Quantum algorithms 2024/2025: Final exam

Benoît Vermersch (benoit.vermersch@lpmmc.cnrs.fr) & Valentin Savin (valentin.savin@cea.fr)
2024 Dec 16th, 10:30-12:30 (2 hours)

- Documents allowed: Slides of the lectures, documents of the exercises, hand-written notes.
- You can only use your laptop to look at the documents from Moodle. **The use of additional resources (Other online material, books, AI tools, etc) is obviously strictly forbidden.**
- You can also use printed versions of these documents.
- The use of smartphones or tablets is not allowed.
- There are two independent exercises. You can decide in which order you want to address them.

1 Hamiltonian simulation via quantum linear algebra

Quantum linear algebra is a recent framework that was introduced to derive quantum algorithms with optimal performances, the most famous example being Hamiltonian Simulation, also known as digital quantum simulation (Lecture 4).

1.1 Introduction to block encodings

We are given a matrix A of dimension $2^n \times 2^n$. A block encoding of A realizes a unitary operation on $m+n$ qubits that satisfies

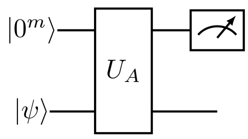
$$U_A |0^m\rangle |\psi\rangle = |0^m\rangle \otimes (A|\psi\rangle) + |\perp\rangle . \tag{1}$$

Here $|\perp\rangle$ has no overlap with the ancilla initial state $|0^m\rangle$, which can be formally expressed as

$$\Pi |\perp\rangle = 0 \tag{2}$$

with $\Pi = |0^m\rangle \langle 0^m| \otimes 1_n$, where 1_n is the identity of n qubits.

1. We realize the following quantum circuit on $m+n$ qubits.



   We denote as $|\psi'\rangle$ the wavefunction of the system before measurement.

   Explain based on what you have learned during the lectures how $|\psi'\rangle$ is projected during the measurement of a bitstring x on the first register (that is made of the first m qubits).

   Solution: *Following Lecture 1, The projection operator is $P_x = |x\rangle \langle x| \otimes 1_n$ on any m-qubit bit string x. A measurement of x occurs with probability $\langle \psi'|P_x|\psi'\rangle$ and the corresponding post-measurement state if*

$$P_x |\psi'\rangle / ||P_x |\psi'\rangle || \tag{3}$$

2. We assume that the measured bitstring is $x = 0^m$. Show that the final state of the circuit is

$$|\psi''\rangle = \frac{|0^m\rangle \otimes A|\psi\rangle}{||A|\psi\rangle ||}, \tag{4}$$

   with $|| |\phi\rangle || = \sqrt{\langle \phi|\phi\rangle}$.

   Solution: *First we note that $|\psi'\rangle = U_A |0^m\rangle |\psi\rangle$. For a measurement $x = 0^m$, we have $P_{0^m} = \Pi$, and therefore the (unnormalized) measured state is*

$$\Pi |\psi'\rangle = \Pi(U_A |0^m\rangle |\psi\rangle) = |0^m\rangle \otimes (A|\psi\rangle), \tag{5}$$

   where we have used that $\Pi |\perp\rangle = 0$, and the normalization factor is

$$||\Pi |\psi'\rangle || = || |0^m\rangle \otimes (A|\psi\rangle)|| = ||A|\psi\rangle || \tag{6}$$

1.2 Qubitization

We have seen that the block encoding U_A allows us to apply the matrix A on a quantum state $|\psi\rangle$. Qubitization is a quantum routine that applies, in a similar way, a non-linear transformation of A.

1. We consider now an Hermitian matrix A, with eigenvalue decomposition

$$A = \sum_i \lambda_i |\nu_i\rangle \langle \nu_i| , \tag{7}$$

where λ_i is real, the set $\{|\nu_i\rangle\}$ is an orthonormal basis, and we also assume for simplicity $\lambda_i \neq \pm 1$. Show that we can write

$$U_A |0^m\rangle |\nu_i\rangle = \lambda_i |0^m\rangle |\nu_i\rangle + \sqrt{1-\lambda_i^2} |\perp_i\rangle \tag{8}$$

where $|\perp_i\rangle$ is normalized, and $\Pi |\perp_i\rangle = 0$.

