Notes on Quantum Computing Algorithms for Natural Language Processing

Leonardo Hügens

l.lobatodiasleitehugens@students.uu.nl

8th December 2021

Contents

1 'Rigorous mathematicians and physicists' **3**

2 Quantum Tomography of 1 qubit states **4**

2.1 Test 1 - determine θ 4

2.2 Test 2 - determine $|\phi|$ 4

2.3 Test 3 - determine $sign\,(\phi)$ 5

3 Expected value $\langle\psi| U |\psi\rangle$ - Hadamard test **6**

4 Attempt at contraction: measuring $\langle\psi| \hat{P} |\psi\rangle$. **8**

4.1 Motivation 8

4.2 Hadamard Test 9

4.3 Bell Basis Test 9

5 Contraction method: Projection on $|\beta_{00}\rangle$. **11**

5.1 3-qubit example 12

5.2 5-qubit example 12

5.3 3-qubit test 14

6 Ambiguous readings on Bob Coeck method **16**

6.1 Using swap gates to generate different contraction 16

6.2 Using control bit to put different readings in superposition 18

7 Thoughts about the usage of Grover's Algorithm **21**

7.1 Quick overview 21

8 Grover's algorithm for semantic analysis **22**

9 Generalization of Grover's Algorithm **26**

9.1 Summary 26

9.2 Detailed explanation 27

9.3 How does this look like in our context 29

9.4 Implementation of *who talks?* 30

1 'Rigorous mathematicians and physicists'

In this section it's shown how two possible different readings of a sentence correspond to different contractions, based on the calculation taken from [3]. The sentence is 'rigorous mathematicians and physicists. The two interpretations are:

- I - (rigorous mathematicians) and physicists
- II - rigorous (mathematicians and physicists)

We start with the representation of the two words in the semantic spaces (using Einstein summation convention)

$$\begin{aligned}
[\![\text{ rigorous }]\!] &= r_{ij}\hat{n}_i \otimes \hat{n}_j \\
[\![\text{ mathematicians }]\!] &= m_k\hat{n}_k \\
[\![\text{ and }]\!] &= a_{lmn}\hat{n}_l \otimes \hat{n}_m \otimes \hat{n}_n \\
[\![\text{ physicists }]\!] &= p_o\hat{n}_o
\end{aligned}$$

Interpretation I:

$$\begin{aligned}
&[\![\text{ rigorous mathematicians }]\!].[\![\text{ and physicists}]\!] \\
&= \{[\![\text{ rigorous }]\!].[\![\text{ mathematicians }]\!]\} . \{[\![\text{ and }]\!].[\![\text{ physicists }]\!]\} \\
&= \{(r_{ij}\hat{n}_i \otimes \hat{n}_j) . (m_k\hat{n}_k)\} . \{(a_{lmn}\hat{n}_l \otimes \hat{n}_m \otimes \hat{n}_n) . (p_o\hat{n}_o)\} \\
&= \{r_{ij}m_k\hat{n}_i\delta_{jk}\} . \{a_{lmn}p_o\hat{n}_l \otimes \hat{n}_m\delta_{no}\} \\
&= \{r_{ij}m_j\hat{n}_i\} . \{a_{lmn}p_n\hat{n}_l \otimes \hat{n}_m\} \\
&= r_{ij}m_ja_{lmn}p_n\delta_{il}\hat{n}_m \\
&= r_{ij}m_ja_{imn}p_n\hat{n}_m
\end{aligned}$$

Interpretation II:

$$\begin{aligned}
&[\![\text{ rigorous }]\!].[\![\text{ mathematicians and physicists}]\!] \\
&= [\![\text{ rigorous }]\!]. \{[\![\text{ mathematicians }]\!]. \{[\![\text{ and }]\!].[\![\text{ physicists }]\!]\}\} \\
&= \{r_{ij}\hat{n}_i \otimes \hat{n}_j\} . \{(m_k\hat{n}_k) . (a_{lmn}p_n\hat{n}_l \otimes \hat{n}_m)\} \\
&= \{r_{ij}\hat{n}_i \otimes \hat{n}_j\} . \{m_ka_{lmn}p_n\delta_{kl}\hat{n}_m\} \\
&= \{r_{ij}\hat{n}_i \otimes \hat{n}_j\} . \{m_la_{lmn}p_n\hat{n}_m\} \\
&= r_{ij}m_la_{lmn}p_n\hat{n}_i\delta_{jm} \\
&= r_{ij}m_la_{ljn}p_n\hat{n}_i
\end{aligned}$$

2 Quantum Tomography of 1 qubit states

Any 1 qubit state can be written in the form

$$|\psi\rangle = e^{i\gamma}\left(\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle\right)$$

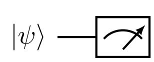
It is intuitive to see that having 3 free parameters makes sense, since we have 4 parameters (real and complex parts of each of the 2 coefficients) but we also have the constraint of the state being normalized, which $|\alpha|^2 + |\beta|^2 = 1$ for a general case $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. However, the global phase should be completely irrelevant for any procedure, so now we'll show 3 tests that can be applied to a quantum state, provided that we can prepare a system in that state as many times as we want, and that enable us to determine θ and ϕ to obtain:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle$$

The intervals for each angle are $\theta \in [0, \pi]$ and $\phi \in [-\pi, \pi)$.

2.1 Test 1 - determine θ

The circuit for this test is:



We know that the probabilities of measuring 0 and 1 (P_0 and P_1) are:

$$P_0 = \cos^2\left(\frac{\theta}{2}\right)$$
$$P_1 = \sin^2\left(\frac{\theta}{2}\right)$$

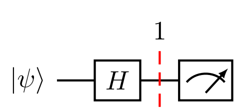
which gives us $\frac{\theta}{2} \in \left[0, \frac{\pi}{2}\right]$:

$$\theta = 2\arccos\left(\sqrt{P_0}\right) = 2\arcsin\left(\sqrt{P_1}\right)$$

If this experiments give $\theta = 0$ or $\theta = \pi$, we'll already know $|\psi\rangle = |1\rangle$ or $|\psi\rangle = |0\rangle$ respectively, so in that case we skip the next tests.

2.2 Test 2 - determine $|\phi|$

The circuit for this test is:



The final state is:

$$
\begin{aligned}
|\psi_1\rangle &= H\left[\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle\right] \\
&= \cos\left(\frac{\theta}{2}\right)\frac{|0\rangle + |1\rangle}{\sqrt{2}} + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\frac{|0\rangle - |1\rangle}{\sqrt{2}} \\
&= \frac{1}{\sqrt{2}}\left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]|0\rangle + \frac{1}{\sqrt{2}}\left[\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]|1\rangle
\end{aligned}
$$

which implies:

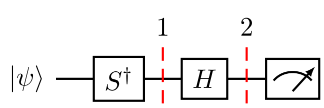
$$
\begin{aligned}
P_0 &= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right|^2 \\
&= \frac{1}{2}\left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]\left[\cos\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{-i\phi}\right] \\
&= \frac{1}{2}\left[1 + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(e^{i\phi} + e^{-i\phi}\right)\right] \\
&= \frac{1}{2}\left[1 + \sin(\theta)\cos(\phi)\right]
\end{aligned}
$$

$$
\begin{aligned}
P_1 &= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right|^2 \\
&= \frac{1}{2}\left[\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]\left[\cos\left(\frac{\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)e^{-i\phi}\right] \\
&= \frac{1}{2}\left[1 - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(e^{i\phi} + e^{-i\phi}\right)\right] \\
&= \frac{1}{2}\left[1 - \sin(\theta)\cos(\phi)\right]
\end{aligned}
$$

We can manipulate this as

$$
\begin{aligned}
P_0 - P_1 &= \sin(\theta)\cos(\phi) \\
\cos(\phi) &= \frac{P_0 - P_1}{\sin(\theta)} \\
\phi &= \pm\arccos\left(\frac{P_0 - P_1}{\sin(\theta)}\right) \\
|\phi| &= \left|\arccos\left(\frac{P_0 - P_1}{\sin(\theta)}\right)\right|
\end{aligned}
$$

2.3 Test 3 - determine $sign(\phi)$



The intermediate and final states are:

$$
\begin{aligned}
|\psi_1\rangle &= S^\dagger\left[\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle\right] \\
&= \cos\left(\frac{\theta}{2}\right)|0\rangle - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_2\rangle &= H\left[\cos\left(\frac{\theta}{2}\right)|0\rangle - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}|1\rangle\right] \\
&= \cos\left(\frac{\theta}{2}\right)\frac{|0\rangle+|1\rangle}{\sqrt{2}} - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\frac{|0\rangle-|1\rangle}{\sqrt{2}} \\
&= \frac{1}{\sqrt{2}}\left[\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]|0\rangle + \frac{1}{\sqrt{2}}\left[\cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]|1\rangle
\end{aligned}
$$

The probabilities are

$$
\begin{aligned}
P_0 &= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right|^2 \\
&= \frac{1}{2}\left[\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]\left[\cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right)e^{-i\phi}\right] \\
&= \frac{1}{2}\left[1 - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(ie^{i\phi} - ie^{-i\phi}\right)\right] \\
&= \frac{1}{2}\left[1 + \sin(\theta)\sin(\phi)\right]
\end{aligned}
$$

$$
\begin{aligned}
P_1 &= \frac{1}{2}\left|\cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right|^2 \\
&= \frac{1}{2}\left[\cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right)e^{i\phi}\right]\left[\cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)e^{-i\phi}\right] \\
&= \frac{1}{2}\left[1 + \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left(ie^{i\phi} - ie^{-i\phi}\right)\right] \\
&= \frac{1}{2}\left[1 - \sin(\theta)\sin(\phi)\right]
\end{aligned}
$$

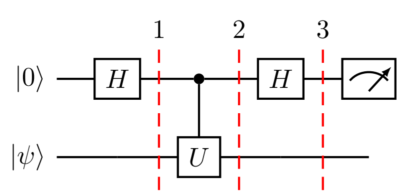
which can be combined to give

$$
\begin{aligned}
P_0 - P_1 &= \sin(\theta)\sin(\phi) \\
\sin(\phi) &= \frac{P_0 - P_1}{\sin(\theta)} \\
sign(\phi) &= sign\left(\arcsin\left(\frac{P_0 - P_1}{\sin(\theta)}\right)\right) \\
sign(\phi) &= sign(P_0 - P_1)
\end{aligned}
$$

where we used that the range of usual principal value or arcsin is $\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ and $\sin(\theta) > 0 \ \forall\theta \in (0, \pi)$.

