

Quantum Algorithms

Computer scientists usually find conventional expositions of quantum computation difficult, since a lot of new concepts have to be learned together to make sense of it all. In this course, we take a different approach, starting from a point where every computer science student is comfortable, and introducing the new concepts one by one into the familiar framework. We hope it will be much easier this way. So let's start with deterministic finite automata!

Chapter 1

Finite automata

1.1 Deterministic model

You already know the stuff in Sipser's book. Note that the transitions of a DFA can be represented as 0-1 matrices, the states can be traced with vectors, and the execution on an input string boils down to multiplying this vector with the corresponding sequence of those matrices.

1.2 Probabilistic model

We define real-time¹ probabilistic finite automata (rtPFAs) by generalizing the matrix definition of rtDFAs to column stochastic transition matrices. Consider a transition graph representation for a moment. It is as if computation flows through many arrows (associated with the same input symbol) parallelly in each step. Under this "zero-error" regime (exact computation) rtPFAs are identical to rtDFAs: Since none of these computational paths can arrive at an incorrect response at the end, tracing any single path is sufficient for seeing what the machine will do. So we convert each rtPFA matrix (which have to contain at least one nonzero entry in each column) to a rtDFA matrix with a 1 in just the position corresponding to the topmost nonzero entry of the rtPFA in that column. The resulting machine is guaranteed to recognize the same language, with the same number of states!

¹A real-time machine is one that consumes its input string from left to right at a rate of one symbol per move, and its runtime is therefore $n+2$, if we allow for endmarker symbols delimiting the input.

A machine M recognizes a language with bounded error if there exists a number $\varepsilon < 1/2$ such that M is guaranteed to give the correct response to any input string with probability at least $1 - \varepsilon$. If you know to build such a machine M_1 for a language for some error bound ε , you can build another machine M_2 for the same language with far smaller error by just letting the M_2 simulate the execution of M_1 on the input string several times, and report the majority response given by these simulations. If the machines under consideration are real-time, this would have to be a parallel simulation. This is a good place to recall the tensor product, which allows one to view several parallel systems as a single combined system. For any positive numbers m and n , and any two matrices A (which is $m \times n$) and B , the tensor product $A \otimes B$ is the matrix

$$\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ \vdots & \ddots & \vdots \\ a_{m,1} & \cdots & a_{m,n} \end{pmatrix} \otimes B = \begin{pmatrix} a_{1,1}B & \cdots & a_{1,n}B \\ \vdots & \ddots & \vdots \\ a_{m,1}B & \cdots & a_{m,n}B \end{pmatrix}.$$

So when running two PFA's with n and m states parallelly, the state vector of the combined machine would be

$$\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ \vdots \\ a_1 b_m \\ a_2 b_1 \\ \vdots \\ a_n b_m \end{pmatrix},$$

and the transition matrices of the resulting machine for each input symbol would be obtained by taking the tensor product of the constituent machines' transition matrices for that symbol. The parallel simulation of multiple copies of a machine for reducing the error can be performed by constructing such a combined machine, whose initial state is the state that corresponds to the collection of start states of the original machines, and whose accept states are those that correspond to collections containing a majority of accept states.

1.3 Quantum model

Quantum physics turns out to allow a more general kind of transformation than the ones seen until now. Here are the new features: Computation

can fork” in two different ways in this new setup. One way is probabilistic branching, with which we are familiar from probabilistic computations. The new way is quantum branching, in which the branches are allowed to interact, merging or even canceling each other out in a novel manner, as we will see. Transition matrices for a rtQFA represent these alternatives as follows: For a k -state machine that can branch at most m ways probabilistically in any single step, we have m $k \times k$ matrices (stack these on each other to obtain an $mk \times k$ rectangle) for each input symbol. The matrices are allowed to contain real numbers in the interval $[-1,1]$ in each entry. The wellformedness condition is that each column in these rectangles should have norm (i.e. the square root of the sum of the squares of the numbers in it) 1, and every pair of different columns should be orthogonal to each other (the sum of the products of the entries in the corresponding rows should be 0). The first step of a rtQFA on its input amounts to multiplying each of the m matrices separately with the initial state vector (containing a 1 for the start state and 0 for the rest) and writing the vectors that are the results of these multiplications as the children of the initial vector in a computation tree. Every subsequent input symbol is handled similarly, adding more generations to this tree, which is completed with the reading of the last input symbol. The probability of acceptance is calculated by squaring each entry corresponding to an accepting state in the last generation and adding these squares up.

The branches of this computation tree correspond to classical probabilistic branching. The square of the norm of a vector, say, v , in, say, the i th level of the tree is the probability $P(v)$ that that node is reached. Ignore all nodes containing all-zero vectors, computation simply does not branch there. Normalize all vectors like v in other nodes (by dividing each entry with the norm of that vector) to obtain v_N . The machine will be in the pure state (i.e. the state vector) described by v_N with probability $P(v)$ after executing the i th step. The overall “mixture” of states at a particular level will be best described by something called a density matrix, to be defined soon. First, let us formalize things a bit:

Definition 1. *A real-time quantum finite automaton (rt-QFA) is a 5-tuple $\{Q, \Sigma, q, \{\mathcal{E}_\sigma\}_{\sigma \in \Sigma}, F\}$ where*

- Q is a finite set of classical states
- Σ is a finite input alphabet
- $q \in Q$ is the initial state

- $F \subset Q$ is the set of accepting states
- $\{\mathcal{E}_\sigma\}_{\sigma \in \Sigma}$ is a finite collection of $|Q|m \times |Q|$ -dimensional matrices, each of which are composed of m $|Q| \times |Q|$ -dimensional matrices (operation elements) $\{E_i | 1 \leq i \leq m\}$ for m a positive integer.

If our knowledge of the current superposition of a quantum system is certain, then the system is said to be in a *pure state*. Sometimes, (e.g. during classical probabilistic computation) we only know that the system is in pure state $|\psi_i\rangle$ with probability p_i for $i > 1$, and with the probabilities adding up to 1. In this case, the system is said to be in a *mixed state*.

When $m=1$, the conditions on the transition matrices, to be discussed soon, turn out to require that they be unitary, and the machine gets weaker, unable to recognize some regular languages.

All observations on quantum systems in our discussion will be done by **projective measurements**. In the case of the rtQFA, this process is particularly simple, since all we wish is to see whether we have ended up in an accept state or not. We just specify a matrix

$$P_a = \sum_{q \in F} |q\rangle\langle q|,$$

where F is the set of accept states, and for any column vector $|v\rangle$, $\langle v|$ denotes the conjugate transpose of $|v\rangle$.

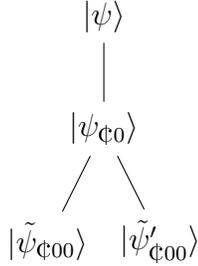
Consider the following quantum finite automaton with states $\{q_1, q_2, q_3\}$ where q_1 is the initial state, input alphabet $\{0\}$, $m=2$. For the only element of the input alphabet, the quantum operator \mathcal{E}_0 consists of matrices

$$E_{0,1} = \begin{matrix} & \begin{matrix} q_1 & q_2 & q_3 \end{matrix} \\ \begin{matrix} q_1 \\ q_2 \\ q_3 \end{matrix} & \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \end{matrix} \quad E_{0,2} = \begin{matrix} & \begin{matrix} q_1 & q_2 & q_3 \end{matrix} \\ \begin{matrix} q_1 \\ q_2 \\ q_3 \end{matrix} & \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{matrix}.$$

Assume that the machine just performs the identity transformation on the left input end-marker \clubsuit . Because q_1 is the initial state, ket vector $|\psi_\clubsuit\rangle = |q_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ represents the initial superposition.

After reading the first 0, the machine reaches new superposition $|\psi_{\clubsuit 0}\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$ without a probabilistic branching.

After reading the second 0, the machine reaches superposition $|\tilde{\psi}_{\phi 00}\rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ in one probabilistic branch, and also reaches superposition $|\tilde{\psi}'_{\phi 00}\rangle = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$ in another probabilistic branch. The machine is in a mixed state which is the ensemble of pure states $|\tilde{\psi}_{\phi 00}\rangle$ and $|\tilde{\psi}'_{\phi 00}\rangle$.



From this point on, $|\tilde{\psi}_{\phi 00}\rangle$ and $|\tilde{\psi}'_{\phi 00}\rangle$ should be considered as separate probabilistic branches and evolution of the machine should be traced by applying the quantum operator to each probabilistic branches separately.

For a long input string, the number of probabilistic branches makes it impossible to trace a simple finite automaton by hand. For this reason, we introduce *density matrix* notation in which an n by n density matrix is enough to keep the state information of machine for any number of probabilistic and quantum branches.

