Equivalence Checking of Quantum Circuits

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Research thrust *Reliability and Trustworthiness*

DEPARTMENT
OF COMPUTER
SCIENCE

This talk is based on joint work[1]

Christian Bøgh Larsen

Simon Brun Olsen

Kim Guldstrand Larsen

INDEPENDENT RESEARCH FUND DENMARK

VILLUM FONDEN

DIREC Digital Research Centre Denmark

[1] C. B. Larsen, S. B. Olsen, K. G. Larsen, and C. Schilling. "Contraction heuristics for tensor decision diagrams". *Entropy* (2024).

Overview

Short overview of quantum computing

Equivalence checking of quantum circuits

Existing approaches to equivalence checking

Tensor networks

Equivalence check based on tensor decision diagrams

Empirical evaluation

Conclusion and future work

Overview

Delimitation

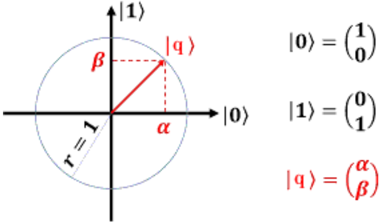
We have an idealized mathematical view, meaning:

- No noise
- No decoherence
- No mixed states

Single qubit

- Basis states $|0\rangle$ and $|1\rangle$
- Superposition $|q\rangle = \alpha|0\rangle + \beta|1\rangle$

  where $\alpha, \beta \in \mathbb{C}$ s.t. $|\alpha|^2 + |\beta|^2 = 1$
- Written as vector: $|q\rangle \equiv \begin{bmatrix}\alpha \\ \beta\end{bmatrix}$



Multiple qubits: Tensor product

$$
\begin{aligned}
|q_0 q_1\rangle &= |q_0\rangle \otimes |q_1\rangle \\
&\equiv \begin{bmatrix} \alpha_0 \\ \beta_0 \end{bmatrix} \otimes \begin{bmatrix} \alpha_1 \\ \beta_1 \end{bmatrix} \\
&\equiv \alpha_0\alpha_1 |00\rangle + \alpha_0\beta_1 |01\rangle + \beta_0\alpha_1 |10\rangle + \beta_0\beta_1 |11\rangle \\
&\equiv \begin{bmatrix} \alpha_0\alpha_1 \\ \alpha_0\beta_1 \\ \beta_0\alpha_1 \\ \beta_0\beta_1 \end{bmatrix}
\end{aligned}
$$

Quantum gates and quantum circuits

- Analogous to classical logic gates and circuits
- Quantum gates transform quantum states

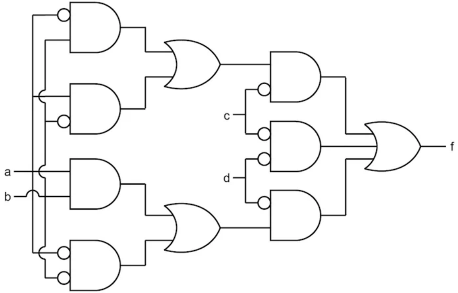
  Equivalent to (unitary) matrix multiplication with state vector

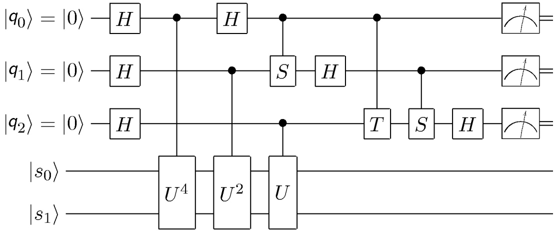
$$|q'\rangle = U\,|q\rangle$$

- Quantum circuits are compositions of multiple gates

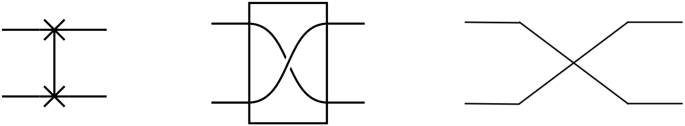
$$|q'\rangle = U_m \cdot U_{m-1} \cdots U_2 \cdot U_1\,|q\rangle$$

Quantum gates and quantum circuits





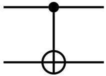
Example: SWAP gate

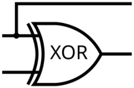


- Swapping of two qubits

$$SWAP(|q_0 q_1\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_0\alpha_1 \\ \alpha_0\beta_1 \\ \beta_0\alpha_1 \\ \beta_0\beta_1 \end{bmatrix} = \begin{bmatrix} \alpha_0\alpha_1 \\ \beta_0\alpha_1 \\ \alpha_0\beta_1 \\ \beta_0\beta_1 \end{bmatrix} = |q_1 q_0\rangle$$

