wins the game by assumption, the classical device can effectively measure the cloned state repeatedly to learn some information hidden in the state. We will show that learning this hidden information is equivalent to solving arbitrary $\oplus\mathsf{L}$ problems. Therefore, whatever kind of classical device solves the interactive graph state problem, it must at least have the power of $\oplus\mathsf{L}$.

This is subtle, so it's worth reiterating. This argument does *not* imply that constant-depth quantum circuits can solve $\oplus\mathsf{L}$ problems. Instead, we show that a *classical* device that can simulate constant-depth quantum circuits can solve $\oplus\mathsf{L}$ problems. Formally, we will show the following theorem:

Theorem 4.26 (Grier, Schaeffer [GS20])**.** *Suppose there is a classical circuit $\mathcal{O}$ solving the interactive graph state measurement problem. Then, $\oplus\mathsf{L} \subseteq (\mathsf{AC}^0)^{\mathcal{O}}$.*

Let's see how we might go about using this theorem to prove separations. Suppose that the circuit $\mathcal{O}$ could be instantiated with an AC^0 circuit. By the theorem, we have

$$\oplus\mathsf{L} \subseteq (\mathsf{AC}^0)^{\mathsf{AC}^0} = \mathsf{AC}^0$$

where the last equality follows from the observation that giving an AC^0 circuit the "additional" ability to solve AC^0 problems doesn't increase its power. The Parity problem (i.e., is the Hamming weight of the input even or odd?) is solvable by a $\oplus\mathsf{L}$ machine, but Parity is not in AC^0 [Ajt83, FSS84, Has86], so it is impossible for AC^0 to contain $\oplus\mathsf{L}$. This contradiction implies that there must not have been an AC^0 circuit to solve the interactive grid measurement problem.

We can generalize this argument to show that not even $\mathsf{AC}^0[p]$ circuits can solve this problem. Once again, invoking the theorem, we get

$$\oplus\mathsf{L} \subseteq (\mathsf{AC}^0)^{\mathsf{AC}^0[p]} = \mathsf{AC}^0[p]$$

since we can replace any oracle access with a constant-depth circuit with MOD_p gates. However, $\oplus\mathsf{L} \not\subseteq \mathsf{AC}^0[q]$ for all primes q [Raz87, Smo87]; Therefore, $\mathcal{O} \notin \mathsf{AC}^0[p]$ for any prime p. In

other words, we have exhibited an interactive game that can be won by QNC^0 circuits but not by $\mathsf{AC}^0[p]$ circuits. We will see much more "impressive" separations later between quantum and classical complexity classes, but these separations will rely on unproven conjectures. This is one of the largest-known *unconditional* separations between natural classes of quantum and classical circuits.

For the purposes of these lecture notes, let's focus on a simpler variant of Theorem 4.26, where we only need to show hardness for NC^1. To show this, we only need to work with graph states corresponding to width-2 grids. That is, we will show that if there is a classical device $\mathcal{O}$ that can solve the interactive graph state measurement problem on the $2 \times n$ grid, then $\mathsf{NC}^1 \subseteq (\mathsf{AC}^0)^{\mathcal{O}}$. All of the separations we claimed previously (e.g., against $\mathsf{AC}^0[p]$ circuits) still hold.

There will be four main ingredients that go into the proof.

Ingredient 1: 2-qubit Clifford circuits are NC^1-hard

Let's start with a 2-qubit modification of the Clifford circuit problem that earlier showed was $\oplus\mathsf{L}$-complete.

2-qubit Clifford Circuit Problem
Input: List of 2-qubit Clifford gates $g_1, g_2, \ldots, g_n$
Output: Their product $g_n g_{n-1} \cdots g_1$

Theorem 4.27. *The 2-qubit Clifford Circuit Problem is NC^1-hard, even under the promise that the output is $I \otimes I$ or $H \otimes H$.*

We omit the proof but note that this is a consequence of Barrington's Theorem, namely that multiplying over the symmetric group S_5 is an NC^1-hard problem. Indeed, there is a subgroup of the Clifford group (the Clifford group mod the Pauli group) that is isomorphic to S_6, so that multiplication over the Clifford gates must be at least as hard as multiplication over S_5.

Ingredient 2: Measurement-Based Quantum Computation

Above, we have presented a problem that seems in some sense inherently sequential, or at the very least cannot be computed in constant depth. However, using the measurement-based quantum computation tricks of Section 4.7 we can show the following special case of Theorem 4.25, where we only wish to use MBQC for Clifford computation:

Corollary 4.28. *For all 2-qubit Clifford gates g, there exists a set of 38 measurements on the 2×20 grid graph state that leaves the unmeasured qubits in the state $Pg\,|00\rangle$ for some Pauli matrix P, where P depends on the outcomes of the measurements.*

As we've seen, you can string these gadgets together, so that if you have a graph state of size $2 \times (20n)$ and a list of gates $g_1, \ldots, g_n$, then there is a set of measurements on the graph state that creates the state

$$P_n g_n P_{n-1} g_{n-1} \ldots P_1 g_1 \,|00\rangle$$

where the Pauli terms $P_1, \ldots, P_n$ depend on the measurement results obtained in each one of the gadgets.

