Equivalence Checking of Quantum Circuits

Christian Schilling

Overview

Overview

Circuit compilation

- When designing (classical or quantum) circuits, it is useful to have many gate types available
- Real hardware only supports a few gates types
- A **compiler** translates a high-level circuit with many gate types to a low-level circuit with few gate types
- Quantum gates incur different amounts of error
- Deeper quantum circuits incur more errors
- Quantum compilers also optimize for reducing errors
- Important that the compiled circuits are **equivalent** (same input $\rightsquigarrow$ same output)
- How can we check equivalence of circuits?

Overview

Qubit

- Ground state $|0\rangle$, excited state $|1\rangle$
- Superposition $|q\rangle = \alpha\,|0\rangle + \beta\,|1\rangle, \quad \alpha, \beta \in \mathbb{C}$
- Written as 2D vector: $|q\rangle \equiv \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$
- Constraint $|\alpha|^2 + |\beta|^2 = 1$
- Ignoring complex numbers,
  a qubit state describes a circle

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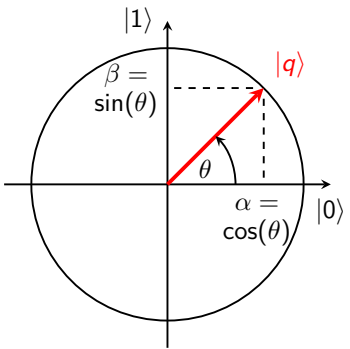
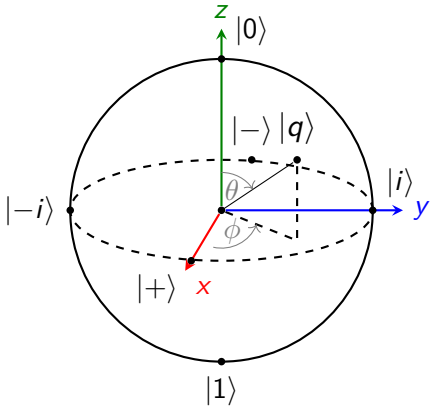


Bloch sphere



- Polar coordinates: $|q\rangle = \underbrace{\cos\frac{\theta}{2}}_{\alpha}|0\rangle + \underbrace{e^{i\phi}\sin\frac{\theta}{2}}_{\beta}|1\rangle$

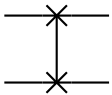
Multiple qubits

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

- Not every multi-qubit state is a product state

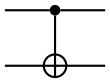
Quantum gates

- Unitary matrix operations
- Example: Swapping of two qubits



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

Another quantum gate: Controlled NOT



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

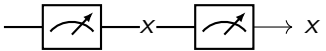
$$= |q_0, q_0 \oplus q_1\rangle$$

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

Measurement

- Probabilistically projects to basis state ($|0\rangle$ or $|1\rangle$)
- Not invertible

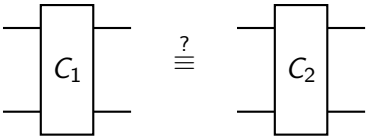
$$|q\rangle \equiv \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$



$$x = \begin{cases} |0\rangle & \text{with probability } |\alpha|^2 \\ |1\rangle & \text{with probability } |\beta|^2 \end{cases}$$

Overview

Black-box equivalence check for classical circuits



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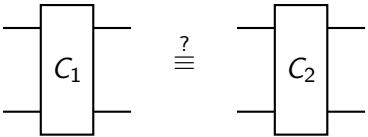

- Classical circuits: Pick an input and execute both circuits

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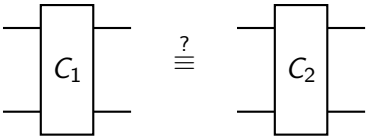
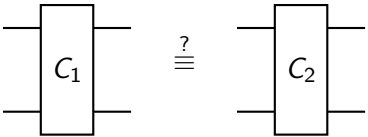