Example: Controlled NOT gate





- Controlled negation of second qubit

$$CNOT(|q_0 q_1\rangle) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha_0\alpha_1 \\ \alpha_0\beta_1 \\ \beta_0\alpha_1 \\ \beta_0\beta_1 \end{bmatrix} = \begin{bmatrix} \alpha_0\alpha_1 \\ \alpha_0\beta_1 \\ \beta_0\beta_1 \\ \beta_0\alpha_1 \end{bmatrix}$$

$$= |q_0\rangle \otimes |q_0 \oplus q_1\rangle$$

where $\oplus$ is addition modulo 2 ("XOR")

Example: Hadamard gate

- Creates a superposition

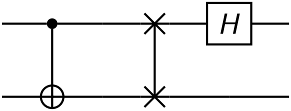
$$H(|q\rangle) = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}\alpha+\beta\\ \alpha-\beta\end{bmatrix}$$

Examples

$$H(|0\rangle) = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix} \equiv \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

$$H(|1\rangle) = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ -1\end{bmatrix} \equiv \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$$

Example: A random circuit



$$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}\left(\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\1&-1\end{bmatrix}\otimes\begin{bmatrix}1&0\\0&1\end{bmatrix}\right)$$

$$=\frac{1}{\sqrt{2}}\begin{bmatrix}1&0&1&0\\1&0&-1&0\\0&1&0&-1\\0&1&0&1\end{bmatrix}$$

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Quantum circuit compilation

- When designing quantum algorithms (= circuits), it is useful to have many types of gates available
- Real quantum computers only support a few types of gates
- A **compiler** translates a high-level circuit with many gate types to a low-level circuit with few gate types

Quantum circuit compilation

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- Different types of gates incur different amounts of error
- Deeper circuits incur more errors
- A compiler also tries to optimize circuits to reduce errors

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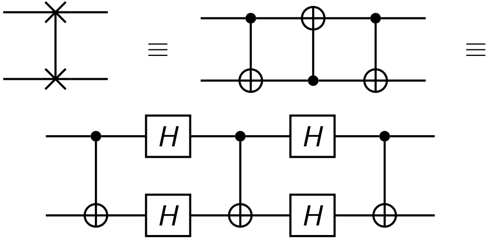
- Important that the compiled circuits are **equivalent** (i.e., compute the same output for the same input)

How to implement a SWAP gate?

- The SWAP gate is **equivalent** to three CNOT gates



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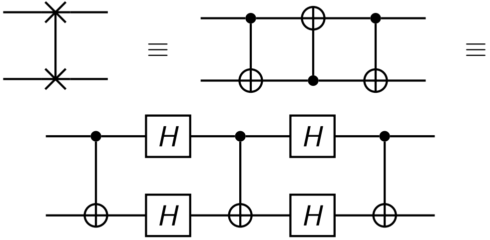

- We can easily prove this by comparing the matrices

$$\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{bmatrix}\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{bmatrix}$$

Algorithm to check equivalence of quantum circuits

- Given, two circuits C_1, C_2
- Question: Are the circuits equivalent ($C_1 \equiv C_2$)?

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  1. Compute matrix representations U_1, U_2
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Algorithm to check equivalence of quantum circuits

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- Problem: Matrices are **exponentially large**

  For n qubits $\rightsquigarrow 2^n \times 2^n$

Equivalence checking is hard

- Checking exact equivalence is NQP-complete[1]
- Checking approximate equivalence is QMA-complete[2,3]
- Problems in these complexity classes are widely believed to require exponential computations in the worst case

[1] Y. Tanaka. "Exact non-identity check is NQP-complete". *Int. J. Quantum Inf.* (2010).
[2] D. Janzing, P. Wocjan, and T. Beth. ""Non-identity-check" is QMA-complete". *Int. J. Quantum Inf.* (2005).
[3] Z. Ji and X. Wu. *Non-identity check remains QMA-complete for short circuits*. 2009. arXiv: 0906.5416.

Overview

Approaches to equivalence checking

- ZX-calculus[1]
- Encoding with decision diagrams[2]
- Tensor network contraction[3]
- Simulation-based approach for the Clifford group[4]
- Weighted model counting[5]

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[1] T. Peham, L. Burgholzer, and R. Wille. "Equivalence checking of quantum circuits with the ZX-calculus". *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).

[2] L. Burgholzer and R. Wille. "Advanced equivalence checking for quantum circuits". *IEEE Trans. Comput. Aided Des. Integr. Circuits Syst.* (2021).

[3] R. Orús. "Tensor networks for complex quantum systems". *Nature Reviews Physics* (2019).

[4] D. Thanos, T. Coopmans, and A. Laarman. "Fast equivalence checking of quantum circuits of Clifford gates". *ATVA*. 2023.

