Fall 2023: Final Project
COM-309: Quantum Information Processing

In this project, you will learn about a quantum algorithm for the computation of the trace of a unitary matrix. It has two parts: the theoretical one shows how the circuit is used in this algorithm and in the practical one, you are asked to implement it and see how it works.

Part I
Theoretical Background

1 Bell states

Let $|B_{00}\rangle_{AB} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Show that $|B_{00}\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} |x\rangle_{A_1\ldots A_n} \otimes |x\rangle_{B_1\ldots B_n}$.

Solution: We may express $|B_{00}\rangle_{AB} = \frac{1}{\sqrt{2}} \sum_{x\in\{0,1\}} |x\rangle_A \otimes |x\rangle_B$. Then,

$$\begin{aligned} |B_{00}\rangle^{\otimes n} &= \frac{1}{2^{n/2}} \sum_{x_1\in\{0,1\}} \cdots \sum_{x_n\in\{0,1\}} |x_1\rangle_{A_1} \otimes \ldots |x_n\rangle_A \otimes |x_1\rangle_B \otimes \ldots |x_n\rangle_B \\ &= \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} |x\rangle_{A_1\ldots A_n} |x\rangle_{B_1\ldots B_n}. \end{aligned}$$

or you may use a proof by induction.

2 An interesting quantum circuit

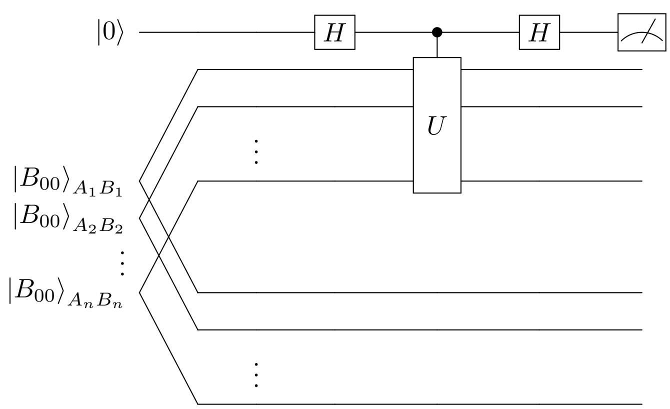

Figure 1: Trace estimation circuit

Figure 1 illustrates a circuit used in the trace estimation algorithm that you will analyze in the following exercise. U is a $2^n \times 2^n$ unitary matrix. This circuit starts with the first qubit in the state $|0\rangle$, and $2n$ qubits in the state $|B_{00}\rangle^{\otimes n}$. A Hadamard gate $H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ is applied to the first qubit. Then, a "controlled unitary"

$$|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$$

is applied from the first qubit to the first n halves of the Bell pairs. That is, the unitary U is applied to the qubits $2, \ldots, n+1$ based on the state of the qubit 1. Another Hadamard gate is applied to the first qubit. Finally, the first qubit is measured in the computational basis $\{|0\rangle, |1\rangle\}$.

1. Compute the probability of measuring the outcome $|0\rangle$ at the end of the circuit shown in Figure 1.

   (a) What is the overall state after the first Hadamard gate?
   Solution:
   $$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |B_{00}\rangle^{\otimes n}$$

   (b) What is the overall state after the controlled unitary? (Hint: use the expression of the Bell state that you proved in question 1)
   Solution:
   $$\frac{1}{\sqrt{2}}\left(|0\rangle \otimes |B_{00}\rangle^{\otimes n} + |1\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U|x\rangle|x\rangle\right)$$

   (c) What is the overall state after the second Hadamard gate?
   Solution:
   $$\begin{aligned}|\psi\rangle = \frac{1}{2}\Bigg(&|0\rangle \otimes |B_{00}\rangle^{\otimes n} + |1\rangle \otimes |B_{00}\rangle^{\otimes n} + |0\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U|x\rangle|x\rangle - |1\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U|x\rangle|x\rangle\Bigg)\\ &= \frac{1}{2^{n/2+1}}\left(|0\rangle \sum_x (|x\rangle + U|x\rangle)|x\rangle + |1\rangle \sum_x (|x\rangle - U|x\rangle)|x\rangle\right)\\ &= \frac{1}{2^{n/2+1}}\left(|0\rangle \sum_x (I+U)\otimes I|x\rangle|x\rangle + |1\rangle \sum_x (I-U)\otimes I|x\rangle|x\rangle\right)\end{aligned}$$