- Classical circuits: Pick an input and execute both circuits
  - One-way result: Disagreement implies different circuits
  - **Exponentially many** classical inputs

Black-box equivalence check for quantum circuits



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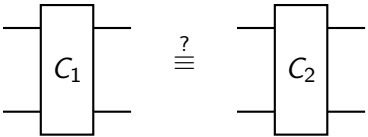

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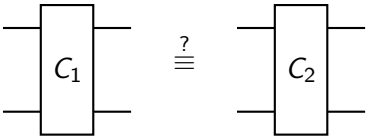

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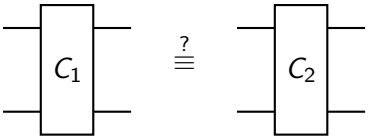

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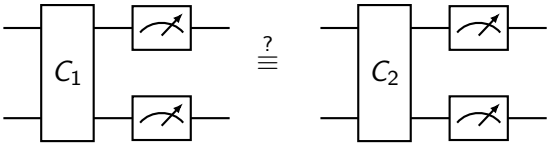

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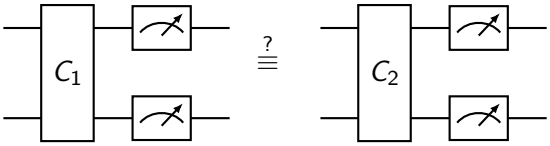

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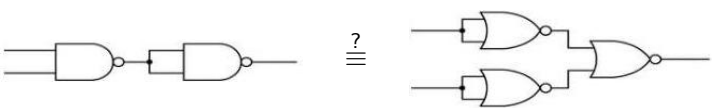
  - Disagreement does **not** imply different circuits
  - **Approximation** by many executions is **expensive**

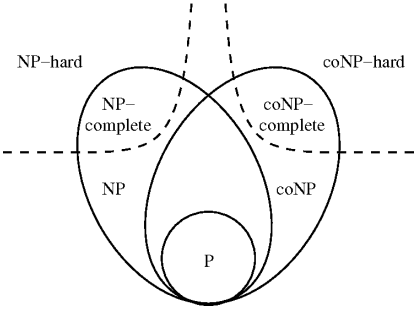
White-box equivalence check for classical circuits

- What if we know the circuits?



White-box equivalence check for classical circuits

- Fundamentally, the problem is likely not easier
- Checking that two classical circuits are equivalent is co-NP-complete
  - Believed to require exponential complexity
  - So no better way than checking all possible inputs



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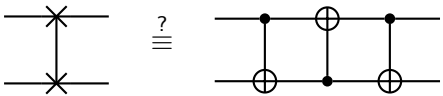
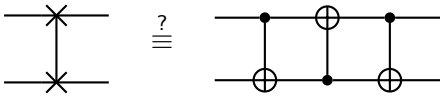


- What if we know the quantum circuits?

White-box equivalence check for quantum circuits



- What if we know the quantum circuits?
- We can check equivalence by comparing the matrices

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

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

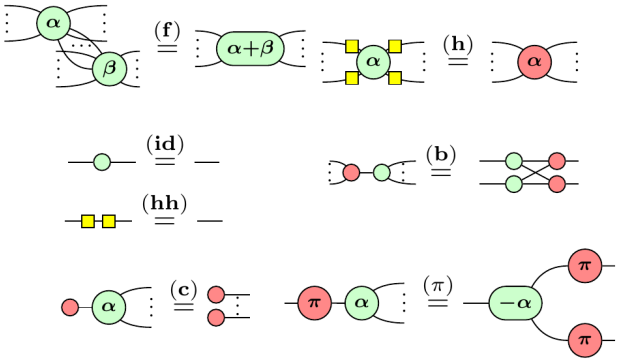
[1] Y. Tanaka. *Int. J. Quantum Inf.* (2010).
[2] D. Janzing, P. Wocjan, and T. Beth. *Int. J. Quantum Inf.* (2005).
[3] Z. Ji and X. Wu. 2009. arXiv: 0906.5416.