[5] J. Mei, T. Coopmans, M. M. Bonsangue, and A. Laarman. "Equivalence checking of quantum circuits by model counting". *IJCAR*. 2024.

Approaches to equivalence checking

- ZX-calculus[1]
- Encoding with decision diagrams[2] ← relevant later
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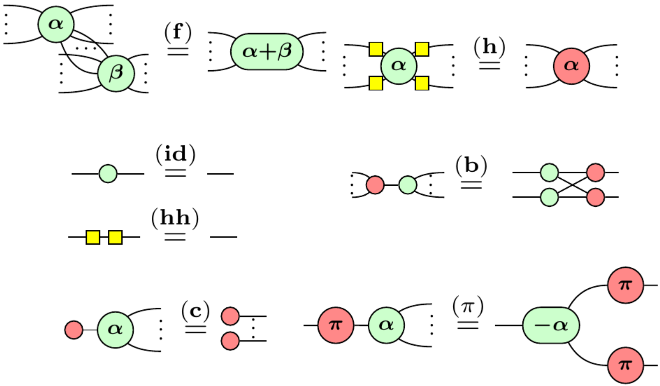
Based on ZX-calculus[1,2]



Axioms

[1] B. Coecke and R. Duncan. "Interacting quantum observables". *ICALP.* 2008.

[2] T. Peham, L. Burgholzer, and R. Wille. "Equivalence checking of quantum circuits with the ZX-calculus". *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).

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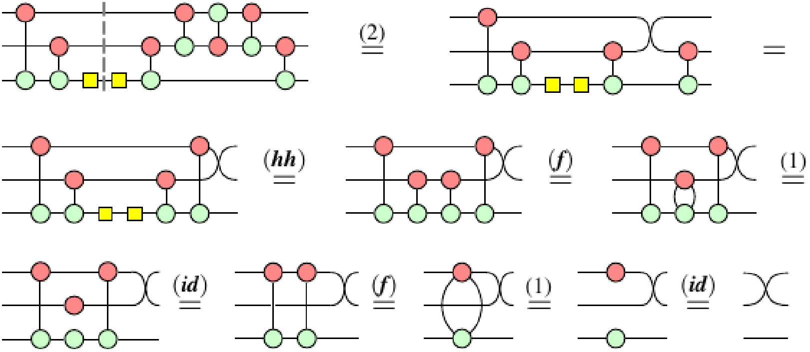
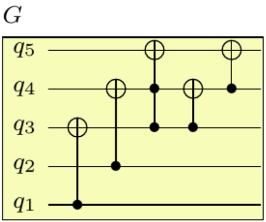


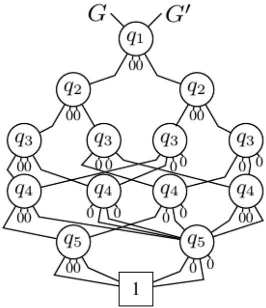
Example proof

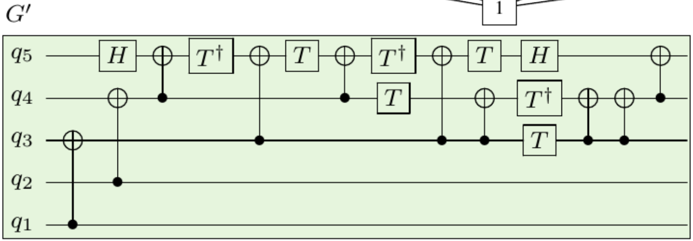
[1] B. Coecke and R. Duncan. "Interacting quantum observables". *ICALP.* 2008.

[2] T. Peham, L. Burgholzer, and R. Wille. "Equivalence checking of quantum circuits with the ZX-calculus". *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).

Based on decision diagrams[1]

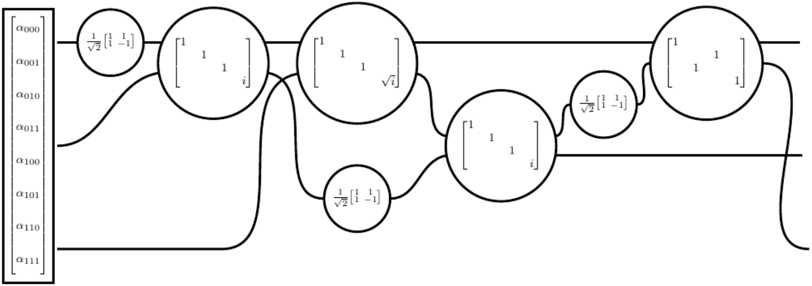






[1] L. Burgholzer and R. Wille. "Advanced equivalence checking for quantum circuits". *IEEE Trans. Comput. Aided Des. Integr. Circuits Syst.* (2021).

Based on tensor network contraction[1,2]



[1] X. Hong, Y. Feng, S. Li, and M. Ying. "Equivalence checking of dynamic quantum circuits". *ICCAD*. 2022.

