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Quantum Abstract Interpretation

Seminar for the **Introduction to Quantum Computing** course

Università di Pisa
Dipartimento di Informatica

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Roadmap

① Introduction

② Preliminaries

Density Matrix

Reduced Density Matrix

③ Abstract Domain

Abstraction and Concretization Functions

Abstract Operations

Assertions



Introduction

As quantum computing advances, we would like to have some means to prove correctness properties on quantum programs, *especially* since quantum programming is counterintuitive.



Reasons

The naive way to check properties of a program is to run it and observe its behaviour.



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No: **exponential** space and time cost.



Example

$$n_{qubits} = 1$$

$$|0\rangle \langle 0|$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$2^2 = 4 \text{ complex numbers}$$



Example

$$n_{\text{qubits}} = 2$$

$$|00\rangle \langle 00|$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$2^4 = 16 \text{ complex numbers}$$



Example

$$n_{\text{qubits}} = 3$$

$$|000\rangle \langle 000|$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$2^6 = 64 \text{ complex numbers}$$



Example

$$n_{\text{qubits}} = 300$$

$$|0\rangle^{\otimes 300} \langle 0|^{\otimes 300}$$

?????



Example

$$n_{\text{qubits}} = 300$$

$$|0\rangle^{\otimes 300} \langle 0|^{\otimes 300}$$

$2^{600} = 41495155688809929585124078636911611510124462322424368$
 $999956573296906528114129081463997070489471037942881978866113$
 $007891823951510754117753078868748341139636870611818034015095$
 23685376

Bigger than the number of atoms in the universe.



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The naive way to check properties of a program is to run it and **observe** its behaviour.

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Could **simulation** on a classical machine solve this issue?

No: **exponential** space and time cost.

Solution: abstract interpretation



Ingredients

- Abstract domain
 - Abstraction function
 - Concretization function
 - Abstract operations
- Assertions



Density Matrix

Instead of dealing with a state $|\phi\rangle$ in vector form, we use its *density matrix*:

$$\rho_\phi = |\phi\rangle \langle\phi| \quad (\text{For a pure state})$$

- positive semi-definite
- $\text{Tr}(\rho) = 1$
- projection ($P = P^\dagger = P^2$)



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- positive semi-definite
- $\text{Tr}(\rho) = 1$
- projection ($P = P^\dagger = P^2$)

Example:

$$\begin{aligned} |\beta_{00}\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \\ \rho_{\beta_{00}} &= |\beta_{00}\rangle \langle\beta_{00}| = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \\ &= \frac{1}{2}(|00\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 00| + |11\rangle \langle 11|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$



Reduced Density Matrix

Suppose we have a composite quantum system $AB = A \otimes B$, and we want to focus our attention on a state $|\phi\rangle \in AB$ with respect to the subsystem A .

$$A = \mathbb{C}^{2^n} \times \mathbb{C}^{2^n} \quad B = \mathbb{C}^{2^m} \times \mathbb{C}^{2^m}$$

$$AB = (\mathbb{C}^{2^n} \times \mathbb{C}^{2^n}) \otimes (\mathbb{C}^{2^m} \times \mathbb{C}^{2^m})$$

$$Tr_B[\rho] : AB \rightarrow A$$

$$Tr_A[\rho] : AB \rightarrow B$$

$$Tr_B[\alpha \otimes \beta] = \alpha \cdot Tr(\beta)$$

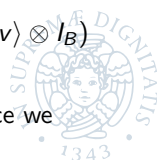
$$Tr_A[\alpha \otimes \beta] = Tr(\alpha) \cdot \beta$$

$$Tr_S[\rho + \sigma] = Tr_S[\rho] + Tr_S[\sigma] \text{ (Linearity)}$$

Alternatively:

$$Tr_B[\rho] = \sum_{v=0}^{2^m} (I_A \otimes \langle v|) \rho (I_A \otimes |v\rangle) \quad Tr_A[\rho] = \sum_{v=0}^{2^n} (\langle v| \otimes I_B) \rho (|v\rangle \otimes I_B)$$

Where v labels vectors of an orthonormal basis of the subspace we are tracing out.