Smarter approaches to equivalence checking

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

[1] T. Peham, L. Burgholzer, and R. Wille. *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).
[2] L. Burgholzer and R. Wille. *ASP-DAC.* 2020.
[3] R. Orús. *Nature Reviews Physics* (2019).
[4] D. Thanos, T. Coopmans, and A. Laarman. *ATVA.* 2023.
[5] J. Mei, T. Coopmans, M. M. Bonsangue, and A. Laarman. *IJCAR.* 2024.

Based on ZX-calculus[1,2]



Axioms

[1] B. Coecke and R. Duncan. *ICALP*. 2008.

[2] T. Peham, L. Burgholzer, and R. Wille. *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).

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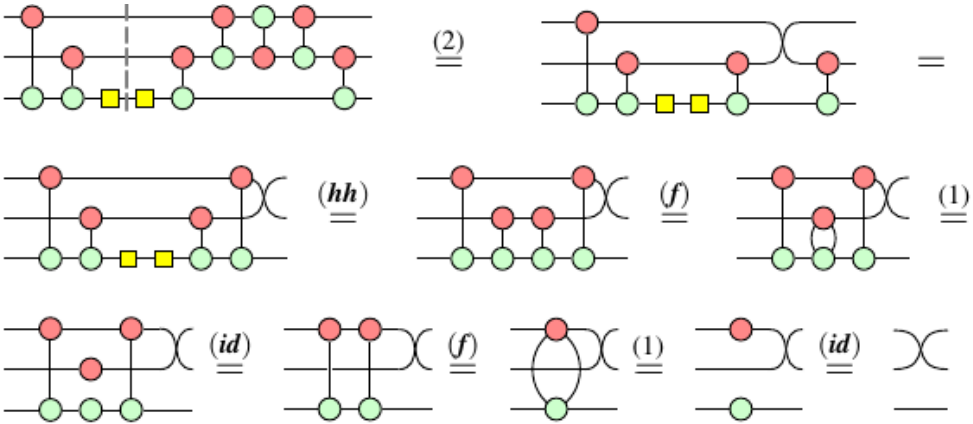

Example proof

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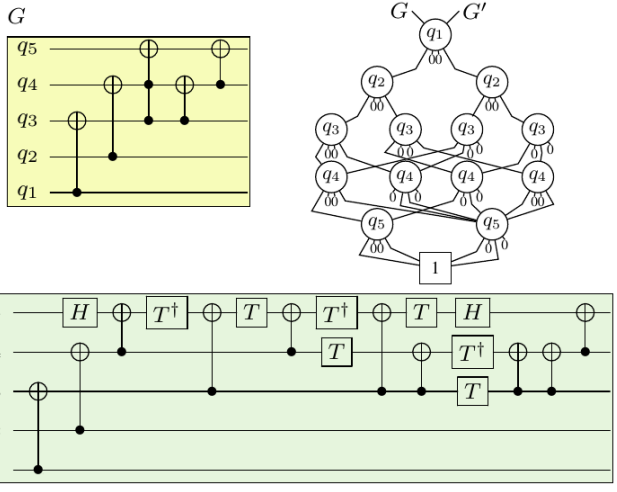
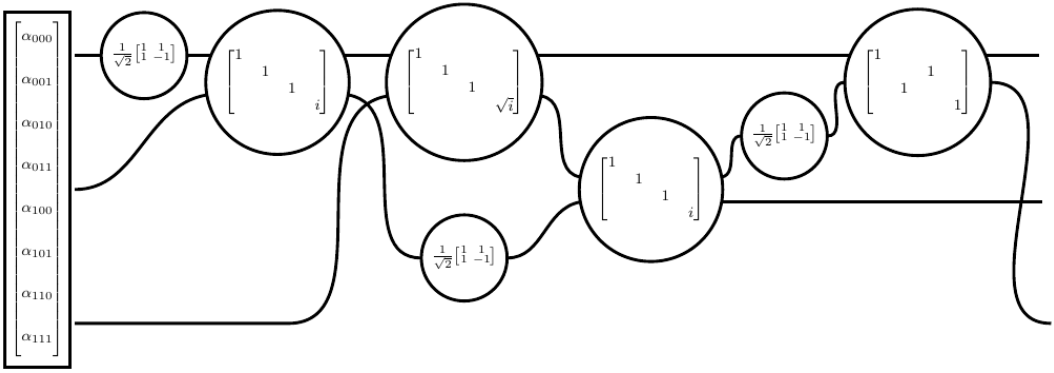
[2] T. Peham, L. Burgholzer, and R. Wille. *IEEE J. Emerg. Sel. Topics Circuits Syst.* (2022).