[2] L. Burgholzer, A. Ploier, and R. Wille. "Simulation paths for quantum circuit simulation with decision diagrams - what to learn from tensor networks, and what not". *IEEE Trans. Comput. Aided Des. Integr. Circuits Syst.* (2023).

Based on a folklore theorem

Theorem 1. *Let U, V be two unitaries on $n \geq 1$ qubits. Then U is equivalent to V if and only if the following conditions hold:*

1. *for all $j \in \{1, 2, \ldots, n\}$, we have $UZ_jU^\dagger = VZ_jV^\dagger$; and*
2. *for all $j \in \{1, 2, \ldots, n\}$, we have $UX_jU^\dagger = VX_jV^\dagger$.*

Here, as before, we have denoted $Z_j = I \otimes \cdots \otimes I \otimes Z \otimes I \otimes \cdots \otimes I$, i.e. an n-fold tensor product of identity gates I with the Pauli Z gate at the j-th position. Analogously, $X_j = I \otimes \cdots \otimes I \otimes X \otimes I \otimes \cdots \otimes I$ where X is the Pauli X gate.

- Reduces to **simulation** for **Clifford circuits**[1]
  - $UZ_jU^\dagger$ is the same as computing $U|0\rangle^{\otimes n}$
  - $UX_jU^\dagger$ is the same as computing $U|+\rangle^{\otimes n}$
- Simulation is generally hard, but it is easy for Clifford circuits
- Extension to general circuits based on encoding as a **weighted model counting** problem[2]

[1] D. Thanos, T. Coopmans, and A. Laarman. "Fast equivalence checking of quantum circuits of Clifford gates". *ATVA*. 2023.

[2] J. Mei, T. Coopmans, M. M. Bonsangue, and A. Laarman. "Equivalence checking of quantum circuits by model counting". *IJCAR*. 2024.

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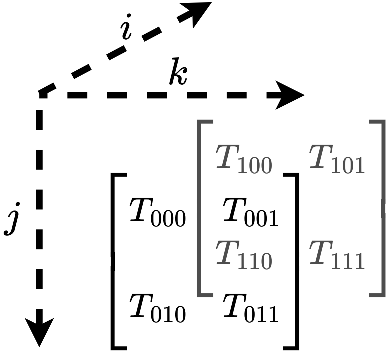
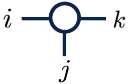
Tensors

- Generalization of vectors / matrices to higher dimensions



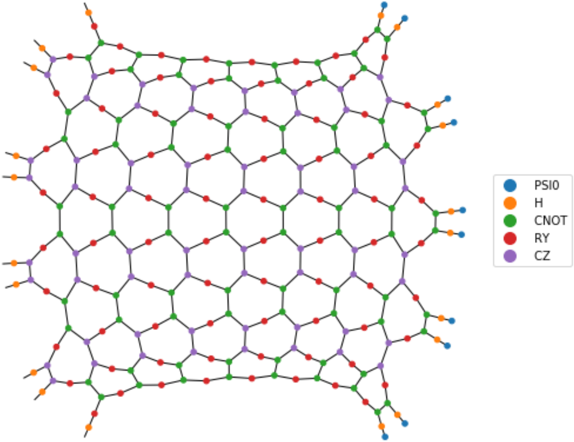
Tensors

- Generalization of vectors / matrices to higher dimensions
- High-level graphical representation as a node with edges

vector	v_j	
matrix	M_{ij}	
3-index tensor	T_{ijk}	

Tensor networks

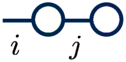
- Tensors can be arranged in a graph



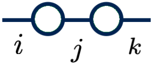
Tensor networks

- Tensors can be arranged in a graph
- Nodes with shared edges can be **contracted** (= merged)

  Corresponds to matrix-vector and matrix-matrix multiplication for special cases



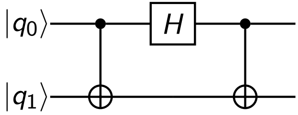
$$= \sum_j A_{ij} v_j$$

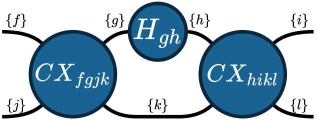


$$= \sum_j A_{ij} B_{jk} = AB$$

Example

1. Initial tensor network has one tensor for each gate
   Three choices for contraction $(\{g\}, \{h\}, \{k\})$





1.