3 Expected value $\langle\psi| U |\psi\rangle$ - Hadamard test

In this section I'll show how to measure the expected value of any unitary operator U on the state $|\psi\rangle$. This can be made through the Hadamard test, whose circuit is, where we can the first qubit in the state $|0\rangle$ the control qubit:



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= |0\rangle \otimes |\psi\rangle \\
|\psi_1\rangle &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\psi\rangle \\
|\psi_2\rangle &= \frac{1}{\sqrt{2}} |0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes U |\psi\rangle \\
|\psi_3\rangle &= \frac{|0\rangle + |1\rangle}{2} \otimes |\psi\rangle + \frac{|0\rangle - |1\rangle}{2} \otimes U |\psi\rangle \\
&= |0\rangle \otimes \frac{1}{2} \left(\mathbb{I} + U\right) |\psi\rangle + |1\rangle \otimes \frac{1}{2} \left(\mathbb{I} - U\right) |\psi\rangle
\end{aligned}
$$

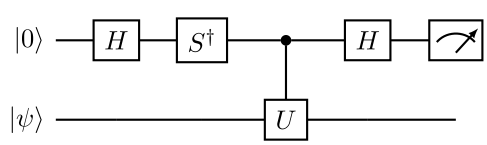
So the probabilities of measuring 0 or 1 of the control bit in the first wire are:

$$
\begin{aligned}
P_0 &= \frac{1}{4} \langle\psi| \left(\mathbb{I} + U^\dagger\right) \left(\mathbb{I} + U\right) |\psi\rangle \\
P_1 &= \frac{1}{4} \langle\psi| \left(\mathbb{I} - U^\dagger\right) \left(\mathbb{I} - U\right) |\psi\rangle
\end{aligned}
$$

which we can manipulate to find

$$
\begin{aligned}
P_0 - P_1 &= \frac{1}{4} \langle\psi| \left[\left(\mathbb{I} + U^\dagger\right) \left(\mathbb{I} + U\right) - \left(\mathbb{I} - U^\dagger\right) \left(\mathbb{I} - U\right)\right] |\psi\rangle \\
&= \frac{1}{4} \langle\psi| \left[\mathbb{I} + U^\dagger + U + U^\dagger U - \left(\mathbb{I} - U^\dagger - U + U^\dagger U\right)\right] |\psi\rangle \\
&= \frac{1}{2} \langle\psi| \left(U^\dagger + U\right) |\psi\rangle \\
&= \mathrm{Re}\left[\langle\psi| U |\psi\rangle\right]
\end{aligned}
$$

Similarly, we can determine the imaginary part of the expectation value (e.g. for the case that U is not hermitian), by applying the same procedure to the circuit:



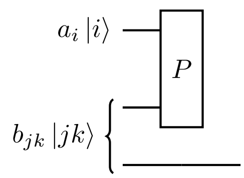
This time we'll have that the imaginary part of the expectation value if the difference of probabilities of measuring the control bit and it being 0 or 1:

$$
P_0 - P_1 = \mathrm{Im}\left[\langle\psi| U |\psi\rangle\right]
$$

4 Attempt at contraction: measuring $\langle\psi|\,\hat{P}\,|\psi\rangle$.

4.1 Motivation

Let's consider the most simple example of a contraction: the 3-qubit contraction $|\psi\rangle = a_i b_{jk}\,|ijk\rangle \to a_i b_{ik}\,|k\rangle$, whose initial configuration in a quantum computer would be:



Let's consider the calculation of the expectation value of the permutation operator P_{01}, as indicated in the circuit. We write the subscript $_{01}$ to indicate that it is the permutation operator between the first two wires, with indices 0 and 1 (for convenience when implementing code).

$$
\begin{aligned}
&\langle\psi|\,\hat{P}_{01}\otimes O_2\,|\psi\rangle \\
=&a^\star_{i'}b^\star_{j'k'}\,\langle i'j'k'|\left(\hat{P}_{01}\otimes O_2\right)|ijk\rangle\,a_i b_{jk} \\
=&a^\star_{i'}b^\star_{j'k'}\,\langle i'j'k'|\,O_2\,|jik\rangle\,a_i b_{jk} \\
=&a^\star_{i'}b^\star_{j'k'}\,\langle i'j'|ji\rangle\,\langle k'|\,O_2\,|k\rangle\,a_i b_{jk} \\
=&a^\star_{i'}b^\star_{j'k'}\delta_{i'j}\delta_{j'i}\,\langle k'|\,O_2\,|k\rangle\,a_i b_{jk} \\
=&a^\star_{j}b^\star_{ik'}\,\langle k'|\,O_2\,|k\rangle\,a_i b_{jk} \\
=&\left[a_i b^\star_{ik'}\,\langle k'|\right]O_2\left[a^\star_j b_{jk}\,|k\rangle\right]
\end{aligned}
$$

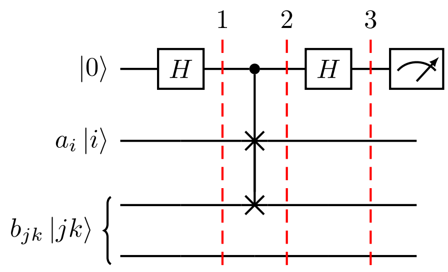
We see that the state that 'appears' to be left in the last qubit is $a^\star_j b_{jk}\,|k\rangle$, which we can compare to the contracted state that we desired $a_j b_{jk}\,|k\rangle$, that they only differ by the complex conjugation of one of the tensors. Just as quick note, these two states we mentioned (conjugation or not) have different probabilities of being measured:

$$
\begin{aligned}
|a_j b_{jk}|^2 &= [a_j b_{jk}]\left[a^\star_{j'}b^\star_{j'k}\right] = a_j b_{jk} a^\star_{j'} b^\star_{j'k} \\
\left|a^\star_j b_{jk}\right|^2 &= \left[a^\star_j b_{jk}\right]\left[a_{j'}b^\star_{j'k}\right] = a^\star_j b_{jk} a_{j'} b^\star_{j'k}
\end{aligned}
$$

Thus, it may seem that measuring this expected value would leave the last bit the pure state $a^\star_j b_{jk}\,|k\rangle$, but this is an artifact of the expected value calculation, which is not equivalent to actually performing the expected value calculation in a quantum circuit, as we shall see in the next sections.

4.2 Hadamard Test

As we saw in a previous section, we can use the Hadamard test to determine the expectation value $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle$, and because this operator is hermitian we have $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle = \mathrm{Re}\left[\langle\psi|\,\hat{P}_{01}\,|\psi\rangle\right]$, so we only need the following circuit:



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= |0\rangle \otimes a_i\,|i\rangle \otimes b_{jk}\,|jk\rangle \\
|\psi_1\rangle &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes a_i\,|i\rangle \otimes b_{jk}\,|jk\rangle \\
|\psi_2\rangle &= \frac{1}{\sqrt{2}}\,|0\rangle \otimes a_i b_{jk}\,|ijk\rangle + \frac{1}{\sqrt{2}}\,|1\rangle \otimes a_i b_{jk}\,|jik\rangle \\
|\psi_3\rangle &= \frac{|0\rangle + |1\rangle}{2} \otimes a_i b_{jk}\,|ijk\rangle + \frac{|0\rangle - |1\rangle}{2} \otimes a_j b_{ik}\,|ijk\rangle \\
&= |0\rangle \otimes \left[\frac{1}{2}\left(a_i b_{jk} + a_j b_{ik}\right)|ijk\rangle\right] + |1\rangle \otimes \left[\frac{1}{2}\left(a_i b_{jk} - a_j b_{ik}\right)|ijk\rangle\right] \\
&= |0\rangle \otimes a_{(i} b_{j)k}\,|ijk\rangle + |1\rangle \otimes a_{[i} b_{j]k}\,|ijk\rangle
\end{aligned}
$$

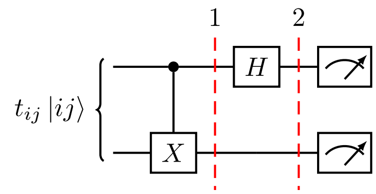
The $a_{(i}b_{j)k}$ and $a_{[i}b_{j]k}$ denote the symmetric and antisymmetric parts of the tensor $a_i b_{jk}$, respectively, w.r.t the indices i and j. We can see that the last qubit was not left in a pure state, contrary to what we desire. Moreover, there is no combination of i, j values and control qubit value s.t. that component would be our desired state (e.g. $|0\rangle \otimes a_i b_{ik}\,|00k\rangle$ would be such a state, but it's not on $|\psi_3\rangle$). This circuit still allows us to determine $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle$ of course, through the probabilities of the control qubit P_0 and P_1, it just does not leave the last qubit in the pure state that we want, to allow for further processing of that state.

4.3 Bell Basis Test

In this section I'll show how to determine $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle$ through a basis transformation into the Bell basis $|\beta_{ij}\rangle$. The relationship between the canonical basis $|ij\rangle$ and the Bell states (a.k.a. EPR pairs) $|\beta_{ij}\rangle$ is:

$$
\begin{aligned}
|\beta_{00}\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right) & |00\rangle &= \frac{1}{\sqrt{2}}\left(|\beta_{00}\rangle + |\beta_{10}\rangle\right) \\
|\beta_{01}\rangle &= \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) & |01\rangle &= \frac{1}{\sqrt{2}}\left(|\beta_{01}\rangle + |\beta_{11}\rangle\right) \\
|\beta_{10}\rangle &= \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right) & |10\rangle &= \frac{1}{\sqrt{2}}\left(|\beta_{01}\rangle - |\beta_{11}\rangle\right) \\
|\beta_{11}\rangle &= \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right) & |11\rangle &= \frac{1}{\sqrt{2}}\left(|\beta_{00}\rangle - |\beta_{10}\rangle\right)
\end{aligned}
$$

The circuit that performs the inverse Bell transformation, i.e. in allows us to measure a states in the Bell basis, is represented bellow:



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= t_{ij}\,|\beta_{ij}\rangle \\
&= t_{0j}\,|\beta_{0j}\rangle + t_{1j}\,|\beta_{1j}\rangle \\
&= \frac{t_{0j}}{\sqrt{2}}\left(|0j\rangle + |1\bar{j}\rangle\right) + \frac{t_{1j}}{\sqrt{2}}\left(|0j\rangle - |1\bar{j}\rangle\right) \\
|\psi_1\rangle &= \frac{t_{0j}}{\sqrt{2}}\left(|0j\rangle + |1j\rangle\right) + \frac{t_{1j}}{\sqrt{2}}\left(|0j\rangle - |1j\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left(t_{0j} + t_{1j}\right)|0j\rangle + \frac{1}{\sqrt{2}}\left(t_{0j} - t_{1j}\right)|1j\rangle \\
|\psi_2\rangle &= \frac{1}{2}\left(t_{0j} + t_{1j}\right)\left(|0j\rangle + |1j\rangle\right) + \frac{1}{2}\left(t_{0j} - t_{1j}\right)\left(|0j\rangle - |1j\rangle\right) \\
&= t_{0j}\,|0j\rangle + t_{1j}\,|1j\rangle \\
&= t_{ij}\,|ij\rangle
\end{aligned}
$$

For example, if initially in the beginning of the circuit we had $|\beta_{ij}\rangle$ then we would measure the state $|ij\rangle$ in the end. Thus, we could think of this circuit as being inside a usual measurement symbol in the circuit, but a measurement in the Bell basis.

To measure $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle$, we would just need to prepare $|\psi\rangle = a_{ij}\,|ij\rangle$ and send it through the circuit, and the expected value would be determine from measures as follows:

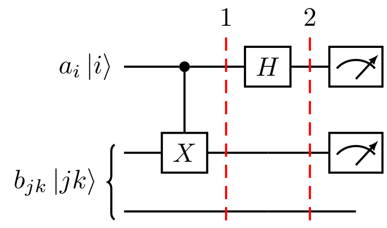
$$
\begin{aligned}
|\psi\rangle &= \langle\beta_{00}|\psi\rangle\,|\beta_{00}\rangle + \langle\beta_{01}|\psi\rangle\,|\beta_{01}\rangle + \langle\beta_{10}|\psi\rangle\,|\beta_{10}\rangle + \langle\beta_{11}|\psi\rangle\,|\beta_{11}\rangle \\
\hat{P}_{01}\,|\psi\rangle &= \langle\beta_{00}|\psi\rangle\,|\beta_{00}\rangle + \langle\beta_{01}|\psi\rangle\,|\beta_{01}\rangle + \langle\beta_{10}|\psi\rangle\,|\beta_{10}\rangle - \langle\beta_{11}|\psi\rangle\,|\beta_{11}\rangle \\
\langle\psi|\,\hat{P}_{01}\,|\psi\rangle &= |\langle\beta_{00}|\psi\rangle|^2 + |\langle\beta_{01}|\psi\rangle|^2 + |\langle\beta_{10}|\psi\rangle|^2 - |\langle\beta_{11}|\psi\rangle|^2
\end{aligned}
$$

which in more practical terms is

$$\langle\psi|\,\hat{P}_{01}\,|\psi\rangle = P_{00} + P_{01} + P_{10} - P_{11}$$

where P_{ij} denotes the probability of measuring $|ij\rangle$ (careful not to mix with the operator $\hat{P}_{ij}$)

Thus, we know now how to measure the expectation value $\langle\psi|\,\hat{P}_{01}\,|\psi\rangle$, by performing an inverse Bell transformation. However, we'll see now that this circuit does not in general leave the last qubit in the pure state that we want. The circuit is



The states along the circuit are:

$$\begin{aligned}\ket{\psi_0} &= a_i b_{jk} \ket{ijk} \\ &= [a_0 \ket{0} + a_1 \ket{1}] \otimes b_{jk} \ket{jk}\end{aligned}$$

$$\begin{aligned}\ket{\psi_1} &= a_0 \ket{0} \otimes b_{jk} \ket{jk} + a_1 \ket{1} \otimes b_{jk} \ket{\bar{j}k} \\ &= a_0 \ket{0} \otimes b_{jk} \ket{jk} + a_1 \ket{1} \otimes b_{\bar{j}k} \ket{jk}\end{aligned}$$

$$\begin{aligned}\ket{\psi_2} &= a_0 H \ket{0} \otimes b_{jk} \ket{jk} + a_1 H \ket{1} \otimes b_{\bar{j}k} \ket{jk} \\ &= a_0 \frac{\ket{0} + \ket{1}}{\sqrt{2}} \otimes b_{jk} \ket{jk} + a_1 \frac{\ket{0} - \ket{1}}{\sqrt{2}} \otimes b_{\bar{j}k} \ket{jk} \\ &= \frac{1}{\sqrt{2}} \left[\left(a_0 b_{jk} + a_1 b_{\bar{j}k} \right) \ket{0jk} \right] + \frac{1}{\sqrt{2}} \left[\left(a_0 b_{jk} - a_1 b_{\bar{j}k} \right) \ket{1jk} \right]\end{aligned}$$

This final state $\ket{\psi_2}$ cannot be written in the form $\ket{\psi} = (\text{any 2 qubit state}) \otimes (a_i b_{ik} \ket{k})$. Thus, both the Hadamard Test and the Inverse Bell Test allow us to measure the expected value of the permutation operator, but don't leave the last qubit in the desired contracted pure state as we hoped from our analytical calculation of that expectation value. In the next section we'll see another way in which we can use the Inverse Bell transformation circuit to force the last qubit to be in our desired pure state by measuring the other qubits.