Definition 2. The *density matrix* representation of $\{(p_i, |\psi_i\rangle) \mid 1 < i \leq M < \infty\}$ is

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (1.1)$$

Given a real-time quantum machine having a set of quantum operators $\{\mathcal{E}_{\sigma \in \Sigma}\}$ where each \mathcal{E}_{σ} is an operator having elements $E_{\sigma,i}$ for each i up to m , the computation can be traced by density matrices for any given input string w . In the equation below, ρ_j denotes the system state after reading the j 'th symbol of input w , that is, w_j .

$$\rho_j = \mathcal{E}_{w_j}(\rho_{j-1}) = \sum_i E_{w_j,i} \rho_{j-1} E_{w_j,i}^\dagger, \quad (1.2)$$

where $\rho_0 = |q_1\rangle\langle q_1|$ is the initial density matrix. The transition operators can be extended easily for any string as

$$\mathcal{E}_{w\sigma} = \mathcal{E}_w \circ \mathcal{E}_\sigma, \quad (1.3)$$

where $\sigma \in \Sigma$, $w \in \Sigma^*$, and $\mathcal{E}_\varepsilon = I$. Note that, if $\mathcal{E} = \{E_i | 1 \leq i \leq k\}$ and $\mathcal{E}' = \{E'_j | 1 \leq j \leq k'\}$, then

$$\mathcal{E}' \circ \mathcal{E} = \{E'_j E_i | 1 \leq i \leq k, 1 \leq j \leq k'\}. \quad (1.4)$$

For the example above, the density matrix representing the machine's state before starting the input is $\rho_\Phi = \sum_{i=1}^1 |\psi\rangle\langle\psi| = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1 \ 0 \ 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$.

Reading the first 0 can be simulated as follows:

$$\begin{aligned} \rho_{\Phi 0} = \mathcal{E}(\rho_\Phi) &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \end{pmatrix} + \\ &\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

After reading two 0's, machine is in the state $|\psi_{\Phi 00}\rangle = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$ with probability $p_1 = \frac{3}{4}$ and it is in the state $|\psi'_{\Phi 00}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ with probability $p_2 = \frac{1}{4}$. Notice that vectors $|\tilde{\psi}_{\Phi 00}\rangle$ and $|\tilde{\psi}'_{\Phi 00}\rangle$ are normalized to obtain $|\psi_{\Phi 00}\rangle$ and $|\psi'_{\Phi 00}\rangle$ so that $\sum_i p_i = 1$. Therefore, density matrix after reading two 0's is

$$\rho_{\Phi 00} = \frac{3}{4} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{2}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}.$$

As a direct result of their definition, being the sum of normalized square matrices reveals three important properties of density matrices:

- Numbers on the diagonal of a density matrix are always real numbers.
- i^{th} diagonal entry $d_{i,i}$ of a density matrix D is equal to the probability of being in state q_i .
- Sum of the diagonal elements (i.e. the trace) of a density matrix is 1.

	c_1	c_2	\dots	$c_{ C }$
c_1	E_1			
c_2				
\vdots				
$c_{ C }$				
c_1	E_2			
c_2				
\vdots				
$c_{ C }$				
c_1	E_3			
c_2				
\vdots				
$c_{ C }$				

\mathcal{E} is represented above by a $|C|m \times |C|$ -dimensional matrix, where $C = \{c_1, c_2, \dots, c_{|Q|}\}$, by concatenating each E_i one under the other. The well-formedness rule dictated by physics is that \mathcal{E} is a superoperator, i.e. that

$$\sum_i E_i^\dagger E_i = I.$$

It can be verified that the above condition is satisfied if and only if the columns of \mathcal{E} form an orthonormal set. Let c_{j_1} and c_{j_2} be two configurations with corresponding columns v_{j_1} and v_{j_2} . For an orthonormal set to be formed, we must have

$$v_{j_1}^\dagger v_{j_2} = \begin{cases} 1 & \text{if } j_1 = j_2, \\ 0 & \text{if } j_1 \neq j_2 \end{cases}$$

for all such pairs.

We can ensure that all such configuration transition matrices are well-formed by preparing the program's matrices $\mathcal{E}_{\sigma \in \tilde{\Sigma}}$ such that their columns are orthonormal.

1.4 Quantum Machines Can Simulate Classical Machines

We prove this result for real-time machines, but the same approach is valid for all higher models.

Theorem 1. *Given a rt-PFA $P = (Q_P, \Sigma, \delta_P, q_{0P}, F_P)$, there exists a corresponding rt-QFA $Q = (Q_P, \Sigma, \mathcal{E}_{\sigma \in \Sigma}, q_{0P}, F_P)$ such that*

$$\begin{aligned} p_Q^{acc}(w) &= p_P^{acc}(w) \\ p_Q^{rej}(w) &= p_P^{rej}(w) \end{aligned}$$

for any given w .

Proof. For machine P , we have transition matrices $P_\sigma = \{p_{j,k} | j, k \in Q_P\}$ describing the transition probabilities among each pair of states of the machine, upon seeing the symbol $\sigma \in \Sigma$. We construct our \mathcal{E}_σ operators having elements $E_{\sigma,(n)}$ for every state q_n such that, for a particular input $\sigma \in \Sigma$;

$$E_{\sigma,(n)}_{i,n} = \sqrt{P_{\sigma i,n}}$$

for all i , and all other positions are 0. □

Do not worry about this not looking like a generalization of PFAs, it is. Given a rtPFA P with k states, build the rtQFA Q corresponding to it by setting m to equal k , using a separate square matrix (with zeros everywhere except in the j 'th column) in Q for the j 'th column of the corresponding matrix of P . That location will contain the square roots of the entries in P 's j 'th column.

1.5 QFA on a problem with one-sided error

Here is an example of a superiority of quantum over classical: Consider the following language that is defined on the alphabet $\Sigma = \{a, b\}$:

$$L = \{\mathbf{w} | \text{the number of } a\text{'s is not equal to the number of } b\text{'s in the input string } \mathbf{w}\}$$

We want to build a machine with one-sided error. It will say "YES" to the members of the language with a non-zero probability, "NO" to the non-members of the language with a $p = 1$.

From our earlier knowledge, we know that complement of a language that can be recognized by a DFA, can also be recognized by some DFA (just swap the accept and reject states). For our convenience let us handle with the task of recognizing:

$$\bar{L} = \{\mathbf{w} | \text{the number of } a\text{'s is equal to the number of } b\text{'s in the input string } \mathbf{w}\}$$

We know that this is not a regular language. Therefore there is no DFA that can recognize it. We also know that this is also the case for a PFA since PFA with one-sided error is equivalent to DFA. (Since every member string has a sequence of nonzero-probability transitions from the start state to an accept state, whereas no nonmember string has such sequences, the machine can just be seen as an NFA.) So let's try to build a QFA.

Our 5-tuple is: $Q = \{q_1, q_2\}$, $\Sigma = \{a, b\}$, q_1 (the initial state), $F = \{q_2\}$ (set of accept states), $\{E_a, E_b\}$ (operators), where E_a is defined as follows:

$$E_a = \begin{bmatrix} 3/5 & -4/5 \\ 4/5 & 3/5 \end{bmatrix}$$

When we have an input string a , our new state will be $E_a|q_1\rangle = \frac{3}{5}|q_1\rangle + \frac{4}{5}|q_2\rangle$. In this case, probability that we are on state q_1 and q_2 are respectively $\frac{9}{25}$, $\frac{16}{25}$. q_2 is our accept state. Our machine will say "yes" to the to the input string a with a non-zero probability. So far it is fine. Our only consideration is that when we give the machine the string ab , it should say "no" with a probability 1.

We have not yet defined a transition matrix for the symbol b . Before constructing this matrix, let's focus on transition matrix for the symbol a . Columns of this matrix should be orthonormal to each other. This is rather a special matrix, a rotation matrix. We can parameterize it as follows:

$$E_a = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

where θ is the angle we rotate our vector in counter-clockwise direction. So every time we see an input symbol a , our state vector rotates by θ angle in the unit circle. When it takes an input symbol b , it should undo this rotation. This can be easily done by defining the same transition matrix but with $-\theta$. If we also select this θ to be an irrational multiple of π , then the machine gives "no" answer with a probability of 1 if and only if the number of a 's are equal to the number of b 's in the input string \mathbf{w} .

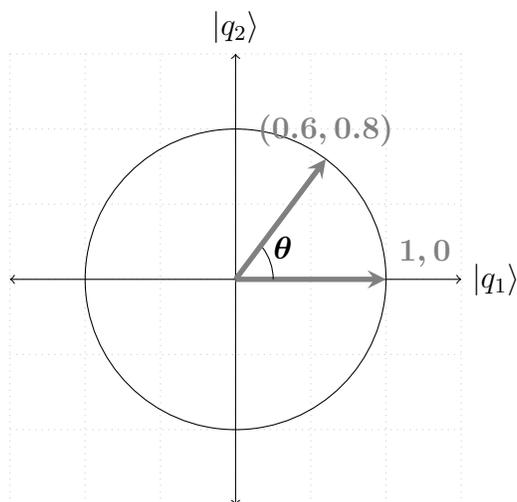


Figure 1.1: Change of vector $|q_1\rangle$ when it is multiplied by a rotation matrix

Why do we need θ to be an irrational multiple of π ? If θ is not an irrational multiple of π , then there is a rational number k such that $k\theta = \pi$. So if our machine will get such an input

$$\underbrace{aa \dots a}_{2k}$$

the initial state will be rotated by $2k\theta = 2\pi$. We can also see that $E_a(0) = E_a(2\pi)$. So our machine will say no with a probability of 1 although the input string is not in our defined language.