Based on decision diagrams[1]



[1] L. Burgholzer and R. Wille. *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. *ICCAD*. 2022.

[2] L. Burgholzer, A. Ploier, and R. Wille. *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 reduction to **weighted model counting**[2]

[1] D. Thanos, T. Coopmans, and A. Laarman. *ATVA*. 2023.

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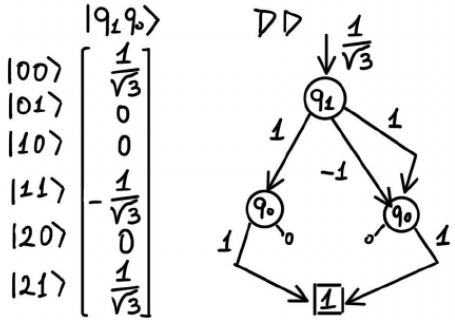
Quantum decision diagrams (QDDs)[1]

- Similar to BDDs, but represent complex numbers
- Available for both vectors and matrices
- Examples below: Mixed qudit systems (≥ 2 bases)



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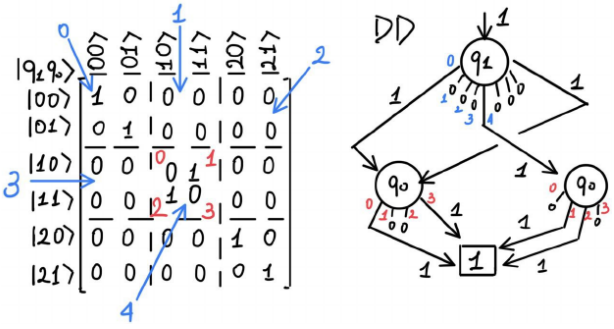

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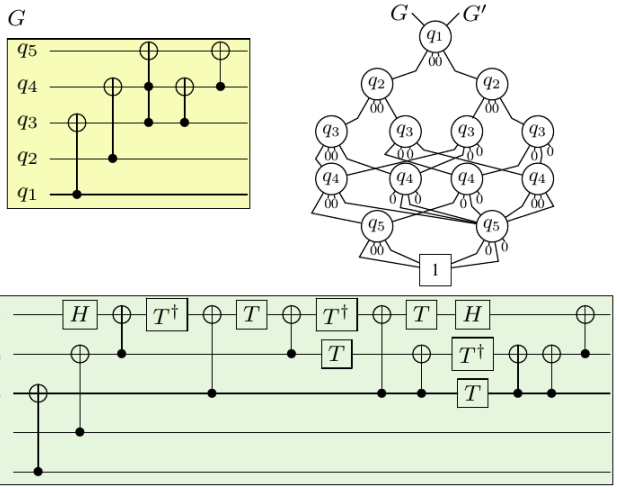
Comparison of circuits after encoding[1]



[1] L. Burgholzer and R. Wille. *ASP-DAC*. 2020.

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. *ICCAD*. 2007.