5 Contraction method: Projection on $\ket{\beta_{00}}$.

We are looking for a method to perform the contraction $a_i b_{jk} \ket{ijk} \rightarrow a_i b_{ik} \ket{k}$ on a quantum computer. Since in practice we cannot simply 'get rid off' two qubits (i and j), the perfect method would perform unitary operations on the initial (not yet contracted) state $\ket{\psi} = a_i b_{jk} \ket{ijk}$ such that the final state could be written in the form.

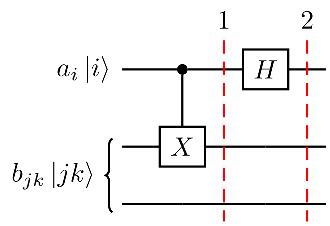
$$\ket{\psi} = (\text{any 2 qubit state}) \otimes (a_i b_{ik} \ket{k})$$

Technically if we found such method, it would mean we found a general method to disentangle a previously entangled qubit from the rest of the qubits, which according to [2] seems to be very difficult to do with certainty.

A method by which it is possible leave the qubit we want a pure state is by measuring all the other qubits. Thus, if we find an algorithm that generates a final state $|\psi\rangle = a_s b_{sk} |ijk\rangle$ for some pair i, j, then we would know that our wanted qubit is in our wanted contracted state if we measured the first 2 qubits to have values i and j. Turn out that one such algorithm is the one that changes the basis to the bell states.

5.1 3-qubit example

The circuit that will perform the contraction as we've specified it is



The states along the circuit are:

$$\begin{aligned} |\psi_0\rangle &= a_i b_{jk} |ijk\rangle \\ &= [a_0 |0\rangle + a_1 |1\rangle] \otimes b_{jk} |jk\rangle \end{aligned}$$

$$\begin{aligned} |\psi_1\rangle &= a_0 |0\rangle \otimes b_{jk} |jk\rangle + a_1 |1\rangle \otimes b_{jk} |\bar{j}k\rangle \\ &= a_0 |0\rangle \otimes b_{jk} |jk\rangle + a_1 |1\rangle \otimes b_{\bar{j}k} |jk\rangle \end{aligned}$$

$$\begin{aligned} |\psi_2\rangle &= a_0 H |0\rangle \otimes b_{jk} |jk\rangle + a_1 H |1\rangle \otimes b_{\bar{j}k} |jk\rangle \\ &= a_0 \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes b_{jk} |jk\rangle + a_1 \frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes b_{\bar{j}k} |jk\rangle \\ &= \frac{1}{\sqrt{2}} \left[\left(a_0 b_{jk} + a_1 b_{\bar{j}k} \right) |0jk\rangle \right] + \frac{1}{\sqrt{2}} \left[\left(a_0 b_{jk} - a_1 b_{\bar{j}k} \right) |1jk\rangle \right] \end{aligned}$$

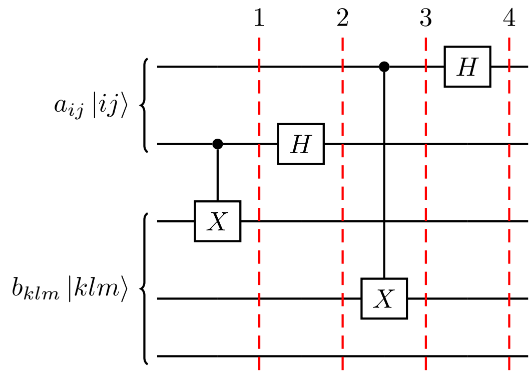
We see that the component with $i = j = 0$ is:

$$\frac{1}{\sqrt{2}} \left(a_0 b_{0k} + a_1 b_{1k} \right) |00k\rangle$$

and the contraction we wanted was $a_i b_{ik} |k\rangle = (a_0 b_{0k} + a_1 b_{1k}) |k\rangle$.

5.2 5-qubit example

In this case, the contraction we hope to perform is $a_{ij} b_{klm} |ijklm\rangle \rightarrow a_{ij} b_{jim} |m\rangle$



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= a_{ij} b_{klm} \, |ijklm\rangle \\
&= (a_{i0} \, |i0\rangle + a_{i1} \, |i1\rangle) \otimes b_{klm} \, |klm\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_1\rangle &= a_{i0} \, |i0\rangle \otimes b_{klm} \, |klm\rangle + a_{i1} \, |i1\rangle \otimes b_{klm} \, \left|\bar{k}lm\right\rangle \\
&= a_{i0} \, |i0\rangle \otimes b_{klm} \, |klm\rangle + a_{i1} \, |i1\rangle \otimes b_{\bar{k}lm} \, |klm\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_2\rangle &= a_{i0} \frac{|i0\rangle + |i1\rangle}{\sqrt{2}} \otimes b_{klm} \, |klm\rangle + a_{i1} \frac{|i0\rangle - |i1\rangle}{\sqrt{2}} \otimes b_{\bar{k}lm} \, |klm\rangle \\
&= \frac{1}{\sqrt{2}} \left(a_{i0} b_{klm} + a_{i1} b_{\bar{k}lm}\right) |i0klm\rangle + \frac{1}{\sqrt{2}} \left(a_{i0} b_{klm} - a_{i1} b_{\bar{k}lm}\right) |i1klm\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_3\rangle = & \frac{1}{\sqrt{2}} \left(a_{00} b_{klm} + a_{01} b_{\bar{k}lm}\right) |00klm\rangle + \frac{1}{\sqrt{2}} \left(a_{00} b_{klm} - a_{01} b_{\bar{k}lm}\right) |01klm\rangle \\
& + \frac{1}{\sqrt{2}} \left(a_{10} b_{k\bar{l}m} + a_{11} b_{\bar{k}\bar{l}m}\right) |10klm\rangle + \frac{1}{\sqrt{2}} \left(a_{10} b_{k\bar{l}m} - a_{11} b_{\bar{k}\bar{l}m}\right) |11klm\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_4\rangle = & \frac{1}{\sqrt{2}} \left(a_{00} b_{klm} + a_{01} b_{\bar{k}lm}\right) \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0klm\rangle \\
& + \frac{1}{\sqrt{2}} \left(a_{00} b_{klm} - a_{01} b_{\bar{k}lm}\right) \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |1klm\rangle \\
& + \frac{1}{\sqrt{2}} \left(a_{10} b_{k\bar{l}m} + a_{11} b_{\bar{k}\bar{l}m}\right) \frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes |0klm\rangle \\
& + \frac{1}{\sqrt{2}} \left(a_{10} b_{k\bar{l}m} - a_{11} b_{\bar{k}\bar{l}m}\right) \frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes |1klm\rangle
\end{aligned}
$$

The component of $|\psi_4\rangle$ that has $i = j = k = l = 0$ is:

$$\begin{aligned}&\frac{1}{2}\left(a_{00}b_{00m} + a_{01}b_{10m} + a_{10}b_{01m} + a_{11}b_{11m}\right)|0000m\rangle \\ =&\frac{1}{2}a_{ij}b_{jim}\,|m\rangle\end{aligned}$$

Thus, up to the factor multiplicative $\frac{1}{2}$, we have the contracted state we wanted on the last qubit given that we measured all others to be $|0\rangle$.

5.3 3-qubit test

In this section I make clear how to test in the simulator/quantum computer if the state in the left over qubit is in fact the contracted state that we desire.

Generate analytical result

First of all, because I want to test it in any general a_i and b_{jk} tensors, I want to have the freedom of doing it without thinking consciously about things like normalization. Thus, I take this procedure:

- Choose any complex-valued tensors A_i and B_j.
- Normalize each of them $A_i \to a_i \;\; B_{jk} \to b_{jk}$, such that the states $a_i\,|i\rangle$ and $b_{jk}\,|jk\rangle$ are both normalized.
- Contract the normalized tensors to obtain the (not necessarily normalized) wanted contraction:

$$|\psi_{\text{wanted}}\rangle = a_s b_{sk}\,|k\rangle$$

- Multiply by the appropriate factor (seems to be $\left(\frac{1}{\sqrt{2}}\right)^n$ where n is the number of contractions:

$$|\psi_{\text{component}}\rangle = \frac{1}{\sqrt{2}}a_s b_{sk}\,|k\rangle$$

- Rotate it such that it is in the (let's call it canonical) form $\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}$, i.e., the first coefficient is real:

$$|\psi_{\text{component canonical}}\rangle = \frac{1}{\sqrt{2}}a'_s b'_{sk}\,|k\rangle$$

Just to make it clear here, the way to put any general state

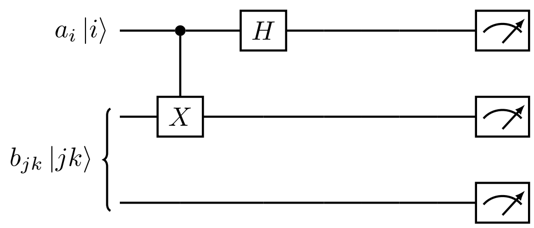
$$|\alpha|\,e^{i\theta_\alpha}\,|0\rangle + |\beta|\,e^{i\theta_\beta}\,|1\rangle$$

in the canonical form is to multiply it by $e^{-i\theta_\alpha}$.

