Foundations of Quantum Programming

Lecture 6: Model-Checking Quantum Systems

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Outline

Quantum Graph Theory
  Basic Definitions
  Bottom Strongly Connected Components
  Decomposition of the State Hilbert Space

Reachability Analysis of Quantum Markov Chains
Outline

Quantum Graph Theory
  Basic Definitions
  Bottom Strongly Connected Components
  Decomposition of the State Hilbert Space

Reachability Analysis of Quantum Markov Chains
Quantum Markov Chains

- A quantum Markov chain is a pair $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$, where:

  1. $\mathcal{H}$ is a finite-dimensional Hilbert space;
  2. $\mathcal{E}$ is a quantum operation (or super-operator) in $\mathcal{H}$.

Behaviour of a quantum Markov chain: if currently the process is in a mixed state $\rho$, then it will be in state $\mathcal{E}(\rho)$ in the next step.

A quantum Markov chain $\langle \mathcal{H}, \mathcal{E} \rangle$ is a discrete-time quantum system of which the state space is $\mathcal{H}$ and the dynamics is described by quantum operation $\mathcal{E}$. 
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Notations

- $\mathcal{D}(\mathcal{H})$ is the set of partial density operators in $\mathcal{H}$; that is, positive operators $\rho$ with trace $tr(\rho) \leq 1$. 
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- For any subset $X$ of $\mathcal{H}$, $\text{span}X$ is the subspace of $\mathcal{H}$ spanned by $X$; that is, it consists of all finite linear combinations of vectors in $X$. 

- The support $\text{supp}(\rho) \in \mathcal{D}(\mathcal{H})$ is the subspace of $\mathcal{H}$ spanned by the eigenvectors of $\rho$ with non-zero eigenvalues.

- Let $\{X_k\}$ be a family of subspaces of $\mathcal{H}$. Then the join of $\{X_k\}$ is $\bigvee_k X_k = \text{span}(\bigcup_k X_k)$.

- The image of a subspace $X$ of $\mathcal{H}$ under a quantum operation $E$ is $E(X) = \bigvee |\psi\rangle \in X \text{ supp}(E(|\psi\rangle\langle\psi|))$. 

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\mathcal{E}(X) = \bigvee_{|\psi\rangle \in X} \text{supp}(\mathcal{E}(|\psi\rangle\langle\psi|)).
\]
Proposition

1. If $\rho = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k|$ where all $\lambda_k > 0$ (but $|\psi_k\rangle$’s are not required to be pairwise orthogonal), then $\text{supp}(\rho) = \text{span}\{|\psi_k\rangle\}$;
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2. \( \text{supp}(\rho + \sigma) = \text{supp}(\rho) \lor \text{supp}(\sigma) \);  

3. If \( E \) has the Kraus operator-sum representation \( E = \sum_{i \in I} E_i \circ E_i^\dagger \), then  
   \[ E(X) = \text{span}\{E_i|\psi\rangle : i \in I \text{ and } |\psi\rangle \in X\}; \]
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4. $\mathcal{E}(X_1 \vee X_2) = \mathcal{E}(X_1) \vee \mathcal{E}(X_2)$. Thus, $X \subseteq Y \Rightarrow \mathcal{E}(X) \subseteq \mathcal{E}(Y)$;
Proposition

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4. $\mathcal{E}(X_1 \lor X_2) = \mathcal{E}(X_1) \lor \mathcal{E}(X_2)$. Thus, $X \subseteq Y \Rightarrow \mathcal{E}(X) \subseteq \mathcal{E}(Y)$;
5. $\mathcal{E}(\text{supp}(\rho)) = \text{supp}(\mathcal{E}(\rho))$. 
Adjacency Relation

Let $C = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain, $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$ be pure states and $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ be mixed states in $\mathcal{H}$. Then

1. $|\varphi\rangle$ is adjacent to $|\psi\rangle$ in $C$, written $|\psi\rangle \rightarrow |\varphi\rangle$, if $|\varphi\rangle \in \text{supp}(\mathcal{E}(|\psi\rangle\langle\psi|))$. 
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2. $|\varphi\rangle$ is adjacent to $\rho$, written $\rho \rightarrow |\varphi\rangle$, if $|\varphi\rangle \in \mathcal{E}(\text{supp}(\rho))$. 
Adjacency Relation

Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain, $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$ be pure states and $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ be mixed states in $\mathcal{H}$. Then

1. $|\varphi\rangle$ is adjacent to $|\psi\rangle$ in $\mathcal{C}$, written $|\psi\rangle \rightarrow |\varphi\rangle$, if $|\varphi\rangle \in \text{supp}(\mathcal{E}(|\psi\rangle\langle\psi|))$.

