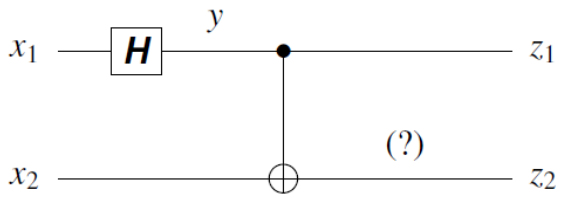
CSE491/596 Lecture Wed. 12/08/21: Large But Feasible Operators, and Measurements

Picking up with the example of a CNOT gate and the basic entangling circuit:



If $x_1 = |0\rangle$, then we can tell exactly what y is: it is the $|+\rangle$ state. And if $x_1 = |1\rangle$, then $y = |-\rangle$. If x_1 is any other qubit state $(a, b) = a|0\rangle + b|1\rangle$, then by linearity we know that $y = a|+\rangle + b|-\rangle$. This expresses y over the transformed basis; in the standard basis it is

$$y = \frac{1}{\sqrt{2}}(a(1,1) + b(1,-1)) = \frac{1}{\sqrt{2}}(a+b, a-b) \ .$$

So we can say exactly what the input coming in to the first "wire" of the CNOT gate is. And the input to the second wire is just whatever x_2 is. But because that gate does entanglement, we cannot specify individual values for the wires coming *out*. The state is an inseparable 2-qubit state:

$$\frac{1}{\sqrt{2}}\big(|00\rangle + |11\rangle\big).$$

This is not the same as the equal +1 superposition of all baskc outcomes for two qubits:

$$|{+}{+}\rangle = \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2}$$

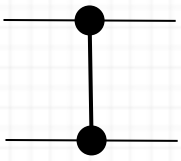
If you measure either qubit individually, you get 0 or 1 with equal probability. This is the same as if you measured the state $|{+}{+}\rangle$. But that state is outwardly as well as inwardly different. When *both* qubits to be measured, it allows 01 and 10 as possible outcomes, whereas measuring the entangled state does not. I've seen papers telling ways to visualize entangled states of 2 or 3 qubits, but none implemented by an applet so far---`quantum-circuit.com` just shows Bloch spheres with the black dot at the center for the "completely mixed state": | ¯_(ツ)_/¯ ⟩.

Call the whole thing U. Then $U = CNOT \cdot (H \otimes I)$. On an arbitrary 4-vector $[a, b, c, d]$ we get $[a, b, c, d]^T = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle = ae_{00} + be_{01} + ce_{10} + de_{11}$

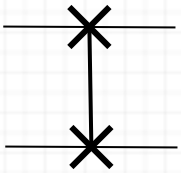
$U[a, b, c, d]^T = aU|00\rangle + bU|01\rangle + cU|10\rangle + dU|11\rangle = aUe_{00} + bUe_{01} + cUe_{10} + dUe_{11}$

Two other 2-qubit gates and their matrix and circuit representations are:

$$\mathbf{CZ} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$



$$\mathbf{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



The $\mathbf{CZ}$ gate is symmetric: note that its results on $|01\rangle$ and on $|10\rangle$ are the same. So are the $\mathbf{CS}$ and $\mathbf{CT}$ gates, which have i and $\omega = e^{i\pi/4} = \sqrt{i}$ in place of the -1. For a general $r \times r$ matrix A, $\mathbf{C}A$ is the $2r \times 2r$ matrix given in block form as $\begin{bmatrix} I & 0 \\ 0 & A \end{bmatrix}$. The circuit convention is to put a black dot on the **control** qubit line and a vertical line extending to A in a box the **target** line(s). Most applets make you do that with $\mathbf{CZ}$ as well as $\mathbf{CS}$ and $\mathbf{CT}$, but it is good to remember that these three (and further ones with roots of ω at bottom right) are symmetric.