Example

$$A = C^2 \times C^2 \quad B = C^2 \times C^2 \quad AB = A \otimes B$$

$$\rho_{\beta_{00}} = |\beta_{00}\rangle \langle \beta_{00}| = \frac{|00\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 00| + |11\rangle \langle 11|}{2}$$

$$\text{Tr}_B[\rho_{\beta_{00}}] =$$



Example

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$$Tr_B[\rho_{\beta_{00}}] = \frac{(Tr_B[|00\rangle \langle 00|] + Tr_B[|00\rangle \langle 11|] + Tr_B[|11\rangle \langle 00|] + Tr_B[|11\rangle \langle 11|])}{2}$$



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$$\begin{aligned} Tr_B[\rho_{\beta_{00}}] &= \frac{(Tr_B[|00\rangle \langle 00|] + Tr_B[|00\rangle \langle 11|] + Tr_B[|11\rangle \langle 00|] + Tr_B[|11\rangle \langle 11|])}{2} \\ &= \frac{(|0\rangle \langle 0| \cdot \langle 0|0\rangle) + (|0\rangle \langle 1| \cdot \langle 0|1\rangle) + (|1\rangle \langle 0| \cdot \langle 1|0\rangle) + (|1\rangle \langle 1| \cdot \langle 1|1\rangle)}{2} \end{aligned}$$



Example

$$A = \mathcal{C}^2 \times \mathcal{C}^2 \quad B = \mathcal{C}^2 \times \mathcal{C}^2 \quad AB = A \otimes B$$

$$\rho_{\beta_{00}} = |\beta_{00}\rangle \langle \beta_{00}| = \frac{|00\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 00| + |11\rangle \langle 11|}{2}$$

$$\begin{aligned} Tr_B[\rho_{\beta_{00}}] &= \frac{(Tr_B[|00\rangle \langle 00|] + Tr_B[|00\rangle \langle 11|] + Tr_B[|11\rangle \langle 00|] + Tr_B[|11\rangle \langle 11|])}{2} \\ &= \frac{(|0\rangle \langle 0| \cdot \langle 0|0\rangle) + (|0\rangle \langle 1| \cdot \langle 0|1\rangle) + (|1\rangle \langle 0| \cdot \langle 1|0\rangle) + (|1\rangle \langle 1| \cdot \langle 1|1\rangle)}{2} \\ &= \frac{|0\rangle \langle 0| + |1\rangle \langle 1|}{2} \end{aligned}$$



Loss of precision

Computing a reduced density matrix **discards information!**

$$\rho_{\beta_{00}} = \frac{|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|}{2} \quad (\text{Pure state})$$

$$\rho_2 = \frac{|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11|}{4} \quad (\text{Mixed state})$$



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$$\text{Tr}_B[\rho_{\beta_{00}}] = \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \text{Tr}_B[\rho_2]$$

The partial traces of two different initial states can be equal.

Moreover, for a state $\rho \in A \otimes B$, even if we know $\text{Tr}_B[\rho]$ and $\text{Tr}_A[\rho]$, we cannot uniquely determine ρ .



Linear Subspaces

Each projection P corresponds to a linear subspace $\{v \mid Pv = v\}$.

The support of a matrix P is the subspace orthogonal to its kernel, i.e., the set $\{v \mid Pv \neq 0\}$.



Abstract Domain

$$\mathcal{D} = \mathbb{C}^{2^n} \otimes \mathbb{C}^{2^n}, \quad S = (s_1, \dots, s_m), \quad 1 \leq m \leq 2^n, \quad s_i \subseteq [n]$$

$$AbsDom(S) = \left\{ (P_{s_1}, \dots, P_{s_m}) \mid P_{s_i} \text{ is a projection in } \mathbb{C}^{2^{|s_i|}} \otimes \mathbb{C}^{2^{|s_i|}} \right\}$$

Intuitively, given a tuple S of sets of qubits, an abstract state $\bar{\sigma} \in AbsDom(S)$ is a tuple of projections over those qubits.

