Foundations of Quantum Programming

Lecture 5: Analysis of Quantum Programs

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Outline

Analysis of Quantum Loops
Quantum while-Loops with Unitary Bodies
General Quantum while-Loops

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- Quantum while-Loops with Unitary Bodies
- General Quantum while-Loops

Quantum **while**-Loops with Unitary Bodies

$$S \equiv \textbf{while}\ M[\overline{q}] = 1\ \textbf{do}\ \overline{q} := U[\overline{q}]\ \textbf{od}$$

where:

- $\overline{q}$ denotes quantum register $q_1, \ldots, q_n$, its state Hilbert space:

$$\mathcal{H} = \bigotimes_{i=1}^{n} \mathcal{H}_{q_i}$$

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- the loop body is unitary transformation $\overline{q} := U[\overline{q}]$ in $\mathcal{H}$;
- the yes-no measurement $M = \{M_0, M_1\}$ in the loop guard is projective: $M_0 = P_{X^\perp}, M_1 = P_X$ with X being a subspace of $\mathcal{H}$, $X^\perp$ being the orthocomplement of X.

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  - The loop continues with probability $p_{NT}^{(1)}(\rho) = 1 - p_T^{(1)}(\rho) = tr(P_X\rho)$. The program state after the measurement:
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  $$\rho_{mid}^{(1)} = \frac{P_X\rho P_X}{p_{NT}^{(1)}(\rho)}.$$
  - $\rho_{mid}^{(1)}$ is fed to the unitary operation U:
  $$\rho_{in}^{(2)} = U\rho_{mid}^{(1)}U^\dagger$$
  is returned. $\rho_{in}^{(2)}$ will be used as the input state in the next step.

- *Induction step*: Suppose the loop has run n steps, it did not terminate at the nth step: $p_{NT}^{(n)} > 0$. If $\rho_{in}^{(n+1)}$ is the program state at the end of the nth step, then in the $(n+1)$th step:

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  - The termination probability: $p_T^{(n+1)}(\rho) = tr(P_{X^\perp}\rho_{in}^{(n+1)})$. The output at this step is

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  - The loop continues to perform the unitary operation U on the post-measurement state

$$\rho_{mid}^{(n+1)} = \frac{P_X\rho_{in}^{(n+1)}P_X}{p_{NT}^{(n+1)}(\rho)}$$

  with probability $p_{NT}^{(n+1)}(\rho) = 1 - p_T^{(n+1)}(\rho) = tr(P_X\rho_{in}^{(n+1)})$. The state $\rho_{in}^{(n+2)} = U\rho_{mid}^{(n+1)}U^\dagger$ will be returned. It will be the input of the $(n+2)$th step.

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where

$$p_{NT}^{(\leq n)}(\rho) = \prod_{i=1}^{n} p_{NT}^{(i)}(\rho)$$

is the probability that the loop does not terminate after n steps.

Terminating

A quantum loop is terminating (resp. almost surely terminating) if it terminates (resp. almost surely terminates) from all input $\rho \in \mathcal{D}(\mathcal{H})$.

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   is the probability that the loop does not terminate after n steps.
3. The loop almost surely terminates from input ρ whenever nontermination probability $p_{NT}(\rho) = 0$.

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A quantum loop is terminating (resp. almost surely terminating) if it terminates (resp. almost surely terminates) from all input $\rho \in \mathcal{D}(\mathcal{H})$.

Computed Function

- The function $\mathcal{F} : \mathcal{D}(\mathcal{H}) \to \mathcal{D}(\mathcal{H})$ computed by the loop:

$$\mathcal{F}(\rho) = \sum_{n=1}^{\infty} p_{NT}^{(\leq n-1)}(\rho) \cdot p_{T}^{(n)}(\rho) \cdot \rho_{out}^{(n)}$$

for each $\rho \in \mathcal{D}(\mathcal{H})$.

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- $$p_{NT}^{(\leq n)}(\rho) = tr(U_X^{n-1} \rho_X U_X^{\dagger n-1})$$
- $$\mathcal{F}(\rho) = P_{X^\perp} \rho P_{X^\perp} + P_{X^\perp} U \left(\sum_{n=0}^{\infty} U_X^n \rho_X U_X^{\dagger n} \right) U^\dagger P_{X^\perp}$$

Termination Analysis

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- A quantum loop is terminating if and only if it terminates from all pure input states.