We should also prove that for our specific choice of θ , there are no integers a, b such that $\frac{\theta}{2\pi} = \frac{a}{b}$. Let us assume that there are such integers a and b . We know that,

$$\cos \theta + i \sin \theta = e^{i\theta}$$

and $i\theta b = ia2\pi$. Then $e^{i\theta b} = 1$.

$$\left(\frac{3}{5} + \frac{4}{5}i\right)^b = 1$$

$$(3 + 4i)^b = 5^b$$

Modulus operation is extended to complex numbers as follows:

$$(x + yi \equiv q + wi \pmod{n}) \triangleq (q \equiv x \pmod{n}) \text{ and } (w \equiv y \pmod{n})$$

If two complex numbers are equal, then we also have $c_1 = c_2 \pmod n$ for any n . We will use this to show that no such b exists that satisfy $(3 + 4i)^b = 5^b$. However,

$$\begin{aligned}(3 + 4i)(3 + 4i) &= -7 + 24i \\ -7 + 24i &\equiv 3 + 4i \pmod 5 \\ (3 + 4i)^b &= 3 + 4i \pmod 5\end{aligned}$$

Therefore,

$$(3 + 4i)^b \not\equiv 5^b \pmod 5$$

So θ is not an irrational multiple of π .

We should note that in order to implement this in real life, one would need to have the ability to carry out the rotation by θ precisely, without even the slightest deviation from that real number, which is not a realistic expectation. Furthermore, the error probability, although less than 0.5, can be arbitrarily close to 0.5, which makes us practically unable to decide on the status of the input when we receive a negative answer, and tensoring multiple copies of the machine would not help, since we can not say that a fixed number of copies guarantees a particular bound (less than 0.5) on the error.

1.6 A Characterization of Regular Languages

Definition 3. Let x and y be strings, and let L be any language. We say that x and y are **distinguishable by L** if some string z exists, whereby exactly one of the strings xz and yz is a member of L . Otherwise, for every string z , we have $xz \in L$ whenever $yz \in L$, and we say that x and y are **indistinguishable by L** . If x and y are indistinguishable by L , we write $x \equiv_L y$.

Proposition 1. \equiv_L is an equivalence relation on the set of all strings.

Definition 4. Let X be a set of strings. X is **pairwise distinguishable by L** if every two distinct strings in X are distinguishable by L .

Definition 5. The **index of L** is the maximum number of elements in any set that is pairwise distinguishable by L .

Proposition 2. If a language L is recognizable by a DFA with k states, it has index at most k .

Proof. Let M be a k -state DFA that recognizes L . Suppose for a contradiction that L has index greater than k . That means some set X with more than k elements is pairwise distinguishable by L . Because M has k states, the pigeonhole principle implies that X contains two distinct strings x and y , where $\delta(q_o, x) = \delta(q_o, y)$. Here $\delta(q_o, x)$ is the state that M is in after starting in the start state q_o and reading input string x . Then, for any string $z \in \Sigma^*$, $\delta(q_o, xz) = \delta(q_o, yz)$. Therefore either both xz and yz are in L or neither are in L . But then x and y aren't distinguishable by L , contradicting our assumption that X is pairwise distinguishable by L . \square

Proposition 3. *If the index of a language L is a finite number k , it is recognized by a DFA with k states.*

Proof. Let $X = \{s_1, \dots, s_k\}$ be pairwise distinguishable by L . We construct DFA $M = (Q, \Sigma, \delta, q_o, F)$ with k states recognizing L . Let $Q = \{q_1, \dots, q_k\}$ and define $\delta(q_i, a)$ to be q_j , where $s_j \equiv_L s_i a$. Note that $s_j \equiv_L s_i a$ for some $s_j \in X$; otherwise, $X \cup s_i a$ would have $k + 1$ elements and would be pairwise distinguishable by L , which would contradict the assumption that L has index k . Let $F = \{q_i | s_i \in L\}$. Let the start state q_o be the q_i such that $s_i \equiv_L \varepsilon$, where ε is the empty string. M is constructed so that, for any state q_i , $\{s | \delta(q_o, s) = q_i\} = \{s | s \equiv_L s_i\}$. Hence M recognizes L . \square

Theorem 2. Myhill-Nerode Theorem *A language L is regular iff it has finite index. Moreover, its index is the size of the smallest DFA recognizing it.*

Proof. (\Rightarrow) Suppose that L is regular and let k be the number of states in a DFA recognizing L . Then by Proposition 2 L has index at most k .

(\Leftarrow) Conversely, if L has index k , then by Proposition 3 it is recognized by a DFA with k states and thus is regular.

To show that the index of L is the size of the smallest DFA accepting it, suppose that L 's index is exactly k . Then, by Proposition 3, there is a k -state DFA accepting L . That is the smallest such DFA because if it were any smaller, then it would follow from Proposition 2 that the index of L is less than k . \square

1.7 Caveat

Zero-error computation as described here² is a fictional concept, because of precision issues. See pages 194-195 of Nielsen and Chuang’s book for the argument that imperfect implementations of operators can approximate the behavior of perfect ones. “Approximate” is the key word here; which means that an actual implementation will involve a slight change in observation (accept/reject) probabilities, thereby destroying “exactness”, and firmly reminding us that very long computations require very precise implementation of amplitudes to even sustain a nonzero error bound.

1.8 Tensor products

A machine M recognizes a language with bounded error if there exists a number $\varepsilon < 1/2$ such that M is guaranteed to give the correct response to any input string with probability at least $1 - \varepsilon$. If you know to build such a machine M_1 for a language for some error bound ε , you can build another machine M_2 for the same language with far smaller error by just letting the M_2 simulate the execution of M_1 on the input string several times, and report the majority response given by these simulations. If the machines under consideration are real-time, this would have to be a parallel simulation. This is a good place to recall the tensor product, which allows one to view several parallel systems as a single combined system. For any positive numbers m and n , and any two matrices A (which is $m \times n$) and B , the tensor product $A \otimes B$ is the matrix

$$\begin{pmatrix} a_{1,1} & \cdots & a_{1,n} \\ \vdots & \ddots & \vdots \\ a_{m,1} & \cdots & a_{m,n} \end{pmatrix} \otimes B = \begin{pmatrix} a_{1,1}B & \cdots & a_{1,n}B \\ \vdots & \ddots & \vdots \\ a_{m,1}B & \cdots & a_{m,n}B \end{pmatrix}.$$

So when running two QFA’s (or PFA’s) with n and m states parallelly,

²The reader should note that this warning also applies to computation with unbounded error or one-sided error.

the state vector of the combined machine would be

$$\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ \vdots \\ a_1 b_m \\ a_2 b_1 \\ \vdots \\ a_n b_m \end{pmatrix},$$

and the transition matrices of the resulting machine would be obtained by taking the tensor products of the operation elements. The parallel simulation of multiple copies of a machine for reducing the error can be performed by constructing such a combined machine, whose initial state is the state that corresponds to the collection of start states of the original machines, and whose accept states are those that correspond to collections containing a majority of accept states.

1.9 Bounded-error QFAs can only recognize regular languages

Let us now show that no nonregular language has a bounded-error rtQFA recognizing it. We will need to talk about “distances” between quantum states, classical distributions, and the relations among these distances.

Define the distance between two quantum states A and B as

$$D(A, B) = \|A - B\|_{tr},$$

where $\|M\|_{tr} = \text{Tr}(\sqrt{MM^\dagger})$. The distance $D(p, q)$ between two classical probability distributions p and q is just the sum of the absolute values of the differences of the probabilities of all the corresponding events in p and q . $D(A, B)$ is known to be an upper bound for the distance among the observation probability distributions from quantum states A and B .

Theorem 3. *The languages recognized by rt-QFA with bounded error are exactly the regular languages.*

Proof. It’s clear that *rt-QFA* can recognize regular languages by simulating DFA. Now we will show that they can’t recognize any other language in

bounded error setting.

Suppose a nonregular language L is recognized by rt - QFA $M = \{Q, \Sigma, q, \{\mathcal{E}_\sigma\}_{\sigma \in \Sigma}, F\}$ with bounded error ϵ . Define an equivalence relation " \equiv_L " on $x, y \in \Sigma^*$ such that $x \equiv_L y$ if for any $z \in \Sigma^*$, $xz \in L$ if and only if $yz \in L$. Then, by Myhill-Nerode theorem, it is sufficient to prove that number of equivalence classes are finite.

Now let $S = \{A \mid \|A\|_{tr} \leq 1, \text{ and } A \text{ is a linear operator on the vector space spanned by vectors corresponding to states in } Q\}$. Then S is a bounded subset from a finite-dimensional space. Let $\rho_x = \mathcal{E}_{x_n} \mathcal{E}_{x_{n-1}} \dots \mathcal{E}_{x_1}(\rho_0)$, then for every input string x , it can be seen that $\rho_x \in S$, because we have $\|\rho_x\|_{tr} = Tr(\rho_x) = 1$.