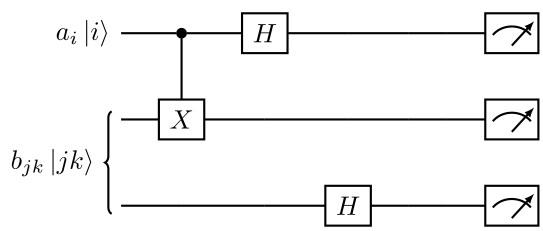
Simulator result

To test if the last qubit is in the pure state (the normalized version of) $a_s b_{sk} |k\rangle$, we need to implement the 3 tests mentioned in the earlier section, namely we'll send the following circuits to qiskit:

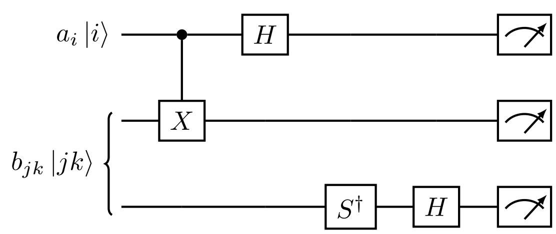
Test 1:



Test 2:



Test 3:



In each test, a dictionary of the following form is generated:

$$\{|000\rangle\ :\ C_{000}\,;\ |001\rangle\ :\ C_{001}\,;\ \ldots\}\,,$$

where C_{ijk} is the number of measures of the state$|ijk\rangle$. We first build the probabilities dictionary of just the last qubit, i.e.:

$$\left\{|0\rangle\ :\ \frac{C_{000}}{C_{000}+C_{001}}\,;\ |1\rangle\ :\ \frac{C_{001}}{C_{000}+C_{001}}\right\}$$

With these probabilities, we reconstruct a normalized canonical state of the form

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|1\rangle$$

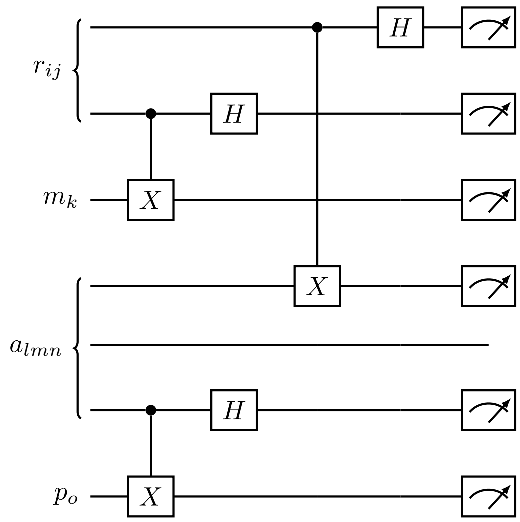
and we need to correct it's norm to the norm of the actual component of the overall 3-qubit state, which is

$$|\psi_{\text{component canonical}}\rangle = \sqrt{\frac{C_{000}+C_{001}}{\sum_{ijk} C_{ijk}}}\left[\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|1\rangle\right]$$

6 Ambiguous readings on Bob Coeck method

6.1 Using swap gates to generate different contraction

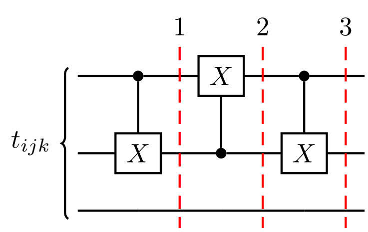
Let's consider the phrase 'rigorous mathematicians and physicists' from the first section. The relevant circuit for interpretation I (only the mathematicians are necessarily rigorous) using the Boeb Coeck method is:



The contraction we obtain with the Bob Coeck method is:

$$|\psi_{\text{component}}\rangle = \frac{1}{2\sqrt{2}} r_{\nu\mu} m_{\mu} a_{\nu m \lambda} p_{\lambda} \, |m\rangle$$

Let's show that we can use two swap gates to generate Interpretation II. The swap gate acts in exactly the same way as the permutation operator: $\hat{P}_{01}\left[t_{ijk}\,|ijk\rangle\right] = t_{ijk}\,|jik\rangle = t_{jik}\,|ijk\rangle$, as we can see, where we decompose the 2-qubit swap gate in terms of more fundamental gates:

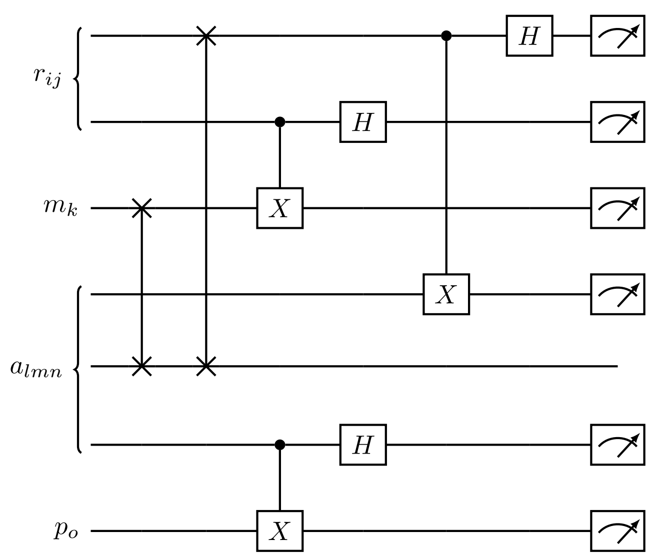


The states along the circuit are:

$$\begin{aligned}
|\psi_0\rangle &= t_{ijk}\,|ijk\rangle \\
&= t_{00k}\,|00k\rangle + t_{01k}\,|01k\rangle + t_{10k}\,|10k\rangle + t_{11k}\,|11k\rangle \\
|\psi_1\rangle &= t_{00k}\,|00k\rangle + t_{01k}\,|01k\rangle + t_{10k}\,|11k\rangle + t_{11k}\,|10k\rangle \\
|\psi_2\rangle &= t_{00k}\,|00k\rangle + t_{01k}\,|11k\rangle + t_{10k}\,|01k\rangle + t_{11k}\,|10k\rangle \\
|\psi_3\rangle &= t_{00k}\,|00k\rangle + t_{01k}\,|10k\rangle + t_{10k}\,|01k\rangle + t_{11k}\,|11k\rangle \\
&= t_{ijk}\,|jik\rangle \\
&= t_{jik}\,|ijk\rangle
\end{aligned}$$

Thus, the action of a swap gate can be expressed by either swapping the indices in the ket or in the coefficients.

The circuit that generates interpretation II is:



Thus, this circuit first does the following:

$$\begin{aligned}
|\psi_0\rangle &= r_{ij} m_k a_{lmn} p_o\,|ijklmno\rangle \\
|\psi_1\rangle &= r_{ij} m_m a_{lkn} p_o\,|ijklmno\rangle \\
|\psi_2\rangle &= r_{mj} m_i a_{lkn} p_o\,|ijklmno\rangle
\end{aligned}$$

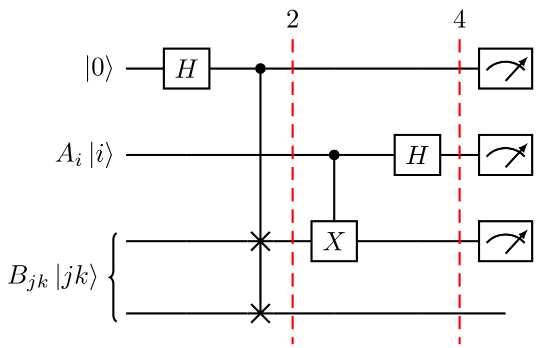
and then the contraction proceeds normally, contracting $(j,k),(i,l),(n,o)$, resulting in

$$|\psi_{\text{component}}\rangle = \frac{1}{2\sqrt{2}} r_{m\mu} m_\nu a_{\nu\mu\lambda} p_\lambda\,|m\rangle$$

which comparing to $r_{ij} m_l a_{ljn} p_n \hat{n}_i$ is the same contraction.

6.2 Using control bit to put different readings in superposition

We can use a control bit in the $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ state to put different readings in superposition. Let's show this by first considering the general 3-qubit example below.



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= |0\rangle \otimes A_i B_{jk} |ijk\rangle \\
|\psi_2\rangle &= |0\rangle \otimes \frac{1}{\sqrt{2}} A_i B_{jk} |ijk\rangle + |1\rangle \otimes \frac{1}{\sqrt{2}} A_i B_{kj} |ijk\rangle \\
|\psi_4\rangle &= \underbrace{|0\rangle}_{\text{control qubit} = 0} \otimes \frac{1}{2} \underbrace{A_\mu B_{\mu k} |00k\rangle}_{\text{reading I}} + \underbrace{|1\rangle}_{\text{control qubit} = 1} \otimes \frac{1}{2} \underbrace{A_\mu B_{k\mu} |00k\rangle}_{\text{reading II}} + \dots
\end{aligned}
$$

Testing this method on a quantum computer simulator, we obtain the results represented in Figure 1.

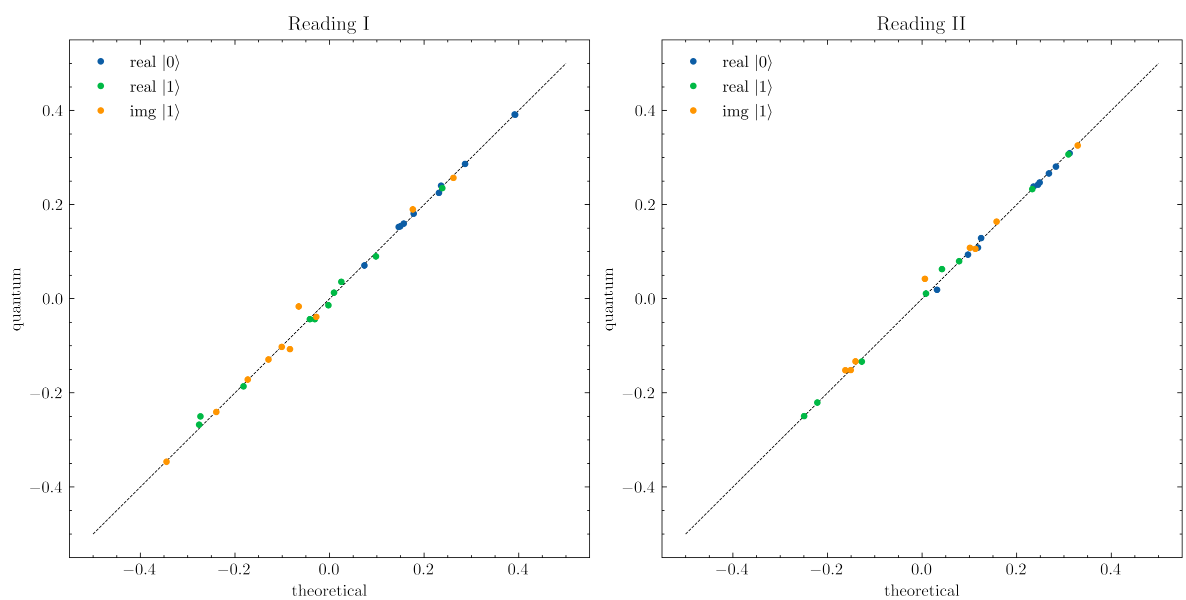


Figure 1: Results of the superposition method in a quantum computer simulator. In this simulation, $N = 8192$ shots were performed for each of the 3 tests mentioned in section 2.

Performing the exact same procedure on an actual quantum computer, with the same amount of shots, we obtain the results represented in Figure 2.