- Let $\{|m_1\rangle, \ldots, |m_l\rangle\}$ be an orthonormal basis of $\mathcal{H}$ such that

$$\sum_{i=1}^{k} |m_i\rangle\langle m_i| = P_X, \quad \sum_{i=k+1}^{l} |m_i\rangle\langle m_i| = P_{X^\perp}$$

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- The loop terminates from pure input state $|\psi\rangle$ if and only if $U_X^n|\psi\rangle_X = \mathbf{0}$ for some nonnegative integer n, where $\mathbf{0}$ is the k-dimensional zero vector.

From Quantum Loop to Classical Loop

- The condition $U_X^n|\psi\rangle_X = \mathbf{0}$ is a termination condition for the loop:

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  2. The classical loop:

$$\textbf{while } \mathbf{v} \neq \mathbf{0} \textbf{ do } \mathbf{v} := (SU_XS^{-1})\mathbf{v} \textbf{ od}$$

     (with $\mathbf{v} \in \mathbf{C}^k$) terminates from input $S\mathbf{v}_0$.

Jordan Normal Form Theorem

For any $(k \times k)$-complex matrix A, there is a nonsingular $(k \times k)$-complex matrix S such that

$$A = SJ(A)S^{-1}$$

where

$$\begin{aligned} J(A) &= \bigoplus_{i=1}^{l} J_{k_i}(\lambda_i) \\ &= diag(J_{k_1}(\lambda_1), J_{k_2}(\lambda_2), \ldots, J_{k_l}(\lambda_l)) \\ &= \begin{pmatrix} J_{k_1}(\lambda_1) & & & & \\ & J_{k_2}(\lambda_2) & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & J_{k_l}(\lambda_l) \end{pmatrix} \end{aligned}$$

is the Jordan normal form of A,

Jordan Normal Form Theorem (Continued)

$\sum_{i=1}^{l} k_i = k$,

$$J_{k_i}(\lambda_i) = \begin{pmatrix} \lambda_i & 1 & & & \\ & \lambda_i & 1 & & \\ & & \ddots & \ddots & \\ & & & \ddots & 1 \\ & & & & \lambda_i \end{pmatrix}$$

is a $(k_i \times k_i)$-Jordan block for each $1 \leq i \leq l$.

Technical Lemma

Let $J_r(\lambda)$ be a $(r \times r)$-Jordan block, $\mathbf{v}$ an r-dimensional complex vector. Then

$$J_r(\lambda)^n \mathbf{v} = \mathbf{0}$$

for some nonnegative integer n if and only if $\lambda = 0$ or $\mathbf{v} = \mathbf{0}$.

Theorem

- The Jordan decomposition of U_X: $U_X = SJ(U_X)S^{-1}$, where

$$J(U_X) = \bigoplus_{i=1}^{l} J_{k_i}(\lambda_i) = diag(J_{k_1}(\lambda_1), J_{k_2}(\lambda_2), \ldots, J_{k_l}(\lambda_l)).$$

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- Let $S^{-1}|\psi\rangle_X$ be divided into l sub-vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_l$ such that the length of $\mathbf{v}_i$ is k_i.

Corollary

The quantum loop is terminating if and only if U_X has only zero eigenvalues.

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- Let $S^{-1}|\psi\rangle_X$ be divided into l sub-vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_l$ such that the length of $\mathbf{v}_i$ is k_i.
- Then: the quantum loop terminates from input $|\psi\rangle$ if and only if for each $1 \leq i \leq l$, $\lambda_i = 0$ or $\mathbf{v}_i = \mathbf{0}$.

Corollary

The quantum loop is terminating if and only if U_X has only zero eigenvalues.

Almost sure termination

- Let $\rho = \sum_i p_i \rho_i$ with $p_i > 0$ for all i. Then the quantum loop almost surely terminates from input ρ if and only if it almost surely terminates from input ρ_i for all i.