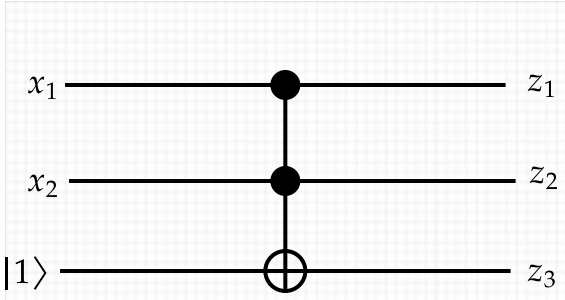
$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \quad T = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{i} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & e^{\pi i/4} \end{bmatrix} \quad \mathbf{CS} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}$$

$$T_{\pi/8} = \begin{bmatrix} 1 & 0 \\ 0 & e^{\pi i/8} \end{bmatrix} \qquad \mathbf{S} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \mathbf{S}^2 = \mathbf{Z} \quad \mathbf{T} = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{i} \end{bmatrix}.$$

Three Qubits and More

The **CNOT** gate by itself has the logical description $z_1 = x_1$ and $z_2 = x_1 \oplus x_2$. This means that if $x_1 = 0$ then $z_2 = x_2$, but if $x_1 = 1$ then $z_2 = \neg x_2$. Since this description is complete for all of the standard basis inputs $x = x_1x_2 = 00, 01, 10, 11$, it extends by linearity to all quantum states. We can use this idea to specify the 3-qubit **Toffoli gate** (**Tof**). It has inputs x_1, x_2, x_3 and symbolic outputs z_1, z_2, z_3 (which, however, might not have individual values in non-basis cases owing to entanglement). Its spec in the basis quantum coordinates is:

$$z_1 = x_1,\ z_2 = x_2, z_3 = x_3 \oplus (x_1 \wedge x_2).$$



	000	001	010	011	100	101	110	111
000	1	0	0	0	0	0	0	0
001	0	1	0	0	0	0	0	0
010	0	0	1	0	0	0	0	0
011	0	0	0	1	0	0	0	0
100	0	0	0	0	1	0	0	0
101	0	0	0	0	0	1	0	0
110	0	0	0	0	0	0	0	1
111	0	0	0	0	0	0	1	0

Of particular note is that if x_3 is fixed to be a constant-1 input, then

$$z_3 \;=\; \neg(x_1 \wedge x_2) \;=\; NAND(x_1, x_2).$$

Thus the Toffoli gate subsumes a classical NAND gate, except that you need an extra "helper wire" to put $x_3 \;=\; 1$ and you gate two extra output wires z_1, z_2 that only compute the identity on x_1, x_2 (in classical logic, that is---the Toffoli effect of switching the 7th and 8th vector components can have knock-on effects). If you have polynomially many Toffoli gates, then you get only polynomial wastage of wires, and you can use the good ones to simulate any polynomial-size Boolean circuit of NAND gates. The m helper wires are like extra tape cells used by a polynomialt-time Turing machine. They are called *ancilla* qubits, from a Latin word meaning (female) "helper."

Because DTIME[$t(n)$] has Boolean circuits of size $\widetilde{O}(t(n))$, and because Toffoli gates are deterministic, we can state an immediate consequence:

Theorem: For fully time-constructible $t(n)$ between linear and exponential,

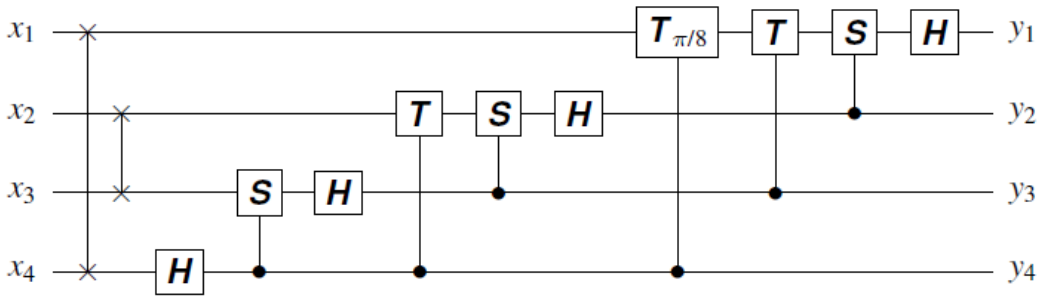
$$\text{DTIME}[t(n)] \;\subseteq\; \text{DQ}\Big[\widetilde{O}(t(n))\Big].$$

In particular, P $\subseteq$ DQP $\subseteq$ BQP, where BQP is to DQP as BPP is to P. (We define BQP formally after saying more about measurements.)