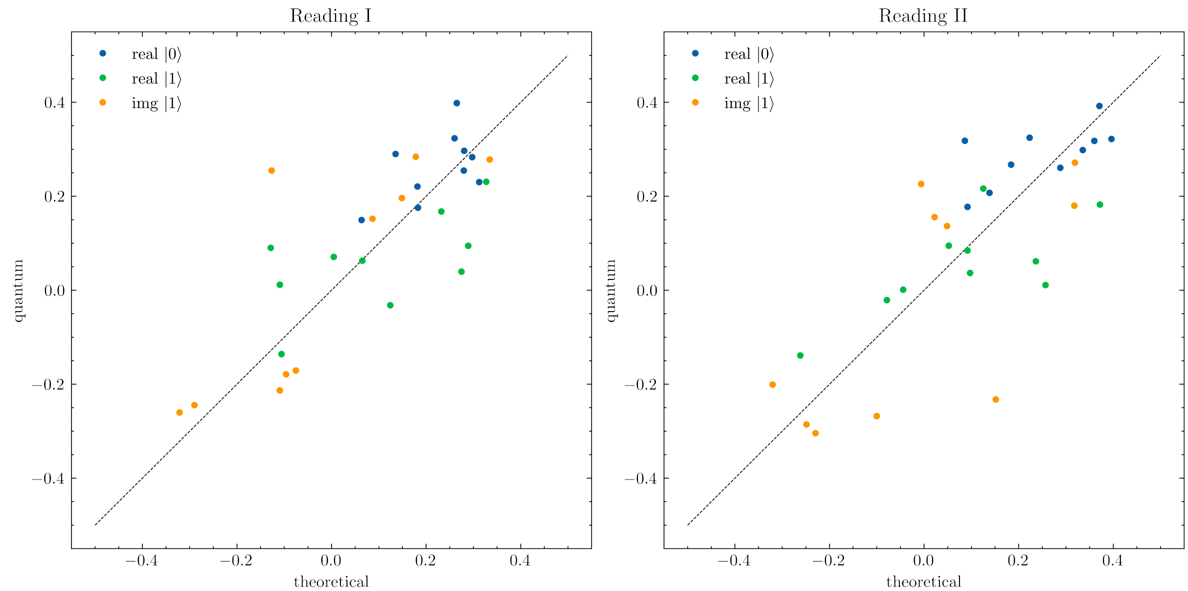
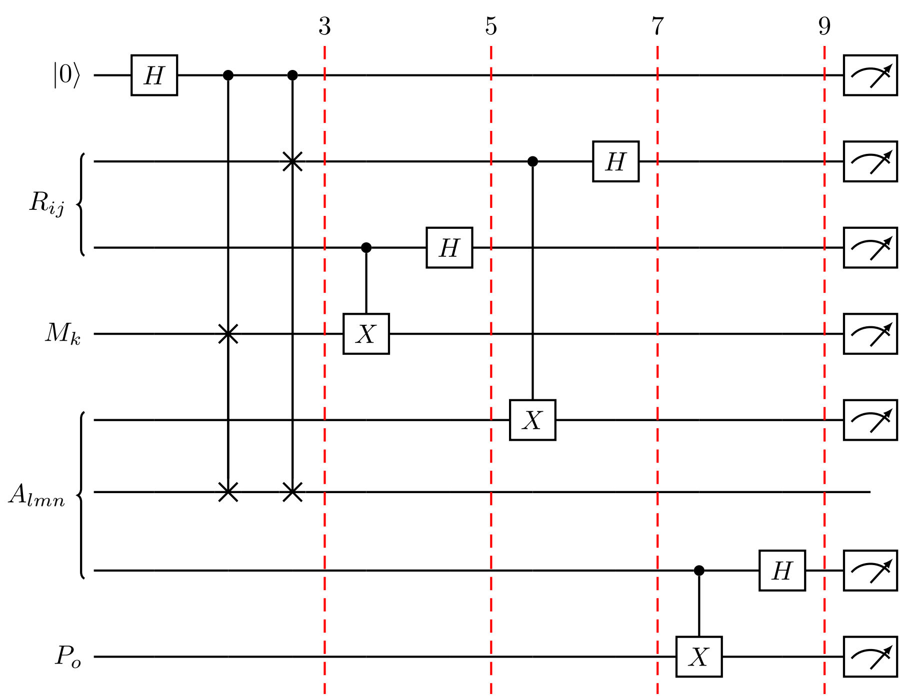


Figure 2: Results of the superposition method in a quantum computer. In this procedure, $N = 8192$ shots were performed for each of the 3 tests mentioned in section 2.

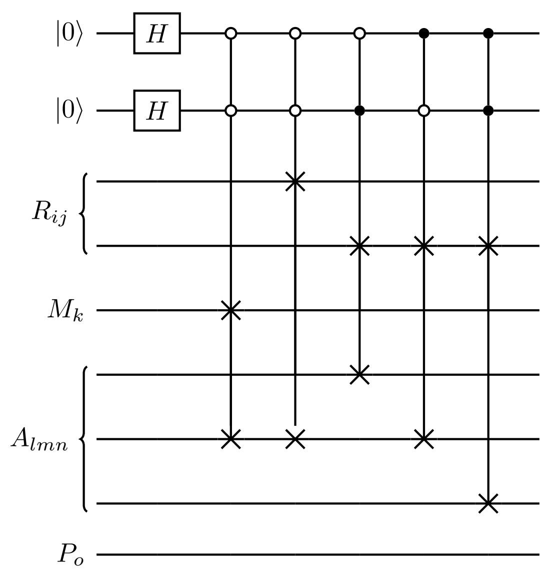
What if we have a more complicated case, like the expression *'rigorous mathematicians and physicists'*? Even if it's not the case, one can imagine that the type complexity of this expression is high enough to generate more than 2 different valid readings, and in that case what would be the proper procedure to put them in superposition? The circuit that performs just one of the valid readings.



The states along the circuit are:

$$
\begin{aligned}
|\psi_0\rangle &= R_{ij} M_k A_{lmn} P_o \, |0ijklmno\rangle \\
|\psi_3\rangle &= \frac{1}{\sqrt{2}} R_{ij} M_k A_{lmn} P_o \, |0ijklmno\rangle + \frac{1}{\sqrt{2}} R_{mj} M_i A_{lkn} P_o \, |1ijklmno\rangle \\
|\psi_5\rangle &= \frac{1}{2} R_{i\mu} M_\mu A_{lmn} P_o \, |0i00lmno\rangle + \frac{1}{2} R_{m\mu} M_i A_{l\mu n} P_o \, |1i00lmno\rangle + \dots \\
|\psi_7\rangle &= \frac{1}{2\sqrt{2}} R_{\nu\mu} M_\mu A_{\nu mn} P_o \, |00000mno\rangle + \frac{1}{2\sqrt{2}} R_{m\mu} M_\nu A_{\nu\mu n} P_o \, |10000mno\rangle + \dots \\
|\psi_9\rangle &= \underbrace{|0\rangle}_{\text{control qubit } = 0} \otimes \frac{1}{4} \underbrace{R_{\nu\mu} M_\mu A_{\nu m\lambda} P_\lambda \, |0000m00\rangle}_{\text{Interpretation I}} + \underbrace{|1\rangle}_{\text{control qubit } = 1} \otimes \frac{1}{4} \underbrace{R_{m\mu} M_\nu A_{\nu\mu\lambda} P_\lambda \, |0000m00\rangle}_{\text{Interpretation II}} + \dots
\end{aligned}
$$

For more than two readings, one idea would be to add more control bits, as in the following circuit:



This circuit generates a final state, after the same contractions of the previous circuit, of the form:

$$
\begin{aligned}
|\psi_{\text{final}}\rangle = |00\rangle &\otimes \frac{1}{\sqrt{2}^5} (\text{reading I}) \, |0000m00\rangle \\
+ |01\rangle &\otimes \frac{1}{\sqrt{2}^5} (\text{reading II}) \, |0000m00\rangle \\
+ |10\rangle &\otimes \frac{1}{\sqrt{2}^5} (\text{reading III}) \, |0000m00\rangle \\
+ |11\rangle &\otimes \frac{1}{\sqrt{2}^5} (\text{reading IV}) \, |0000m00\rangle + \dots
\end{aligned}
$$

One problem that seems to arise is that the probability to measure one of this valid states (there are a lot of invalid states hidden in the '...') drops exponentially, as expected, since each control qubit we add results in a doubling of possible basis states. For a quick analysis, let's assume that we want to perform a general contraction in which we leave only one qubit in the end of the circuit. Let C be the number of index contractions for each interpretation, and 2^r the number of possible readings.

Then the probability of measuring a contraction we want C_i, where the left over qubit has index k, is:

$$P_{\text{valid}} = \frac{1}{2^{C+r}} \sum_{i=0}^{2^n} |C_{ik}|^2$$

So, if we can conveniently afford to perform 2^n shots in a quantum computer, on average we'll have

$$N_{\text{valid}} = 2^{n-C-r} \sum_{i=0}^{2^n} |C_{ik}|^2$$

valid shots, and because the sum is always less than 1, we have:

$$N_{\text{valid}} \leq 2^{n-C-r}$$

For the simple example 'rigorous mathematicians and physicists', we have $C = 3$ and $r = 1$, so if we can afford $2^{13} = 8192$ shots, so $n = 13$, we would on average observe $N_{\text{valid}} \leq 2^9 = 512$ valid shots.

7 Thoughts about the usage of Grover's Algorithm

7.1 Quick overview

In his 1996 paper *'A fast quantum mechanical algorithm for database search'*, Grover showed the existence of a (the fastest actually) algorithm that identified a record satisfying a particular property, in an unsorted database containing N records. One necessary procedure in this algorithm is the creation of a configuration in which the amplitude of the system being in any of the 2^n basis state is equal, which is:

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{2^n}} \sum_{\sigma_i \in \{0,1\}^n} |\sigma_i\rangle$$

where σ_i is a certain n-bit string, so writing this more clearly for $n = 3$:

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{2^3}} \left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right]$$

To apply Grover's Algorithm to a $N = 2^n$ record database, one needs to associate each record S_i to a bit string, so for example

$$S_0 \equiv |000\rangle$$

$$S_1 \equiv |001\rangle$$

$$\ldots \equiv \ldots$$

$$S_i \equiv |\sigma_i\rangle$$

The way the algorithm know how to pick the desired record involves the usage of an *Oracle*, which acts on each basis state in the following way:

$$|x\rangle \xrightarrow{O} (-1)^{f(x)}|x\rangle$$

where $f(x) = 1$ if x is a desired state, and $f(x) = 0$ otherwise.

8 Grover's algorithm for semantic analysis

In this section I'll analyze section 4.3 of [3], to gain a deeper understanding of it. After a circuit that contracts a certain state, for example as explained in section 5, let's suppose the contracted form (let's forget normalizations for now), is:

$$|\psi_{\text{initial}}\rangle = \sum_{aij} W_i^a t_{ij} |a\rangle |s_j\rangle$$

Each ket $|a\rangle$ represents the index of a word, e.g. if we had 4 possible answers {dog, cat, eagle, mouse}, these $|a\rangle$ states could be:

$$|\text{dog}\rangle = |00\rangle$$

$$|\text{cat}\rangle = |01\rangle$$

$$|\text{eagle}\rangle = |10\rangle$$

$$|\text{mouse}\rangle = |11\rangle$$

and the $|s_j\rangle$ would be a 1-qubit ket, with $|\text{false}\rangle = |0\rangle$ and $|\text{true}\rangle = |1\rangle$.

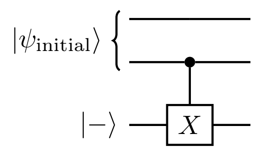
The general assumption is that the representation of the words in the the form of the tensors W_i^a and t_{ij} is such that:

$$\sum_i W_i^a t_{ij} = \begin{cases} 1 & \text{if the pairing } (a, s_j) \text{ is correct} \\ 0 & \text{otherwise} \end{cases}$$

So for example if the question was ‘Is it a bird?’, $|\psi_{\text{initial}}\rangle$ would be

$$
\begin{aligned}
|\psi_{\text{initial}}\rangle &= \frac{1}{\sqrt{4}}\left(|00\rangle \otimes |0\rangle + |01\rangle \otimes |0\rangle + |10\rangle \otimes |1\rangle + |11\rangle \otimes |0\rangle\right) \\
&= \frac{1}{\sqrt{4}}\left(|\text{dog}\rangle \otimes |\text{false}\rangle + |\text{cat}\rangle \otimes |\text{false}\rangle + |\text{eagle}\rangle \otimes |\text{true}\rangle + |\text{mouse}\rangle \otimes |\text{false}\rangle\right)
\end{aligned}
$$

We want to use Grover’s algorithm on this state in order to measure words with $|s_j\rangle = |\text{true}\rangle$, in our case $|\text{eagle}\rangle$, with high probability. The oracle $\hat{O}$ for this problem is very simple:



where the qubit $|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$ is part of the oracle workspace. However, our initial state $|\psi_{\text{initial}}\rangle$ is the usual initial state in Grover’s algorithm, as was mentioned in section 7.