Special case:

$$T = ([n]) \Rightarrow AbsDom(T) = \mathcal{D}$$



Fineness Relation

Let $S = (s_1, \dots, s_m)$ and $T = (t_1, \dots, t_m)$ (with $1 \leq m \leq 2^n$), then:

$$\underbrace{S \sqsubseteq T}_{\text{"T is finer than S"}} \triangleq \forall i \in [m]. s_i \subseteq t_i$$

T is “more concrete” than S .

Least element: $\perp = (\emptyset, \dots, \emptyset)$.

Greatest element: $\top = ([n], \dots, [n])$.

$AbsDom(\top)$ corresponds to a state so abstract that it holds no information at all.

$AbsDom(\top)$ corresponds to tuples where every projection is a concrete state.



Abstraction Function

$$S \sqsubseteq T \triangleq \forall i \in [m]. s_i \subseteq t_i$$

$$\alpha_{T \rightarrow S} : AbsDom(T) \rightarrow AbsDom(S)$$

$$\alpha_{T \rightarrow S}(Q_{t_1}, \dots, Q_{t_m}) = (P_{s_1}, \dots, P_{s_m})$$

$$P_{s_i} = \bigcap_{t_j. s_i \subseteq t_j} supp(Tr_{t_j \setminus s_i}[Q_{t_j}])$$

Given an abstract state $\bar{\tau} \in AbsDom(T) = (Q_{t_1}, \dots, Q_{t_m})$, we want to compute $\bar{\sigma} \in AbsDom(S) = (P_{s_1}, \dots, P_{s_m})$. For each $i \in [m]$:

- ① Find all Q_{t_j} s such that $s_i \subseteq t_j$. We know that at least one exists (for $j = i$), since $S \sqsubseteq T$.
- ② For each Q_{t_j} found, trace out the bits in t_j that are not in s_i .
- ③ Compute the support of the traced matrices (to preserve the structure of projections).
- ④ Compute the intersection of the supports.



Concretization Function

$$S \sqsubseteq T \triangleq \forall i \in [m]. s_i \subseteq t_i$$

$$\gamma_{S \rightarrow T} : AbsDom(S) \rightarrow AbsDom(T)$$

$$\gamma_{S \rightarrow T}(P_{s_1}, \dots, P_{s_m}) = (Q_{t_1}, \dots, Q_{t_m})$$

$$Q_{t_j} = \bigcap_{s_i. s_i \subseteq t_j} P_{s_i} \otimes I_{t_j \setminus s_i}$$

Given an abstract state $\bar{\sigma} \in AbsDom(S) = (P_{s_1}, \dots, P_{s_m})$, we want to compute $\bar{\tau} \in AbsDom(T) = (Q_{t_1}, \dots, Q_{t_m})$. For each $j \in [m]$:

- ① Find all P_{s_i} s such that $s_i \subseteq t_j$. We know at least one exists (for $i = j$), since $S \sqsubseteq T$.
- ② Extend the projection to the space of all qubits in t_j , by computing the tensor product with the identity matrix.
- ③ Compute the intersection of the extended projections.



Order Relation on Abstract States

$$1 \leq m \leq 2^n, \quad S = (s_1, \dots, s_m), \quad \forall i \in [m]. s_i \subseteq [n]$$

$$\bar{\sigma} \in \text{AbsDom}(S) = (P_{s_1}, \dots, P_{s_m}), \quad \bar{\tau} \in \text{AbsDom}(S) = (Q_{s_1}, \dots, Q_{s_m})$$

$$\bar{\sigma} \sqsubseteq \bar{\tau} \triangleq \forall i \in [m]. \underbrace{P_{s_i} \subseteq Q_{s_i}}$$