Suppose $x \not\equiv_L y$, that is there exists a $z \in \Sigma^*$ such that $xz \in L$ and $yz \notin L$. Then we have

$$Tr(P_{acc}\mathcal{E}_z(\rho_x)) \geq 1 - \epsilon \text{ and } Tr(P_{acc}\mathcal{E}_z(\rho_y)) \leq \epsilon.$$

Therefore, we have

$$\begin{aligned} \|\mathcal{E}_z(\rho_x) - \mathcal{E}_z(\rho_y)\|_{tr} &\geq |Tr(P_{acc}\mathcal{E}_z(\rho_x)) - Tr(P_{acc}\mathcal{E}_z(\rho_y))| + \\ &\quad |Tr(P_{rej}\mathcal{E}_z(\rho_x)) - Tr(P_{rej}\mathcal{E}_z(\rho_y))| \\ &\geq 1 - 2\epsilon. \end{aligned}$$

we also have $\|\rho_x - \rho_y\|_{tr} \geq \|\mathcal{E}_z(\rho_x) - \mathcal{E}_z(\rho_y)\|_{tr}$ from the fact that applying the same operator on two different operators doesn't increase the distance between them. By combining these two formulas, we get

$$\|\rho_x - \rho_y\|_{tr} \geq 1 - 2\epsilon$$

This formula says that there should be at least $1 - 2\epsilon$ difference between each ρ_x and ρ_y satisfying $x \not\equiv_L y$ and from the Myhill-Nerode theorem, we know there should be infinite number of such x and y 's so that they construct infinite number of equivalence classes for L to be nonregular. Call the representatives of these classes x_1, x_2, \dots . Since S is bounded in a finite-dimensional space, one can extract a Cauchy sequence (a convergent subsequence) from this sequence to find an x and a y such that $x \not\equiv_L y$ and yet $\|\rho_x - \rho_y\|_{tr} \leq 1 - 2\epsilon$. This leads to a contradiction. Therefore, there is no such nonregular language L recognized by rt - QFA in bounded error setting. \square

1.10 Two Way Deterministic Finite Automata

We will distinguish between the **real-time**, **one-way**, and **two-way** modes of tape head movement. A tape with real-time access is scanned by its head in a single sweep from the left end to the right end with a new symbol scanned at every computational step. One-way access is more general, in the sense that pausing the head on the same square for some steps in the single left-to-right scan is also allowed. Finally, the head can move to the left, as well as to the right, in the case of two-way access.

Definition 6. A two-way deterministic finite automaton **2DFA** is a quintuple $M = (Q, \Sigma, \delta, q_0, F_a, F_r)$ where Q , Σ and q_0 are defined as in the case of the usual real-time DFA, F_a and F_r are the sets of accept and reject states, with the remaining states designated to be non-halting as in the case of TMs, and δ is a map from $Q \times \Sigma$ to $Q \times \{L, R\}$. If $\delta(q, a) = (p, L)$ then in state q , scanning input symbol a , the 2DFA enters state p and moves its input tape head one square to the left. If $\delta(q, a) = (p, R)$, the 2DFA enters state p and moves its head one square to the right.

We assume throughout the course that the input string is written on a read-only tape, sandwiched between a left end-marker symbol and a right end-marker symbol, which are not members of the input alphabet. Earlier definitions of 2DFAs involved no end-markers, and the machine was said to accept when the input head fell off the right end of the input. Our convention, with acceptance based on states, is equivalent to this from a language recognition power point of view, though not from the point of view of state economy. (It is important in our convention to assume that the head never visits the squares beyond the end-markers.)

- Let $L_m = \{a^k \mid k \equiv 0 \pmod{m}\}$ where $m > 1$. The smallest DFA recognizing L_m has m states. A 2DFA with much fewer than $2 \times 3 \times 5 \times 7 \times 11 \times 13 \times 17 \times 19$ states exists for the language $L_{(2 \times 3 \times 5 \times 7 \times 11 \times 13 \times 17 \times 19)}$: In the first pass, while going from the left to the right, the 2DFA checks whether the string is in L_2 . In the second pass, while going from the right to the left, 2DFA checks whether the string is in L_3 , and continuing this way, it is able to determine whether the string is in L_m in 8 passes.

1.11 The Reduction of 2DFA to 1DFA

Theorem 4. *2DFA can recognize only regular languages.*

Proof. Let M be a 2DFA with set of states S recognizing language L . For every string $w \in \Sigma^*$, define a function $\tau_w : \{\bar{s}_0\} \cup S \rightarrow \{0\} \cup S$. For $s \in S$, $\tau_w(s)$ describes the ultimate result of the motion of M when started in state s on the rightmost symbol of w , i.e. if with these initial conditions M ultimately leaves w from the right in the state s' then $\tau_w(s) = s'$, on the other hand if M never leaves w , or leaves w from the left, then $\tau_w(s) = 0$. $\tau_w(\bar{s}_0)$ describes the result of the motion when M is started in the initial state s_0 on the leftmost symbol of w . Now it is easy to see that if $\tau_{w_1} = \tau_{w_2}$ then $w_1 \equiv_L w_2$. But if n is the number of states of M there are at most $(n+1)^{(n+1)}$ distinct τ_w . Then by the Myhill-Nerode Theorem, we conclude that L is regular, since L has finite index. \square

Construction of 1DFA from 2DFA: Let M be a 2DFA recognizing language L . We create a 1DFA M' recognizing the same language L as follows:

- As the state set of M' we take different functions τ_w which arise for $w \in \Sigma^*$.
- We define the initial state of M' to be τ_ε so that $\tau_\varepsilon(\bar{s}_0) = s_0$ and $\tau_\varepsilon(s) = 0$ for all $s \in S$.
- In order to learn the function τ_w for some $w \in \Sigma^*$, we start the machine from each state on the rightmost symbol of w . For each new function τ_w , we add a new state to the state set of M' . We can detect infinite loops since there are finite number of configurations (i.e. state/head-position pairs). If the machine does not move off w , either accepting or rejecting it in less than $|w| \times (n+2)$ units of time, then some configuration is repeated, and the machine has entered an infinite loop, which means that w will not be accepted.
- Use the method of Proposition 3 to construct the transition function.
- We define the accept states of M' by simulating the 2DFA with a member string from each equivalence class of the relation associated with L . If the string is accepted, the state representing the class becomes an accept state of M' .

1.12 2pfa's

2-way PFA's can recognize some nonregular languages with bounded error. See <http://www.dmtcs.org/dmtcs-ojs/index.php/dmtcs/article/view/1457/3371>, (Section 6) for an example.

It is, however, known that 2PFA's cannot recognize nonregular languages in polynomial expected time:

THEOREM: For any polynomial p , 2pfa's with expected runtime $O(p(n))$ recognize only the regular languages with bounded error.

Proof. One starts by defining a quantitative measure of the nonregularity of a language $L \subseteq \Sigma^*$. For a positive integer n , two strings $w, w' \in \Sigma^*$ are n -dissimilar, written $w \approx_{L,n} w'$, if $|w| \leq n$, $|w'| \leq n$, and there exists a *distinguishing string* $v \in \Sigma^*$ with $|wv| \leq n$, $|w'v| \leq n$, and $wv \in L$ iff $w'v \notin L$. Let $N_L(n)$ be the maximum k such that there exist k distinct strings that are pairwise $\approx_{L,n}$. It can be shown that

FACT (*): If L is not regular, then $N_L(n) \geq \frac{n}{2} + 1$ for infinitely many n .

In the rest of the proof, one develops a technique for constructing a Markov chain $P_{A,xy}$ with $2c$ states that models the computation of a given 2pfa A with c states on the concatenated string xy , where x and y are given strings. State 1 of the Markov chain corresponds to A being at the beginning of its computation on the last symbol of $\$x$. (Note that every 2pfa can be modified to start here, without changing the recognized language. The non-halting states of the modified 2pfa are $\{q_1, q_2, \dots, q_{c-1}\}$.) For $1 \leq j \leq c-1$, state j of the Markov chain corresponds to A being in the configuration with the machine in state q_j and the head on the last symbol of $\$x$, and state $c+j-1$ corresponds to A being in the configuration with the machine in state q_j and the head on the first symbol of $y\$$. State $2c-1$ corresponds to a disjunction of rejection, infinite loop with the head never leaving the region $\$x$, and infinite loop within the region $y\$$. State $2c$ corresponds to acceptance. The probability that $P_{A,xy}$ is absorbed in state $2c$ when started in state 1 equals the probability that A accepts xy .

The proof then considers any 2pfa M that recognizes language L in expected time $T(n)$, and proceeds to establish a lower bound, in terms of $N_L(n)$, on $T(n)$. This is accomplished by showing that, for sufficiently large values of n , if the desired lower bound does not exist, then there must be two pairwise $\approx_{L,n}$ strings w and w' , with distinguishing string v , such that the Markov chains $P_{M,wv}$ and $P_{M,w'v}$ are "too close" according to a notion of closeness

defined in It is proven that, if $P_{M,wv}$ and $P_{M,w'v}$ are so close, and if it is guaranteed that both Markov chains are absorbed to state $2c - 1$ or $2c$ with total probability 1 within expected time $T(n)$, then the acceptance probabilities of wv and $w'v$ must be so close that they must both be members (or non-members) of L , contradicting their n -dissimilarity, thereby establishing the desired bound on $T(n)$. The Theorem statement is then obtained by combining this result with Fact (*).

□

1.13 2qfa's (in fact, even a 2pfa plus just one qubit) can recognize some nonregular language with bounded error in polynomial time

Here is how such a machine can recognize a nonregular language with bounded error in polynomial expected time:

After an easy deterministic check on the input w , this 2qfa enters an infinite loop where each iteration compares the number of a's (i) with the number of b's (j). This is achieved by first rotating the qubit counterclockwise for exactly as many times as there are a's, then rotating it clockwise for the b's, and finally checking whether it has returned to its original orientation $|q_0\rangle$. Since the rotation angle is an irrational multiple of π , the probability r_i that the machine will reject at the line marked (I) in Figure 1.2 is zero if and only if there are exactly as many a's as there are b's. Otherwise, r_i will be at least (see the paper "Two-way finite automata with quantum and classical states, where the proof claims a slightly stronger result)

$$\frac{1}{2(i-j)^2 + 1} > \frac{1}{2(i+j)^2}.$$

We therefore conclude that any input string w with unequal numbers of a's and b's which has survived the deterministic check in the beginning will be rejected with a probability greater than $\frac{1}{2|w|^2}$ in each iteration of the infinite loop.

