Automata-Based Fully Automated Analysis of Quantum Programs with AutoQ

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joint work with
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Lukáš Holík, Min-Hsiu Hsieh, Wei-Jia Huang, Jyun-Ao Lin, Fang-Yi Lo,
Ramanathan S. Thinniyam, Wei-Lun Tsai, Di-De Yen

WQS'25

Verification of Classical Programs

Verification of classical programs:

- (pre/post-condition based, a.k.a. Floyd-Hoare style)

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Meaning:

- If S is executed from a state from *Pre*
- and the execution of S terminates,
- then the program state after S terminates is in *Post*.

Verification of Quantum Circuits

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- *Pre* and *Post* denote sets of **quantum** states

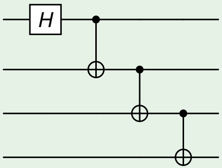
Meaning:

- If C is executed from a quantum state from *Pre*
- then the quantum state after C terminates is in *Post*.
- (termination is implicit)

Verification of Quantum Circuits

Example (GHZ)

$\{|w\rangle : w \in \{0,1\}^4\}$



$\{\frac{1}{\sqrt{2}}|0b_2b_3b_4\rangle \pm \frac{1}{\sqrt{2}}|1\bar{b}_2\bar{b}_3\bar{b}_4\rangle :$
$b_2b_3b_4 \in \{0,1\}^3\}$

Pre Circuit *Post*

$$Pre = \{|0000\rangle, |0001\rangle, \ldots, |1111\rangle\}$$

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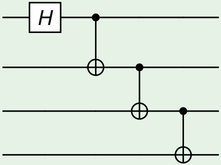

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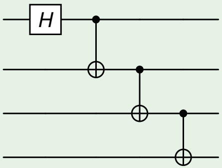

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How to efficiently represent sets of quantum states *Pre* and *Post*?

- naively $\rightsquigarrow$ double exponential size

Quantum States are Trees

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…and quantum gates are tree operations

Quantum States are Trees

x	y	z	*amp*
0	**0**	**0**	**½**
0	0	1	0
0	1	0	0
0	**1**	**1**	**½**
1	**0**	**0**	**½ i**
1	0	1	0
1	1	0	0
1	**1**	**1**	**½ i**

$\Rightarrow$

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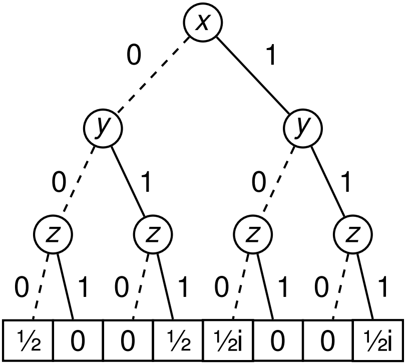

- perfect tree of height n (the number of qubits) $\rightsquigarrow$ 2^n leaves

Quantum Gates are Tree Operations

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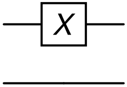
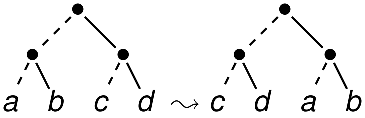


$$X_1 = \overbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}^{X} \otimes \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}^{I}$$



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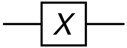

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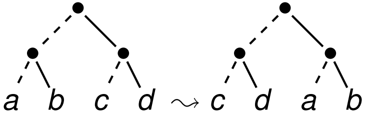
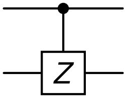
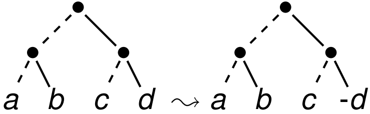




$$CZ_2^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$



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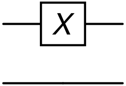

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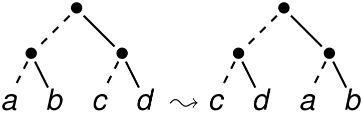

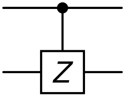

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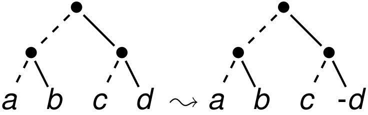
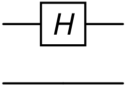
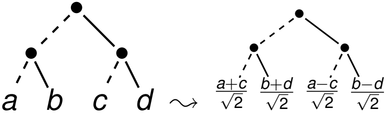




$$H_1 = \overbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}}^{H} \otimes \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}^{I}$$