Next, recall that the Pauli matrices are a normal subgroup of the Clifford group (i.e., conjugating a Pauli operator by a Clifford operator yields another Pauli). This implies that you can "push" Pauli elements through Clifford elements:

$$gP = gP(g^\dagger g) = (gPg^\dagger)g = P'g$$

where P' is just some other Pauli operator. Using this idea, we can propagate all the Pauli operators to the front of our expression:

$$P_n g_n \dots P_1 g_1 = P'_n P'_{n-1} \dots P'_1 g_n \dots g_1 = P^* g_n g_{n-1} \dots g_1 \left|00\right\rangle$$

for some Pauli operator P^*.

Recall that we can use the promise that $g_n g_{n-1} \cdots g_1$ is either $I \otimes I$ or $H \otimes H$. By our previous observation, we just need to distinguish between these cases where the state has been corrupted by some unknown Pauli P^*. (Note that in principle, one could compute P^* from the measurement outcomes. Unfortunately, this computation is itself NC^1-hard, so we can't do this in our reduction).

To circumvent this issue, let's first consider the stabilizer groups for our ending state $|00\rangle$ and $|{+}{+}\rangle$, respectively:

$$\begin{pmatrix} I\,I \\ Z\,I \\ I\,Z \\ Z\,Z \end{pmatrix}, \qquad \begin{pmatrix} I\,I \\ X\,I \\ I\,X \\ X\,X \end{pmatrix}$$

Finally, applying P^* to the state is equivalent to conjugating by P^* in the stabilizer group. The key fact is that conjugation by Pauli matrices can only change the sign. In particular, the output of the measurement based quantum computation is

$$\begin{pmatrix} I\,I \\ a\,P\,I \\ b\,I\,P \\ ab\,P\,P \end{pmatrix}$$

for some $P \in \{X, Z\}$ and $a, b \in \{\pm 1\}$. Our goal then is to distinguish between $P = X$ and $P = Z$.

Ingredient 3: Randomizing the Output

In the next two sections, we will treat the player in the interactive graph state measurement problem as a sort of adversary. Recall that our claim is that we can leverage the simulator to solve the Clifford multiplication problem. In particular, this should be true regardless of which answers the simulator gives us. Therefore, we should expect that the simulator gives us the maximally useless answers at all times. Or, in other words, that the simulator is acting adversarially. To be clear, the simulator must still be correct, but it can still try to answer correctly, without being useful.

Unfortunately, it will turn out that if we only have two possible outcomes (the $I \otimes I$ outcome and the $H \otimes H$ outcome), then adversarial outcomes will prevent us from learning which state we have. To overcome this, let us briefly describe how we can "randomize" the

output of the previous step. Before we compute $g_n \cdots g_1$, we can generate random Clifford gates $h_0, \ldots, h_n$ and redefine $g'_i = h_i g_i h_{i-1}^{-1}$. Then,

$$g'_n g'_{n-1} \ldots g'_1 = h_n g_n h_{n-1}^{-1} h_{n-1} g_{n-1} h_{n-2}^{-1} \ldots h_1 g_1 h_0^{-1} = h_n g_n g_{n-1} \ldots g_1 h_0^{-1}$$

Thus, rather than the two specific stabilizer groups above, we now must distinguish between two stabilizer groups that are random! Since we chose h_i, we know which outcome with correspond to $I \otimes I$ and $H \otimes H$, but what we have essentially done is made the input uniformly random among all sets of n Clifford gates. The adversary does not know.

Ingredient 4: The Magic Square

Our goal is to measure our unknown 2-qubit state to learn what it is. It will turn out that any single measurement cannot give us enough information to determine this state. So, this is the first place we will use interactivity and the rewinding ingredient shown earlier. Still, even with many measurements, it's a bit unclear which measurements we should make.

Our measurements will correspond to the rows/columns of the following matrix called the *Magic Square*:

$$\begin{pmatrix} XX & YY & ZZ \\ YZ & ZX & XY \\ ZY & XZ & YX \end{pmatrix}$$

Let's note some important properties of this arrangement of Pauli operations:

1. The Pauli operators within each column and row commute. This means that we can "measure" all 3 Pauli operations simultaneously, i.e., rotate to the Z-basis and then measure.

2. The product of each row is $-II$. That is, the sum of measurement results on a row must be odd.

3. The product of each column is II. That is, the sum of measurement results on a column must be even.

We now need two key observations:

Fact 4.29. *If a measured Pauli operator happens to be in the stabilizer group of the unknown state, then the measurement result for that Pauli is equal to the sign of the Pauli in the stabilizer group (This is just a generalization of Lemma 4.16 from the previous lecture).*

Fact 4.30. *There is no consistent way to label a 3×3 matrix with $0/1$ values such that the sum of each row is odd and the sum of each column is even.*

Therefore, if we make all measurements corresponding to each row and each column, there must be some measurement output which was different for a particular Pauli (Fact 4.30). On the other hand, if we happened to measure some Pauli that was in the stabilizer group, then we could not have gotten different results. Together, the 6 measurements reveal at least one Pauli element which is *not* in the stabilizer group of the measured state.