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- The quantum loop almost surely terminates from pure input state $|\psi\rangle$ if and only if

$$\lim_{n\to\infty} ||U_X^n|\psi\rangle|| = 0.$$

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- The quantum loop almost surely terminates from input $|\psi\rangle$ if and only if for each $1 \leq i \leq l$, $|\lambda_i| < 1$ or $\mathbf{v}_i = \mathbf{0}$.

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- The quantum loop almost surely terminates from input $|\psi\rangle$ if and only if for each $1 \leq i \leq l$, $|\lambda_i| < 1$ or $\mathbf{v}_i = \mathbf{0}$.
- The quantum loop is almost surely terminating if and only if all the eigenvalues of U_X have norms less than 1.

General Quantum **while**-Loops

$$\textbf{while } M[\overline{q}] = 1 \textbf{ do } S \textbf{ od}$$

where:

- $M = \{M_0, M_1\}$ is a yes-no measurement;

$$\textbf{while } M[\overline{q}] = 1 \textbf{ do } \overline{q} := \mathcal{E}[\overline{q}] \textbf{ od}.$$

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- $\overline{q}$ is a quantum register;

$$\textbf{while } M[\overline{q}] = 1 \textbf{ do } \overline{q} := \mathcal{E}[\overline{q}] \textbf{ od}.$$

Notation

For $i = 0, 1$, define quantum operation $\mathcal{E}_i$:

$$\mathcal{E}_i(\sigma) = M_i \sigma M_i^\dagger$$

General Quantum **while**-Loops

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where:

- $M = \{M_0, M_1\}$ is a yes-no measurement;
- $\overline{q}$ is a quantum register;
- the loop body S is a general quantum program.

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Execution of Loops

Initial step: Perform the termination measurement $\{M_0, M_1\}$ on the input state ρ.

- The probability that the program terminates (the measurement outcome is 0):

  $$p_T^{(1)}(\rho) = tr[\mathcal{E}_0(\rho)].$$

  The program state after termination:

  $$\rho_{out}^{(1)} = \mathcal{E}_0(\rho)/p_T^{(1)}(\rho).$$

  Encode probability $p_T^{(1)}(\rho)$ and density operator $\rho_{out}^{(1)}$ into a partial density operator

  $$p_T^{(1)}(\rho)\rho_{out}^{(1)} = \mathcal{E}_0(\rho).$$

  So, $\mathcal{E}_0(\rho)$ is the partial output state at the first step.

Execution of Loops (Continued)

- The probability that the program does not terminate (the measurement outcome is 1):

$$p_{NT}^{(1)}(\rho) = tr[\mathcal{E}_1(\rho)]$$

The program state after the outcome 1 is obtained:

$$\rho_{mid}^{(1)} = \mathcal{E}_1(\rho)/p_{NT}^{(1)}(\rho).$$

It is transformed by the loop body $\mathcal{E}$ to

$$\rho_{in}^{(2)} = (\mathcal{E} \circ \mathcal{E}_1)(\rho)/p_{NT}^{(1)}(\rho),$$

upon which the second step will be executed.
Combine $p_{NT}^{(1)}$ and $\rho_{in}^{(2)}$ into a partial density operator

$$p_{NT}^{(1)}(\rho)\rho_{in}^{(2)} = (\mathcal{E} \circ \mathcal{E}_1)(\rho).$$

Execution of Loops (Continued)

Induction step: Write $p_{NT}^{(\leq n)} = \prod_{i=1}^{n} p_{NT}^{(i)}$ for the probability that the program does not terminate within n steps, where $p_{NT}^{(i)}$ is the probability that the program does not terminate at the ith step for every $1 \leq i \leq n$.

The program state after the nth measurement with outcome 1:

$$\rho_{mid}^{(n)} = \frac{\left[\mathcal{E}_1 \circ (\mathcal{E} \circ \mathcal{E}_1)^{n-1}\right](\rho)}{p_{NT}^{(\leq n)}}$$

It is transformed by the loop body $\mathcal{E}$ into

$$\rho_{in}^{(n+1)} = \frac{(\mathcal{E} \circ \mathcal{E}_1)^n(\rho)}{p_{NT}^{(\leq n)}}.$$