We first need to say more broadly what it means for quantum computations to be (polynomially) **feasible**. The community convention is simply to count up gates of 1, 2, or 3 qubits as constant cost. Gates involving more qubits are OK if they can be built up out of the small gates:

- We have already seen that $H^{\otimes n}$ is just n binary Hadamard gates laid out in parallel.
- The n-qubit **quantum Fourier transform** (QFT) can be built up out of $O\big(n^2\big)$ smaller gates---examples for $n \;=\; 3$ or 4 are a presentation option.

There is one thing that needs to be said about the QFT. The usual recursive way to build it via $O\big(n^2\big)$ unary and binary gates uses controlled rotations by exponentially tiny angles. This is already evident from the four-qubit illustration in the textbook (where the two gates on the left are :



Here $T_{\pi/8} = \begin{bmatrix} 1 & 0 \\ 0 & \omega' \end{bmatrix}$ with $\omega' = e^{i\pi/8}$ not $\omega = e^{i\pi/4}$ as with the T-gate. So ω' has a phase angle one-sixteenth of a circle. For $n = 5$ the next bank uses $1/32$, then $1/64$, and soon the angles would be physically impossible so the gates could never be engineered. Those super-tiny angles are in the definition of the QFT itself. For any n, it takes $\omega_n = e^{2\pi i/N}$ where $N = 2^n$. With $n = 3$, the matrix together with its quantum coordinates is:

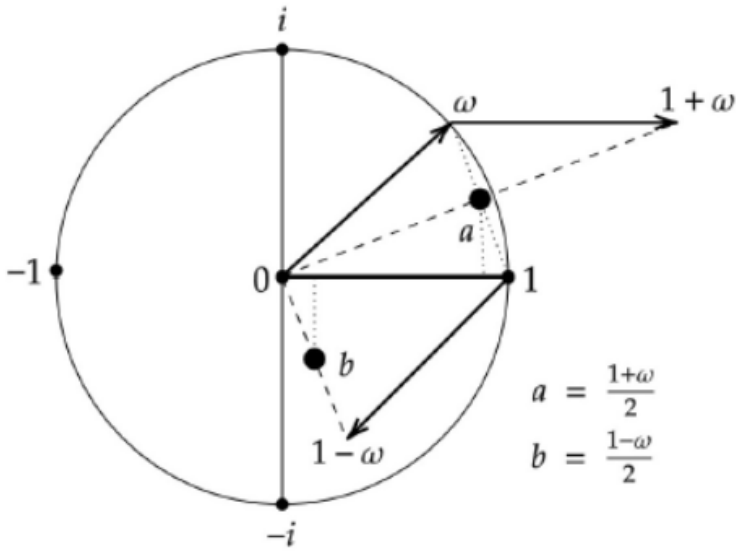
	000	001	010	011	100	101	110	111
000	1	1	1	1	1	1	1	1
001	1	ω	i	$i\omega$	-1	$-\omega$	$-i$	$-i\omega$
010	1	i	-1	$-i$	1	i	-1	$-i$
011	1	$i\omega$	$-i$	ω	-1	$-i\omega$	i	$-\omega$
100	1	-1	1	-1	1	-1	1	-1
101	1	$-\omega$	i	$-i\omega$	-1	ω	$-i$	$i\omega$
110	1	$-i$	-1	i	1	$-i$	-1	i
111	1	$-i\omega$	$-i$	$-\omega$	-1	$i\omega$	i	ω

