Quantum Graph Reachability Problem

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Outline

Introduction

Basics of Quantum Theory

Graphs defined by Quantum Dynamics

Decomposition of the State Space

Algorithms for Computing Reachability in Quantum Graphs

Conclusion
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Conclusion
Graph reachability problem is everywhere

- **Databases**

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- *Databases*
  

- *Algorithms and complexity*
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- Databases
- Algorithms and complexity
- Model-checking
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- **Program analysis and verification**
Graph reachability problem is everywhere

- Databases
  
  [1] M. Yannakakis, Graph-theoretic methods in database theory, 
  PODS’1990

- Algorithms and complexity

- Model-checking

- Program analysis and verification

- Testing of digit circuits and communication protocols
Graph reachability problem is everywhere

- **Databases**
  

- **Algorithms and complexity**

- **Model-checking**

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- **Testing of digit circuits and communication protocols**

- **More ............**
Why quantum graph reachability problem?

- **Model checking quantum systems**
  
  
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- **Model checking quantum systems**

- **Analysis and verification of quantum programs**
Quantum programming environment: Q|SI>

- A quantum programming language
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- Compiler: IBM QASM 2.0
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- Compiler: IBM QASM 2.0  
- Simulator: Sunway Taihu Light — 45 qubits  
- Termination analysis: reachability problem  
- Verification: a theorem prover for quantum Hoare logic — Isabelle/HOL
Possible applications of quantum graph reachability problem to Data Science in future quantum computing era???
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Quantum states

- The state space of a quantum system is a Hilbert space $\mathcal{H}$: a complex vector space with an inner product, complete — every Cauchy sequence has a limit.
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- For finite \( n \), an \( n \)-dimensional Hilbert space is essentially the space \( \mathbb{C}^n \) of complex vectors.
- A pure quantum state is represented by a unit vector — a vector with length 1.
- Dirac’s notation: \( |\varphi\rangle, |\psi\rangle, \ldots \) denote pure states.
Qubits

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with \(|\alpha|^2 + |\beta|^2 = 1\).
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- A qubit can also be in a superposition of \(|0\rangle, |1\rangle\), e.g.

\[ |+\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \]

\[ |--\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \]
Mixed states

- A *mixed state* is represented by an *ensemble*

  \[ \{(p_1, |\psi_1\rangle), \ldots, (p_k, |\psi_k\rangle)\} \]
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- **Intuition:** the system is in state $|\psi_i\rangle$ with probability $p_i$ — a quantum generalisation of a probability distribution over states.
Density operators

- In the $n$-dimensional Hilbert space $\mathbb{C}^n$, an operator is represented by an $n \times n$ complex matrix $A$. 

- Trace of an operator $A$: \[ \text{tr}(A) = \sum_{i} A_{ii} \] (the sum of the entries on the main diagonal).

- Density operator: a positive semidefinite matrix $r$, $\text{tr}(r) = 1$. 
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Mixed states = density operators

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  \rho = \sum_{i} p_i |\psi_i\rangle\langle\psi_i|
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  \rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|.
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- In particular, a pure state $|\psi\rangle$ is identified with the density operator $\rho = |\psi\rangle\langle\psi|$.
Mixed states = density operators

- Mixed state of a qubit:

\[
\left\{ \frac{2}{3}, |0\rangle, \frac{1}{3}, |\psi\rangle \right\}
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- Density matrix:

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\rho = \frac{2}{3} |0\rangle \langle 0| + \frac{1}{3} |\rangle \langle \rangle = \frac{1}{6} \begin{pmatrix} 5 & -1 \\ -1 & 1 \end{pmatrix}
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Unitary operators

- *Dynamics* of a closed quantum system is described by the Schrödinger equation:

\[ ih \frac{d|\psi\rangle}{dt} = H|\psi\rangle \]
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\[ U^\dagger U = UU^\dagger = I \]

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- *unitary transformation*:

\[ |\psi\rangle \mapsto U|\psi\rangle \]
Quantum gates – one-qubit gates

- Pauli gates:

\[
X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
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  \[ H|0\rangle = |+\rangle, \quad H|1\rangle = |-\rangle \]