Combine $p_{NT}^{(\leq n)}$ and $\rho_{in}^{(n+1)}$ into a partial density operator

$$p_{NT}^{(\leq n)}(\rho)\rho_{in}^{(n+1)} = (\mathcal{E} \circ \mathcal{E}_1)^n(\rho).$$

Execution of Loops (Continued)

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  - The probability that the program terminates at the $(n+1)$st step:

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$$p_T^{(n+1)}(\rho) = tr\left[\mathcal{E}_0\left(\rho_{in}^{(n+1)}\right)\right].$$

  - The probability that the program does not terminate within n steps but it terminates at the $(n+1)$st step:

$$q_T^{(n+1)}(\rho) = tr\left(\left[\mathcal{E}_0 \circ (\mathcal{E} \circ \mathcal{E}_1)^n\right](\rho)\right).$$

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  - The program state after the termination:

$$\rho_{out}^{(n+1)} = [\mathcal{E}_0 \circ (\mathcal{E} \circ \mathcal{E}_1)^n](\rho)/q_T^{(n+1)}(\rho).$$

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  - Combining $q_T^{(n+1)}(\rho)$ and $\rho_{out}^{(n+1)}$ yields the partial output state of the program at the $(n+1)$st step:

$$q_T^{(n+1)}(\rho)\rho_{out}^{(n+1)} = [\mathcal{E}_0 \circ (\mathcal{E} \circ \mathcal{E}_1)^n](\rho).$$

Execution of Loops (Continued)

- The probability that the program does not terminate within $(n+1)$ steps:

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Termination

1. The quantum loop terminates from input state ρ if probability $p_{NT}^{(n)}(\rho) = 0$ for some positive integer n.
2. The loop almost surely terminates from input state ρ if nontermination probability

$$p_{NT}(\rho) = \lim_{n\to\infty} p_{NT}^{(\leq n)}(\rho) = 0$$

where $p_{NT}^{(\leq n)}$ is the probability that the program does not terminate within n steps.

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The quantum loop is terminating (resp. almost surely terminating) if it terminates (resp. almost surely terminates) from any input ρ.

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Computed Function

The function $\mathcal{F} : \mathcal{D}(H) \rightarrow \mathcal{D}(H)$ computed by the quantum loop:

$$\mathcal{F}(\rho) = \sum_{n=1}^{\infty} q_T^{(n)}(\rho)\rho_{out}^{(n)} = \sum_{n=0}^{\infty} \left[\mathcal{E}_0 \circ (\mathcal{E} \circ \mathcal{E}_1)^n\right](\rho)$$

for each $\rho \in \mathcal{D}(\mathcal{H})$, where

$$q_T^{(n)} = p_{NT}^{(\leq n-1)} p_T^{(n)}$$

is the probability that the program does not terminate within $n-1$ steps but it terminate at the nth step.

Recursive Characterisation of Computed Function

The quantum operation $\mathcal{F}$ computed by a loop satisfies the recursive equation:

$$\mathcal{F}(\rho) = \mathcal{E}_0(\rho) + \mathcal{F}[(\mathcal{E} \circ \mathcal{E}_1)(\rho)].$$

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Matrix Representation of Quantum Operations

Suppose quantum operation $\mathcal{E}$ in a d-dimensional Hilbert space $\mathcal{H}$ has the Kraus operator-sum representation:

$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger.$$

Then the matrix representation of $\mathcal{E}$ is the $d^2 \times d^2$ matrix:

$$M = \sum_i E_i \otimes E_i^*,$$

where A^* stands for the conjugate of matrix A.

Lemma

Write $|\Phi\rangle = \sum_j |jj\rangle$ for the (unnormalized) maximally entangled state in $\mathcal{H} \otimes \mathcal{H}$, where $\{|j\rangle\}$ is an orthonormal basis of $\mathcal{H}$. Let M be the matrix representation of quantum operaion $\mathcal{E}$. Then for any $d \times d$ matrix A:

$$(\mathcal{E}(A) \otimes I)|\Phi\rangle = M(A \otimes I)|\Phi\rangle.$$

Notations

- Let the quantum operation $\mathcal{E}$ in the loop body has the operator-sum representation:

$$\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger.$$

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- Write $\mathcal{G}$ for the composition of $\mathcal{E}$ and $\mathcal{E}_1$: $\mathcal{G} = \mathcal{E} \circ \mathcal{E}_1$.