$\mathbf{QFT}[i, j] = \omega^{ij}$

$=$

	0	1	2	3	4	5	6	7
0	1	1	1	1	1	1	1	1
1	1	ω	ω^2	ω^3	-1	ω^5	ω^6	ω^7
2	1	ω^2	ω^4	ω^6	1	ω^2	ω^4	ω^6
3	1	ω^3	ω^6	ω	-1	ω^7	ω^2	ω^5
4	1	-1	1	-1	1	-1	1	-1
5	1	ω^5	ω^2	ω^7	-1	ω	ω^6	ω^3
6	1	ω^6	ω^4	ω^2	1	ω^6	ω^4	ω^2
7	1	ω^7	ω^6	ω^5	-1	ω^3	ω^2	ω

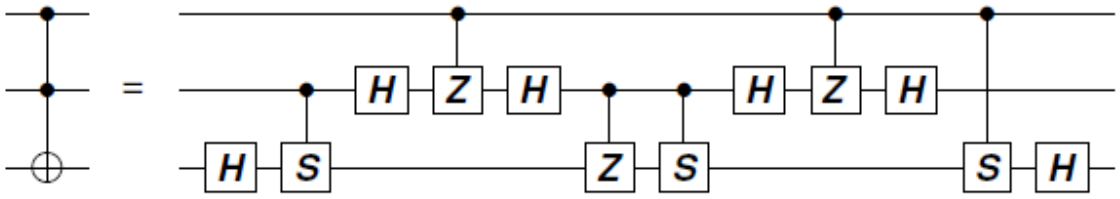
For $\mathbf{QFT}_N$ we raise ω_N with its tiny phase to exponentially many different powers. How can this possibly be feasible? Leonid Levin among others raised this objection. Here are several answers:



- Basic gates can fabricate quantum states having finer phases. This is already hinted by the diagram in the case of $\mathbf{HTH}$. Try composing $\mathbf{HTHT^*H}$ and $\mathbf{HTHT^*HTHT^*H}$. The *Solovay-Kitaev theorem* enables approximating operators with exponentially fine angles by polynomially many gates of phases that are multiples of ω (using **CNOT** to extend this to multiple-qubit operators).
- The Toffoli and Hadamard gates by themselves, which have phases only $+1$ and -1, can simulate the real parts and imaginary parts of quantum computations separately via binary code, in a way that allows re-creating all measurement probabilities. (This is undertaken in exercises

7.8--7.14 with a preview in the solved exercise 3.8.)

- The **CNOT** and Hadamard gates do not suffice for this, even when the so-called "phase gate" $\mathbf{S} = \mathbf{T}^2 = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$ is added. The Pauli $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ gates and also $\mathbf{CZ}$ can be built from these, but quantum circuits of these gates can be simulated in deterministic ("classical") polynomial time. However, $\mathbf{CS}$ suffices to build the Toffoli gate, per the diagram below (which is also a presentation option). So Hadamard + $\mathbf{CS}$ is a universal set using only quarter phases.
- The signature application of the QFT, which is *Shor's algorithm* showing that factoring belongs to BQP, may only require coarsed-grained approximations to $\mathbf{QFT}_N$.



For these reasons, $\mathbf{QFT}_N$ is considered feasible even though $N = 2^n$ is exponential. Not every $N \times N$ unitary matrix U is feasible---the Solovay-Kitaev theorem relies on U having a small exact formulation to begin with. But if we fix a finite **universal gate set** (such as $\mathbf{H + T + CNOT}$, $\mathbf{H + Tof}$, or $\mathbf{H + CS}$ above) and use only matrices that are compositions and tensor products of these gates, then we can use the simple gate-counting metric as the main complexity measure.

Outputs and Measurements

There are various conventions about what it means for a family $[C_n]$ of quantum circuits to compute a function f on $\{0,1\}^*$, where f is an ensemble of functions f_n on $\{0,1\}^n$ and each C_n computes f_n. I like supposing that $f(x)$ is coded in $\{0,1\}^r$ where r depends only on n and giving C_n r-many output qubits separate from the n input qubits, plus some number m of ancilla qubits. (It is traditional, IMHO weirdly, to consider that the primordial input is always $\mathbf{0}^n$ and that for any other x, **NOT** gates are prepended onto the circuit for those lines i where $x_i = 1$.)