Subspace interpretation
of projections



Monotonicity

$$S \trianglelefteq T$$

$$\forall \bar{\sigma}, \bar{\tau} \in \text{AbsDom}(T). \quad \bar{\sigma} \sqsubseteq \bar{\tau} \Rightarrow \alpha_{T \rightarrow S}(\bar{\sigma}) \sqsubseteq \alpha_{T \rightarrow S}(\bar{\tau})$$

$$\forall \bar{\sigma}, \bar{\tau} \in \text{AbsDom}(T). \quad \bar{\sigma} \sqsubseteq \bar{\tau} \Rightarrow \gamma_{T \rightarrow S}(\bar{\sigma}) \sqsubseteq \gamma_{T \rightarrow S}(\bar{\tau})$$



Galois connection

$$\begin{aligned}
 & S \trianglelefteq T \\
 & \forall \bar{\sigma} \in \text{AbsDom}(S). \forall \bar{\tau} \in \text{AbsDom}(T). \\
 & \left(\begin{array}{c} \bar{\tau} \sqsubseteq \gamma_{S \rightarrow T}(\bar{\sigma}) \Rightarrow \alpha_{T \rightarrow S}(\bar{\tau}) \sqsubseteq \bar{\sigma} \\ \wedge \\ (\exists \bar{\rho} \in \text{AbsDom}([n]^m). \bar{\tau} = \alpha_{[n]^m \rightarrow T}(\bar{\rho})) \Rightarrow \bar{\tau} \sqsubseteq \gamma_{S \rightarrow T}(\bar{\sigma}) \Leftrightarrow \alpha_{T \rightarrow S}(\bar{\tau}) \sqsubseteq \bar{\sigma} \end{array} \right)
 \end{aligned}$$

$$\begin{aligned}
 & \forall \bar{\sigma} \in \text{AbsDom}(S). \forall \bar{\tau} \in \text{AbsDom}([n]^m). \\
 & \bar{\tau} \sqsubseteq \gamma_{S \rightarrow [n]^m}(\bar{\sigma}) \Leftrightarrow \alpha_{[n]^m \rightarrow S}(\bar{\tau}) \sqsubseteq \bar{\sigma}
 \end{aligned}$$



Abstract Operations

Operations on the concrete domain are unitary operators U .

To apply them to a concrete state ρ we compute $U\rho U^\dagger$.

We want to define $U^\sharp : AbsDom(S) \rightarrow AbsDom(S)$.

Let $T = (t_1, \dots, t_m)$ s.t. $t_i = s_i \cup s_U$, where s_U denotes the set of qubits that matrix U acts on.

Let $U^{cg}(\bar{\sigma}) = (UT_{t_1}U^\dagger, \dots, UT_{t_m}U^\dagger)$, then

$$U^\sharp = \alpha_{T \rightarrow S} \circ U^{cg} \circ \gamma_{S \rightarrow T}$$

We first concretize to a new, finer domain with sufficient precision to accurately represent the operation, then abstract back to the original abstract domain to keep the representation more compact.



Assertions

We want to check that a state of a program lies in the span of two vectors.

We define an assertion as:

$$A = \text{span}\{v_1 = |a_1\rangle \dots |a_n\rangle, v_2 = |b_1\rangle \dots |b_n\rangle\}$$

And a projection $\text{proj}(A)$ onto this subspace, such that:

$$\text{proj}(A)v_1 = v_1 \quad \text{proj}(A)v_2 = v_2$$



Connectivity

$$S = (s_1, \dots, s_m)$$

S is connected $\triangleq \forall k \in [n-1]. \exists r \in [m]. k \in s_r \wedge k+1 \in s_r$



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Example:

$$n = 5, \quad m = 3$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



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Example:

$$n = 5, \quad m = 3$$

$$0, 1 \in \{0, 1, 2\}$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



Connectivity

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Example:

$$n = 5, \quad m = 3$$

$$1, 2 \in \{0, 1, 2\}$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



Connectivity

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Example:

$$n = 5, \quad m = 3$$

$$2, 3 \in \{0, 2, 3\}$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



Connectivity

$$S = (s_1, \dots, s_m)$$

S is connected $\triangleq \forall k \in [n-1]. \exists r \in [m]. k \in s_r \wedge k+1 \in s_r$