Putting It All Together

Let's first consider the problem from the perspective of the quantum algorithm. In round 1, it uses measurement-based quantum computation (ingredient 2) to prepare the state $P^* g_n \dots g_1 |00\rangle$ in constant depth. The gates $g_1, \dots, g_n$ correspond to the input of some 2-qubit Clifford multiplication problem (ingredient 1). In round 2, it measures that state in the specified basis.

Now consider a classical simulator achieving the same output as the quantum algorithm. After round 1, the simulator has some classical internal state which captures the true quantum state $P^* g_n \dots g_1 |00\rangle$. Using the "rewinding" technique on this intermediate state, it can make many possible measurements in round 2. Armed with this power, it measures all the magic square Paulis (ingredient 4). In this process, it learns some non-stabilizer of the state.

Since we randomized our inputs (ingredient 3), this non-stabilizer will appear in one of the two stabilizer groups for the states we are trying to distinguish with some constant probability. In this case, we learn exactly which one of our two states we have, and so we have solved the Clifford multiplication problem.

There are many details left to check here, but this is most of the main ideas. For example, we must check that this reduction can indeed be done with AC^0 circuits, which upon closer inspection are actually randomized, and so there are more subtleties to handle.

Chapter 5

Quantum Computational Advantage

In this chapter, we move on from quantum advantage against low-depth classical circuits to consider what is sometimes called "quantum supremacy" or "quantum computational advantage." In this setting, we want to devise some task that can be solved efficiently by a quantum computer, but for which there is no analogous efficient classical algorithm. We will not concern ourselves that the task is "useful" in the way that, say, Shor's algorithm is useful in cryptographic contexts. We merely want to show that there is any quantum problem that lies outside of classical polynomial time.

In some sense, the question we are asking is whether or not we can use complexity theory to show that our physical world is quantum mechanical. That is, if we could build a quantum device to perform some task that no classical computer could solve, then nature's laws are at least not simulatable on a classical computer.

With such a lofty goal, we will need to have suitably realistic expectations. For one, as we sketched in Chapter 2, proving that P is distinct from BQP necessarily implies that P is separate from PSPACE, which is a longstanding open question in classical complexity theory. Therefore, we will have to content ourselves with a separation between quantum and classical computers that is predicated on some kind of assumption.

It would be fantastic if our quantum-classical separation only required the assumption that $\mathsf{P} \neq \mathsf{PSPACE}$. This would give strong evidence that classical and quantum computation are indeed different. Unfortunately, as we shall soon see, we will actually require conjectures that are quite a bit stronger. Moreover, as we define tasks that are more likely to be physically realizable by experiments, we will require conjectures that are stronger.

We begin our search for such problems with a discussion of classical complexity, and a review of what sorts of classical complexity assumptions we can use as a basis for our separation results.

5.1 Complexity classes in the polynomial hierarchy

We start by defining a hierarchy of classes that lie between P and PSPACE. To see when we might need such a generalization, consider the following problem:

Minimum Equivalent Formula

Input:	Polynomial-size formula φ and integer k (expressed in unary)
Question:	Is there a formula of size at most k that is equivalent to φ?

We haven't been explicit about how the formula is represented, but let's make the reasonable assumption that if the formula has size 0, then it evaluates to false. We can now easily see that if we had an oracle to solve the Minimum Equivalent Formula problem, then we could immediately solve any problem in NP. To see this, consider some NP-hard formula φ and query the oracle on φ and $k = 0$. If the formula is unsatisfiable, it is always false, so there is an equivalent formula of size 0; otherwise, it must be satisfiable.

On the other hand, it's not clear how you could use an NP oracle to solve the Minimum Equivalent Formula problem. Indeed, you can use your NP oracle to search for a smaller formula, but then you have to check it on *all* inputs to see if it's equivalent to the input formula. If your NP machine itself had an oracle for NP, then it could search for a small formula and then use the oracle to check that there are no inputs which distinguish the two formulas. In other words, we've shown that Minimum Equivalent Formula is in $\mathsf{NP}^{\mathsf{NP}}$. In fact, this problem is $\mathsf{NP}^{\mathsf{NP}}$-complete [Uma01].

Let's now define a hierarchy of NP and coNP machines that have oracle access to more NP machines.

Polynomial-Time Hierarchy (PH)
Complexity classes recursively defined as follows:

- Base case: $\Sigma_0^{\mathsf{P}} = \Pi_0^{\mathsf{P}} = \mathsf{P}$
- Recursive case: $\Sigma_i = \mathsf{NP}^{\Sigma_{i-1}^{\mathsf{P}}}$ and $\Pi_i = \mathsf{coNP}^{\Sigma_{i-1}^{\mathsf{P}}}$

The polynomial hierarchy is defined as the union of these classes: $\mathsf{PH} = \bigcup_i \Sigma_i^{\mathsf{P}}$.