For *languages*, this means that the yes/no verdict comes on qubit $n+1$. Many references say to measure line 1 instead. (Using a swap gate between lines 1 and $n+1$ can show these conventions to be equivalent, but I prefer reserving lines 1 to n for *potential* use of the "copy-uncompute" trick, which is covered in section 6.3 and is a presentation option.) Even for languages, however, one evidently cannot get the most power if you need always to rig the circuit so that on any input $x \in \{0,1\}^n$, the output line always has a (standard-)basis value, i.e., is $\mathbf{0}$ with certainty or is $\mathbf{1}$ with certainty. Instead, one must **measure** it, whereupon the value $\mathbf{0}$ is given with some probability p, $\mathbf{1}$ with probability $1 - p$.

The math of measurements (at least of the kind of *pure states* we get in completely-specified circuits) is simple. At the end we have a quantum state Ψ of $n + r + m$ qubits, counting the output and any ancilla

lines. It "is" a vector $(v_1, v_2, \ldots v_Q) \in \mathbb{C}^Q$ where $Q = 2^{n+r+m}$. Numbering $\{0,1\}^{n+r+m}$ in canonical order as $z_1, \ldots, z_S$, an **all-qubits measurement** gives any z_j with probability $|v_j|^2$. If we focus on just the r output lines, then any $y \in \{0,1\}^r$ occurs with probability

$$\sum_{j:\, z_j \text{ agrees with } y \text{ on the } r \text{ output lines}} |v_j|^2.$$

When $r = 1$ and $y = 0$ the sum is over all binary strings z_j that have a 0 in the corresponding places. It is a postulate of quantum mechanics that we could do the measurement in such a way that the new state Ψ' stays "coherent" on qubit lines outside the r lines that were measured, but we will not care about this---we will be OK doing an all-qubits measurement (which "collapses" the system down to $|z_j\rangle$ for whatever basis state z_j is yielded) and then re-starting the whole circuit to do multiple trials, if necessary. What can make them necessary is the simple "unamplified" definition of BQP along lines of the definition given for BPP. To simplify the notartion, let p_x denote the probability of measuring 1 on the output qubit line. The notion of uniformity is similar to that for ordinary Boolean circuits: it means that C_n can be written down in $n^{O(1)}$ (classical) time.

Definition: A language L belongs to BQP if there is a uniform family $[C_n]$ of polynomial-sized quantum circuits such that for all n and inputs $x \in \{0,1\}^n$,

$$\begin{aligned} x \in L &\implies p_x \geq 3/4; \\ x \notin L &\implies p_x \leq 1/4. \end{aligned}$$

With the help of ideas grouped under the term "**principle of deferred measurement**", the idea of amplifying the difference in probabilities by repeated trials and majority vote of the outcomes can be internalized within the circuits. This needs polynomially more ancilla qubits but allows doing only one measurement, which will then be guaranteed to give the correct answer with probability supremely close to 1 rather than probability $3/4$. However, it is (IMHO) more helpful to think instead of quantum circuits as objects that can be ***sampled***, and that a final classical post-processing routine gives the final answer as a function of the results of the samples. This is how Simon's algorithm, Shor's algorithm, and (general forms of) Grover's algorithm are usually conceived. The same approach of assembling a value $g(x)$ from multiple sample results can likewise be used for defining how functions g are computed.