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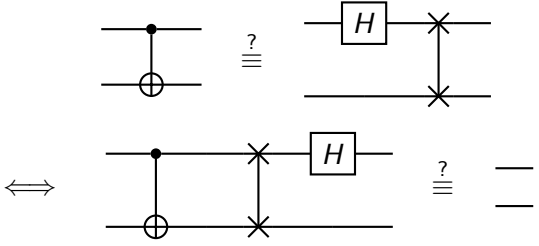

(Coincidentally, the swap and Hadamard gates are self-inverse)

[1] G. F. Viamontes, I. L. Markov, and J. P. Hayes. *ICCAD*. 2007.

Reverse scheme "inside out" with QDDs[1]

- Motivation: Identity matrix has a small QDD encoding
- Start from identity matrix
- Multiply with some gates from first circuit
- Multiply with some gates from second circuit
- Repeat
- In the example (next slide), the QDD never gets above 9 nodes (compared to 13 nodes for each gate)

[1] L. Burgholzer and R. Wille. *ASP-DAC*. 2020.

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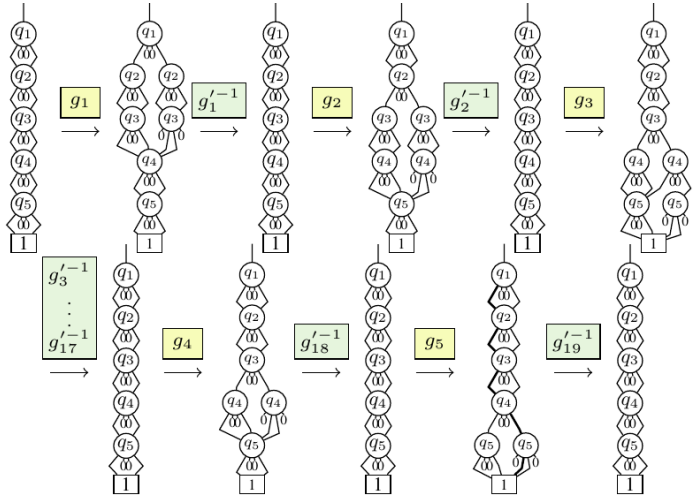

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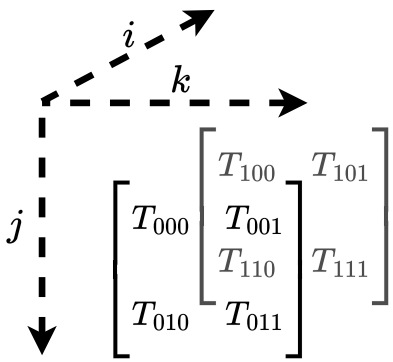
Overview

Tensors

- Generalization of vectors / matrices to higher dimensions



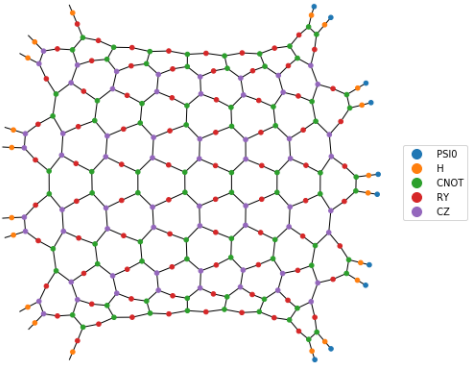
Tensors

- 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

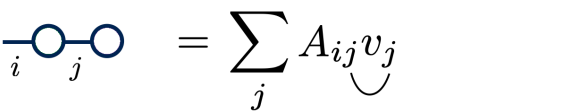
- Tensors can be arranged in a graph



Tensor networks

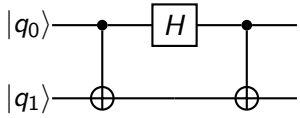
- Tensors can be arranged in a graph
- Nodes with shared edges can be **contracted** (= merged)