2. $|\varphi\rangle$ is adjacent to $\rho$, written $\rho \rightarrow |\varphi\rangle$, if $|\varphi\rangle \in \mathcal{E}(\text{supp}(\rho))$.

3. $\sigma$ is adjacent to $\rho$, written $\rho \rightarrow \sigma$, if $\text{supp}(\sigma) \subseteq \mathcal{E}(\text{supp}(\rho))$. 
Reachability

1. A path from $\rho$ to $\sigma$ in a quantum Markov chain $C$ is a sequence

$$\pi = \rho_0 \rightarrow \rho_1 \rightarrow \cdots \rightarrow \rho_n \ (n \geq 0)$$

of adjacent density operators in $C$ such that $\text{supp}(\rho_0) \subseteq \text{supp}(\rho)$ and $\rho_n = \sigma$. 

Reachable Space

Let $C = \langle H, E \rangle$ be a quantum Markov chain. For any $\rho \in \mathcal{D}(H)$, its reachable space in $C$ is:

$$\mathcal{R}_C(\rho) = \text{span}\{ |\psi\rangle \in H : |\psi\rangle \text{ is reachable from } \rho \text{ in } C \}.$$
Reachability

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of adjacent density operators in $C$ such that $supp(\rho_0) \subseteq supp(\rho)$ and $\rho_n = \sigma$.

2. For any density operators $\rho$ and $\sigma$, if there is a path from $\rho$ to $\sigma$ then $\sigma$ is reachable from $\rho$ in $C$.

Reachable Space

Let $C = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain. For any $\rho \in \mathcal{D}(\mathcal{H})$, its reachable space in $C$ is:

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Transitivity of Reachability
For any $\rho, \sigma \in \mathcal{D}(\mathcal{H})$, if $\text{supp}(\rho) \subseteq \mathcal{R}_C(\sigma)$, then $\mathcal{R}_C(\rho) \subseteq \mathcal{R}_C(\sigma)$.

Theorem
Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain. If $d = \dim \mathcal{H}$, then for any $\rho \in \mathcal{D}(\mathcal{H})$, we have

$$\mathcal{R}_C(\rho) = \bigvee_{i=0}^{d-1} \text{supp} \left( \mathcal{E}^i(\rho) \right)$$

where $\mathcal{E}^i$ is the $i$th power of $\mathcal{E}$; that is, $\mathcal{E}^0 = \mathbb{I}$ and $\mathcal{E}^{i+1} = \mathcal{E} \circ \mathcal{E}^i$ for $i \geq 0$. 
**Strong Connectivity**

- Let $X$ be a subspace of $\mathcal{H}$ and $\mathcal{E}$ a quantum operation in $\mathcal{H}$. Then the restriction of $\mathcal{E}$ on $X$ is defined by

$$\mathcal{E}_X(\rho) = P_X \mathcal{E}(\rho) P_X$$

for all $\rho \in \mathcal{D}(X)$. 
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- Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain. A subspace $X$ of $\mathcal{H}$ is strongly connected in $\mathcal{C}$ if for any $|\varphi\rangle, |\psi\rangle \in X$:

$$|\varphi\rangle \in \mathcal{R}_{\mathcal{C}_X}(\psi) \text{ and } |\psi\rangle \in \mathcal{R}_{\mathcal{C}_X}(\varphi)$$

where $\varphi = |\varphi\rangle\langle\varphi|$ and $\psi = |\psi\rangle\langle\psi|$, quantum Markov chain $\mathcal{C}_X = \langle X, \mathcal{E}_X \rangle$ is the restriction of $\mathcal{C}$ on $X$. 
Inductive Partial Order

- Let \((L, \sqsubseteq)\) be a partial order. If any two elements \(x, y \in L\) are comparable; that is, either \(x \sqsubseteq y\) or \(y \sqsubseteq x\), then \(L\) is linearly ordered by \(\sqsubseteq\).
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- A partial order \((L, \sqsubseteq)\) is inductive if for any subset \(K\) of \(L\) that is linearly ordered by \(\sqsubseteq\), the least upper bound \(\bigcup K\) exists in \(L\).