Solution: *Because U_A is a block encoding*

$$U_A |0^m\rangle |\nu_i\rangle = \lambda_i |0^m\rangle |\nu_i\rangle + |\tilde{\perp}_i\rangle \tag{9}$$

with $\Pi |\tilde{\perp}_i\rangle = 0$.

As $\lambda_i^2 \neq 1$, we can now define $|\perp_i\rangle$ such that $|\tilde{\perp}_i\rangle = \sqrt{1-\lambda_i^2} |\perp_i\rangle$ The norm of $U_A |0^m\rangle |\nu_i\rangle$ being one, we have in addition

$$1 = \lambda_i^2 + (1-\lambda_i^2) \langle \perp_i \mid \perp_i\rangle \tag{10}$$

which gives $\langle \perp_i \mid \perp_i\rangle = 1$, i.e such state is normalized.

Note: If $\lambda_i^2 = 1$, the norm of $U_A |0^m\rangle |\nu_i\rangle$, being one, we also have that

$$1 = 1 + \langle \tilde{\perp}_i | \tilde{\perp}_i\rangle , \tag{11}$$

i.e we have that $|\tilde{\perp}_i\rangle = 0$, which we can also write as $\sqrt{1-\lambda_i^2} |\perp_i\rangle$, with $|\perp_i\rangle$ arbitrary normalized state.

2. We assume that U_A is Hermitian, i.e. $U_A = U_A^\dagger$.
Using $U_A^2 = 1_{m+n}$, write an expression for $U_A |\perp_i\rangle$ as a function of $|0^m\rangle |\nu_i\rangle$ and $|\perp_i\rangle$.

Solution: *Multiplying the equation shown in the last question by U_A, we obtain*

$$\begin{aligned} U_A^2 |0^m\rangle |\nu_i\rangle &= \lambda_i U_A |0^m\rangle |\nu_i\rangle + \sqrt{1-\lambda_i^2} U_A |\perp_i\rangle \\ |0^m\rangle |\nu_i\rangle &= \lambda_i^2 |0^m\rangle |\nu_i\rangle + \lambda_i \sqrt{1-\lambda_i^2} |\perp_i\rangle + \sqrt{1-\lambda_i^2} U_A |\perp_i\rangle \end{aligned} \tag{12}$$

As $\lambda_i^2 \neq 1$, we have that

$$U_A |\perp_i\rangle = \sqrt{1-\lambda_i^2} |0^m\rangle |\nu_i\rangle - \lambda_i |\perp_i\rangle . \tag{13}$$

3. Show that the matrix U_A restricted in the subspace B_i formed by the two states $|0^m\rangle |\nu_i\rangle$ and $|\perp_i\rangle$ can be written as

$$U_A = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix} \tag{14}$$

Note: We talk about qubitization of the operator A in this context because we can describe effectively the action on U_A for each eigenstate $|\nu_i\rangle$ using a two-dimensional Hilbert space.

Solution: *Simply combining the results of the last two questions, we obtain in matrix form in the subspace $\{|0^m\rangle |\nu_i\rangle , |\perp_i\rangle\}$*

$$U_A = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix} \tag{15}$$

4. We introduce the m-qubit phase operator $Z = (2|0^m\rangle \langle 0^m| - 1_m) \otimes 1_n = 2\Pi - 1_{m+n}$. Show that Z is unitary, and write its expression in the subspace B_i as a 2×2 matrix.

Solution: *Z is unitary because*

$$ZZ^\dagger = Z^2 = 4\Pi^2 - 4\Pi + 1 = 1 \tag{16}$$

where we have used that $\Pi^2 = \Pi$.