If the input w has not been rejected after the rotation procedure described above, the 2qcfa makes two consecutive random walks starting on the first

Check if the input is of the form a^+b^+ , otherwise REJECT.
 LOOP:
 Move the head right to the next a .
 Set the qubit to $|q_0\rangle$.
 While the currently scanned symbol is a :
 Rotate the qubit with angle $\sqrt{2}\pi$.
 Move the head to the right.
 While the currently scanned symbol is b :
 Rotate the qubit with angle $-\sqrt{2}\pi$.
 Move the head to the right.
 Measure the qubit. If the result is q_1 , REJECT. (I)
 (The currently scanned symbol is the right end-marker.)
 Repeat twice:
 Move the tape head to the first input symbol.
 While the currently scanned symbol is not an end-marker, do the following:
 Simulate a classical coin flip. If the result is heads, move right. Otherwise, move left.
 If the process ended at the right end-marker both times, and k more coin flips all turn out heads, goto EXIT.
 Move the head to the left end-marker, and goto LOOP.
 EXIT:
 ACCEPT the input.

Figure 1.2: A 2qfa

input symbol, and ending at an end-marker. The probability that both these walks will end at the right end-marker, and the subsequent coin tosses all yield heads, leading to acceptance in this iteration of the infinite loop, is $\frac{1}{2^k(|w|+1)^2}$, and the expected runtime for this stage is $O(|w|^2)$. This means that the machine will halt within $O(|w|^2)$ expected iterations of the loop, leading to an overall expected runtime of $O(|w|^4)$.

To conclude, the 2qcfa of Figure 1.2 will accept any string in $\{a^n b^n : n \geq 1\}$ with probability 1. On the other hand, any w not in this language that makes it into the loop has a rejection probability that is much larger than its acceptance probability in each iteration, and therefore will be rejected with great probability, where one can pull the error as near to zero as one wants by tuning the parameter k .

1.14 The Hadamard and Toffoli gates

Until now, whenever we constructed some well-formed superoperator for our finite automata, let's say on 10 states, we just assumed that some kind person

in the quantum physics lab would implement it physically, working out all the angles, polarizations and whatnot. This is not fair, as it assumes that this job is equally easy for all matrices. A better approach is to allow ourselves to use only a fixed number of “elementary” operators, or “gates”, and let the burden of specifying how all the quantum transformations will be realized in terms of these gates fall on the programmer (i.e. us). (It is similar to what’s going on with Boolean circuits and the “universal” sets of gates like $\{AND, NOT\}$.) A set of quantum gates is said to be universal if any quantum transformation on any number of qubits can be approximated by the application of a particular sequence of these gates on selected qubits.³ Among many others, the set consisting of the Toffoli and Hadamard gates is known to be universal:

The Hadamard operation works on a single quantum bit, with the 2X2 transition

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix},$$

and the Toffoli operation works on three qubits, with transition

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

(so when you perform it on three bits with values x , y and z , it transforms them to x , y , and $(z \text{ XOR } (x \text{ AND } y))$). (I’m assuming that you are familiar with tensor products. If you have a system of four qubits, and you apply Hadamard to the first one, and Toffoli to the second, third and fourth ones in that order, say, just take the tensor product of these two matrices to see what the overall transformation on the whole system looks like.)

(Toffoli alone is known to be universal for classical computation, so if you need to implement a classical subroutine on a quantum computer, for

³The classical algorithm described in <http://arxiv.org/pdf/quant-ph/0505030v2.pdf> can be used to compile a quantum program using arbitrary single-qubit operations to one approximating it using only operators from a fixed set efficiently.

instance, to run it on all possible inputs simultaneously using quantum parallelism you can do it.) Toffoli, Hadamard and CNOT (which work on two qubits) gates are self-inverse, and can appear in quantum circuits to represent quantum algorithms. We are assuming that the error correction issues, which we routinely ignore in classical computation, are solved and the matrices are implemented perfectly.

1.15 The no-cloning theorem and BB84

The no-cloning theorem forbids a universal copying program. Proof is by contradiction: Assume that there is a unitary transformation C which takes two registers and sets the second register to a perfect copy of the state of the first register, while leaving the first register intact, i.e.

$$C(|\psi\rangle \otimes |s\rangle) = |\psi\rangle \otimes |\psi\rangle$$

But then one has

$$\begin{aligned} C((\alpha|0\rangle + \beta|1\rangle) \otimes |s\rangle) &= (\alpha|0\rangle + \beta|1\rangle) \otimes (\alpha|0\rangle + \beta|1\rangle) \\ &= \alpha^2|00\rangle + \alpha\beta|01\rangle + \alpha\beta|10\rangle + \beta^2|11\rangle \end{aligned}$$

However, we also have

$$\begin{aligned} C((\alpha|0\rangle + \beta|1\rangle) \otimes |s\rangle) &= C(\alpha|0\rangle \otimes |s\rangle) + C(\beta|1\rangle \otimes |s\rangle) \\ &= (\alpha|0\rangle \otimes \alpha|0\rangle) + (\beta|1\rangle \otimes \beta|1\rangle) = \alpha^2|00\rangle + \beta^2|11\rangle \end{aligned}$$

So such a copier cannot exist if you are copying superpositions. (It is OK but trivial if α or β is zero.)

Using this theorem, the BB84 quantum key distribution protocol enables Alice and Bob to remotely decide on a one-time pad and be sure that no eavesdropping occurred while they were doing it.

1.16 Superdense coding

Note that on a two qubit register, $H(1)$ followed by $CNOT(1,2)$ performs a transform from the computational basis to the Bell basis, i.e., from $|00\rangle$ to $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$, from $|01\rangle$ to $\frac{|01\rangle+|10\rangle}{\sqrt{2}}$, from $|10\rangle$ to $\frac{|00\rangle-|11\rangle}{\sqrt{2}}$, and from $|11\rangle$ to $\frac{|01\rangle-|10\rangle}{\sqrt{2}}$. Since both H and $CNOT$ are self inverse, a measurement in the Bell basis is equivalent to a $CNOT(1,2)$, followed by a $H(1)$, followed by a measurement in the computational basis.

A single Hadamard does a similar thing for a one-qubit register. Bell states are entangled and Einstein did not like this.

The NOT (X) operation works on a single quantum bit, with the 2X2 transition

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and the Z operation works on a single quantum bit, with the 2X2 transition

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In the superdense coding protocol, Alice and Bob share a Bell pair in state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$. Alice then performs an operation (based on which two-bit string she wants to send) on her qubit:

If she wants to send 00, she does nothing, and the two-qubit system is in state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$.

If she wants to send 01, she performs a NOT gate, and the two-qubit system is in state $\frac{|01\rangle+|10\rangle}{\sqrt{2}}$.

If she wants to send 10, she performs a Z gate, and the two-qubit system is in state $\frac{|00\rangle-|11\rangle}{\sqrt{2}}$.

If she wants to send 11, she performs a Z gate followed by an X gate, (note that the matrix is XZ, which is

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}),$$

and the two-qubit system is in state $\frac{|10\rangle-|01\rangle}{\sqrt{2}}$.

Alice then sends her qubit to Bob, who measures the system in the Bell basis as described above. He sees the intended message with probability 1 in each case.

1.17 Teleportation

Alice has a qubit (lets call it qubit 1) in state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. She also shares a Bell pair in state $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ with Bob. (Lets call those qubits 2 and 3, Alice has 2, Bob has 3.) Alice then performs the operations CNOT(1,2) and H(1), and measures qubits 1 and 2.

Let us follow the 3-qubit system state. At the beginning:

$$\frac{1}{\sqrt{2}}(\alpha|0\rangle \otimes (|00\rangle + |11\rangle) + \beta|1\rangle \otimes (|00\rangle + |11\rangle))$$

After CNOT(1,2):

$$\frac{1}{\sqrt{2}}(\alpha|0\rangle \otimes (|00\rangle + |11\rangle) + \beta|1\rangle \otimes (|10\rangle + |01\rangle))$$

After H(1):

$$\begin{aligned} & \frac{1}{2}(\alpha(|0\rangle + |1\rangle) \otimes (|00\rangle + |11\rangle) + \beta(|0\rangle - |1\rangle) \otimes (|10\rangle + |01\rangle)) \\ &= \frac{1}{2}(\alpha|000\rangle + \alpha|011\rangle + \alpha|100\rangle + \alpha|111\rangle + \beta|010\rangle + \beta|001\rangle - \beta|110\rangle - \beta|101\rangle) \\ &= \frac{1}{2}(|00\rangle \otimes (\alpha|0\rangle + \beta|1\rangle) + |01\rangle \otimes (\alpha|1\rangle + \beta|0\rangle)) + |10\rangle \otimes (\alpha|0\rangle - \beta|1\rangle) + \\ & |11\rangle \otimes (\alpha|1\rangle - \beta|0\rangle) \end{aligned}$$

So Alice observes each two-bit string equiprobably, meaning that the physical system that is qubit 1 is now at a completely random state. Where has its previous state information gone?