- Rotation about \( x \)-axis of the Bloch sphere:
  \[ R_x(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \]
Quantum gates – two-qubit gate

- The controlled-NOT (CNOT) gate:

\[
\text{CNOT} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]

CNOT generates entanglement: separable state \(|+0\rangle_i\) is transformed to EPR (Einstein-Podolsky-Rosen) pair:

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Super-operators

- **Dynamics** of an open quantum system is described by master equation, Langevin equation, stochastic differential equation, e.g. the Lindblad form:

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\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] + \sum_j [2L_j \rho L_j^\dagger - \{L_j^\dagger L_j, \rho\}]
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$$\rho \mapsto \mathcal{E}(\rho)$$
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- *Intuition*: a super-operator can be seen as a quantum counterpart of a transformation between probability distributions.
Kraus representation

- **Notation** — Löwner order: $A \sqsubseteq B$ if and only if $B - A$ is positive semidefinite.
Kraus representation

- **Notation** — Löwner order: \( A \subseteq B \) if and only if \( B - A \) is positive semidefinite.

- **Kraus Theorem**: Each super-operator \( \mathcal{E} \) has a Kraus representation:

\[
\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger
\]

for all density operators \( \rho \), where the set \( \{E_i\} \) of operators satisfies the sub-normalisation condition: \( \sum_i E_i^\dagger E_i \subseteq I \).
Example

The *bit flip channel* in quantum communication:

- It flips the state of a qubit from $|0\rangle$ to $|1\rangle$ and vice versa, with probability $1 - p$, $0 \leq p \leq 1$. 

For example, $r = \frac{2}{3}|0\rangle - \frac{1}{3}|1\rangle$ is transformed by $E$ to $E(r) = \frac{1}{6} + \frac{2}{3}p\frac{1}{6}$. 

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- The channel is modelled by super-operator:

$$
\mathcal{E}(\rho) = E_0 \rho E_0 + E_1 \rho E_1
$$

where $E_0 = \sqrt{p}I$, $E_1 = \sqrt{1-p}X$.  

For example, $r = \frac{2}{3} |0\rangle + \frac{1}{3} |1\rangle$ is transformed by $\mathcal{E}$ to $\mathcal{E}(r) = \frac{1}{6} + \frac{2}{3} p \frac{1}{3}$. 

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- For example,

$$\rho = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|\rangle\langle \rangle = \frac{1}{6} \begin{pmatrix} 5 & -1 \\ -1 & 1 \end{pmatrix}$$

is transformed by $\mathcal{E}$ to

$$\mathcal{E}(\rho) = \begin{pmatrix} \frac{1}{6} + \frac{2p}{3} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{5}{6} - \frac{2p}{3} \end{pmatrix}$$
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Adjacency relation

Given a quantum system $G = \langle H, E \rangle$, where

- $H$ is a finite-dimensional Hilbert space, the state space of $G$;

**Definition**: $\rho, \sigma$ are two (mixed) states in $H$.

**Notations**: 

$\text{span } X = \bigoplus_{i=0}^{n} a_i |y_i \rangle \in X; a_i \in \mathbb{C}$, $n \geq 1$. 

$\text{supp}(\rho) = \text{span} \{ \text{eigen vectors of } \rho \text{ with nonzero eigen values} \}$. 
Adjacency relation

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- $\sigma$ is adjacent to $\rho$, written $\rho \rightarrow \sigma$, if

$$\text{supp}(\sigma) \subseteq \mathcal{E}(\text{supp}(\rho)).$$

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Reachability

- A sequence

\[ \rho_0 \rightarrow \rho_1 \rightarrow \cdots \rightarrow \rho_n \]

of adjacent density operators is a path from \( \rho_0 \) to \( \rho_n \).
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  of adjacent density operators is a **path** from \( \rho_0 \) to \( \rho_n \).
- If there is a path from \( \rho \) to \( \sigma \) then \( \sigma \) is **reachable** from \( \rho \).
- The **reachable space** of \( \rho \) in \( \mathcal{G} \) is
  \[ \mathcal{R}_G(\rho) = \text{span}\{ |\psi\rangle \in \mathcal{H} : |\psi\rangle \text{ is reachable from } \rho \text{ in } \mathcal{G} \} \].
Theorem (Transitive Closure)

\[ \mathcal{R}_G(\rho) = \bigvee_{i=0}^{d-1} \text{supp}(\mathcal{E}^i(\rho)) \]

where \( d = \dim \mathcal{H} \).