For example, $\Sigma_1^{\mathsf{P}} = \mathsf{NP}$ and $\Sigma_2^{\mathsf{P}} = \mathsf{NP}^{\mathsf{NP}}$. We've seen with the Minimum Equivalent Formula problem that there is a problem in Σ_2^{P} that doesn't appear to be in Σ_1^{P}. One reasonable question is whether or not this phenomenon exists for all levels of the polynomial hierarchy. Could it be that after some number of levels, adding an additional NP oracle doesn't help? It is widely believe that this is not true:

Conjecture 5.1. *The polynomial hierarchy is infinite:* $\Sigma_i^{\mathsf{P}} \subsetneq \Sigma_j^{\mathsf{P}}$ *for all* $i < j$.

This will be one of the central assumptions in our proofs of quantum computational advantage, though we will see exactly how this becomes relevant later.

For now, let's turn to ways to upper bound the power of the polynomial hierarchy. The first claim is that $\mathsf{PH} \subseteq \mathsf{PSPACE}$. To see this, notice that any language in PH can be solved with k nested NP oracles for some $k \in \mathbb{N}$. Each one of these oracles is some polynomially verifiable search problem. Furthermore, solving the search problem is possibly with polynomial space by simply iterating over all possible solutions. Since k is a constant (k does not grow with the input size), the nested search problems can be solved in polynomial space.

As it turns out, however, PSPACE is not the tightest upper bound on the complexity of the polynomial hierarchy that we know, though improved upper bounds are significantly harder to prove:

Theorem 5.2 (Toda's Theorem)**.** $\mathsf{PH} \subseteq \mathsf{P}^{\mathsf{PP}}$.

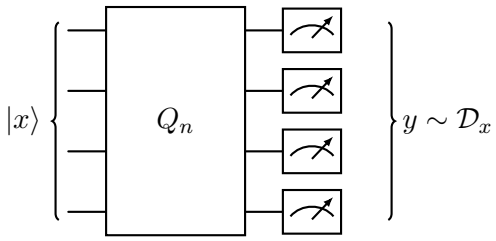
Finally, we note that polynomial-time randomized computation is not *too* powerful in the sense that it is still contained within some finite level of the polynomial hierarchy:

Theorem 5.3 (Sipser-Gács-Lautemann theorem [Sip83, Lau83])**.** $\mathsf{BPP} \subseteq \Sigma_2^{\mathsf{P}} \cap \Pi_2^{\mathsf{P}}$.

5.2 The hardness of exactly simulating quantum circuits

Our goal is to show that there are distributions that quantum circuits can sample from that efficient classical computers cannot sample from. Formally, a sampling problem is defined by a suite of distributions $\{\mathcal{D}_x\}_{x\in\{0,1\}^*}$. An *exact sampler* is any procedure that, given an input $x \in \{0,1\}^n$, samples an outcome $y \sim \mathcal{D}_x$ from the distribution. Note that this is a harder task than the relation problems that were used to show quantum advantage with Clifford circuits (see Section 4.4). There, the goal in some sense was to output *any* element in the support of the distribution. Now, the probabilities of the output of the sampler must exactly reproduce the entire distribution.

One way to make sure that a quantum circuit is able to solve some sampling problem is just to define the sampling problem with respect to what some family of quantum circuits is already doing. That is, for some family of quantum circuits $\{Q_n\}_{n=1}^{\infty}$, we define the distribution $\mathcal{D}_x$ for a given input $x \in \{0,1\}^n$ simply as what you would obtain by measuring some number of the output qubits of Q_n:



We want to show that no polynomial-size classical circuit can sample from the same distribution. While we won't be able to show such a separation unconditionally, we will be able to base the hardness of classical sampling on a standard complexity-theoretic assumption.

Let's start by considering a somewhat weird model of quantum circuits that will be surprisingly relevant to our proof. In particular, let's consider a model of "postselected" quantum computation where we get to choose or *postselect* which measurement outcome we get from any measurement. That is, even if the actual probabiltiy of measuring a some outcome is incredibly small (so that we'd never see it in a real quantum experiment), we can still choose to see that outcome. Formally, we define the following complexity class:

Postselected BQP **(**PostBQP**)**
Languages L such that there is a poly-uniform family of polynomial-size quantum circuits $\{Q_n\}_{n=1}^{\infty}$ such that for all $x \in \{0,1\}^n$:

- The probability of measuring $|1\rangle$ on the first qubit of $Q_n |x\rangle |0\cdots 0\rangle$ is nonzero.
- If $x \in L$, then conditioned on the first qubit being $|1\rangle$, the probability of measuring $|1\rangle$ on the second qubit is at least $2/3$.
- If $x \notin L$, then conditioned on the first qubit being $|1\rangle$, the probability of measuring $|1\rangle$ on the second qubit is at most $1/3$.