Alice sends her measurement result to Bob.

If Bob receives 00, he does nothing.

If Bob receives 01, he does X(3).

If Bob receives 10, he does Z(3).

If Bob receives 11, he does X(3) followed by Z(3), i.e. he applies ZX to his qubit.

In all cases, qubit 3 ends up in the state $\alpha|0\rangle + \beta|1\rangle$!

1.18 The Deutsch-Jozsa Algorithm

The Deutsch-Jozsa algorithm is a simple example of running a classical subroutine on a quantum computer on all possible inputs parallelly.

But what about matrices with imaginary entries? No worries. Complex numbers can be represented by 2X2 matrices of reals. It is easy to simulate the complex numbers with use of real numbers by replacing every complex number $a + bi$ with the real valued 2×2 matrix

$$\begin{pmatrix} a & b \\ -b & a \end{pmatrix}$$

in all our transition matrices. Our machines could have been defined with complex amplitudes all along, with the necessary generalizations of the well-formedness conditions.

The two most famous quantum algorithms are Grover's and Shor's algorithms. They can be described in terms of QTMs, or in other equivalent formalisms.

1.19 Grover's Search Algorithm

Determining whether a given boolean formula is satisfiable or not is an NP-Complete problem. The corresponding language recognition problem refers to the language below:

$$SAT = \{f \mid f \text{ is a satisfiable boolean formula} \}$$

The best known classical algorithm for solving SAT runs in $poly(n)2^n$ time where n denotes the number of boolean variables occurring in the input formula. Grover's algorithm to be introduced below runs in $poly(n)2^{n/2}$ time and hence it provides a quadratic speedup over the best known classical algorithm for a related task.

Theorem 5. *There is a quantum algorithm that given any polynomial time computable function $f : \{0, 1\}^n \rightarrow \{0, 1\}$ (i.e., represented as a circuit computing f) as input, where $f(a) = 1$ for just one input string a , returns a in $poly(n)2^{n/2}$ time.*

Proof. Before giving the details of the algorithm we will be defining two vectors.

- $u = \frac{1}{2^{n/2}} \sum_{w \in \{0,1\}^n} |w\rangle$ represents the equal superposition of the vectors for all strings of length n
- $e = \sum_{w \in \{0,1\}^n, w \neq a} |w\rangle$ represents the sum of vectors for all strings of length n which are mapped to 0 by the function f .

Note that $|a\rangle$ and e are orthogonal. The two-dimensional space spanned by $|a\rangle$ and e will be useful in visualization of the working of the algorithm.

The algorithm runs on a quantum register of $n + 1 + m$ qubits where the last m bits are the auxiliary bits used in the quantum implementation of the circuit part for computing f , and since f is polynomially computable, m is not large. Therefore the algorithm will be described on the first $n + 1$ bits initially prepared in the state $|0^{n+1}\rangle$. In the following x will be used to denote the state of the first n qubits and σ will be used to denote the state of the $(n + 1)$ st qubit. See Algorithm 1 for the details of Grover's search.

Step 2.2.2 can be achieved by a one-qubit operation which leaves the $n+1$ 'st bit unchanged if it is initially 0, and multiplies it by -1 if it is 1.

Algorithm 1 Grover's Search Algorithm

Runs on $n + 1$ qubit register initially prepared to $|0^n0\rangle$.

- **Initialization:** Apply Hadamard transformation on the first n qubits.
 - **Loop:** Repeat $Round(\frac{\arccos(\frac{1}{2^{n/2}})}{2\arcsin(\frac{1}{2^{n/2}})})$ times:
 - Step 1: Reflect the vector in the first n qubits around $e = \sum_{w \in \{0,1\}^n, w \neq a} |w\rangle$:
 - 1.1: On qubit $n+1$, run an X and an H gate, yielding the state $\frac{|0\rangle - |1\rangle}{\sqrt{2}}$
 - 1.2: On the first $n+1$ qubits, compute $|x\sigma\rangle \rightarrow |x(\sigma \oplus f(x))\rangle$ (this has the effect of multiplying $|x\rangle$ by -1 iff $f(x) = 1$)
 - 1.3: On qubit $n+1$, run an H and an X gate, setting it back to $|0\rangle$
 - Step 2: Reflect the vector in the first n qubits around $u = \frac{1}{2^{n/2}} \sum_{w \in \{0,1\}^n} |w\rangle$:
 - 2.1: Apply Hadamard transformation on the first n qubits.
 - 2.2: Reflect around $|0^n\rangle$:
 - 2.2.1: If the first n qubits are not all zero, flip the $n+1$ st qubit
 - 2.2.2: If $\sigma = 1$ then multiply $|x\rangle$ by -1
 - 2.2.3: If the first n qubits are not all zero, flip the $n+1$ st qubit
 - 2.3: Apply Hadamard transformation on the first n qubits.
 - **Measurement:** Measure x and compute $f(x)$. If the result is 1, return x . Otherwise repeat the algorithm.
-

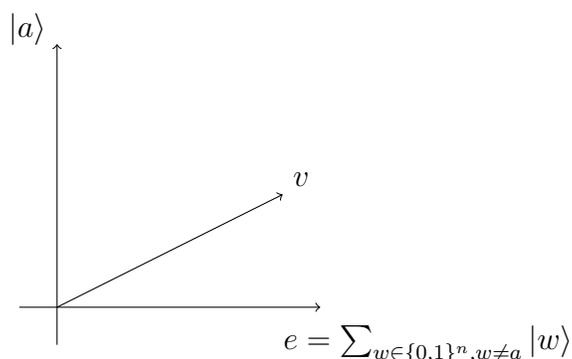


Figure 1.3: Two dimensional space spanned by $|a\rangle$ and e .

Rotation around a vector $|\psi\rangle$ can be obtained by multiplication with the matrix $(2|\psi\rangle\langle\psi| - I)$. Note that Step 2 is based on the fact that $H(2|0\rangle\langle 0| - I)H = 2|u\rangle\langle u| - I$, where the letters indicate the n -fold tensored versions of the single-bit gates with those names.

In the following parts we will be showing how Grover's algorithm operates on the state vectors and how it comes up with a satisfying assignment. We will visualize the change in the state vectors represented in the two dimensional space spanned by $|a\rangle$ and e . In doing so we will use

- $\mathbf{x}_{i,0}$ to denote the state of the first n bits at the beginning of the i 'th iteration of the algorithm,
- $\mathbf{x}_{i,1}$ to denote the state of the first n bits at i 'th iteration after step 1 and
- $\mathbf{x}_{i,2}$ to denote the state of the first n bits at i 'th iteration after step 2.

Let's see how x evolves during the execution of the algorithm. At the beginning the first n bits are initialized to the equal superposition of all strings of length n by Hadamard transformation. Therefore we have $x_{1,0} = u$.

Then comes the first iteration of the loop where the states $x_{1,1}$ and $x_{1,2}$ are computed as shown in Figure 1.5.

Figure 1.5 suggests that first iteration of the Grover loop which moves the state x of the first n bits from $x_{1,0}$ to $x_{1,2}$ cuts the angular distance between a and x by 2θ . Figure 1.6 will show that further iterations of the loop will

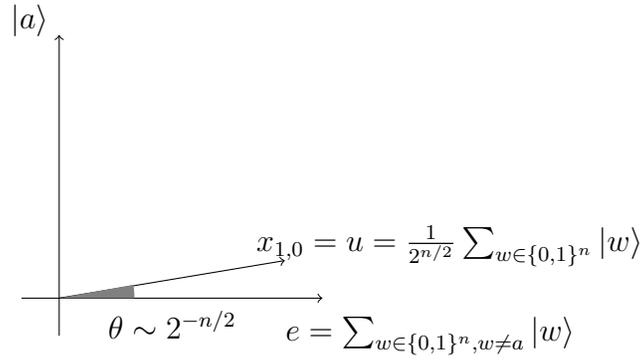


Figure 1.4: x is initialized to equal superposition of all strings of length n .

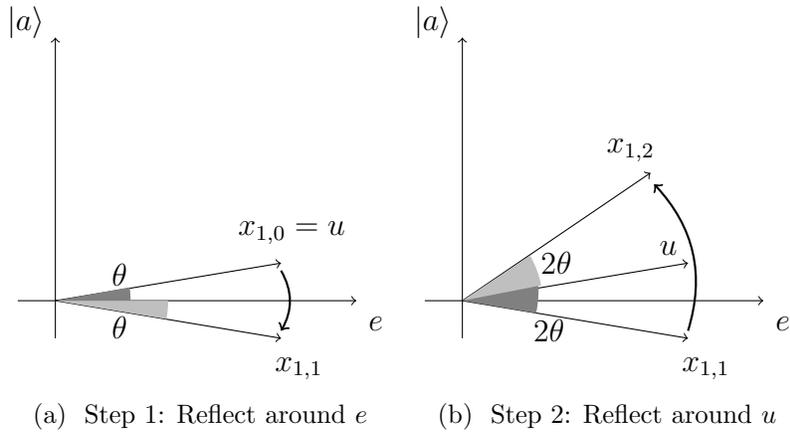


Figure 1.5: The first iteration of the Grover loop

continue to do the same.