With that said, the idea of computing a function $f(x) = y$ with y represented literally within a quantum (basis) state is often applied a different way. Given a circuit C computing y on lines $n+1, \ldots, n+r$ that way---and using "copy-uncompute" to restore x on lines $1, \ldots, n$---make C' by prepending $\mathbf{H}^{\otimes n}$ on the first n lines. Give $C'|0^n\rangle$ as the actual input. The resulting state is

$$s_f = \sum_{x \in \{0,1\}^n} |x\rangle|f(x)\rangle.$$

Although each individual term $|x\rangle|f(x)\rangle$ is separable---indeed, it is the basis state $\mathbf{e_x} \otimes \mathbf{e_y} = \mathbf{e_{xy}}$ where $y = f(x)$---the sum is usually majorly entangled. Our text calls this the **functional superposition** of f over the domain $\{0,1\}^n$. In **Shor's algorithm** for a product $M = pq$ of two primes, first a seed $a < M$ is chosen randomly from the $\rho = (p-1)(q-1)$ numbers that are not multiples of p or q. Then $f(x)$ is the function $a^x \bmod M$, where x is redundantly allowed to go as high as $Q-1$ with Q being a power of 2 between M^2 and $2M^2$. That makes enough room for the periodicity of the powering mod M to make enough waves for the QFT to do what Joseph Fourier knew it would 198 years ago: it transforms the waves' period, which divides ρ, into a peak. Repeated runs and measurements eventually give enough information about ρ to infer p and q.

Thus Shor's algorithm invokes *both* the "input x, output $f(x)$" view of what a quantum circuit does and the randomized sampling view. The latter is the external algorithm, and its input is not "x" but rather C, which in turn comes from the factoring problem instance M and the random seed a. In lieu of covering the full details in chapters 11 and 12, we can state:

Shor's Theorem: FACTORING is in BQP.

At present, I accept that s_f is feasible to build and the QFT is feasible to apply---at least with sufficient approximation for Shor's algorithm to work. However, I am chary of the account given under the Many Worlds Hypothesis. As told by David Deutsch and others, each Hadamard gate branches into two universes. If the n Hadamards stayed separate to make n pairs that might be reasonable, but building s_f seems to entail piggy-backing them to make 2^n universes, all harnessed together by the QFT.

Reckoning and Visualizing Circuits and Measurements

There are basically three ways to "reckon" a quantum circuit computation:

1. Multiply the $Q \times Q$ matrices together---using *sparse-matrix techniques* as far as possible. If BQP $\neq$ P and you try this on a problem in the difference then the sparse-matrix techniques must blow up at some (early) point. The downside is that the exponential blowup is paid early; the upside is that once you pay it, the matrix multiplications don't get any worse, no matter how more complex the gates become. This is often called a "Schrödinger-style" simulation.
2. Any product of s-many $Q \times Q$ matrices can be written as a single big sum of s-fold products. For instance, if A, B, C, D are four such matrices and u is a length-Q vector, then
$$ABCDu[i] = \sum_{j,k,l,m=1}^{Q} A[i,j] \cdot B[j,k] \cdot C[k,l] \cdot D[l,m] \cdot u[m] \ .$$
Every (*nonzero*) product of this form can be called a (*legal*) **path** through the system. [As hinted before, in a quantum circuit, u will be at left---on an input x, it will be the basis vector $\mathbf{e_{x0^{r+m}}} = |x0^{r+m}\rangle$ under the convention that 0s are used to initialize the output and ancilla lines---and D will be the first matrix from gate(s) in the circuit as you read left-to-right. Thus the

output will come out of A, which is why it is best to visualize the path as coming in from the top of the column vector u, going out at some row m (where u_m is nonzero---for a standard basis vector, there is only one such m), then coming in at column m of D, choosing some row l to exit (where the entry $D[l, m]$ is nonzero), then coming in at column l of C, and so on until exiting at the designated row i of A. This is the discrete form of Richard Feynman's **sum-over-paths** formalism which he originally used to represent integrals over quantum fields (often with respect to infinite-dimensional Hilbert spaces). The upside is that each individual path has size $O(s)$ which is linear not exponential in the circuit size. The downside is that the number of nonzero terms in the sum can be far worse than Q and doubles each time a Hadamard gate (or other nondeterministic gate) is added to the circuit.

3. Find a way to formulate the matrix product so that the answer comes out of symbolic linear algebra---if possible!