Of course, such a postselected model is not unique to quantum computation. We can consider a similar variant of BPP where we can to postselect on certain random outcomes:

Postselected BPP **(**PostBPP **or** $\mathsf{BPP}_{\mathsf{path}}$**)**
Languages L such that there is poly-uniform family of two-output polynomial-size classical circuits $\{C_n\}_{n=1}^{\infty}$ such that for all $x \in \{0,1\}^n$:

- Postselect strings: $\mathcal{R}_x := \{r \in \{0,1\}^{\mathsf{poly}(n)} : \text{first output of } C_n(x,r) \text{ is } 1\} \neq \emptyset$
- If $x \in L$, the second output of $C_n(x,r)$ is 1 for at least $2/3$ fraction of strings in $r \in \mathcal{R}_x$.
- If $x \notin L$, the second output of $C_n(x,r)$ is 1 for at most $1/3$ fraction of strings in $r \in \mathcal{R}_x$.

The key insight we will use is that if there is an exact classical sampler for any polynomial-size quantum circuit, then it must be the case that postselected classical computation is the same as postselected quantum computation, i.e., PostBPP = PostBQP. Indeed, if the output distribution of a quantum and classical circuit are the same, then the marginal distributions on the first and second (qu)bits must also be the same. However, this is where we can attempt to prove a contradiction—postselected quantum computation is *extremely* powerful, whereas postselected classical computation is only moderately powerful.

Formally, a result of Aaronson shows that PostBQP = PP [Aar05]. Therefore, by Toda's theorem, we have that poly-time computation with query access to a PostBQP device can solve any problem in the polynomial hierarchy:

$$\mathsf{P}^{\mathsf{PostBQP}} = \mathsf{P}^{\mathsf{PP}} \supseteq \mathsf{PH}.$$

Meanwhile, postselected classical computation is relatively less powerful. In particular, PostBPP $\subseteq$ $\mathsf{BPP}^{\mathsf{NP}}$ [HHT97]. Combined with the Sipser-Gács-Lautemann theorem, we have that

$$\mathsf{PostBPP} \subseteq \mathsf{NP}^{\mathsf{NP}^{\mathsf{NP}}} = \Sigma_3^{\mathsf{P}}.$$

Assuming that PostBPP = PostBQP, we can combine the above to get the following sequence of conclusions:

$$\mathsf{PH} \subseteq \mathsf{P}^{\mathsf{PostBQP}} = \mathsf{P}^{\mathsf{PostBPP}} = \mathsf{P}^{\Sigma_3^{\mathsf{P}}} = \Sigma_3^{\mathsf{P}}.$$

We've arrived the following theorem:

Theorem 5.4 (Hardness of exact sampling)**.** *Suppose that every family of* BQP *circuits can be exactly sampled with a family of* BPP *circuits. Then, the polynomial hierarchy collapses to the third level:* $\mathsf{PH} \subseteq \Sigma_3^{\mathsf{P}}$.

Because the non-collapse of the polynomial hierarchy is a widely accepted conjecture in complexity theory, the above theorem is strong evidence that there is no efficient classical method to sample exactly from the output distributions of polynomial-size quantum circuits.

5.3 Hardness of multiplicative approximations

While exact hardness of sampling results provide very strong evidence for quantum advantage, they are nevertheless somewhat disappointing. To state the obvious, exact sampling is an *extremely* stringent requirement. The distribution that we are asking the classical simulator to sample from has an exponential support with exponentially small probabilities. Indeed, if we designed a "real" quantum device to perform the same task, it is unlikely that it would sample from that same distribution.

Therefore, we would like to relax the sampling condition. Can we show that approximately sampling from quantum circuits is still hard? We will start to answer this question with *multiplicative* approximations, which is still a very strong requirement, but will nevertheless help us build up our tool chest for tackling more realistic notions of approximations. Moreover, we will eventually require stronger conjectures in order to weaken our notion of approximation. For multiplicative approximations, we can still use the same conjecture that we used for exact sampling hardness.

For some $c \geq 1$, we say that $\hat{z} \in \mathbb{R}$ is a multiplicative c-approximation of $z \in \mathbb{R}$ if

$$c^{-1}z \leq \hat{z} \leq cz.$$

We say a distribution multiplicatively c-approximates another distribution if it multiplicatively c-approximates every output probability. We are interested in classical algorithms that can multiplicatively c-approximate the output of a quantum circuit.

To show hardness of approximation, we are once again going to exploit a key difference between classical and quantum samplers—in this case, the difference between probabilities (which are always positive) and amplitudes (which can be both positive and negative). The complexity-theoretic distinction here can be boiled down to the difference between approximation in two different counting complexity classes.

Counting classes

Counting classes are a specific kind of function complexity class where functions are defined in terms out of how many inputs cause a machine to accept. Our discussion will center around two complexity classes where the goal is the count the number of accepting solutions for some polynomial time computation.

Counting Polynomial Time (#P)
Functions $f\colon \{0,1\}^* \to \mathbb{N}$ such that there exists a poly-time Turing machine M and polynomial q such that, on input $x \in \{0,1\}^n$, f counts the number of strings $r \in \{0,1\}^{q(n)}$ causing M to accept x. That is, for all $x \in \{0,1\}^n$

$$f(x) = |\{r \in \{0,1\}^{q(n)} : M(x,r) = 1\}|.$$

That natural complete problem for #P (pronounced "sharp P") is counting the number of inputs that cause some poly-sized circuit to output 1. In other words, #P is about *counting* the number of satisfying solutions, whereas a decision class like NP is about deciding if there is at least one satisfying solution.