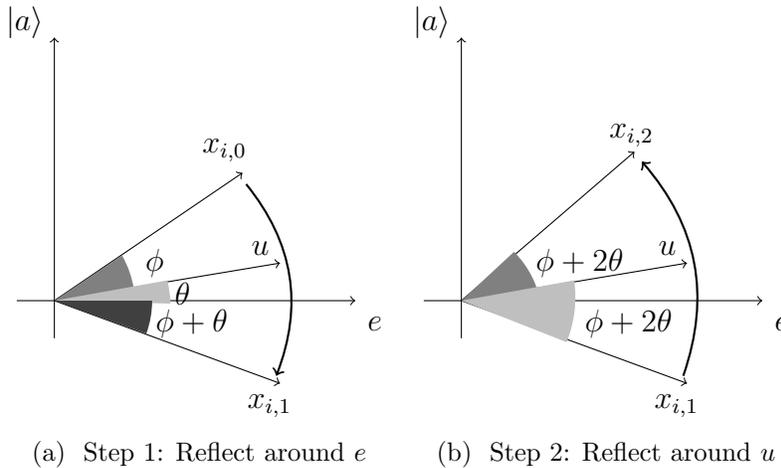


Figure 1.6: The i 'th iteration of the Grover loop

Figure 1.5 and Figure 1.6 provide sufficient means to conclude that each iteration of the Grover loop will decrease the angle (which is originally $\arccos(\frac{1}{2^{n/2}})$) between a and x by 2θ radians. In order to maximize the probability of observing a in the measurement step one should terminate the loop at the point where distance between x and a is as small as possible.

For large values of n , the number of iterations is $O(2^{n/2})$ (the numerator tends to $\pi/2$, whereas the denominator tends to $2\frac{1}{2^{n/2}}$, since $\sin(x)=x$ for small x). \square

1.20 Shor's Algorithm

In 1994, Peter Shor formulated a quantum algorithm for integer factorization: Given an integer N , which is promised to be the product of at most two prime numbers, find those primes.

The algorithm has two parts:

1. A reduction, which can be efficiently done on a classical computer, of the factoring problem to the problem of order finding.

2. A quantum algorithm to solve the order finding problem.

1.20.1 Factoring reduces to order finding

Algorithm 2 Reduction of factoring to order finding

Given N , find a prime factor of N :

- **Step 1:** Check if N is a prime itself, if so print N .
 - **Step 2:** Check if N is a perfect power, i.e. $N = C^D$ for some $C, D \in \mathbb{Z}$. If so, call this algorithm on C .
 - **Step 3:** Randomly choose A in $[2, \dots, N - 1]$
 - **Step 4:** $g = \gcd(A, N)$. If $g > 1$, call this algorithm on g .
 - **Step 5:** Run Shor's algorithm on A and N to obtain a number r such that $A^r \equiv 1 \pmod{N}$.
 - **Step 6:** If r is odd, then go to step 3 to pick another A .
 - **Step 7:** Let $y = A^{\frac{r}{2}} \pmod{N}$, if $y = -1$, then go to step 3.
 - **Step 8:** Let $z = \gcd(y - 1, N)$, if $z = 1$ then r was not the order, go to step 5 to try to obtain a correct r .
 - **Step 9:** Run this algorithm on z .
-

For step 1, we know that $PRIMES \in P$, so we can efficiently check the primality of N on a classical computer. In step 2, we know that the binary representation of our input N has length $n = \log(N)$ and if $N = C^D$, then we know that $n = D \log(C)$, therefore the value of D can be at most the length of our input, thus it can be computed efficiently that if N is a perfect power by exhaustively going through all candidate values of D and using binary search to see if the D 'th root for this D is an integer. For step 5, we want to find the smallest r (order), such that $r \leq N$.

Lemma 1. For every N and $y \in \{1, \dots, N - 1\}$, if $y^2 \equiv 1 \pmod{N}$ but $y \pmod{N} \notin \{-1, +1\}$, then $\gcd(y - 1, N) \notin \{1, N\}$.

Proof. N divides $y^2 - 1 = (y + 1)(y - 1)$ but does not divide neither $(y - 1)$ nor $(y + 1)$. However, this means $\gcd(y - 1, N) > 1$, since if $y - 1$ and N were co-primes, then since N divides $(y - 1)(y + 1)$, it would have to divide $(y + 1)$. \square

Lemma 2. *For every nonprime N that is not a prime power, the probability that a random element A of $\mathcal{Z}_N^* = \{A \in \{0, \dots, N - 1\} | \gcd(A, N) = 1\}$ has an even order r and furthermore, $A^{\frac{r}{2}} \neq -1 \pmod{N}$, is at least $\frac{1}{4}$.*

Proof. If $N = PQ$ where P and Q are primes, following the Chinese Remainder Theorem, we know that choosing a random $A \in \mathcal{Z}_N^*$ is equivalent to choosing two random numbers Y, Z in \mathcal{Z}_P^* and \mathcal{Z}_Q^* respectively, and setting A to be the unique number corresponding to the pair $\langle Y, Z \rangle$. For every k , $A^k \pmod{N}$ is isomorphic to $\langle Y^k \pmod{P}, Z^k \pmod{Q} \rangle$ and so the order of A is the least common multiple of the orders of Y and Z modulo P and Q respectively.

Let us show that;

- **A** - with probability at least $\frac{1}{2}$, the order of Y is even : $2^k \cdot c$ for $k \geq 1$ and c is odd.
- **B** - with probability at least $\frac{1}{2}$, the order of Z has the form $2^l \cdot d$ for d is odd and $l \neq k$.

Proof. A - The set of numbers in \mathcal{Z}_P^* with odd order is a subgroup of \mathcal{Z}_P^* , since if Y, Y' have odd orders r, r' , then $\langle Y, Y' \rangle^{rr'} = 1 \pmod{P}$ which means that the order of YY' divides the odd number rr' . Consider -1 which has even order, so not everyone has odd order. \mathcal{Z}_P^* with odd order is a proper subgroup, meaning at most $\frac{1}{2}$ of the population will be odd. \square

Proof. B - For every l , define G_l to be the subset of \mathcal{Z}_Q^* whose order modulo Q is of the form $2^j \cdot d$ where $j \leq l$ and d is odd. For every l , G_l is a subgroup of G_{l+1} . Since Q is prime, the mapping $x \rightarrow x^2 \pmod{Q}$ is two-to-one and maps G_{l+1} to G_l , so;

$$|G_l| \geq \frac{|G_{l+1}|}{2}$$

Let l_0 name the largest number such that G_{l_0} is a proper subgroup of \mathcal{Z}_Q^* . Then

$$|G_{l_0}| = \frac{|\mathcal{Z}_Q^*|}{2}.$$

So with probability exactly $\frac{1}{2}$, the order of a random $Z \in \mathcal{Z}_Q^*$ is a number of the form $2^l \cdot d$ for $l \leq l_0$. We conclude that for a specific k , the order being of the form $2^k \cdot d$ has probability at most $\frac{1}{2}$. \square

This implies that, with probability at least $\frac{1}{4}$, the order of A is $r = 2^{\max(k,l)} \cdot \text{lcm}(c, d)$, for $k \neq l$. $A^{\frac{r}{2}}$ will therefore be isomorphic to a pair which has at least one 1 in it. We know that -1 is isomorphic to the pair $\langle -1, -1 \rangle$, which leads to a contradiction for the case that $A^{\frac{r}{2}} = -1 \pmod{N}$.

This argument can be generalized to any composite N which is not a prime power. \square

1.20.2 Order finding

We can now introduce Shor's actual contribution, the polynomial time order finding algorithm. (Consult the pseudocode.)

Modular exponentiation has an efficient classical algorithm.

We know the Fourier Transform:

$$\tilde{f}(x) = \frac{1}{\sqrt{M}} \sum_{y \in \mathcal{Z}_M} f(y) \omega^{xy}$$

where $\omega = e^{\frac{2\pi i}{M}}$, an M^{th} root of unity.

The quantum version does this transformation on the amplitudes, mapping $\sum_{x \in \mathcal{Z}_M} f(x) |x\rangle$ to $\sum_{x \in \mathcal{Z}_M} \tilde{f}(x) |x\rangle$.

The QFT on m bits ($2^m = M$ states) can be implemented efficiently by noting that its action on a basis state

$$|x\rangle \rightarrow \frac{1}{\sqrt{M}} \sum_{y=0}^{M-1} e^{\frac{2\pi i xy}{N}} |y\rangle$$

can be rewritten in terms of the action on individual bits as

$$|x_1, \dots, x_n\rangle \rightarrow \frac{(|0\rangle + e^{2\pi i 0 \cdot x_n} |1\rangle)(|0\rangle + e^{2\pi i 0 \cdot x_{n-1} x_n} |1\rangle) \dots (|0\rangle + e^{2\pi i 0 \cdot x_1 x_2 \dots x_n} |1\rangle)}{2^{\frac{n}{2}}}$$

This formulation leads to an implementation using gates of the form

$$R_k = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^k}} \end{pmatrix},$$

Algorithm 3 Shor's algorithm for order finding

Given numbers A and N , such that $A < N$, N is written in n bits, and $\gcd(A, N) = 1$, find a number r , such that $A^r = 1(\text{mod}N)$. We will call the first $m = \lceil 5\log(N) \rceil$ bits of the tape 'the first register'. The n bits after that are called 'the second register'. Let $M = 2^m$.