Notations:

- \( \bigvee_i X_i = \text{span} \ (\bigcup_i X_i) \).
Strong connectivity

A subspace $X$ of $\mathcal{H}$ is **strongly connected** in $\mathcal{G}$ if for any $|\phi\rangle, |\psi\rangle \in X$,

$$|\phi\rangle \in \mathcal{R}_{G_X}(\psi) \text{ and } |\psi\rangle \in \mathcal{R}_{G_X}(\phi)$$
Strong connectivity
A subspace $X$ of $\mathcal{H}$ is strongly connected in $\mathcal{G}$ if for any $|\varphi\rangle, |\psi\rangle \in X$, $|\varphi\rangle \in \mathcal{R}_{\mathcal{G}_X}(\psi)$ and $|\psi\rangle \in \mathcal{R}_{\mathcal{G}_X}(\varphi)$

Strongly Connected Components
A maximal strongly connected subspace is a strongly connected component (SCC). [Zorn’s Lemma $\Rightarrow$ Existence]
Strong connectivity
A subspace $X$ of $\mathcal{H}$ is strongly connected in $\mathcal{G}$ if for any $|\varphi\rangle, |\psi\rangle \in X$,

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Strongly Connected Components
A maximal strongly connected subspace is a strongly connected component (SCC). [Zorn’s Lemma $\Rightarrow$ Existence]

Bottom Strongly Connected Component
A subspace $X$ of $\mathcal{H}$ is a bottom strongly connected component (BSCC) if it is a SCC and invariant in $\mathcal{E}$:

$$\mathcal{E}(X) \subseteq X.$$
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- **Finite-state Markov chain**: a state is transient if and only if the probability at this state will eventually become 0.
Transient Subspaces

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- A subspace $X \subseteq \mathcal{H}$ is transient in $\mathcal{G} = \langle \mathcal{H}, \mathcal{E} \rangle$ if

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

for all $\rho$. 
Largest Transient Subspace

Notation: The asymptotic average of a super-operator \( \mathcal{E} \):

\[
\mathcal{E}_\infty = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \mathcal{E}^n.
\]

Theorem

\[
\mathcal{H} = \mathcal{E}_\infty(\mathcal{H}) \oplus \mathcal{E}_\infty(\mathcal{H})^\perp.
\]

\[
T_\mathcal{E} := \mathcal{E}_\infty(\mathcal{H})^\perp
\]

is the largest transient subspace.
Decomposition Theorem

\[ \mathcal{E}_\infty(\mathcal{H}) \]

can be decomposed into the direct sum of some orthogonal BSCCs.

Corollary

The state space \( \mathcal{H} \) can be decomposed into

\[ \mathcal{H} = B_1 \oplus \cdots \oplus B_u \oplus T_\varepsilon \]

where \( B_i \)'s are orthogonal BSCCs.
Theorem (Weak Unique Decomposition)

Let
\[ \mathcal{H} = B_1 \oplus \cdots \oplus B_u \oplus T_\varepsilon = D_1 \oplus \cdots \oplus D_v \oplus T_\varepsilon \]

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Graphs defined by Quantum Dynamics

Decomposition of the State Space

Algorithms for Computing Reachability in Quantum Graphs

Conclusion
Decomposition Algorithm

BSCC decomposition in time $O(d^8)$, where $d = \dim \mathcal{H}$. 

Why Classical Algorithms, DFS, BFS, etc. Don’t Work?

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- Iteration of super-operator \( \Rightarrow \) multiplication of matrix:

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- Connections to “non-commutative graphs”?

Thank You!
Quantum measurements

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- The measurement on a qubit in the computational basis \{\ket{0}, \ket{1}\} is \( M = \{M_0, M_1\} \):

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M_0 = \ket{0}\bra{0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad M_1 = \ket{1}\bra{1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
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