   (d) Show that the probability of getting the outcome $|0\rangle$ is $\frac{1}{2} + \frac{1}{2}\frac{1}{2^n}\mathbf{Re}\{\mathrm{Tr}[U]\}$.
   Solution: Write $U = U_R + iU_I$. The probability of getting the outcome $|0\rangle$ is
   $$\begin{aligned}\langle\psi|\,|0\rangle\langle 0| \otimes I\,|\psi\rangle &= \frac{1}{2^{n+2}} \sum_{x,x'} \langle x|\langle x|\, I \otimes (I+U^\dagger)(I+U) \otimes I\,|x'\rangle|x'\rangle\\ &= \frac{1}{2^{n+2}} \sum_x \langle x|(I+U^\dagger)(I+U)|x\rangle\\ &= \frac{1}{2^{n+2}} \sum_x (2 + \langle x|U^\dagger|x\rangle + \langle x|U|x\rangle)\\ &= \frac{1}{2} + \frac{1}{2^{n+2}}(\mathrm{Tr}[U_R^T - iU_I^T + U_R + iU_I])\\ &= \frac{1}{2} + \frac{1}{2}\frac{1}{2^n}\mathbf{Re}\{\mathrm{Tr}[U]\}\end{aligned}$$

2. Discuss how the normalized real part of the trace $\frac{1}{2^n}\mathbf{Re}\{\mathrm{Tr}[U]\}$ can be computed using this circuit. **Solution:** To estimate the normalized real part of the trace, we can run the circuit N times and record $N_Z = \#$zero outcomes. We can then obtain an estimate of the probability of getting the outcome $|0\rangle$, $\hat{p}_0 = \frac{N_Z}{N}$. The larger N is, the better the estimate. Then, we compute the estimate of the normalized real part of the trace as $2\hat{p}_0 - 1$.

3. Check that the matrix $S = \begin{bmatrix}1 & 0\\ 0 & -i\end{bmatrix}$ represents a valid quantum operation. **Solution:** We can check that $SS^\dagger = S^\dagger S = I$, thus S represents valid unitary evolution.

4. We will modify the circuit in Figure 1 and apply S to the first qubit right after the first Hadamard gate (right before the controlled-unitary). Show how to use the new circuit to compute $\frac{1}{2^n}\mathbf{Im}\{\mathrm{Tr}[U]\}$.

Solution: The state evolution in the modified circuit is described below.
After the first Hadamard:

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |B_{00}\rangle^{\otimes n}.$$

After the application of S:

$$\frac{1}{\sqrt{2}}(|0\rangle - i\,|1\rangle) \otimes |B_{00}\rangle^{\otimes n}.$$

After the controlled unitary:

$$\frac{1}{\sqrt{2}}\Bigg(|0\rangle \otimes |B_{00}\rangle^{\otimes n} - i\,|1\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U\,|x\rangle\,|x\rangle\Bigg).$$

After the second Hadamard gate:

$$\begin{aligned}
|\psi\rangle = \frac{1}{2}\Bigg(|0\rangle \otimes |B_{00}\rangle^{\otimes n} + |1\rangle \otimes |B_{00}\rangle^{\otimes n} - i\,|0\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U\,|x\rangle\,|x\rangle + i\,|1\rangle \frac{1}{2^{n/2}} \sum_{x\in\{0,1\}^n} U\,|x\rangle\,|x\rangle\Bigg) \\
= \frac{1}{2^{n/2+1}}\Bigg(|0\rangle \sum_x (|x\rangle - iU\,|x\rangle)\,|x\rangle + |1\rangle \sum_x (|x\rangle + iU\,|x\rangle)\,|x\rangle\Bigg) \\
= \frac{1}{2^{n/2+1}}\Bigg(|0\rangle \sum_x (I - iU)\otimes I\,|x\rangle\,|x\rangle + |1\rangle \sum_x (I + iU)\otimes I\,|x\rangle\,|x\rangle\Bigg).
\end{aligned}$$

Now we compute the probability of getting the outcome $|0\rangle$

$$\begin{aligned}
\langle\psi|\,|0\rangle\,\langle 0| \otimes I\,|\psi\rangle &= \frac{1}{2^{n+2}} \sum_{x,x'} \langle x|\,\langle x|\, I \otimes (I + iU^\dagger)(I - iU) \otimes I\,|x'\rangle\,|x'\rangle \\
&= \frac{1}{2^{n+2}} \sum_x \langle x|\,(I + iU^\dagger)(I - iU)\,|x\rangle \\
&= \frac{1}{2^{n+2}} \sum_x (2 + i\,\langle x|\,U^\dagger\,|x\rangle - i\,\langle x|\,U\,|x\rangle) \\
&= \frac{1}{2} + \frac{1}{2^{n+2}}(\mathrm{Tr}[iU_R^T + U_I^T - iU_R + U_I]) \\
&= \frac{1}{2} + \frac{1}{2}\frac{1}{2^n}\mathbf{Im}\{\mathrm{Tr}[U]\}
\end{aligned}$$

To estimate the normalized imaginary part of the trace, we follow a similar idea as the one used for estimating the real part. We run the modified circuit N times and record $N_Z^{(I)} = \#$zero outcomes. We can then obtain an estimate of the probability of getting the outcome $|0\rangle$, $\hat{p}_0^{(I)} = \frac{N_Z^{(I)}}{N}$. The larger N is, the better the estimate. Then, we compute the estimate of the normalized imaginary part of the trace as $2\hat{p}_0^{(I)} - 1$.