Sets of Quantum States are Sets of Trees

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  - finite-state automata representing sets of finite trees
  - extension of standard finite automata for regular languages

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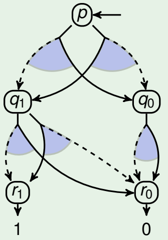
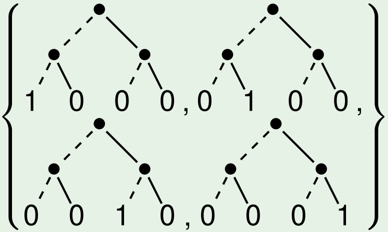
Example



represents the set
$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} =$



Representing *Pre* and *Post* with Tree Automata

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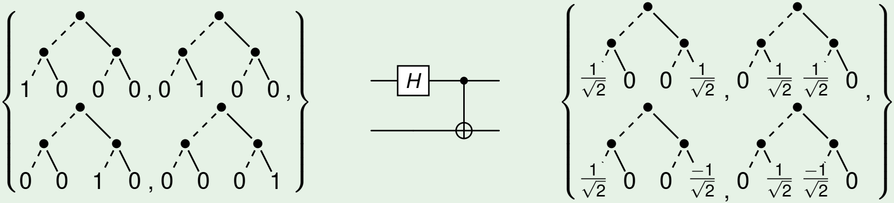

$\mathcal{L}(\mathcal{A}_{Pre})$ $\mathcal{L}(\mathcal{A}_{Post})$

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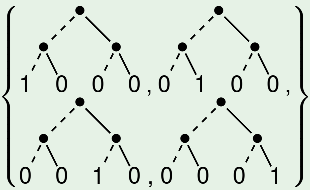

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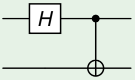
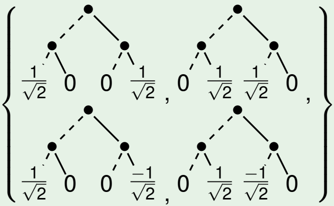




$\mathcal{L}(\mathcal{A}_{Post})$

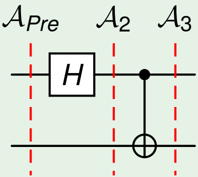
- $\mathcal{A}$'s size can be small
  - e.g., $\mathcal{A}$ for $\{|w\rangle : w \in \{0,1\}^n\}$ needs $\mathcal{O}(n)$ states/transitions

Verification with Tree Automata

$$\overset{\textit{precondition}}{\{\mathcal{A}_{Pre}\}} \quad \underset{\textit{circuit}}{C} \quad \overset{\textit{postcondition}}{\{\mathcal{A}_{Post}\}}$$

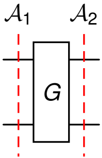
- Run C with $\mathcal{A}_{Pre}$:

Example



- ... and test $\mathcal{L}(\mathcal{A}_3) \subseteq \mathcal{L}(\mathcal{A}_{Post})$
  - (standard tree automata inclusion is **EXPTIME**-complete)

Abstract Transformers for Quantum Gates



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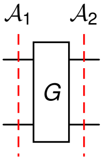

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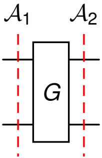

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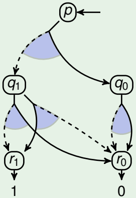
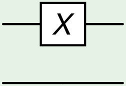
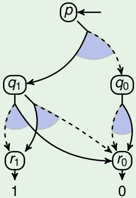


$\{|00\rangle, |01\rangle\}$





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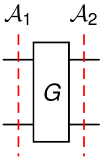
Abstract Transformers for Quantum Gates



- Supported gate types:
  - (anti-)diagonal: X, Y, Z, S, T, R_z, controls ($CNOT, CZ, Toffoli, \ldots$)
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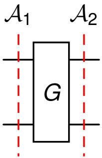

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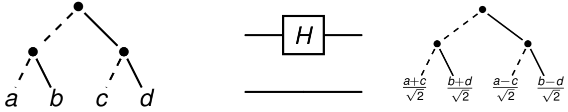
    - simple manipulation with automaton: $\mathcal{O}(|\mathcal{A}_1|)$
  - general: $H, R_x, R_y, \ldots$
    - need to synchronize subtrees of the same tree



    - standard tree automata: $\mathcal{O}(2^{|\mathcal{A}_1|})$
    - level-synchronized tree automata: $\mathcal{O}(|\mathcal{A}_1|^2)$

Quantum Circuit Verification Algorithm

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- Algorithm:
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  3. Test $\mathcal{L}(\mathcal{A}_C) \subseteq \mathcal{L}(\mathcal{A}_{Post})$.