The salient feature of #P for our purposes is that solutions only add up, rather than cancel each other out. Let's contrast #P with another function class called GapP, where we do not have this property.

Gap P (GapP)
Functions $f\colon \{0,1\}^* \to \mathbb{N}$ such that there exists a poly-time Turing machine M and polynomial q such that, on input $x \in \{0,1\}^n$, f counts the difference in the number of strings $r \in \{0,1\}^{q(n)}$ that cause M to accept and reject. That is, for all $x \in \{0,1\}^n$

$$f(x) = |\{r \in \{0,1\}^{q(n)} : M(x,r) = 1\}| - |\{r \in \{0,1\}^{q(n)} : M(x,r) = 0\}|.$$

Equivalently, GapP is the closure of #P under addition and subtraction.

At first glance, these two complexity classes don't seem meaningfully different. Indeed, with some trivial post-processing, we can compute a GapP function given the ability to compute a #P function. That is, if k of the 2^m strings in $\{0,1\}^m$ cause a Turing machine to accept, then the number of strings causing rejection is $2^m - k$, and so the number of accepting minus rejecting strings is $2k - 2^m$. This shows that $\mathsf{P}^{\#\mathsf{P}} = \mathsf{P}^{\mathsf{GapP}}$.

The key difference is when *approximating* these two kinds of functions. We start with approximating #P functions:

Theorem 5.5 (Stockmeyer counting)**.** *There is a* $\mathsf{BPP}^{\mathsf{NP}}$ *algorithm to multiplicatively approximate any function in* #P *to error* $1 + 1/\mathsf{poly}(n)$.

In other words, Stockmeyer counting essentially says that the ability to *detect* a solution (i.e., with the NP oracle) confers the ability to approximately count the number of solutions.

Proof sketch. While some details need to be worked out, the idea is fairly simple. Let's suppose we're trying to count the number of solutions to some poly-time computable function $f\colon \{0,1\}^n \to \{0,1\}$. First use your NP oracle to detect if there is a solution. If there are no solutions, then you are done immediately since 0 is a perfect count of the number of solutions. Otherwise, generate a random hash function $h_1\colon \{0,1\}^n \to \{0,1\}$ using your BPP capabilities. Now create a new function $f_1(x) := f(x) \wedge h_1(x)$, which only accepts if both the original function f and the new hash function h_1 accept. With high probability, this will cut the number of solutions roughly in half.

Once again, run your solution detection algorithm. If the number of solutions is still greater than zero, then consider $f_2(x) := f(x) \wedge h_1(x) \wedge h_2(x)$ for another hash function h_2, which cuts the solution space in half yet again. Continue cutting the space of solutions in half like this until the NP oracle detects that there are 0 solutions remaining. If we've used m total hash functions, then the number of solutions is approximately $2^m - 1$. Formally checking the details of this process will show that it yields a multiplicative 2-approximation. To get an approximation factor polynomially close to 1 consider the following modification of the original #P function f you are trying to approximate:

$$g(x_1, x_2, \ldots, x_m) = f(x_1) \wedge f(x_2) \wedge \cdots \wedge f(x_m)$$

Notice that if f is computable in polynomial time, then g is also certainly computable in polynomial time if $m = \mathsf{poly}(n)$. Furthermore, if f had k solutions, then g has k^m solutions. A 2-approximation $\hat{k}$ to the number of solutions to g implies

$$\frac{1}{2}k^m \leq \hat{k} \leq 2k^m \implies \frac{1}{2^{1/m}}k \leq \hat{k}^{1/m} \leq 2^{1/m}k.$$

Since $2^{1/m} < 1 + 1/m$, we get that $\hat{k}^{1/m}$ is a $1 + 1/m$ approximation to k. □

Let's now consider the analogous approximate computation of functions in GapP. For some intuition, consider a function where the number of solutions is extremely close to the number of non-solutions. Since we're aiming for a multiplicative approximation, we must be able to detect with 100% probability when the number of solutions is exactly equal to the

number of non-solutions. This looks like a problem that requires a PP oracle rather than a NP oracle. It is possible to formalize this intuition to show that multiplicatively approximating a GapP function it itself a GapP-hard problem:

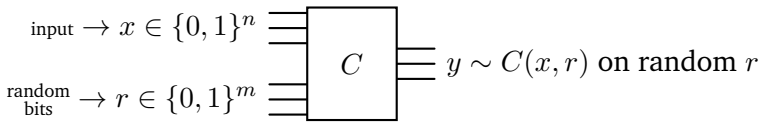
Theorem 5.6. *Exactly computing* GapP *functions is poly-time reducible to multiplicatively approximating* GapP *functions. Formally, let $\mathcal{O}$ be an oracle that can multiplicatively approximate* GapP *functions to* any *non-zero error. Then* $\mathsf{P}^{\mathsf{GapP}} \subseteq \mathsf{P}^{\mathcal{O}}$.