It turns out that if we make the change

$$
\left(2\,|\psi\rangle\,\langle\psi| - \hat{1}\right)\hat{O} \longrightarrow \left(2\,|\psi_{\text{initial}}\rangle\,\langle\psi_{\text{initial}}| - \hat{1}\right)\hat{O}
$$

or expressed in a different way,

$$
H^{\otimes n}\left(2\,|0\rangle\,\langle 0| - \hat{1}\right)H^{\otimes n}\hat{O} \longrightarrow U\left(2\,|0\rangle\,\langle 0| - \hat{1}\right)U^{\dagger}\hat{O}
$$

where $U\,|0\rangle = |\psi_{\text{initial}}\rangle$. Let’s also express $|\psi_{\text{initial}}\rangle$ in the usual way. Firstly, we define the following states:

$$
\begin{aligned}
|\alpha\rangle &= \frac{1}{\sqrt{P-Q}}\sum_{x}|x\rangle \\
|\beta\rangle &= \frac{1}{\sqrt{Q}}\sum_{x'}|x'\rangle
\end{aligned}
$$

where $|x\rangle = |a\rangle \otimes |0\rangle$ and $|x'\rangle = |a\rangle \otimes |1\rangle$. Thus we can write:

$$
\begin{aligned}
|\psi_{\text{initial}}\rangle &= \frac{1}{\sqrt{4}}\left(|00\rangle \otimes |0\rangle + |01\rangle \otimes |0\rangle + |10\rangle \otimes |1\rangle + |11\rangle \otimes |0\rangle\right) \\
&= \frac{\sqrt{3}}{\sqrt{4}}\frac{1}{\sqrt{3}}\left[|00\rangle + |01\rangle + |11\rangle\right] \otimes |0\rangle + \frac{1}{\sqrt{4}}|10\rangle \otimes |1\rangle \\
&= \frac{\sqrt{3}}{\sqrt{4}}|\alpha 0\rangle + \frac{1}{\sqrt{4}}|\beta 1\rangle \\
&= \cos\left(\frac{\theta}{2}\right)|\alpha 0\rangle + \sin\left(\frac{\theta}{2}\right)|\beta 1\rangle
\end{aligned}
$$

This allows us recover the same computation that was happening in the usual Grover's algorithm:

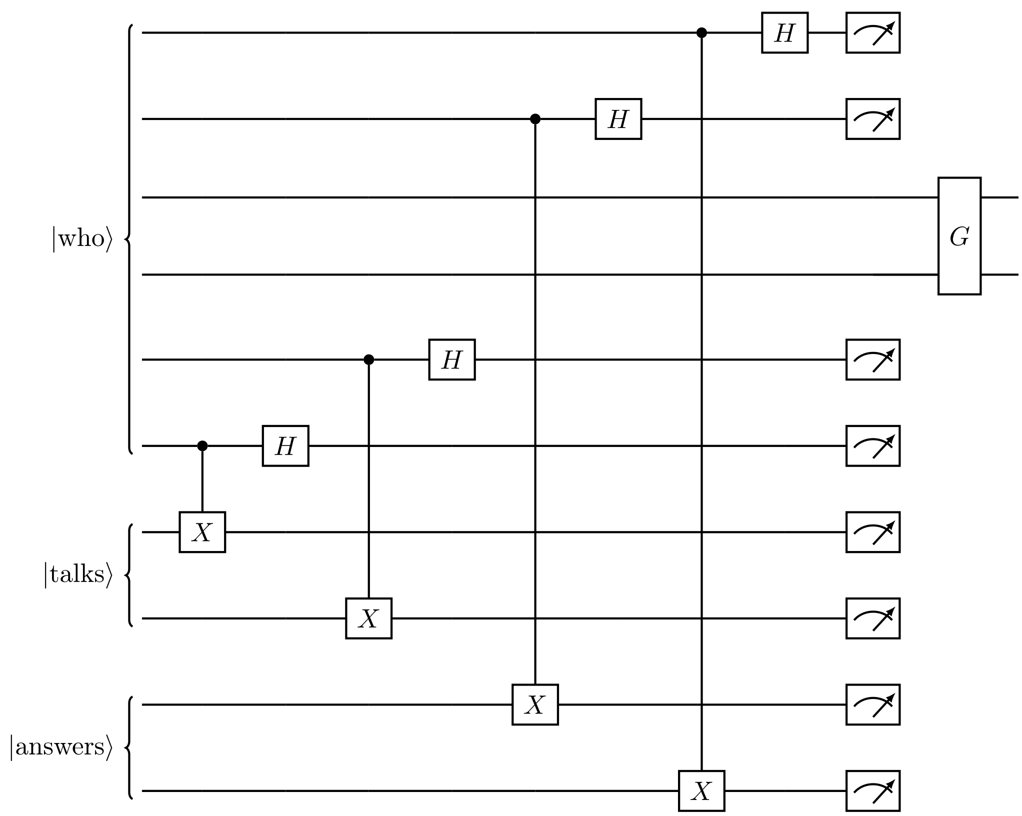
$$
\begin{aligned}
&\left(2\left|\psi_{\text{initial}}\right\rangle\left\langle\psi_{\text{initial}}\right|-\hat{1}\right)\hat{O}\left|\psi_{\text{initial}}\right\rangle\\
=&\left[2\left(\cos\left(\frac{\theta}{2}\right)\langle\alpha 0|+\sin\left(\frac{\theta}{2}\right)\langle\beta 1|\right)\left(\cos\left(\frac{\theta}{2}\right)|\alpha 0\rangle+\sin\left(\frac{\theta}{2}\right)|\beta 1\rangle\right)-\hat{1}\right]\left[\cos\left(\frac{\theta}{2}\right)|\alpha 0\rangle-\sin\left(\frac{\theta}{2}\right)|\beta 1\rangle\right]\\
=&\ldots\\
=&\cos\left(\frac{3\theta}{2}\right)|\alpha 0\rangle+\sin\left(\frac{3\theta}{2}\right)|\beta 1\rangle
\end{aligned}
$$

Thus the proof of convergence of this altered Grover's algorithm is the same as the usual one. The missing piece of the puzzle is: how do we build U, s.t. $U|0\rangle = |\psi_{\text{initial}}\rangle$, at 'runtime'?

In my view, some observations worth mentioning are:

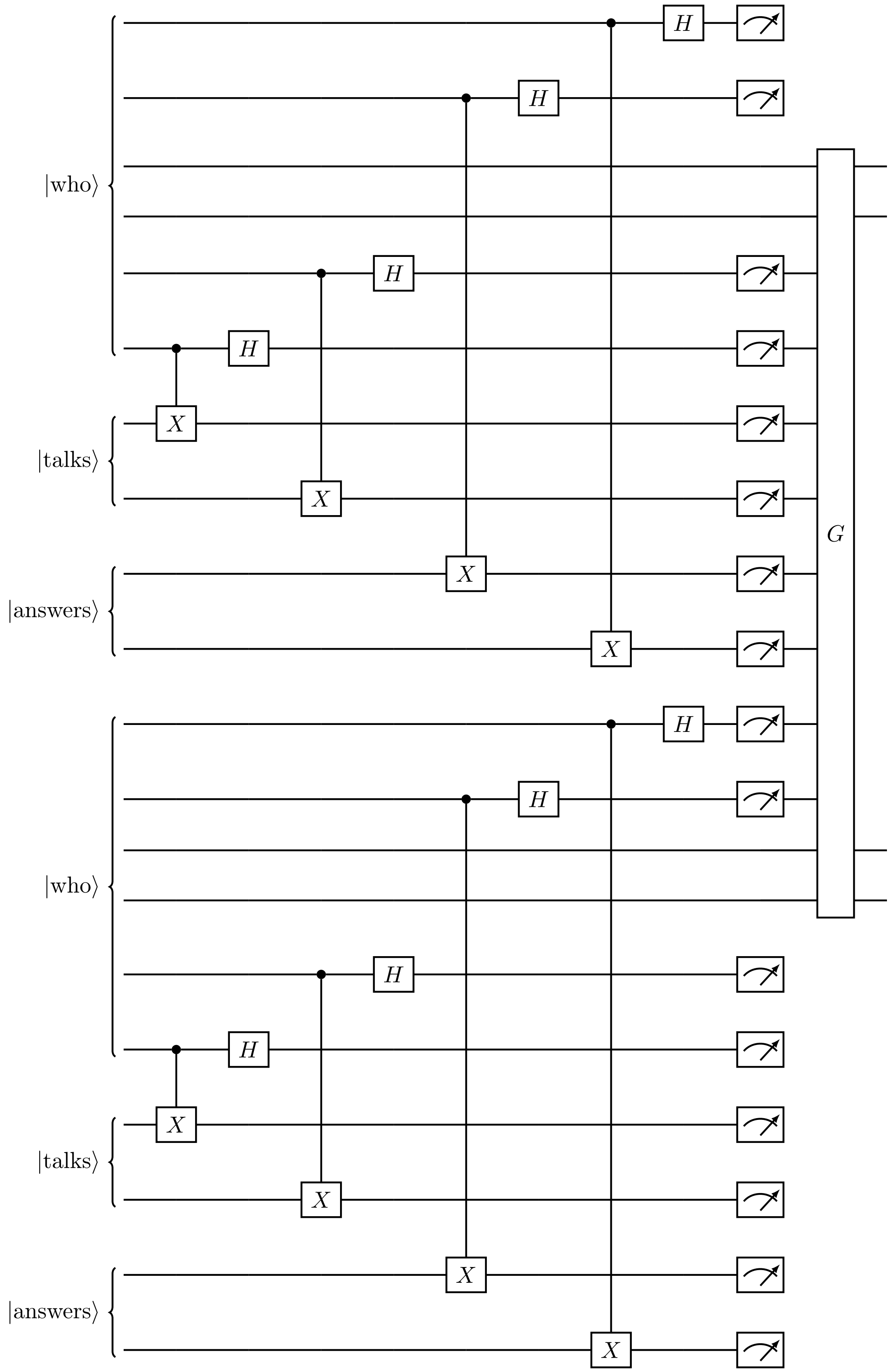
1. We are trying to find one circuit that does two things: take initial words represented in quantum states and contract them into $|\psi_{\text{initial}}\rangle$; take $|\psi_{\text{initial}}\rangle$ and apply the operator $U\left(2|0\rangle\langle 0|-\hat{1}\right)U^{\dagger}\hat{O}$ several times, until we can measure a state with truth value $s_j = 1$ with high probability.

2. If we choose to keep the size of the total qubit space, for example as in the following picture:



Then we would have to know what exactly $|\psi_{\text{initial}}\rangle$ is even before running the circuit, such that we can build U. But because we don't know that (the circuit itself will calculate $|\psi_{\text{initial}}\rangle$), we can't build U.

3. Another option that comes to mind would be that of duplicating the qubit space, and have half of it only contract the state and use it as a control to apply U, like this:



To make this idea work, we would have to come up with a procedure U that performs $U\left(|\psi_{\text{initial}}\rangle \otimes |0\rangle\right) = |\psi_{\text{initial}}\rangle \otimes |\psi_{\text{initial}}\rangle$ (or some other standard pure state $|g\rangle$ in place of $|0\rangle$). Let's suppose there is such a unitary operator U that performs that copy. If we have two different initial states (for example, cause by asking a different question) $|\psi_{\text{initial}}\rangle$ and $|\phi_{\text{initial}}\rangle$, then we have:

$$U\left(|\psi_{\text{initial}}\rangle \otimes |0\rangle\right) = |\psi_{\text{initial}}\rangle \otimes |\psi_{\text{initial}}\rangle$$
$$U\left(|\phi_{\text{initial}}\rangle \otimes |0\rangle\right) = |\phi_{\text{initial}}\rangle \otimes |\phi_{\text{initial}}\rangle$$

and we take the inner product of both expressions, we have:

$$\begin{aligned}\left[\left(\langle\phi_{\text{initial}}| \otimes \langle 0|\right) U^\dagger\right]\left[U\left(|\psi_{\text{initial}}\rangle \otimes |0\rangle\right)\right] &= \left[\langle\phi_{\text{initial}}| \otimes \langle\phi_{\text{initial}}|\right]\left[|\psi_{\text{initial}}\rangle \otimes |\psi_{\text{initial}}\rangle\right] \\ \left(\langle\phi_{\text{initial}}| \otimes \langle 0|\right)\left(|\psi_{\text{initial}}\rangle \otimes |0\rangle\right) &= \langle\phi_{\text{initial}}|\,\psi_{\text{initial}}\rangle^2 \\ \langle\phi_{\text{initial}}|\,\psi_{\text{initial}}\rangle &= \langle\phi_{\text{initial}}|\,\psi_{\text{initial}}\rangle^2\end{aligned}$$

which implies $\langle\phi_{\text{initial}}|\,\psi_{\text{initial}}\rangle = 0$ or $\langle\phi_{\text{initial}}|\,\psi_{\text{initial}}\rangle = 1$, meaning either $|\psi_{\text{initial}}\rangle$ and $|\phi_{\text{initial}}\rangle$ are orthogonal, or $|\psi_{\text{initial}}\rangle = |\phi_{\text{initial}}\rangle$. This is the no cloning theorem: a *general* quantum cloning device is impossible. Thus, in principle, the idea in this point cannot be implemented.