Lemm

Write \(SC(\mathcal{C})\) for the set of all strongly connected subspaces of \(\mathcal{H}\) in \(\mathcal{C}\). Then partial order \((SC(\mathcal{C}), \subseteq)\) is inductive.
Zorn Lemma
Every inductive partial order has (at least one) maximal elements.
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Strongly Connected Components
A maximal element of \((\text{SC}(\mathcal{C}), \subseteq)\) is a strongly connected component (SCC) of \(\mathcal{C}\).

Invariants
A subspace \(X\) of \(\mathcal{H}\) is invariant under a quantum operation \(\mathcal{E}\) if \(\mathcal{E}(X) \subseteq X\).
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A maximal element of $(SC(\mathcal C), \subseteq)$ is a strongly connected component (SCC) of $\mathcal C$.

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A subspace $X$ of $\mathcal H$ is invariant under a quantum operation $\mathcal E$ if $\mathcal E(X) \subseteq X$.

Theorem
Let $\mathcal C = \langle \mathcal H, \mathcal E \rangle$ be a quantum Markov chain. If subspace $X$ of $\mathcal H$ is invariant under $\mathcal E$, then:

$$tr(P_X E(\rho)) \geq tr(P_X \rho)$$

for all $\rho \in \mathcal D(\mathcal H)$. 
Bottom Strongly Connected Components

Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain. Then a subspace $X$ of $\mathcal{H}$ is a bottom strongly connected component (BSCC) of $\mathcal{C}$ if it is an SCC of $\mathcal{C}$ and it is invariant under $\mathcal{E}$.

Characterisation of BSCCs, I

A subspace $X$ is a BSCC of quantum Markov chain $\mathcal{C}$ if and only if $\mathcal{R}_{\mathcal{C}}(\langle \varphi \rangle ) = X$ for any $\langle \varphi \rangle \in X$. 
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Characterisations of BSCCs, II

▶ A density operator $\rho$ in $\mathcal{H}$ is a fixed point state of quantum operation $\mathcal{E}$ if $\mathcal{E}(\rho) = \rho$. 

▶ A fixed point state $\rho$ of quantum operation $\mathcal{E}$ is minimal if for any fixed point state $\sigma$ of $\mathcal{E}$, $\text{supp}(\sigma) \subseteq \text{supp}(\rho)$ implies $\sigma = \rho$.

▶ If $\rho$ is a fixed point state of $\mathcal{E}$, then $\text{supp}(\rho)$ is invariant under $\mathcal{E}$. Conversely, if $X$ is invariant under $\mathcal{E}$, then there exists a fixed point state $\rho_X$ of $\mathcal{E}$ such that $\text{supp}(\rho_X) \subseteq X$.

▶ A subspace $X$ is a BSCC of quantum Markov chain $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ if and only if there exists a minimal fixed point state $\rho$ of $\mathcal{E}$ such that $\text{supp}(\rho) = X$. 

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- A subspace $X$ is a BSCC of quantum Markov chain $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ if and only if there exists a minimal fixed point state $\rho$ of $\mathcal{E}$ such that $\text{supp}(\rho) = X$. 
Lemma

1. For any two different BSCCs $X$ and $Y$ of quantum Markov chain $\mathcal{C}$: $X \cap Y = \{0\}$ (0-dimensional Hilbert space).
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2. If $X$ and $Y$ are two BSCCs of $\mathcal{C}$ with $\dim X \neq \dim Y$, then they are orthogonal: $X \perp Y$. 
Transient Subspaces

A subspace $X \subseteq \mathcal{H}$ is transient in a quantum Markov chain $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ if

$$\lim_{k \to \infty} tr \left( P_X \mathcal{E}^k (\rho) \right) = 0$$

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

Asymptotic Average

Let $\mathcal{E}$ be a quantum operation in $\mathcal{H}$. Then its asymptotic average is $\mathcal{E}^\infty = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \mathcal{E}^n$. 
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Asymptotic Average

Let $\mathcal{E}$ be a quantum operation in $\mathcal{H}$. Then its asymptotic average is

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Lemma

1. For any density operator \( \rho \), \( \mathcal{E}_\infty(\rho) \) is a fixed point state of \( \mathcal{E} \);
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1. For any density operator $\rho$, $\mathcal{E}_\infty(\rho)$ is a fixed point state of $\mathcal{E}$;
2. For any fixed point state $\sigma$: $\text{supp}(\sigma) \subseteq \mathcal{E}_\infty(\mathcal{H})$.