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- The matrix representations of $\mathcal{E}_0$ and $\mathcal{G}$ are:

$$N_0 = M_0 \otimes M_0^*,$$
$$R = \sum_i (E_i M_1) \otimes (E_i M_1)^*.$$

Lemma

- Suppose that the Jordan decomposition of R is

$$R = SJ(R)S^{-1}$$

where S is a nonsingular matrix, and $J(R)$ is the Jordan normal form of R:

$$J(R) = \bigoplus_{i=1}^{l} J_{k_i}(\lambda_i) = diag(J_{k_1}(\lambda_1), J_{k_2}(\lambda_2), \cdots, J_{k_l}(\lambda_l)).$$

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1. $|\lambda_s| \leq 1$ for all $1 \leq s \leq l$.
2. If $|\lambda_s| = 1$ then the sth Jordan block is 1-dimensional; that is, $k_s = 1$.

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2. Quantum loop is almost surely terminating if and only if $|\Phi\rangle$ is orthogonal to all eigenvectors of $R^\dagger$ corresponding to eigenvalues λ with $|\lambda| = 1$.

Expectation of Observables at the Outputs

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where R is the matrix representation of $\mathcal{G} = \mathcal{E} \circ \mathcal{E}_1$.
- This series may not converge when some eigenvalues of R has module 1.
- *Idea to overcome this objection*: modify the Jordan normal form $J(R)$ of R by vanishing the Jordan blocks corresponding to those eigenvalues with module 1: $N = SJ(N)S^{-1}$

$$J(N) = diag(J_1', J_2', \cdots, J_3'),$$

$$J_s' = \begin{cases} 0 & \text{if } |\lambda_s| = 1, \\ J_{k_s}(\lambda_s) & \text{otherwise.} \end{cases}$$

Lemma

For any integer $n \geq 0$:

$$N_0 R^n = N_0 N^n,$$

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Theorem

The expectation of observable P in the output state $\mathcal{F}(\rho)$ of quantum loop with input state ρ:

$$tr(P\mathcal{F}(\rho)) = \langle\Phi|(P \otimes I)N_0(I \otimes I - N)^{-1}(\rho \otimes I)|\Phi\rangle.$$

Average Running Time

- The average running time loop with input state ρ:

$$\sum_{n=1}^{\infty} n p_T^{(n)}$$

where for each $n \geq 1$,

$$p_T^{(n)} = tr\left[\left(\mathcal{E}_0 \circ (\mathcal{E} \circ \mathcal{E}_1)^{n-1}\right)(\rho)\right] = tr\left[\left(\mathcal{E}_0 \circ \mathcal{G}^{n-1}\right)(\rho)\right]$$

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Theorem

The average running time of quantum loop with input state ρ:

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- Let $\mathcal{H}_d$ be the direction space — a 2-dimensional Hilbert space with orthonormal basis state $|L\rangle$ and $|R\rangle$, indicating directions Left and Right.

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- The state space of the quantum walk: $\mathcal{H} = \mathcal{H}_d \otimes \mathcal{H}_p$.
- The initial state: $|L\rangle|0\rangle$.
- This walk has an absorbing boundary at position 1.

Example: Quantum Walk on a Circle, Continued

Eeach step of the walk consists of:

1. Measure the position of the system to see whether the current position is 1. If the outcome is "yes", then the walk terminates; otherwise, it continues. This measurement models the absorbing boundary:

$$M = \{M_{yes} = I_d \otimes |1\rangle\langle 1|, M_{no} = I - M_{yes}\}.$$

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

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3. A shift operator

$$S = \sum_{i=0}^{n-1} |L\rangle\langle L| \otimes |i \ominus 1\rangle\langle i| + \sum_{i=0}^{n-1} |R\rangle\langle R| \otimes |i \oplus 1\rangle\langle i|$$

is performed in the space $\mathcal{H}$.

Example: Quantum Walk on a Circle, Continued

- Quantum **while**-loop:

$$\textbf{while } M[d,p] = yes \textbf{ do } d,p := W[d,p] \textbf{ od}$$

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- *Question*: The average running time is n for all $n \geq 30$?