5. How many addition operations does a naive classical trace computation need to do to compute the trace of a unitary acting on n qubits? **Solution:** A unitary acting on n qubits is a matrix of size $2^n \times 2^n$. To compute the trace, a straightforward way is to sum up all the elements on the diagonal of the unitary. Since there are 2^n elements on the diagonal, we will need to perform $2^n - 1$ (complex) addition operations, or $2(2^n - 1)$ real additions , i.e., $\mathcal{O}(2^n)$ addition operations.

Part II
Practical Implementation

For this part of the project, you will use IBM's quantum computing simulators and a quantum computing software development kit Qiskit, available at `https://lab.quantum-computing.ibm.com/`. Fill in your solutions and code in the accompanying Jupyter notebook.

3 A random unitary and a quantum device

1. Generate a random unitary by generating a random circuit over $n = 5$ qubits with depth (i.e., number of circuit time steps) $= 3$ using Qiskit.

2. Compute the trace of this unitary "classically".

3. Run the trace estimation circuit on a quantum simulator. Compare the trace estimate from the quantum circuit and the classical trace computation.

4 A mystery

You are given a unitary $U_{\text{mystery}} = e^{i\theta(X \otimes X)}$. You do not know the angle θ.

1. How can you use the trace estimation circuit in Figure 1 to estimate θ? (Hint: use the Euler identity for matrices M such that $M^2 = I$.) **Solution:** Using the Euler identity, we can write

$$U_{\text{mystery}} = e^{i\theta(X \otimes X)} = \cos\theta(I \otimes I) + i \sin\theta(X \otimes X).$$

   Note that

$$\mathrm{Tr}[U_{\text{mystery}}] = \cos\theta \mathrm{Tr}[I \otimes I] + i \sin\theta \mathrm{Tr}[X \otimes X] = 4\cos\theta.$$

   Then, we may use the trace estimation circuit to obtain an estimate $\hat{e}$ for $\frac{1}{4}\mathbf{Re}\{\mathrm{Tr}[U_{\text{mystery}}]\} = \cos\theta$. Then, we may compute the estimate for θ; $\hat{\theta} = \cos^{-1}(\hat{e})$.

2. Generate angles $\in [0, 2\pi]$, and run the trace estimation circuit on Qiskit. Plot the estimates vs. θ.

5 Confidence intervals

Suppose we would like to understand how many times you need to run the trace estimation to be close enough to real value. One of the estimates which characterizes this is a confidence interval (CI).

Let $X_1, \ldots, X_k$ be a random sample from a probability distribution p_θ with a parameter θ. Then, $(L(X), U(X))$ is a CI at confidence level γ if for any θ,

$$\mathbb{P}_{X \sim p_\theta}\left(L(X) < \theta < U(X)\right) = \gamma.$$

That is, $L(X)$ and $U(X)$ are 'numbers' (or statistics) computed from the random variable X such that, with probability γ, the true value of the parameter θ should lie between them. Typically, one considers γ close to 1, e.g. $\gamma = 0.95$ or $\gamma = 0.99$. When the interval is "narrow" enough, with some degree of confidence, we can think that the value of the parameter chosen from it is not too different from the real one. Often, it is hard to construct a CI at the exact confidence level γ; one is then satisfied with approximate equality.

One of the ways to derive (an approximate) CI is by application of the central limit theorem (CLT). Let $X_1, \ldots, X_k$ be an i.i.d. sample with $\mathbb{E}\left[X_i\right] = \mu$ and $\mathrm{Var}\left[X_i\right] = \sigma^2 < \infty, \sigma^2 > 0$, and suppose we want to find CI for μ. According to CLT – more precisely, one of its corollaries – if $\overline{X} := \frac{1}{k}\sum_{i=1}^{k} X_i$ is sample mean and $S_k^2 := \frac{1}{k}\sum_{i=1}^{k}\left(X_i - \overline{X}\right)^2$ is sample variance, $\frac{\sqrt{k}(\overline{X} - \mu)}{S_k} \to \mathcal{N}(0,1)$ converges in distribution when $k \to \infty$.