Level-Synchronized Tree Automata

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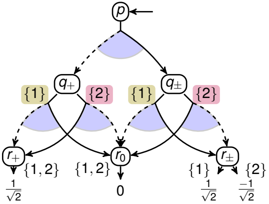
Level-Synchronized Tree Automata

- allow synchronization across subtrees



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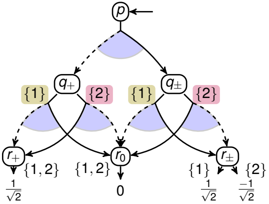

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  - general gates: $\mathcal{O}(|\mathcal{A}|^2)$ (improved from $\mathcal{O}(2^{|\mathcal{A}|})$)

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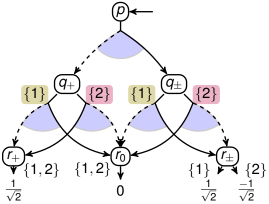

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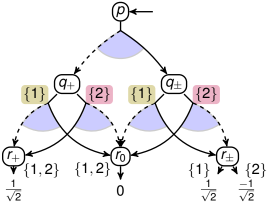

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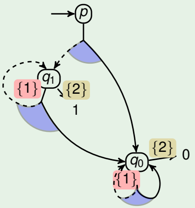
- incomparable to basic TAs
  - cannot express “all trees”
- language operations:
  - emptiness: **PSPACE**-complete
  - inclusion/equivalence: **PSPACE**-hard, in **EXPSPACE**

Level-Synchronized Tree Automata (LSTAs)

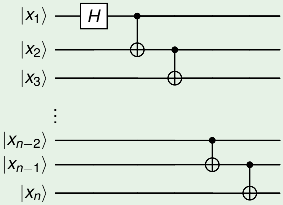
Level-Synchronized Tree Automata

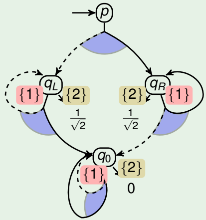
- enable basic parameterized verification

Example (GHZ)



$\{|0^n\rangle : n \geq 1\}$





$\{\frac{1}{\sqrt{2}}|0^n\rangle + \frac{1}{\sqrt{2}}|1^n\rangle : n \geq 1\}$

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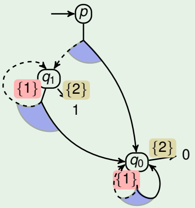

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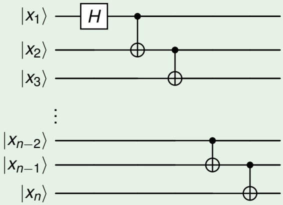

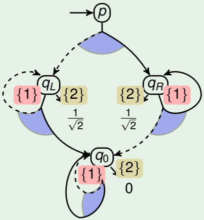

$\{\frac{1}{\sqrt{2}}|0^n\rangle + \frac{1}{\sqrt{2}}|1^n\rangle : n \geq 1\}$

- GHZ, fermionic unitary evolution (single/double fermionic excitation)

Weighted Level-Synchronized Tree Automata

$\rightsquigarrow$ in Yu-Fang's talk

What can we verify?

- (parameterized versions of) Bernstein-Vazirani, multi-control Toffoli
- Grover's algorithm:
  - pre/post with precise sets of quantum states
  - single/all oracles
  - $P(solution) > 0.9$ (symbolic TAs)
  - one iteration increases probability (symbolic TAs)
  - equivalence of parameterized one loop (WLSTAs)
  - weakly-measured version (symbolic TAs + measurements)
- repeat until success circuits (found bugs!)
- circuits from **RevLib**, **Feynman**, **Random**
- parameterized GHZ
- parameterized fermionic unitary evolution (LSTAs)

Takeaways and Future Directions

Takeaways

Quantum ♡ Automata

Future Directions

- a good specification language
  - expressive, user-friendly
  - can compile to (*)TAs quickly
- parameterized verification of circuits with QFT
- Go go go ... transducers!
- How to represent quantum circuits efficiently?
  - algebra over trees? logic?

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Thank you!