Example

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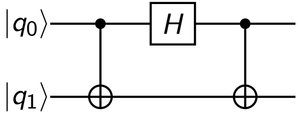
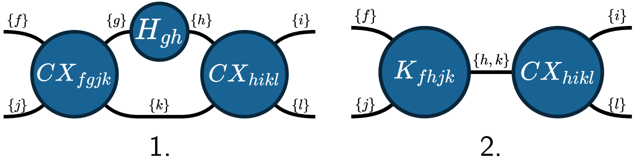
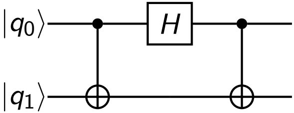
2. Contraction of CX_{fgjk} and H_{gh} via $\{g\}$

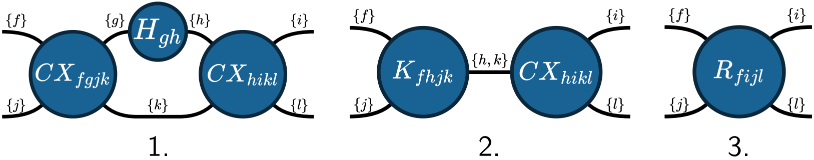




Example

1. Initial tensor network has one tensor for each gate
   Three choices for contraction ($\{g\}, \{h\}, \{k\}$)
2. Contraction of CX_{fgjk} and H_{gh} via $\{g\}$
3. Contraction of remaining two tensors





Application: Quantum simulation on classical computer[2]

- Contract tensors in smart orders
- Different contraction heuristics to minimize floating-point operations, size, etc.[1]

[1] J. Gray and S. Kourtis. "Hyper-optimized tensor network contraction". *Quantum* (2021).

[2] I. L. Markov and Y. Shi. "Simulating quantum computation by contracting tensor networks". *SIAM J. Comput.* (2008).

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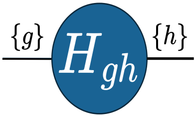
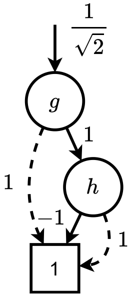
Tensor decision diagrams (TDDs)

- Alternative, unique representation of a tensor
- Informal introduction by example

Example: Hadamard gate, tensor, and TDD

$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$





Alternative "reverse scheme" for equivalence[1]

$$C_1 \equiv C_2 \overset{\text{def}}{\iff} \exists\theta\colon U_1 = e^{i\theta} \cdot U_2$$

$$\iff \exists\theta\colon U_1 \cdot U_2^{\dagger} = e^{i\theta} \cdot I \overset{\text{def}}{\iff} C_1 C_2^{-1} \equiv C_I$$

- C_2^{-1} is the inverted C_2 (reversed and each gate inverted)
- Allows to combine both circuits

[1] G. F. Viamontes, I. L. Markov, and J. P. Hayes. "Checking equivalence of quantum circuits and states". *ICCAD*. 2007.

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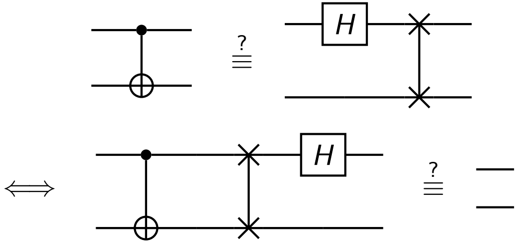


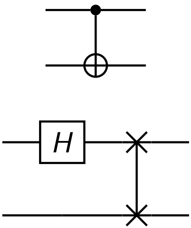
- (Coincidentally, the swap and Hadamard gates are self-inverse)

[1] G. F. Viamontes, I. L. Markov, and J. P. Hayes. "Checking equivalence of quantum circuits and states". *ICCAD*. 2007.

New algorithm for equivalence checking

Algorithm combines reverse scheme, tensor networks, and TDDs

Given: Quantum circuits C_1, C_2



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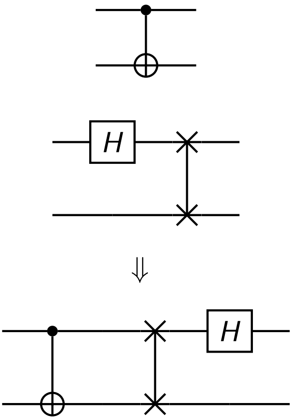
1. Construct circuit $C_1 C_2^{-1}$