Theorem - Largest Transient Subspace

Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain. Then

$$T_{\mathcal{E}} = \mathcal{E}_\infty(\mathcal{H})^\perp$$

is the largest transient subspace in $\mathcal{C}$, where $^\perp$ stands for orthocomplement.
Lemma
Let $\rho$ and $\sigma$ be two fixed point state of $\mathcal{E}$, $\text{supp}(\sigma) \subset \text{supp}(\rho)$. Then there exists another fixed point state $\eta$ such that

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Lemma
Let $\rho$ and $\sigma$ be two fixed point state of $\mathcal{E}$, $\text{supp}(\sigma) \subsetneq \text{supp}(\rho)$. Then there exists another fixed point state $\eta$ such that

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2. $\text{supp}(\rho) = \text{supp}(\eta) \oplus \text{supp}(\sigma)$.

Theorem - BSCC Decomposition

$\langle H, \mathcal{E} \rangle$ be a quantum Markov chain. Then $\mathcal{E}_\infty(H)$ can be decomposed into the direct sum of orthogonal BSCCs of $C$. The Hilbert space of a quantum Markov chain $\langle H, \mathcal{E} \rangle$ can be decomposed into:

$$H = B_1 \oplus \cdots \oplus B_u \oplus T_E$$

where $B_i$'s are orthogonal BSCCs of $C$, $T_E$ is the largest transient subspace.
Lemma
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Lemma
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where $B_i$’s are orthogonal BSCCs of $\mathcal{C}$, $T_\mathcal{E}$ is the largest transient subspace.
Theorem - (Weak) Uniqueness of BSCC Decomposition

Let $\mathcal{C} = \langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain,

$$\mathcal{H} = B_1 \oplus \cdots \oplus B_u \oplus T_\mathcal{E} = D_1 \oplus \cdots \oplus D_v \oplus T_\mathcal{E}$$

be two BSCC decompositions, $B_i$s and $D_i$s are arranged, respectively, according to the increasing order of the dimensions. Then

1. $u = v$; and
Theorem - (Weak) Uniqueness of BSCC Decomposition

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be two BSCC decompositions, $B_i$s and $D_i$s are arranged, respectively, according to the increasing order of the dimensions. Then

1. $u = v$; and
2. $\dim B_i = \dim D_i$ for each $1 \leq i \leq u$.

Theorem - Decomposition Algorithm

Given a quantum Markov chain $\langle \mathcal{H}, \mathcal{E} \rangle$, Algorithm QDECOM decomposes the Hilbert space $\mathcal{H}$ into the direct sum of a family of orthogonal BSCCs and a transient subspace of $\mathcal{C}$ in time $O(d^8)$, where $d = \dim \mathcal{H}$. 
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Quantum Graph Theory
  Basic Definitions
  Bottom Strongly Connected Components
  Decomposition of the State Hilbert Space

Reachability Analysis of Quantum Markov Chains
Reachability Probability

Let $\langle \mathcal{H}, \mathcal{E} \rangle$ be a quantum Markov chain, $\rho \in \mathcal{D}(\mathcal{H})$ an initial state, and $X \subseteq \mathcal{H}$ a subspace. Then the probability of reaching $X$, starting from $\rho$, is

$$\Pr(\rho \vdash \diamond X) = \lim_{i \to \infty} tr\left( P_X \tilde{E}^i(\rho) \right)$$

where $\tilde{E}^i$ is the composition of $i$ copies of $\tilde{E}$, and $\tilde{E}$ is the quantum operation defined by

$$\tilde{E}(\sigma) = P_X \sigma P_X + \mathcal{E} (P_X \perp \sigma P_X \perp)$$

for all density operator $\sigma$. 
Lemma
Let \( \{B_i\} \) be a BSCC decomposition of \( \mathcal{E}_\infty(\mathcal{H}) \), \( P_{B_i} \) the projection onto \( B_i \). Then for each \( i \), we have

\[
\lim_{k \to \infty} tr \left( P_{B_i} \mathcal{E}^k(\rho) \right) = tr \left( P_{B_i} \mathcal{E}_\infty(\rho) \right)
\]

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

Theorem - Computing Reachability Probability
Let \( \langle \mathcal{H}, \mathcal{E} \rangle \) be a quantum Markov chain, \( \rho \in \mathcal{D}(\mathcal{H}) \), \( X \subseteq \mathcal{H} \) a subspace. Then

\[
\Pr(\rho \models \diamond X) = tr \left( P_X \tilde{\mathcal{E}}_\infty(\rho) \right),
\]

and this probability can be computed in time \( O(d^8) \) where \( d = \dim(\mathcal{H}) \).