Suppose we want a CI at confidence level $1 - \alpha$. We denote z_p as a p-quantile of standard normal distribution, i.e. if $Y \sim \mathcal{N}(0,1)$, z_p is a such value that $\mathbb{P}\left(Y \leq z_p\right) = p$. Then, for sufficiently large k,

$$\mathbb{P}\left(z_{\frac{\alpha}{2}} \leq \frac{\mu - \overline{X}}{S_k/\sqrt{k}} \leq z_{1-\frac{\alpha}{2}}\right) = \mathbb{P}\left(\frac{\mu - \overline{X}}{S_k/\sqrt{k}} \leq z_{1-\frac{\alpha}{2}}\right) - \mathbb{P}\left(\frac{\mu - \overline{X}}{S_k/\sqrt{k}} < z_{\frac{\alpha}{2}}\right) \approx \left(1 - \frac{\alpha}{2}\right) - \frac{\alpha}{2} = 1 - \alpha,$$

or

$$\mathbb{P}\left(\overline{X} + z_{\frac{\alpha}{2}}\frac{S_k}{\sqrt{k}} \leq \mu \leq \overline{X} + z_{1-\frac{\alpha}{2}} \cdot \frac{S_k}{\sqrt{k}}\right) \approx 1 - \alpha.$$

As $z_{\frac{\alpha}{2}} = -z_{1-\frac{\alpha}{2}}$, the CI bounds for μ would be $\overline{X} \pm z_{1-\frac{\alpha}{2}} \cdot \frac{S_k}{\sqrt{k}}$. If we would like to have 95% confidence level, i.e. $\alpha = 0.05$, we would take $z_{1-\frac{\alpha}{2}} = z_{0.975} \approx 1.96$.

Now, you will apply this theory to the trace estimation algorithm.

1. Let X_i be a random variable equal to 1 if i-th measurement gave $|0\rangle$ and 0 otherwise. Suppose we ran the circuit k times, and k_0 times the result of measurement was $|0\rangle$. Let $\hat{p} = \frac{k_0}{k}$. Show that $\overline{X} = \hat{p}$ and $S_k = \sqrt{\hat{p}(1-\hat{p})}$.

   Solution:
$$\overline{X} = \frac{1}{k}\sum_{i=1}^{k} X_i = \frac{1}{k}\sum_{i=1}^{k} \mathbb{1}\{i\text{-th measurement was } |0\rangle\} = \frac{k_0}{k},$$
   and
$$S_k^2 = \frac{1}{k}\sum_{i=1}^{k}\left(X_i - \overline{X}\right)^2 = \underbrace{\frac{1}{k}\sum_{i=1}^{k} X_i^2}_{=\frac{1}{k}\sum_{i=1}^{k} X_i = \overline{X}} - 2\overline{X}\cdot \underbrace{\frac{1}{k}\sum_{i=1}^{k} X_i}_{=\overline{X}} + \overline{X}^2 = \overline{X} - \overline{X}^2 = \overline{X}(1-\overline{X}) = \hat{p}(1-\hat{p}).$$

2. Write down CI for $\mathbb{E}[X_i]$ at level $1-\alpha$. Derive from it a CI for $\mathbf{Re}\{\mathrm{Tr}[U]\}$ at level $1-\alpha$ with bounds $2^{n+1}\left(\hat{p} - \frac{1}{2} \pm z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}}\right)$. Which value of $\hat{p}$ gives the widest interval?

   Solution: Let $p := \frac{1}{2} + \frac{1}{2^{n+1}}\mathbf{Re}\{\mathrm{Tr}[U]\}$.
   Then, $\mathbb{E}[X_i] = \mathbb{E}[\mathbb{1}\{i\text{-th measurement was } |0\rangle\}] = \mathbb{P}(i\text{-th measurement was } |0\rangle) = p$. Knowing that, we can write:
$$\mathbb{P}\left(\hat{p} - z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}} \le p \le \hat{p} + z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}}\right) \approx 1-\alpha.$$
   Now, as $\mathbf{Re}\{\mathrm{Tr}[U]\} = 2^{n+1}\left(p - \frac{1}{2}\right)$
$$\mathbb{P}\left(2^{n+1}\left(\hat{p} - \frac{1}{2} - z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}}\right) \le \mathbf{Re}\{\mathrm{Tr}[U]\} \le 2^{n+1}\left(\hat{p} - \frac{1}{2} + z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}}\right)\right) \approx 1-\alpha.$$
   Width of this interval is $2^{n+2} z_{1-\frac{\alpha}{2}} \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{k}}$; it is the widest when $\hat{p} = \frac{1}{2}$, which is more typical for p close to $\frac{1}{2}$, i.e. $\mathbf{Re}\{\mathrm{Tr}[U]\}$ close to 0.

3. Take the circuit from Ex. 3 (the random one). For different values of k, run the trace estimation circuit k times and compute 1) the previously derived single value estimate of $\mathbf{Re}\{\mathrm{Tr}[U]\}$ and 2) the CI you got in this exercise at level 95%.
   Then, plot the real value of $\mathbf{Re}\{\mathrm{Tr}[U]\}$, the single-value estimate of it, and the CI against k.