Example:

$$n = 5, \quad m = 3$$

$$3, 4 \in \{3, 4, 5\}$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



Connectivity

$$S = (s_1, \dots, s_m)$$

S is connected $\triangleq \forall k \in [n-1]. \exists r \in [m]. k \in s_r \wedge k+1 \in s_r$

Example:

$$n = 5, \quad m = 3$$

$$4, 5 \in \{3, 4, 5\}$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$



Connectivity

$$S = (s_1, \dots, s_m)$$

$$S \text{ is connected} \triangleq \forall k \in [n-1]. \exists r \in [m]. k \in s_r \wedge k+1 \in s_r$$

Example:

$$n = 5, \quad m = 3$$

$$S = (\{0, 2, 3\}, \{0, 1, 2\}, \{3, 4, 5\})$$

For an assertion A , if S is connected, then:

$$proj(A) = \gamma_{S \rightarrow [n]^m}(\alpha_{[n]^m \rightarrow S}(proj(A)))$$



Assertion Checking

Given an assertion A , if the final state of a computation is v and the final abstract state of the abstract interpretation is $\bar{v} \in \text{AbsDom}(S)$, with S connected, then:

$$\bar{v} \sqsubseteq \alpha_{[n]^m \rightarrow S}(\text{proj}(A)) \quad \Rightarrow \quad v \in A$$



Choice of Tuple S

Fundamental choice for the shape of the abstract domain and, in turn, the success of the analysis.



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Type of S	Pros	Cons
Less, smaller sets	Less computational cost and memory footprint	Less precision
More, bigger sets	More computational cost and memory footprint	More precision



Choice of Tuple S

Fundamental choice for the shape of the abstract domain and, in turn, the success of the analysis.

Type of S	Pros	Cons
Less, smaller sets	Less computational cost and memory footprint	Less precision
More, bigger sets	More computational cost and memory footprint	More precision

Example:

- $S_1 = \text{all } \binom{n}{k} \text{ combinations of } k \text{ qubits}$
- $S_2 = \text{sets that contain qubits used by at least two 3-qubit gates}$
- ...



Assertion Checking Example

We want to check (partial) correctness of Grover's algorithm.

Grover's algorithm steps:

- 1 Prepare the initial state $|\phi\rangle^{(0)}$
- 2 Repeat approx. $\frac{\pi}{4}\sqrt{N}$ times $|\phi\rangle^{(t+1)} = G|\phi\rangle^{(t)}$.
- 3 Measure in the computational basis.

With this abstract interpretation framework, we can prove the loop invariant:

$$|\phi\rangle^{(t)} \in A = \text{span}\{|\beta\rangle, |\phi\rangle\}$$



Computing the Projection of a Support

To compute a projection corresponding to $\text{supp}(A)$, we:

- 1 take the rows $\{r_1, \dots, r_n\}$ of A ;
- 2 extract an orthonormal set of vectors $\{b_1, \dots, b_n\}$ that span the same subspace as the rows;
- 3 create the matrix $B = \begin{pmatrix} b_1 \\ \dots \\ b_n \end{pmatrix}$;
- 4 return BB^\dagger .



Computing the Projection of an Intersection

$$\{P_1, \dots, P_k\}, \quad \forall i \in [k]. \ P_i = C^n \times C^n$$
$$\bigcap_{i \in [k]} P_i \triangleq I_n - \text{supp}(kl_n - \sum_{i \in [k]} P_i)$$



Computing the Assertion Projection

Given two vectors

$$v_1 = |a_1\rangle \dots |a_n\rangle$$

$$v_2 = |b_1\rangle \dots |b_n\rangle$$

① Create a matrix $P = \begin{pmatrix} v_1^T \\ v_2^T \\ \mathbf{0} \\ \dots \\ \mathbf{0} \end{pmatrix}$

② Return $\text{supp}(P)$