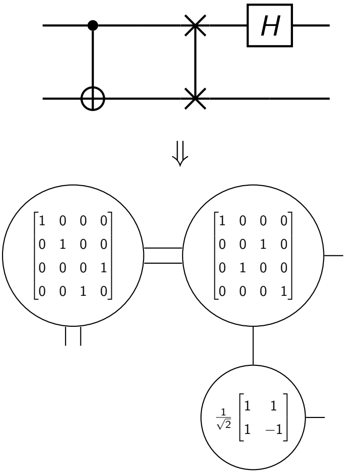


New algorithm for equivalence checking

Algorithm combines reverse scheme, tensor networks, and TDDs

Given: Quantum circuits C_1, C_2

1. Construct circuit $C_1 C_2^{-1}$
2. Convert $C_1 C_2^{-1}$ to tensor network



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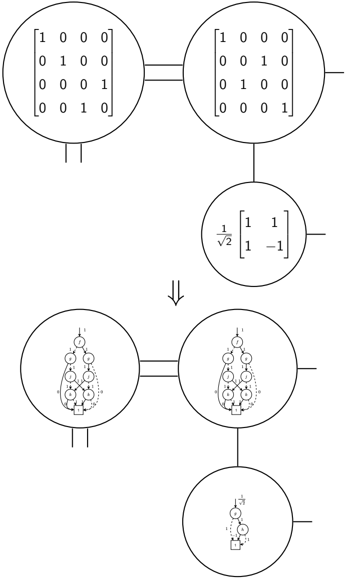

(TDDs on the right are only exemplary)

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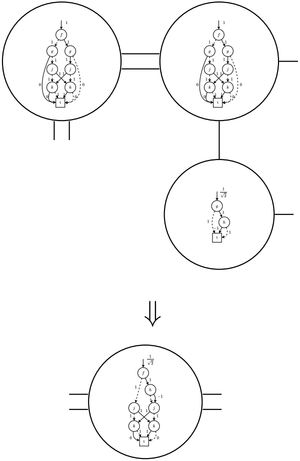

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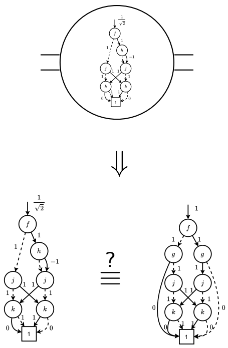

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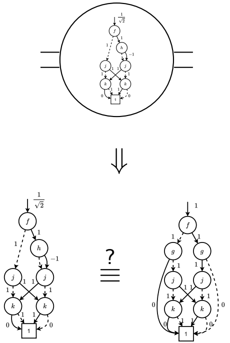
4. **Contract TDD network** $\leftarrow$ how?
5. Compare TDD to identity TDD



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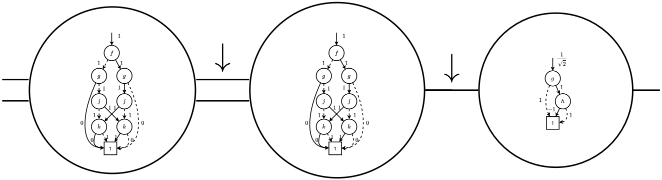
Lookahead heuristic for TDD contraction

- Greedy algorithm (finds a local optimum)
- In each contraction step:
  1. Evaluate all possible contractions



Lookahead heuristic for TDD contraction

- Greedy algorithm (finds a local optimum)
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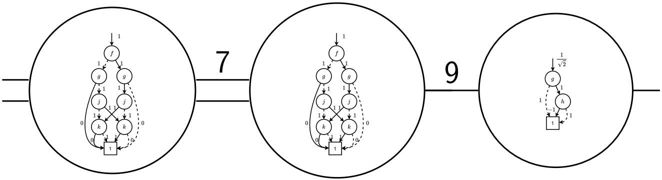
  2. Measure size of resulting TDDs



Lookahead heuristic for TDD contraction

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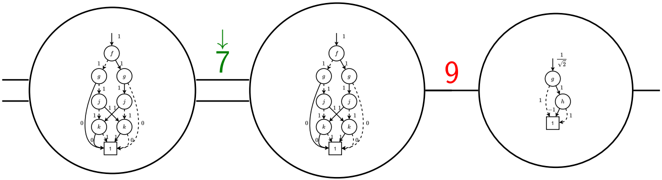

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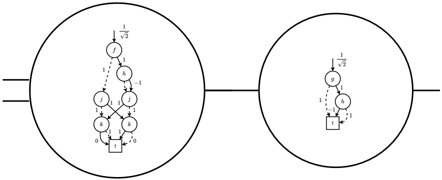

Lookahead heuristic for TDD contraction

- Greedy algorithm (finds a local optimum)
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  1. Evaluate all possible contractions
  2. Measure size of resulting TDDs
  3. Execute a contraction with smallest output
- Why should this scale?
  - Network is sparsely connected
  - Initial contractions (with many tensors) are cheap
  - Results can be stored for later iterations
- Still, step 1. is quite expensive

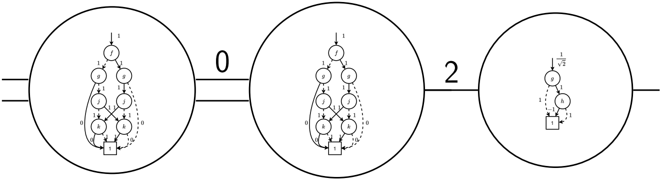
Counting heuristic for TDD contraction

- Goal: Imitate lookahead heuristic without expensive step 1
- Empirical observation: Lookahead heuristic prefers to distribute the contractions over the tensor network