References

- Chen, Chung, Lengál, Lin, Tsai, Yen. An Automata-Based Framework for Verification and Bug Hunting in Quantum Circuits. PLDI'23.
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Symbolic Amplitudes

Introducing Symbolic Amplitudes

- So far, we only used finite numbers of amplitudes

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- But what about verifying a property like this?

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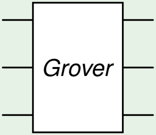
$$\{h\,|000\rangle + \ell\,|w\rangle : w \in \{0,1\}^3 \setminus \{000\}\}$$



$$\{h'\,|000\rangle + \ell'\,|w\rangle : w \in \{0,1\}^3 \setminus \{000\}\}$$

global constraint:

$$h, h', \ell, \ell' \in \mathbb{C} \land |h'|^2 \geq |h|^2 \land |\ell'|^2 \leq |\ell|^2 \land$$
$$|h|^2 \geq |\ell|^2 \land |h|^2 + 7|\ell|^2 = 1 \land |h'|^2 + 7|\ell'|^2 = 1$$

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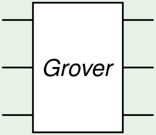

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- uncountably many quantum states

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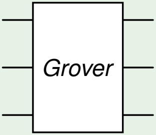

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- uncountably many amplitueds
- uncountably many quantum states
- $\rightsquigarrow$ symbolic amplitudes!

Verifying Quantum Circuits using Symbolic Amplitudes

Modifications to the verification algorithm:

- (L-S) tree automata $\rightsquigarrow$ symbolic (L-S) tree automata
  - alphabet contains symbolic values, terms, and predicates

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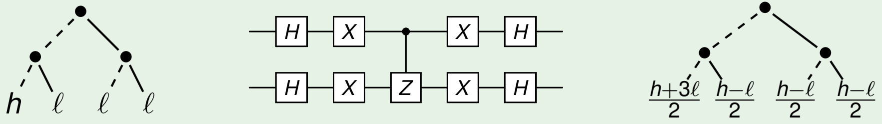

Grover's diffusion operator

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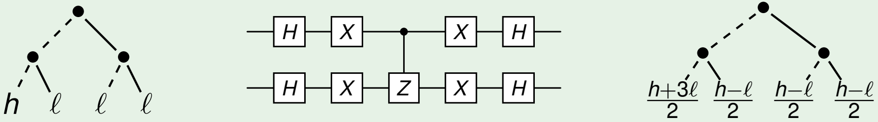

Grover's diffusion operator

- modified language inclusion test

Verification of Quantum Circuits with Loops

- Common structure of quantum programs:

$$\textbf{while}\ \ (M(x_i) = 0)\\ \quad C;$$

Algorithm 6: A Weakly Measured Version of Grover's algorithm (solution $s = 0^n$)

Pre: $\{1\left|0^{n+2}\right\rangle + 0\left|*\right\rangle\}$;
$H_3;\ H_4;\ \ldots;\ H_{n+2};$
$O_{2,\ldots,(n+2)}; CK_1^2; O_{2,\ldots,(n+2)};$
Inv: $\{v_{sol1}\left|000^n\right\rangle + v_k\left|000^{n-1}1\right\rangle + \cdots +$
$\quad v_k\left|001^n\right\rangle + v_{sol2}\left|100^n\right\rangle + 0\left|*\right\rangle\}$;
while $M_1 = 0$ **do**
$\quad \{\mathcal{G}_{2,\ldots,(n+2)}; O_{2,\ldots,(n+2)}; CK_1^2; O_{2,\ldots,(n+2)}\}$;
Post: $\{1\left|10s\right\rangle + 0\left|*\right\rangle\}$;

- repeat-until-success, weakly measured Grover

Verification of Quantum Circuits with Loops

- Common structure of quantum programs:

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H_3; H_4; ...; H_{n+2};
O_{2,...,(n+2)}; CK_1^2; O_{2,...,(n+2)};
Inv: {v_{sol1} |000^n⟩ + v_k |000^{n-1}1⟩ + ··· +
        v_k |001^n⟩ + v_{sol2} |100^n⟩ + 0 |*⟩};
while M_1 = 0 do
  | {G_{2,...,(n+2)}; O_{2,...,(n+2)}; CK_1^2; O_{2,...,(n+2)}};
Post: {1 |10s⟩ + 0 |*⟩};
```

- repeat-until-success, weakly measured Grover
- symbolic (L-S)TAs + measurements