We have that $Z |0^m\rangle |\nu_i\rangle = |0^m\rangle |\nu_i\rangle$, and

$$Z |\perp_i\rangle = 2\Pi |\perp_i\rangle - |\perp_i\rangle = - |\perp_i\rangle \tag{17}$$

leading to the matrix expression in the subspace B_i

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{18}$$

5. Write the "Walk operator" $O = U_A Z$ in the subspace B_i as a 2×2 matrix.

   Solution:

$$O = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix} \tag{19}$$

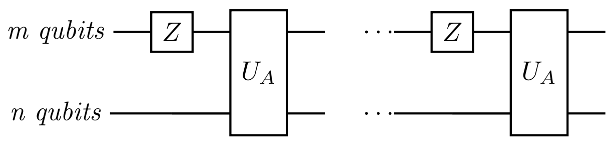
6. We admit now that we can write (still in the B_i subspace)

$$O^k = \begin{pmatrix} T_k(\lambda_i) & -\alpha_k(\lambda_i) \\ \alpha_k(\lambda_i) & * \end{pmatrix} \tag{20}$$

   where $T_k(\lambda_i)$ is a so-called Chebyshev polynomial, $\alpha_k(\lambda_i)$ is a function of λ_i (whose specific form is not important), and $*$ denotes an irrelevant term.

7. Represent the circuit O^k graphically.

   Solution:



8. Let us consider the matrix $T_k(A) = \sum_i T_k(\lambda_i) |\nu_i\rangle \langle\nu_i|$, show that

$$T_k(A) |\psi\rangle = \sum_i c_i T_k(\lambda_i) |\nu_i\rangle , \tag{21}$$

   where $|\psi\rangle$ is an arbitrary n-qubit state, and $c_i = \langle\nu_i|\psi\rangle$.

   Solution:

$$T_k(A) |\psi\rangle = \sum_i T_k(\lambda_i) |\nu_i\rangle \langle\nu_i| |\psi\rangle = \sum_i c_i T_k(\lambda_i) |\nu_i\rangle \tag{22}$$

9. Show that O^k implements a block-encoding of the matrix $T_k(A)$.

   Tip: To evaluate $O^k |0^m\rangle |\psi\rangle$, use the eigenstate decomposition $|\psi\rangle = \sum_i c_i |\nu_i\rangle$.

   Solution:

$$\begin{aligned} O^k |0^m\rangle |\psi\rangle &= \sum_i c_i O^k |0^m\rangle |\nu_i\rangle = \sum_i c_i \left(T_k(\lambda_i) |0^m\rangle |\nu_i\rangle + \alpha_k(\lambda_i) |\perp_i\rangle\right) \\ &= |0^m\rangle \otimes (T_k(A) |\psi\rangle) + |\perp'\rangle , \end{aligned} \tag{23}$$

   with $|\perp'\rangle = \sum_i c_i \alpha_k(\lambda_i) |\perp_i\rangle$ *Finally we have*

$$\Pi |\perp'\rangle = \sum_i c_i \alpha_k(\lambda_i) \Pi |\perp_i\rangle = 0 \tag{24}$$

   Therefore according to the definition given in Eq (1), O^k *is a block encoding for* $T_k(A)$.

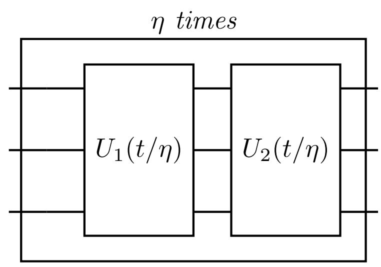
1.3 Hamiltonian simulation

1. We consider the implementation of the time-evolution operator $U(t) = \exp(-iHt)$ associated with an Hamiltonian H on a quantum computer. We assume $H = H_1 + H_2$ and that we have the ability to implement any circuit of the form $U_1(t_1) = \exp(-iH_1 t_1)$, and $U_2(t_2) = \exp(-iH_2 t_2)$. Explain how to realize $U(t)$ up to arbitrary accuracy using the Trotter approach described in our lectures, and draw the corresponding quantum circuit.