[1] We set one edge to "2" to get an interesting example

Counting heuristic for TDD contraction

- Goal: Imitate lookahead heuristic without expensive step 1
- Empirical observation: Lookahead heuristic prefers to distribute the contractions over the tensor network
- In each contraction step:
    1. Select a pair of nodes with longest non-usage[1]



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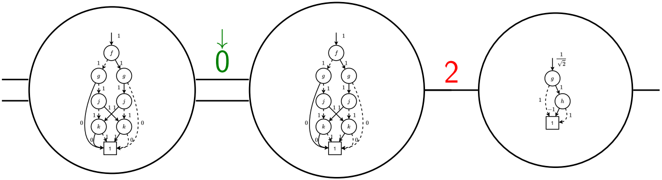

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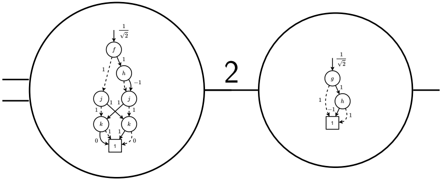

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Counting heuristic for TDD contraction

- Goal: Imitate lookahead heuristic without expensive step 1
- Empirical observation: Lookahead heuristic prefers to distribute the contractions over the tensor network
- In each contraction step:
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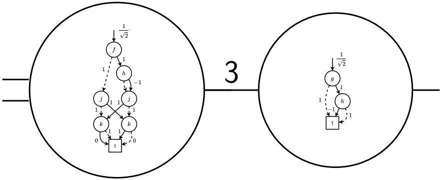
  2. Update usage statistics of neighboring edges



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Overview

Quantum circuits in evaluation

- Circuits from MQT Bench[1] with varying number of qubits at two compilation levels (level 1 and 3 (out of 4)) with significantly different gate sets and layouts
  - Deutsch-Jozsa algorithm (DJ)
  - Greenberger-Horne-Zeilinger state preparation (GHZ)
  - Graph state preparation (GS)
  - Quantum Fourier transformation (entangled qubits) (QFTE)
  - Real amplitudes ansatz with random parameters (RAR)
  - W state preparation (WS)

[1] N. Quetschlich, L. Burgholzer, and R. Wille. "MQT Bench: Benchmarking software and design automation tools for quantum computing". *Quantum* (2023).

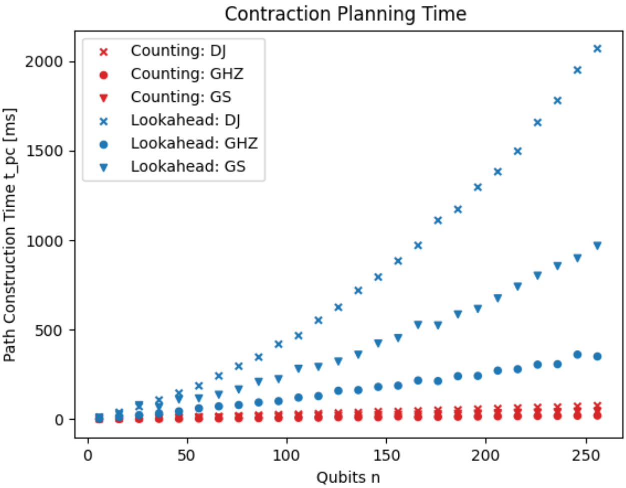
Types of experiments

1. Compare heuristics to each other
2. Compare heuristics to heuristics from cotengra[1]
3. Compare heuristics to QCEC[2] (decision diagrams)

[1] J. Gray and S. Kourtis. "Hyper-optimized tensor network contraction". *Quantum* (2021).

[2] L. Burgholzer and R. Wille. "QCEC: A JKQ tool for quantum circuit equivalence checking". *Softw. Impacts* (2021).