- **Step 0:** Initialize $m+n$ qubits to $|0^m0^n\rangle$.
 - **Step 1:** Apply Hadamards to each qubit in the first register.
 - **Step 2:** Compute modular exponentiation, i.e. $|x\rangle|y\rangle \rightarrow |x\rangle|y \oplus (A^x \text{ mod } N)\rangle$.
 - **Step 3:** Measure the second register to obtain a y_0 .
 - **Step 4:** Apply Quantum Fourier Transform to the first register.
 - **Step 5:** Observe the first register to obtain an x . Let $z=0$.
 - **Step 6:** Find a rational approximation $\frac{a}{b}$ with $\gcd(a, b) = 1$ and $b < N$, that approximates the number $\frac{x}{2^m-z}$ within $\frac{1}{10 \times 2^{m-z}}$ accuracy. If this approximation satisfies $A^{2^z b} = 1(\text{mod}N)$, then output $2^z b$ and terminate. If $z > 3n$, terminate. Otherwise, increment z and go to the beginning of Step 6.
-

which was shown in class. The Solovay-Kitaev theorem guarantees the existence of an algorithm which we can use to approximate these gates efficiently in terms of our fixed set of quantum operations.

Step 6 is classical. The efficient continued fractions algorithm generates a sequence of better and better approximations of the form a/b with bigger and bigger values of b to the number $x/2^{m-z}$ as long as $b < N$.

Step 1 computes

$$\frac{1}{\sqrt{M}} \sum_{x \in \mathcal{Z}_M} |x\rangle |0^n\rangle$$

after which every amplitude is set to $\frac{1}{\sqrt{M}}$.

In step 2, we're doing the modular exponentiation, which transforms the second register by computing

$$\frac{1}{\sqrt{M}} \sum_{x \in \mathcal{Z}_M} |x\rangle |A^x(\text{mod } N)\rangle$$

After the step 3, i.e. the measurement of the second register, the first register partially collapses

$$\frac{1}{\sqrt{K}} \sum_{l=0}^{K-1} |x_0 + lr\rangle |y_0\rangle$$

such that x_0 is the smallest number such that $A^{x_0} = y_0(\text{mod } N)$ and $K = \lfloor \frac{M-1-x_0}{r} \rfloor + 1$.

After the Quantum Fourier Transform in step 4, we have

$$\frac{1}{\sqrt{MK}} \left(\sum_{x \in \mathcal{Z}_M} \sum_{l=0}^{K-1} \omega^{(x_0+lr)x} |x\rangle \right) |y_0\rangle$$

Observing the first register, we obtain a value x . There are two cases here:

1 - r divides M .

If $M=rc$ for some integer c , then the absolute value of the amplitude of $|x\rangle$ before the measurement is $\frac{1}{\sqrt{Mc}} \left| \sum_{l=0}^{c-1} \omega^{lrx} \right|$. If c does not divide x , then $\sum_{l=0}^{c-1} \omega^{lrx} = 0$ (since ω^r is a c 'th root of unity by our assumptions, and

the formula for the sum of a finite geometric series can be applied since the denominator is not zero). If $x=ca$ for some a , then $\sum_{l=0}^{c-1} \omega^{lrx} = \sum_{l=0}^{c-1} \omega^{lrca} = \sum_{l=0}^{c-1} \omega^{lMa} = c$. For all the r possible values in $\{0, 1, \dots, r-1\}$ of a , the probability that such an x will be observed is thus $c/M=1/r$.

So the observed x will satisfy $x/M=a/r$ for some randomly selected a in that set. Since there are $\Omega(\frac{r}{\log r})$ prime numbers less than r , and at most $\log r$ of these are factors of r , we can put a lower bound on the probability that a/r will not be "simplified", and the continued fractions algorithm will print r .

2 - The measured value x doesn't satisfy that M divides xr .

Lemma 3. *There exists $\Omega(\frac{r}{\log r})$ values $x \in \mathcal{Z}_M$ such that*

1. $0 < xr' \pmod{M'} < \frac{r'}{10}$
2. $\lfloor \frac{xr'}{M'} \rfloor$ and r' are coprime,

where $r' = r/\gcd(r, M)$ and $M' = M/\gcd(r, M)$.

Proof. Let $\gcd(r, M) = d$. Then $r' = r/d$ and $M' = M/d$, and $x \rightarrow r'x \pmod{M'}$ is a permutation of $\mathcal{Z}'_{M'}$. There are at least $\Omega(\frac{r}{d \log r})$ numbers in $[1, \dots, \frac{r'}{10}]$ that are coprime to r' . So at least $\Omega(\frac{r}{d \log r})$ numbers x exist such that $r'x \pmod{M'} = xr' - \lfloor \frac{xr'}{M'} \rfloor M'$ is in $[1, \dots, \frac{r'}{10}]$ and is coprime to r' , and for these values of x , $\lfloor \frac{xr'}{M'} \rfloor$ and r' have to be coprime, since if these two have a shared factor, that factor would be shared with $r'x \pmod{M'}$ as well. Since $r'x = r'(x+cM')$ modulo M' for any c , we have a total of $\Omega(\frac{r}{\log r})$ such numbers $x \in \mathcal{Z}_M$ with $xr' \pmod{M'} < \frac{r'}{10}$. \square

Lemma 4. *If x satisfies $0 < xr' \pmod{M'} < \frac{r'}{10}$, where r' is a factor of r greater than 1, then the coefficient of $|x\rangle$ is at least $\Omega(\frac{1}{\sqrt{r}})$.*

Proof. The absolute value of $|x\rangle$'s amplitude is

$$\frac{1}{\sqrt{MK}} \left| \sum_{l=0}^{K-1} \omega^{lrx} \right| \tag{1.5}$$

We have $\frac{M}{2r} < K \leq \frac{M}{r}$ since $x_0 < N \ll M$.

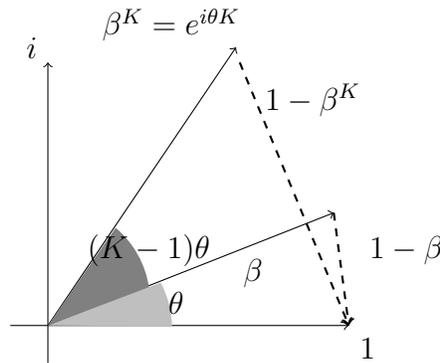
Let $\beta = \omega^{rx}$. Note that $\beta \neq 1$, since x doesn't satisfy that M divides xr . Using the formula for the sum of a geometric series, (1.5) is at least

$$\frac{\sqrt{r}}{M} \left| \frac{1 - \beta^K}{1 - \beta} \right|,$$

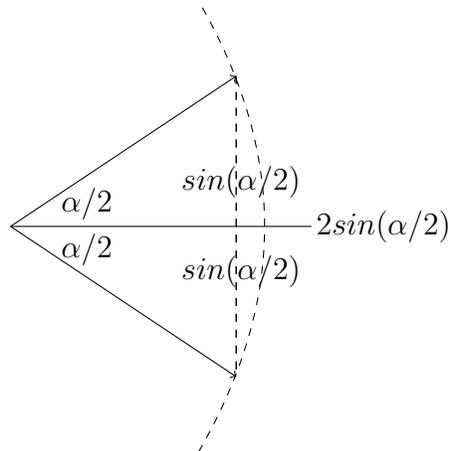
and at most

$$\frac{\sqrt{2r}}{M} \left| \frac{1 - \beta^K}{1 - \beta} \right|.$$

Letting $\theta = 2\pi \frac{rx(\text{mod}M)}{M}$ be the angle such that $\beta = e^{i\theta}$, the following figure shows the relationship between these variables in the complex plane:



Furthermore, it can be seen from the figure below that if the angle between the lines decreases, the length of the chord length approximates $2\sin\frac{\alpha}{2}$.



But then the amplitude under consideration is

$$\Theta\left(\frac{\sqrt{r} \sin(\frac{K\theta}{2})}{M \sin(\frac{\theta}{2})}\right).$$

Note that, if $xr'(\bmod M') < \frac{r'}{10}$, then $xr(\bmod M) < \frac{r}{10}$. Since $K \leq M/r$, $\theta = 2\pi \frac{rx(\bmod M)}{M}$, and $xr(\bmod M) < \frac{r}{10}$, we have $K\theta/2 < \pi/10$. Since small angles can be approximated with their sines, the amplitude is $\Theta(\frac{\sqrt{r}}{M} \lceil \frac{M}{r} \rceil) = \Theta(\frac{1}{\sqrt{r}})$. \square

Combining these two lemmas, we conclude that, with probability $\Omega(\frac{1}{\log r})$, the measured value of x will satisfy $xr' - cM' < r'/10$ for $c = \lfloor \frac{xr'}{M'} \rfloor$, meaning $|\frac{x}{M'} - \frac{c}{r'}| < \frac{1}{10M}$.

So if we hit on the correct value of M' (which is $M/2^z$ for some z , recalling that M is a power of 2) by dividing M repeatedly by 2, c/r' won't "simplify further" and will approximate x/M' closely enough that it will be the fraction found by the continued fractions algorithm when it runs. Since r equals $2^z r'$, it will be found as a result of the subsequent checks. Since $z = O(\log N)$, the repetitions add up to polynomial runtime.

[1]

Bibliography

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