   Solution: *Cf Lecture 4, we use*

$$\exp(-iHt) \approx \left(U_2(t/\eta) U_1(t/\eta)\right)^\eta , \tag{25}$$

   where the depth η *can be increased at will to reach a certain accuracy.*



2. The block encoding formalism has been shown recently to allow for Hamiltonian simulation with less ressources compared to the Trotter approach. While the optimal scenario is based on "quantum signal processing" (QSP), we will use here as illustration a less optimal method known as linear combination of unitaries (LCU).

   Consider a $2^n \times 2^n$ matrix $A = \sum_{j=0}^{2^r-1} g_j A_j$, with g_j real positive coefficients, and assume that we know how to block encode each term A_j of size $2^n \times 2^n$ via a unitary matrix U_j acting on $m+n$ qubits. Let us define

$$S = \sum_j |j\rangle \langle j| \otimes U_j \tag{26}$$

   in a combined system of $r+m+n$ qubits, with j a sum of all possible 2^r bitstrings. We also consider P acting on the first r qubits as

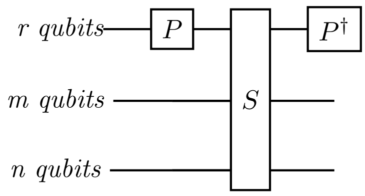
$$P|0^r\rangle = \frac{1}{\sqrt{g}} \sum_j \sqrt{g_j}\, |j\rangle \,. \tag{27}$$

   with $g = \sum_j |g_j|$.

   We admit here that $W = (P^\dagger \otimes 1_{m+n}) S (P \otimes 1_{m+n})$ is a block encoding for the matrix A/g (proof in the corrections)

   Represent graphically the circuit associated with the unitary operator W

   Solution:



   Proof that W is a block-encoding for A/g

$$\begin{aligned}
W|0^r\rangle|0^m\rangle|\psi\rangle &= \frac{1}{\sqrt{g}} \sum_j \sqrt{g_j} (P^\dagger \otimes 1_{m+n}) S |j\rangle |0^m\rangle |\psi\rangle \\
&= \frac{1}{\sqrt{g}} \sum_j \sqrt{g_j} (P^\dagger \otimes 1_{m+n}) |j\rangle U_j |0^m\rangle |\psi\rangle \\
&= \frac{1}{\sqrt{g}} \sum_j \sqrt{g_j} (\sum_{j'} |j'\rangle \langle j'|) P^\dagger \otimes 1_{m+n}) |j\rangle U_j |0^m\rangle |\psi\rangle \\
&= \frac{1}{g} \sum_j g_j |0^r\rangle U_j |0^m\rangle |\psi\rangle + |\perp\rangle \\
&= \frac{1}{g} \sum_j g_j |0^r\rangle A_j |0^m\rangle |\psi\rangle + |\perp'\rangle \\
&= \frac{1}{g} |0^r\rangle A |0^m\rangle |\psi\rangle + |\perp'\rangle
\end{aligned} \tag{28}$$

   where we have broken the sum in two terms $j' = 0^r$, $j' \neq 0^r$, and we have then that $\Pi^{(r)}|\perp\rangle = 0$, with $\Pi^{(r)} = |0^r\rangle\langle 0^r|$. In the second to last line, we gather all terms orthogonal such that $\Pi^{(r+m)}|\perp'\rangle = 0$,. using the fact that U_j block encodes A_j,

3. Let us consider a Chebyshev decomposition of the exponential function

$$e^{-iHt} = \sum_k g_k T_k(Ht). \tag{29}$$

   Let also consider that we know the circuit U_A that block-encodes $A = Ht$

   Explain without further calculations how one could realize Hamiltonian simulation combining qubitization and linear combination of unitaries.

   Solution: *In the qubitization part of the exercise, we have seen how to realize block-encodings O^k of the Chebyshev polynomial $T_k(Ht)$, we can then form a block encoding for $e^{-iHt} = \sum_k g_k T_k(Ht)$, using linear combination of unitaries.*