What about doing the contractions classically? This presents some advantages:

- We know a exact expression for $|\psi_{\text{initial}}\rangle$, which would allow us to come up with a particular gate U' s.t. $U'|0\rangle = |\psi_{\text{initial}}\rangle$. We would just need to initialize $|\psi_{\text{initial}}\rangle$ by 'hand' and then apply Grover's to it.
- We wouldn't have to perform a lot of 'shots' until we measure 0's in all the non-remaining wires.
- In terms of doing proofs of concept, this would make that easier since we can easily build a state like $|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{4}}\left(|00\rangle \otimes |0\rangle + |01\rangle \otimes |0\rangle + |10\rangle \otimes |1\rangle + |11\rangle \otimes |0\rangle\right)$ without having to find special tensors W and t such that $\sum_i W_i^a t_{ij} = 0, 1$.

But also some disadvantages:

- Contracting classically probably makes using Grover's algorithm worthless, since building contracting the state and building the matrix U' is probably of higher complexity than $O(N)$. At least building the matrix is $O(N)$.

9 Generalization of Grover's Algorithm

9.1 Summary

In the paper *Quantum Amplitude Amplification and Estimation* [1], it's shown that if one has a state $|\psi\rangle$ that was generated by a unitary transformation as $|\psi\rangle = \mathcal{A}|0\rangle$, and it can be written as $|\psi\rangle = |\psi_1\rangle + |\psi_0\rangle$, where it is our goal to amplify the state $|\psi_1\rangle$ (i.e. shift more probability mass to it s.t. it is measured with higher probability), then that can be done by repeated application of the operator $Q = -\mathcal{A}S_0\mathcal{A}^\dagger S_\chi$, where S_0 flips the sign only of the zero state and S_χ flips the sign only of the desired state. This works because the m^{th} iteration is:

$$Q^m |\psi\rangle = \frac{1}{\sqrt{a}} \sin\left((2m+1)\,\theta_a\right)|\psi_1\rangle + \frac{1}{\sqrt{1-a}} \cos\left((2m+1)\,\theta_a\right)|\psi_0\rangle$$

where $\theta_a \in \left[0, \frac{\pi}{2}\right]$ is defined s.t. $\sin(\theta_a) = a = \langle\psi_1|\psi_1\rangle$, which means that $|\psi_1\rangle$ will be measured with probability $\sin^2\left((2j+1)\,\theta_a\right)$. It is desired that this probability is close to 1, and that can be achieved by setting $m = \lfloor\frac{\pi}{4\theta_a}\rfloor$, which will produce a good outcome with probability *at least* $\max(1-a, a)$.

9.2 Detailed explanation

In his original 1996 paper [4], Grover formulated his algorithm to work on an initial state consisting of a equal superposition of all basis states, which for the 3-qubit case would be, for clarity:

$$|\psi_{\text{G}}\rangle = \frac{1}{\sqrt{2^3}}\left[|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right]$$

But what if we still wanted to use the same mechanism to amplify a certain part of the state, i.e. shift probability mass into that certain part, but our $|\psi_{\text{initial}}\rangle$ was not the same as $|\psi_{\text{G}}\rangle$? In *Quantum Amplitude Amplification and Estimation* [1], a generalization of Grover's algorithm is achieved, which will be explained in this section.

Consider:

- A Boolean function of the form $\chi : X \to \{0, 1\}$

$$\chi(x) = \begin{cases} 1 \text{ if } x \text{ is } \textit{good} \\ 0 \text{ if } x \text{ is } \textit{bad} \end{cases}$$

- A Hilbert space $\mathcal{H}$.

- A unitary operator $\mathcal{A}$, and a state $|\psi\rangle = \mathcal{A}|0\rangle$.

Because the function χ induces a partition of $\mathcal{H}$ into a direct sum $\mathcal{H}_{good} \oplus \mathcal{H}_{bad}$, any arbitrary state $|\gamma\rangle \in \mathcal{H}$ can be written in the form

$$|\gamma\rangle = |\gamma_1\rangle + |\gamma_0\rangle,$$

where $|\gamma_1\rangle \in \mathcal{H}_{good}$ and $|\gamma_0\rangle \in \mathcal{H}_{bad}$ ($|\gamma_1\rangle$ and $|\gamma_0\rangle$ are in general not normalized states). If we just measured $|\gamma\rangle$, the probability of having a good state as outcome is

$$a = \langle\gamma_1|\gamma_1\rangle$$

The amplification process, which will allow us to measure a good state with much higher probability, consists in repeatedly applying the following operator:

$$Q = -\mathcal{A}S_0\mathcal{A}^{-1}S_\chi$$

where:

$$S_0 |x\rangle = \begin{cases} -|x\rangle \text{ if } x = 0 \\ \\ \quad |x\rangle \text{ otherwise} \end{cases}$$

$$S_\chi |x\rangle = \begin{cases} -|x\rangle \text{ if } x \text{ is } \textit{good} \\ \\ \quad |x\rangle \text{ otherwise} \end{cases}$$

This operator can also be written in a more intuitive way:

$$\begin{aligned} Q &= -\mathcal{A}S_0\mathcal{A}^{-1}S_\chi \\ &= -\mathcal{A}\left(1 - 2|0\rangle\langle 0|\right)\mathcal{A}^{-1}\left(2\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|\psi_0\rangle} - 1\right) \\ &= \left(1 - 2|\psi\rangle\langle\psi|\right)\left(1 - \frac{2}{1-a}|\psi_0\rangle\langle\psi_0|\right) \\ &= U_\psi U_{\psi_0} \end{aligned}$$

which consists in two reflections: first through $|\psi_0\rangle$ and then through $|\psi\rangle$.

Let's denote $\mathcal{H}_\psi$ the subspace spanned by $|\psi_1\rangle$ and $|\psi_0\rangle$. We see that it is stable under Q:

$$\mathrm{Q}|\Psi_1\rangle = (1-2a)|\Psi_1\rangle - 2a|\Psi_0\rangle$$

$$\mathrm{Q}|\Psi_0\rangle = 2(1-a)|\Psi_1\rangle + (1-2a)|\Psi_0\rangle .$$

We can also see that the operator $\mathcal{A}S_0\mathcal{A}^{-1} = 1 - 2|\psi\rangle\langle\psi|$ acts as the identity on $\mathcal{H}_\psi^\perp$, the orthogonal complement of $\mathcal{H}_\psi$, which implies Q acts as $-S_\chi$ on $\mathcal{H}_\psi^\perp$. Thus, Q^2 acts as the identity on $\mathcal{H}_\psi^\perp$, which implies every eigenvector of Q on $\mathcal{H}_\psi^\perp$ has eigenvalue ± 1. Thus, to understand the action of Q in any arbitrary $|\gamma\rangle \in \mathcal{H}$, we only need to consider it's projection onto $\mathcal{H}_\psi$.

Since Q is unitary, the subspace $\mathcal{H}_\psi$ has an orthonormal basis consisting of two eigenvectors of Q:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{a}}|\psi_1\rangle \pm \frac{i}{\sqrt{1-a}}|\psi_0\rangle\right)$$

and their eigenvalues are $\lambda_\pm = e^{\pm i2\theta_a}$. Our initial state $|\psi\rangle$ is written in this basis as

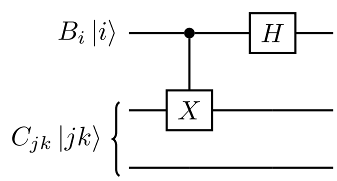
$$|\psi\rangle = \frac{-i}{\sqrt{2}}\left(e^{i\theta_a}|\psi_+\rangle - e^{-i\theta_a}|\psi_-\rangle\right)$$

which implies

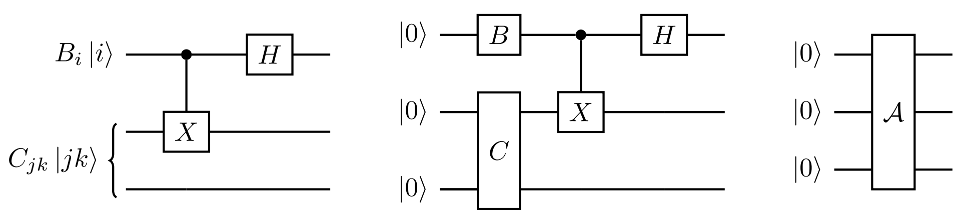
$$
\begin{aligned}
Q^m |\psi\rangle &= \frac{-i}{\sqrt{2}} \left(e^{i(2m+1)\theta_a} |\psi_+\rangle - e^{-i(2j+1)\theta_a} |\psi_-\rangle \right) \\
&= \frac{1}{\sqrt{a}} \sin\left((2m+1)\,\theta_a \right) |\psi_1\rangle + \frac{1}{\sqrt{1-a}} \cos\left((2m+1)\,\theta_a \right) |\psi_0\rangle
\end{aligned}
$$

9.3 How does this look like in our context

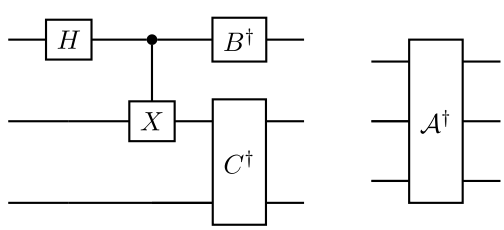
Let's illustrate how this general method applies in our case. For this, let's again consider the simplest contraction possible: the 3-qubit example, given by the circuit:



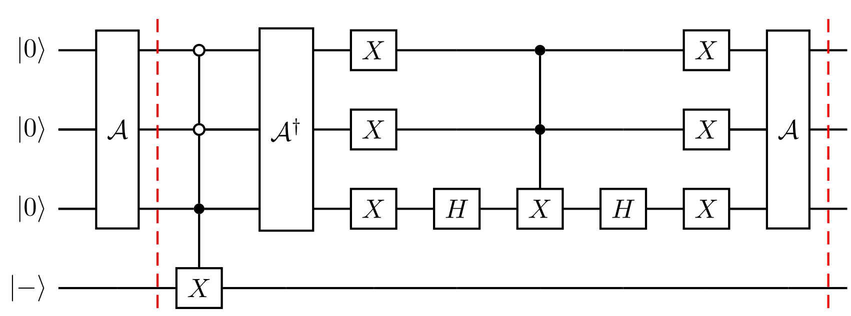
which is equivalent (by definition) to all the following circuits:



where $B|0\rangle = B_i|i\rangle$ and $C|00\rangle = C_{jk}|jk\rangle$ are unitary operators. We also need the operator $\mathcal{A}^\dagger$, which is:



The first iteration of this method thus looks like the following circuit, where algorithm Q is inside the red dashed lines:



In this simple example, our desired basis state is $|001\rangle$, because the component where the two first qubits are 0 has our correct contraction, and the final qubit in this example works as the truth value of the contraction (it corresponds to the $|s_j\rangle$ qubit in the $|\Psi_{\text{initial}}\ \rangle = \sum_{aij} W_{ia} t_{ij} |a\rangle_3 \, |s_j\rangle_4$ of [3].

