0.0.1 NP-Completeness

Consider SAT, the prototypical example of an NP-complete problem. An instance of this problem consists of a Boolean function \( f(x_1, \ldots, x_n) = c_1 \land \ldots \land c_m \); the SAT problem asks you to determine whether there exists a satisfying assignment—that is, an input \((a_1, \ldots, a_n)\) such that \(f(a_1, \ldots, a_n) = 1\). UNIQUE-SAT is a variant of SAT that poses the same problem with the restriction that \( f \) must have zero or one satisfying assignments, but no more. As it turns out, there is a randomized reduction from SAT to UNIQUE-SAT; thus, the two problems are equally hard.

We’ll use the black box model when considering this problem. In this model, we know that either \( f \equiv 0 \) or there exists exactly one \( a \) such that \( f(a) = 1 \), where \( a \) is chosen uniformly at random. That is, \( f \) is treated as a black box; we can make queries to \( f \), but we have no access to the Boolean formula itself. Equivalently we can represent \( f \) by a table of \( N = 2^n \) entries where either none or exactly one entry is 1. Ideally we want a quantum algorithm that solves this problem in time \( O(\text{poly}(n)) = O(\text{poly} - \text{log}(n)) \).

Can a quantum computer solve this problem by going into a superposition of all exponentially many possible truth assignments? To answer this question precisely, let us define the black box query model:

0.0.2 The quantum black box model

Here’s the problem: You are given a boolean function \( f : \{1, \ldots, N\} \to \{0, 1\} \), and are promised that for exactly one \( a \in \{1, \ldots, N\} \), \( f(a) = 1 \). Think of this as a table of size \( N \), where exactly one element has value 1, and all the others are 0. Since we assume \( f \) can be computed classically in polynomial time, we can also compute it in superposition:

\[
\sum_x \alpha_x |x\rangle |0\rangle \rightarrow \sum_x \alpha_x |x\rangle |f(x)\rangle
\]

Another way we can implement \( f \) is put the answer register in superposition:

\[
\sum_x \alpha_x |x\rangle \left( \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right) \rightarrow \sum_x \alpha_x \left( \frac{|x\rangle |f(x)\rangle - |x\rangle |f(x)\rangle}{\sqrt{2}} \right)
= \sum_x \alpha_x |x\rangle \left( \frac{|f(x)\rangle - |f(x)\rangle}{\sqrt{2}} \right)
= \sum_x \alpha_x |x\rangle (-1)^{f(x)} \left( \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right)
\]

Now, we might as well assume \( f \) is a black box or oracle. All we need to do is design an algorithm that finds \( a : f(a) = 1 \).
0.0.3 The Hybrid Argument

For the purposes of this discussion, we want to separate the quantum algorithm itself from the function $f$. We assume that the quantum algorithm is infinitely powerful (i.e., it can do any computation in one step) and focus instead on the number of queries it must make to $f$. All queries to $f$ occur in superposition; that is, a single query on $\sum \alpha_t |x_t\rangle |0\rangle$ yields the output $\sum \alpha_t |x_t\rangle |f(x_t)\rangle$.

**Theorem 10.1:** In the black box model, any quantum algorithm for determining whether there exist $x_1, \ldots, x_n$ such that $f(x_1, \ldots, x_n) = 1$ must make $\Omega(\sqrt{N})$ queries to $f$.

**Proof:**

Consider any quantum algorithm $A$ for solving this search problem. First do a test run of $A$ on the function $f \equiv 0$. Let $T$ be the number of queries that $A$ makes to $f$, and let $\alpha_{t,j}$ be the amplitude with which $A$ queries $x$ at time $t$ (that is, the query at time $t$ is $\sum \alpha_{t,j} |x_t\rangle$). Now, define the query magnitude of $x$ to be $\sum |\alpha_{t,j}|^2$. The expectation value of the query magnitude of $x$ is $E_x (\sum |\alpha_{t,j}|^2) = \frac{T}{N}$. Thus, $\min \sum |\alpha_{t,j}|^2 \leq \frac{T}{N}$. Let $z$ be the input at which this minimum occurs; then by the Cauchy-Schwarz inequality, $\sum |\alpha_{t,j}| \leq \frac{T}{\sqrt{N}}$.\[\square\]

Let $|\phi_t\rangle$ be the states of $A_x$ after the $t$-th step. Now run the algorithm $A$ on the function $g$ such that $g(z) = 1$ and for all $y \neq z$, $g(y) = 0$. Suppose the final state of $A_g$ is $|\psi_f\rangle$. By the claim that follows, $|\phi_T\rangle = |\psi_f\rangle = |E_0\rangle + \ldots + |E_{T-1}\rangle$ where $||E_i|| \leq \sqrt{2} |\alpha_{t,j}|$. Using the triangle inequality and the inequality proved above, we have $|||\phi_T\rangle - |\psi_f\rangle|| \leq \sum_i ||E_i|| \leq \sqrt{2} \sum |\alpha_{t,j}| \leq \frac{T}{\sqrt{2}/N}$. This implies that the two states can be distinguished with probability at most $O(T/\sqrt{N})$ by any measurement. Thus any quantum algorithm that distinguishes $f$ from $g$ with constant probability of success must make $\Omega(\sqrt{N})$ queries.