Comparison of own heuristics



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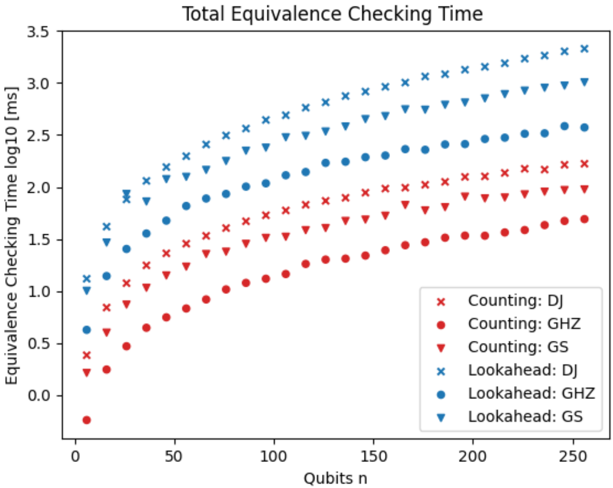
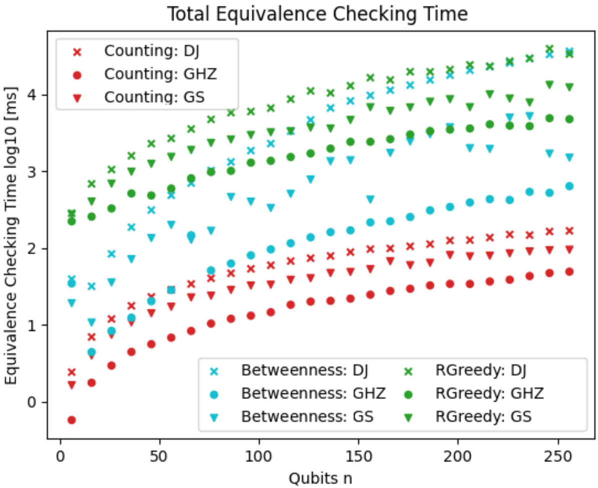


Comparison to cotengra



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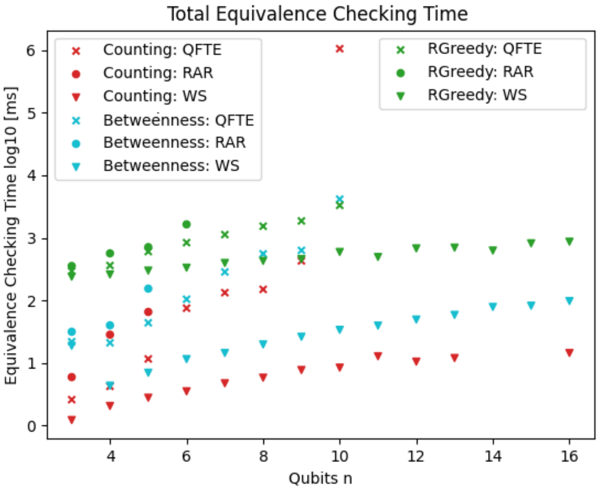
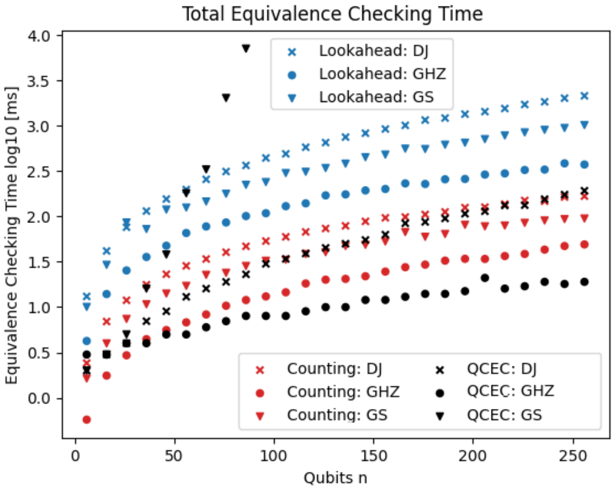


Comparison to QCEC



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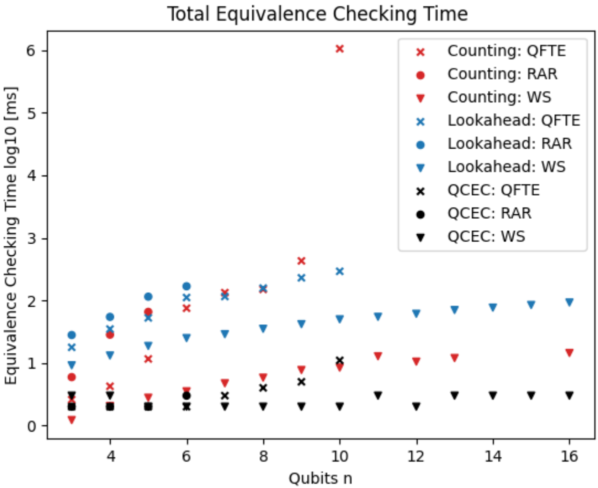

Overview

Conclusion

- Integration of “reverse scheme” and TDD networks
- Lookahead heuristic (greedy)
- Counting heuristic (cheap approximation)
- Evaluation:
  - Outperforms cotengra’s heuristics
  - Often keeps up with QCEC

Future work

- Evaluate beyond equivalence checking
- Exploit parallelization (CPU, GPU)
- Find other heuristics
  - Generalize tensor network heuristics to TDD networks
  - Identify equivalent subcomponents (modularity)
  - Employ machine learning
- New PhD project since December 2024

DeiC