9.4 Implementation of *who talks?*

In this section we apply this algorithm to the *'who talks?'* in [3]. First of all, we have to make a specific choice of tensors to be contracted. After contractions, the state in the remaining wires should be

$$|\psi_{\text{initial}}\rangle = \sum_{aij} W_{ia} t_{ij} \, |as_j\rangle \, .$$

Let's suppose that we have two possible answers, $|\text{dog}\rangle = |1\rangle$ and $|\text{cat}\rangle = |0\rangle$, and that $|\text{dog}\rangle$ is a correct answer to the question *'who talks?'*, and $|\text{cat}\rangle$ is not. Thus, this state would become:

$$\begin{aligned} |\psi_{\text{initial}}\rangle &= |\text{cat}\rangle \otimes |\text{false}\rangle + |\text{dog}\rangle \otimes |\text{true}\rangle \\ &= |00\rangle + |11\rangle \, . \end{aligned}$$

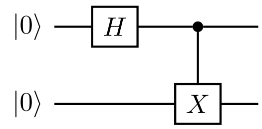
Thus, we have to find tensors W_{ia} and t_{ij} that contract this way. This can be achieved by setting $W_{ij} = \frac{\delta_{ij}}{\sqrt{2}}$ and $t_{ij} = \frac{\delta_{ij}}{\sqrt{2}}$ (the normalization factors need to be there because initial states are generated with these tensors):

$$\begin{aligned} |\psi_{\text{initial}}\rangle &= \sum_{aij} W_{ia} t_{ij} \, |as_j\rangle \\ &= \frac{1}{2} \sum_{aij} \delta_{ia} \delta_{ij} \, |as_j\rangle \\ &= \frac{1}{2} \delta_{00} \delta_{00} \, |00\rangle + \frac{1}{2} \delta_{11} \delta_{11} \, |11\rangle \\ &= \frac{1}{2} \left(|00\rangle + |11\rangle \right) \end{aligned}$$

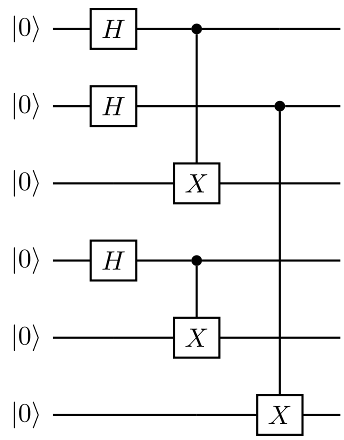
This implies that our (explicit) initial states are:

$$\begin{aligned} |\text{talks}\rangle &= t_{mn} \, |n_m s_n\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right) \\ |\text{answers}\rangle &= W_{pb} \, |n_p b\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right) \\ |\text{who}\rangle &= \frac{1}{\sqrt{8}} \sum_{ail} |a n_i a s_j s_j n_i\rangle \\ &= \frac{1}{\sqrt{8}} \left[|000000\rangle + |000110\rangle + |010001\rangle + |010111\rangle + |101000\rangle + |101110\rangle + |111001\rangle + |111111\rangle \right] \end{aligned}$$

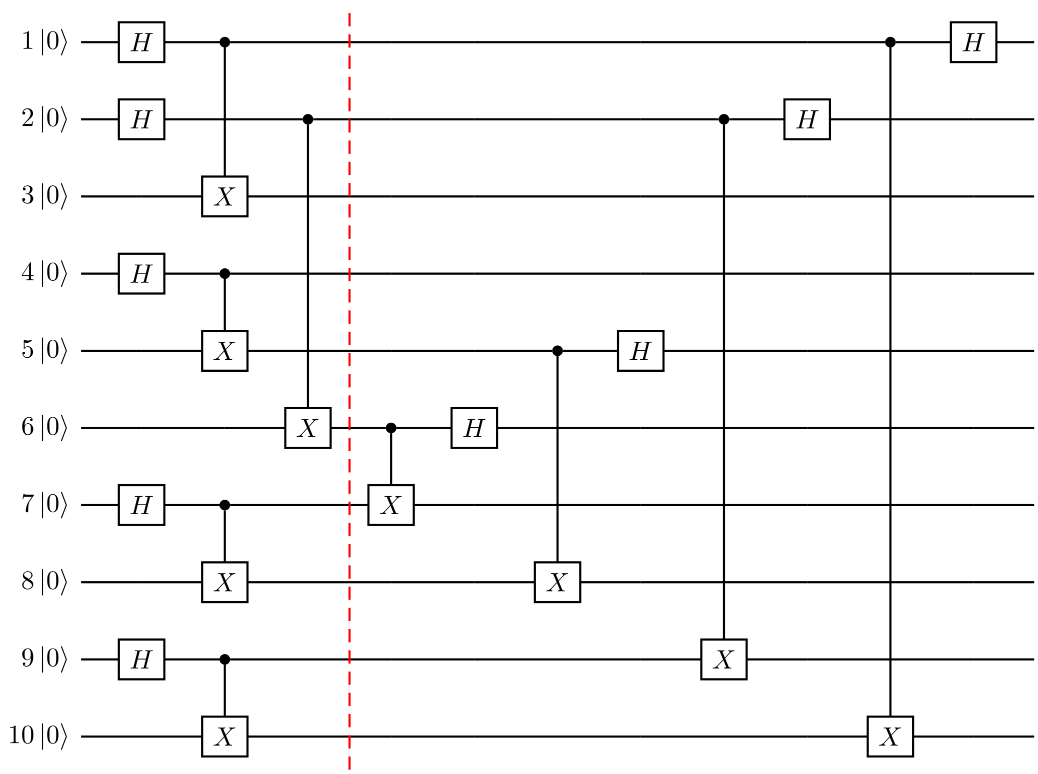
The circuit that generates both $|\text{talks}\rangle$ and $|\text{answers}\rangle$ is:



The circuit that generates $|\text{who}\rangle$ is:



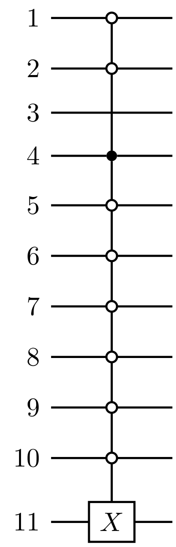
Thus, algorithm $\mathcal{A}$ in this case is:



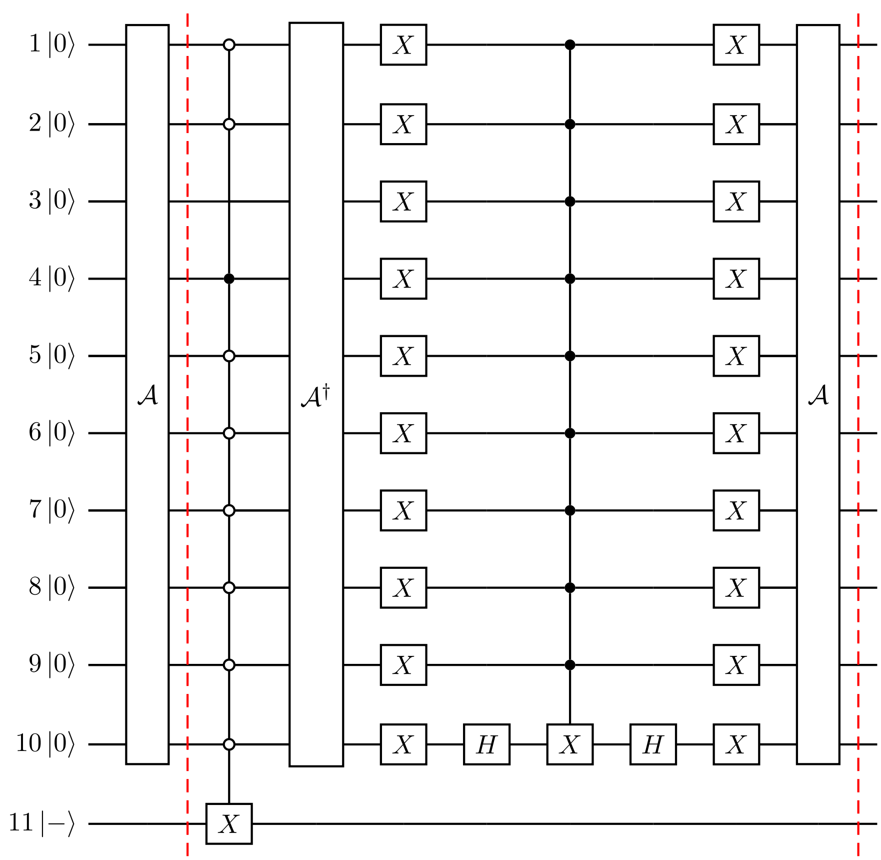
To the left of the red line, we have the initialization of $|\text{who}\rangle$ in wires 1-6, $|\text{talks}\rangle$ in wires 7-8 and $|\text{talks}\rangle$ in wires 9-10. To the right of the red line, we have the contraction algorithm, which hold the right contraction in all states of the form $|00..000000\rangle$, where qubits that have the dot '.' can have any value (and in this case will hold the right contraction).

In the context of the amplification algorithm, the basis states that are allowed to be in the linear superposition $|\psi_1\rangle$ are of the form $|00.1000000\rangle$, because not only we are only interested in the components that have the right contraction ($|00..000000\rangle$)

but we are also interested in keeping the correct answer to the question *'who talks?'*, which means that we also want the qubit in wire 4 to have value of 1. Thus, our oracle operator looks like this:



where the qubit in wire 11 is initially prepared in the $|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$ state. To make everything clear, this is the first iteration of the algorithm:



Performing the simulation, and plotting the probability of finding a desired state, which is

$$P_m = \frac{\langle\psi_1| Q^m |\psi\rangle}{\langle\psi_1|\psi_1\rangle}$$

and theoretically it should be $\sin^2((2m+1)\theta_a)$, we obtain:

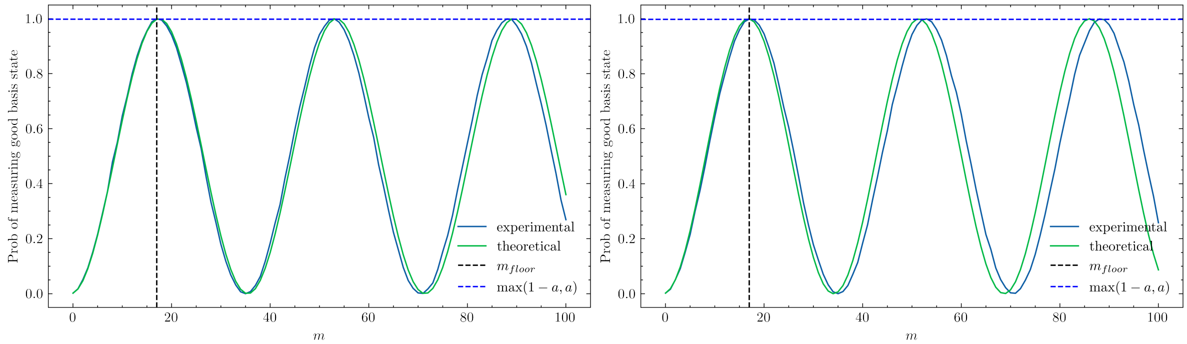


Figure 3: Results of the amplification method in a quantum computer simulator. In this simulation, $N = 8192$ shots were performed for each of the circuits. In our specific *'who talks?'* case, the only desired state is $|0011000000\rangle$, whose probability of being measured is in the y-axis. In the left figure, 1 ancillary bit was used for the oracle, whereas in the right figure no ancillary bits where used.

We can see that after the predicted number of iterations $m_{floor} = \lfloor \frac{\pi}{4\theta_a} \rfloor$, the probability of measuring a desired state is very close to 1, i.e. we would measure the qubit 3 to be 1, which is the index of the correct answer $|\mathrm{dog}\rangle$.

References

[1] Gilles Brassard, Peter HÃžyer, Michele Mosca, and Alain Tapp. Quantum amplitude amplification and estimation. *Quantum Computation and Information*, 2002.

[2] VladimÃr BuÅŸek and Mark Hillery. Quantum disentanglers. *Physical Review A*, 62(5), Oct 2000.

[3] A. D. Correia, M. Moortgat, and H. T. C. Stoof. Grover's algorithm for question answering, 2021.

[4] Lov K Grover. A fast quantum mechanical algorithm for database search. pages 212–219, 1996.

[5] Isaac L. Chuang Michael A. Nielsen. *Quantum computation and quantum information*. Cambridge Series on Information and the Natural Sciences. Cambridge University Press, 1 edition, 2004.