Proof. Let $f\colon \{0,1\}^n \to \{0,1\}$ be a poly-time computable function, and let $\Delta_f := |f^{-1}(0)| - |f^{-1}(1)|$ be the number of solutions minus the number of non-solutions to f. Recall that computing Δ_f is a GapP-complete problem. We will use the fact that if we can multiplicatively approximate Δ_f (to *any* multiplicative factor), then we can detect if Δ_f is positive, negative, or zero. Let's also use that GapP is the closure of #P under addition and subtraction. In particular, from f, we can create a new poly-time computable function g such that $\Delta_g = \Delta_f \pm c$ for any poly-time computable number c.

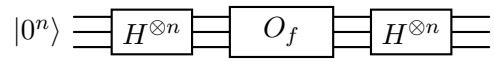
This gives us a relatively straightforward way to binary search for the exact value of Δ_f. A priori, we have that Δ_f is in the interval $[-2^n, 2^n]$. A multiplicative approximation to Δ_f reveals that it is either 0 or in one of the two intervals $[-2^n, 0]$ or $[0, 2^n]$. That is, we either learn Δ_f exactly or we cut the possible interval in which Δ_f can live in half. If, say, $\Delta_f \in [-2^n, 0]$, add 2^{n-1} so that it lies in the interval $[-2^{n-1}, 2^{n-1}]$ and recurse. □

Approximately computing probabilities in quantum and classical circuits

Computing output probabilities in classical circuits is almost a #P task by definition—to compute the probability of outputting $y \in \{0,1\}^n$, count how many settings of the random bits $r \in \{0,1\}^m$ cause the circuit to output 1:



Does computing the output probabilities of quantum circuits naturally correspond to GapP-complete problems? Consider the following quantum circuit that applies a classical function $f\colon \{0,1\}^n \to \{0,1\}$ in superposition via the phase oracle (see Section 3.1):



The final state is given by

$$|0^n\rangle \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle \xrightarrow{O_f} \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} (-1)^{f(x)} |x\rangle \xrightarrow{H^{\otimes n}} \frac{1}{2^n} \sum_{y\in\{0,1\}^n} \sum_{x\in\{0,1\}^n} (-1)^{f(x)+x\cdot y} |y\rangle$$

so the amplitude on the all-zeroes state is given by

$$\langle 0^n| H^{\otimes n} O_f H^{\otimes n} |0^n\rangle = \frac{1}{2^n} \sum_{x\in\{0,1\}^n} (-1)^{f(x)} = \frac{\Delta_f}{2^n}.$$

In other words, computing quantum amplitudes is at least as hard as computing Δ_f, which is a GapP-hard function! Unfortunately, we now run into the distinction between computing amplitudes and probabilities. Importantly, if we have a sampler for a quantum circuit, we have a proxy for computing *probabilities*, not amplitudes. That is, a multiplicative classical sampler we allow us to estimate the absolute value of Δ_f, rather than Δ_f itself. We seem to need a version of Theorem 5.6 wherein the multiplicative approximation only tells us whether or not Δ_f is zero or non-zero. Thankfully, there is a decision variant of GapP that does just that:

Exact-Counting Polynomial-Time ($\mathsf{C_{=}P}$)
Languages L such that there exists a poly-time Turing machine M and a polynomial q such that for all $x \in \{0,1\}^n$, $x \in L$ iff

$$|r \in \{0,1\}^{q(x)} : M(x,r) = 0\}| = |r \in \{0,1\}^{q(x)} : M(x,r) = 1\}|.$$

In summary, the construction above shows that multiplicative approximating the outputs of a classical circuit is equivalent to deciding problems in $\mathsf{C_{=}P}$. A variant of Toda's theorem, shows that this is still an extremely powerful primitive:

Theorem 5.7 (Toda and Ogiwara [TO92])**.** $\mathsf{PH} \subseteq \mathsf{BPP}^{\mathsf{C_{=}P}}$.

Multiplicative approximations imply polynomial hierarchy collapses

We are finally ready to piece together all of the above results to show that multiplicatively sampling from the outputs of quantum circuits implies that the polynomial hierarchy collapses. The proof outline is more-or-less identical to the one for exact sampling. Let's start with the assumption that there is a polynomial-time classical sampling algorithm that can multiplicatively sample from the output distribution of a given quantum circuit. Let $\mathcal{O}$ be the oracle for multiplicative approximations of the output probabilities given polynomial-size quantum circuits. On the one hand, since we have a classical sampler, we can use Stockmeyer counting to conclude that $\mathcal{O} \subseteq \mathsf{BPP}^{\mathsf{NP}}$, and so

$$\mathsf{BPP}^{\mathcal{O}} \subseteq \mathsf{BPP}^{\mathsf{BPP}^{\mathsf{NP}}} \subseteq \mathsf{BPP}^{\mathsf{NP}} \subseteq \Sigma_3^{\mathsf{P}}.$$

On the other hand, we've just shown that multiplicative approximations imply algorithms for problems $\mathsf{C_{=}P}$, so we get

$$\mathsf{BPP}^{\mathcal{O}} \supseteq \mathsf{BPP}^{\mathsf{C_{=}P}} \supseteq \mathsf{PH}$$

and so once again combining the two cases, we get that the polynomial hierarchy collapses to the third level:

$$\mathsf{PH} \subseteq \Sigma_3^{\mathsf{P}}.$$

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Appendix A

Classical complexity

In this appendix, we review some of the important concepts from classical complexity theory.