$|\psi_f\rangle = |\phi_T\rangle = |E_0\rangle + |E_1\rangle + \ldots + |E_{T-1}\rangle$, where $||E_i|| \leq \sqrt{2} |\alpha_{t,j}|$.

**Proof:**

Consider two runs of the algorithm $A$, which differ only on the $t$-th step. The first run queries the function $f$ on the first $t$ steps and queries $g$ for the remaining $T-t$ steps; the second run queries $f$ on the first $t-1$ steps and $g$ for the remaining $T-t+1$ steps. After the first $t-1$ steps, both runs are in state $|\phi_t\rangle$. On the $t$-th step, one run queries $f$ and the other queries $g$. The outputs of these queries differ only on the amplitude of the two basis vectors $|z\rangle |0\rangle$ and $|z\rangle |1\rangle$, so overall the output vectors differ by at most $\sqrt{2} |\alpha_{t,j}|$. Thus, at the end of the $t$-th step, the state of the first run is $|\phi_t\rangle$, whereas the state of the second run is $|\phi_t\rangle + |F_t\rangle$, where $||F_t|| \leq \sqrt{2} |\alpha_{t,j}|$. Now if $U$ is the unitary transform describing the remaining $T-t$ steps (of both runs), then the final state after $T$ steps for the two runs are $U|\phi_t\rangle$ and $U(|\phi_t\rangle + |F_t\rangle)$, respectively. The latter state can be written as $U|\phi_t\rangle + |E_t\rangle$, where $|E_t\rangle = U|F_t\rangle$. Since unitary transformations preserve length, we know that $||E_t|| \leq \sqrt{2} |\alpha_{t,j}|$. Thus, the effect of switching the queried function only on the $t$-th step can be described by an “error” $|E_t\rangle$ in the final state of the algorithm, where $||E_t|| \leq \sqrt{2} |\alpha_{t,j}|$.

We can transform the run $A_f$ to $A_g$ by a succession of $T$ changes of the kind described above. Overall, the difference between the final states of $A_f$ and $A_g$ is $|E_0\rangle + |E_1\rangle + \ldots + |E_{T-1}\rangle$, where $||E_t|| \leq \sqrt{2} |\alpha_{t,j}|$.

Finally, it is useful to consider where this factor of $\sqrt{N}$ comes from. In the worst case, we query $z$ with amplitude $1/\sqrt{N}$ at each time step. The vectors that indicate the differences at each step could all be orthogonal, in which case the total distance is the sum of the squares of each vector’s length, which is about $N$. However, if all vectors are in the same direction, the total distance is the sum of the length of each vector, which is approximately $\sqrt{N}$. Grover’s

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1The Cauchy-Schwarz inequality says that for two vectors $a$ and $b$ of length $T$, $(\sum a_t b_t)^2 \leq (\sum a_t^2) (\sum b_t^2)$. If we let $b_t = 1$ for all $t$, then we have $(\sum a_t)^2 \leq T \sum a_t^2$. Thus, if $\sum |\alpha_{t,j}|^2 \leq T/N$, then $(\sum |\alpha_{t,j}|)^2 \leq T^2/N$.\[\square\]
algorithm, which we will describe next, demonstrates that it is possible to align all of these vectors and achieve the factor of $\sqrt{N}$.

### 0.0.4 Grover’s algorithm

Grover’s algorithm finds $a$ in $O(\sqrt{N})$ steps. Consider the two dimensional subspace that consists of two states: $|a\rangle$ and $|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle$. Let $\theta$ be the angle between $|\psi_0\rangle$ and $|e\rangle$, where $|e\rangle$ is the vector that is orthogonal to $|a\rangle$ in the direction of $|\psi_0\rangle$ in this subspace. See Figure 0.1 for an illustration of these vectors.

$|a\rangle$ is the target, so we want to increase $\theta$. But how?

One way to rotate a vector is to make two reflections. In particular, we can rotate a vector $|v\rangle$ by $2\theta$ by reflecting about $|e\rangle$ and then reflecting about $|\psi_0\rangle$. This transformation is also illustrated in Figure 0.1.

Each step of our algorithm is a rotation by $2\theta$ (we discuss the implementation below). This means that we need $\frac{\pi/2}{2\theta}$ iterations for the algorithm to complete. Now, what’s $\theta$?

$$\langle \psi_0 | a \rangle = \cos(\pi/2 - \theta) = \sin(\theta) = \frac{1}{\sqrt{N}}$$

Since $\sin \theta \approx \theta$, we know that $\theta \approx \frac{1}{\sqrt{N}}$. Thus, we need $O(\sqrt{N})$ iterations for the algorithm to complete. In the end, we get very close to $|a\rangle$, and then with high probability, a measurement of the state yields $a$.

How do you implement the two reflections?

1. Reflection about $|e\rangle$ is easy. All we need to do is flip the phase of the component in the direction of $|a\rangle$; to accomplish this, we just use the second implementation of $f$ that we showed earlier.
2. For the reflection about $|\psi_0\rangle$, we use the Diffusion operator $D$ (assume $N = 2^n$), which works as follows. First, apply $H_{2^n}$, which maps $|\psi_0\rangle \mapsto |00\ldots0\rangle$. Then reflect around $|00\ldots0\rangle$. Finally, apply $H_{2^n}$ to return to the original basis. (Note that this is simply a reflection around the zero vector in the Hadamard basis.)