A.1 Complexity classes for decision problems

A *language* $L \subseteq \{0,1\}^*$ is simply a set of strings over the binary alphabet. The *decision problem* corresponding to a language L is the task of computing membership in the language. That is, given input $x \in \{0,1\}^*$, output "YES" if $x \in L$ and output "NO" if $x \notin L$.

A *complexity class* is a collection of languages recognized by a particular model of computation. The complexity classes below are defined in terms of classical Turing machines. The more resources we give the Turing machine (e.g., time, space, randomness, or nondeterminism), the more languages that model of Turing machine can recognize.

Polynomial Time (P):
Languages L such that there exists a deterministic poly-time Turing machine M such that $M(x)$ accepts iff $x \in L$.

Non-deterministic Polynomial Time (NP):
Language L such that there exists deterministic poly-time Turing machine M and polynomial q such that for all $x \in \{0,1\}^n$

- If $x \in L$, $\exists y \in \{0,1\}^{q(n)}$ such that $M(x,y)$ accepts
- If $x \notin L$, $\forall y \in \{0,1\}^{q(n)}$, $M(x,y)$ rejects.

NP is a generalization of P (just forget about the witness string y), so P $\subseteq$ NP. It is widely conjectured that P $\neq$ NP, but we do not have a proof!

Bounded-error Probabalistic Polynomial Time (BPP):
Languages L such that there exists a deterministic poly-time Turing machine M and polynomial q such that for all $x \in \{0,1\}^n$

- If $x \in L$, then $M(x,y)$ accepts for at least $2/3$ of the strings $y \in \{0,1\}^{q(n)}$.
- If $x \notin L$, then $M(x,y)$ accepts for at most $1/3$ of the strings $y \in \{0,1\}^{q(n)}$.

That is, y is a random string given to the Turing machine. Once again, it is clear that $\mathsf{P} \subseteq \mathsf{BPP}$ since we can just forget about the extra random bits. However, we do not know if $\mathsf{BPP} \subseteq \mathsf{NP}$ or if $\mathsf{NP} \subseteq \mathsf{BPP}$, though it is widely conjectured that $\mathsf{P} = \mathsf{BPP}$.

Probabilistic Polynomial Time (PP):
Languages L such that there exists a deterministic poly-time Turing machine M and polynomial q such that for all $x \in \{0,1\}^n$

- If $x \in L$, then $M(x,y)$ accepts for more than $1/2$ of strings $y \in \{0,1\}^{q(n)}$.
- If $x \notin L$, then $M(x,y)$ accepts at most $1/2$ of strings $y \in \{0,1\}^{q(n)}$.

Notice that the definition PP to identical to that of BPP except with a smaller gap between acceptance and rejection probabilities. Therefore, we have that $\mathsf{BPP} \subseteq \mathsf{PP}$. In fact, PP is powerful enough even to contain NP. To see this, take any NP machine M, and alter it in the following way. If $M(x,y)$ accepts, then accept. If $M(x,y)$ rejects, then flip an unbiased coin (to be completely rigorous, one would need to extend the length of the random string y)—if heads, accept, and if tails, reject. Notice that if there are no accepting y for the original machine, then the new machine accepts with exactly 50% probability. However, if there is any accepting y, then the new machine accepts with greater than 50%, and so the inclusion $\mathsf{NP} \subseteq \mathsf{PP}$ follows.

Polynomial Space (PSPACE):
Languages L such that there exists a deterministic Turing machine M that uses at most polynomial space and M accepts x iff $x \in L$.

We have that $\mathsf{PP} \subseteq \mathsf{PSPACE}$ since a PSPACE machine can simply count all the $y \in \{0,1\}^{q(n)}$ that make a poly-time Turing machine accept. There are exponentially many such y, but this is not an issue since we can erase the previous computation as we are enumerating over all the y.

Exponential Time (EXP):
Languages L such that there exists a deterministic Turing machine M and a polynomial q such M halts in $2^{q(n)}$ time and M accepts x iff $x \in L$.

We have that $\mathsf{PSPACE} \subseteq \mathsf{EXP}$ because a Turing machine that uses polynomial space can only have exponentially many configurations. And, if you were to reach the same configuration twice, then you will be in an infinite loop, so you might as well halt.

Figure A.1 shows a summary of how the complexity classes introduced above relate to each other.

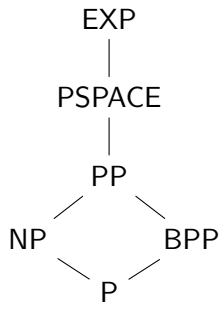

Figure A.1: Inclusion diagram of classical complexity classes. A is below B if $A \subseteq B$.