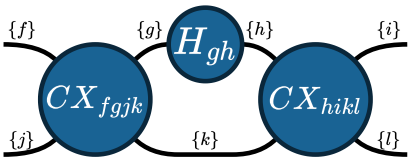
  Corresponds to matrix-vector and matrix-matrix multiplication for special cases



Example

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

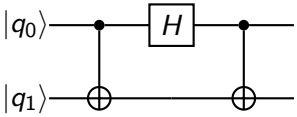


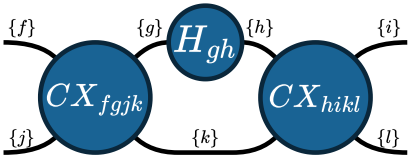


1.

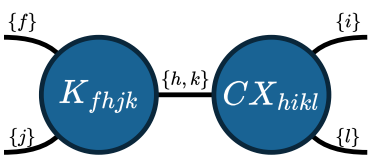
Example

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 $\{g\}$





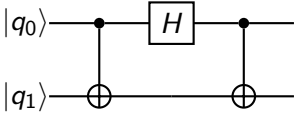
1.

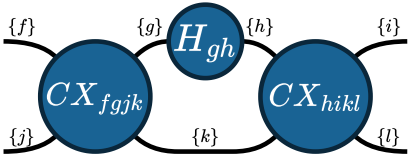


2.

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





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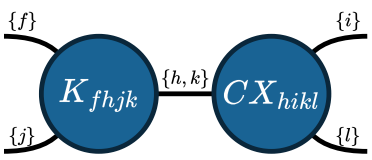
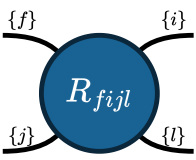


2.



3.

Application: Quantum simulation on classical computer[2]

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

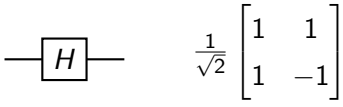
[1] J. Gray and S. Kourtis. *Quantum* (2021).
[2] I. L. Markov and Y. Shi. *SIAM J. Comput.* (2008).

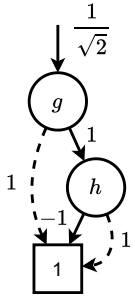
Overview

Tensor decision diagrams (TDDs)

- Alternative representation of tensors

Example: Hadamard gate with matrix, tensor, and TDD

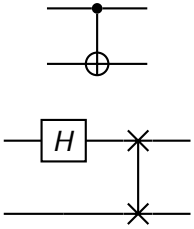




TDD-based algorithm for equivalence checking[1]

Algorithm combines reverse scheme, tensor networks, and TDDs

Given: Quantum circuits C_1, C_2



[1] C. B. Larsen, S. B. Olsen, K. G. Larsen, and C. Schilling. *Entropy* (2024).

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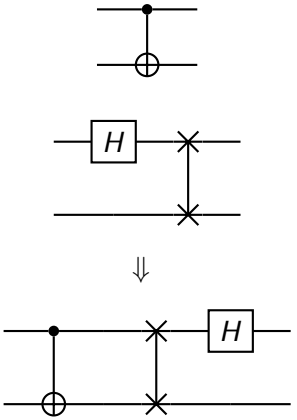
Algorithm combines reverse scheme, tensor networks, and TDDs

Given: Quantum circuits C_1, C_2

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



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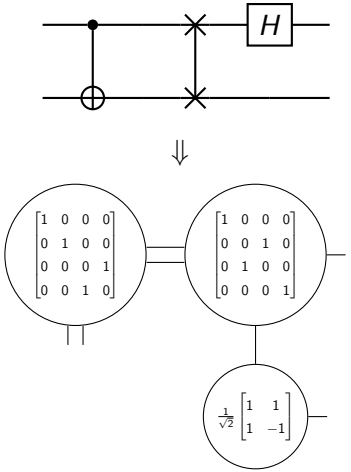
TDD-based algorithm for equivalence checking[1]

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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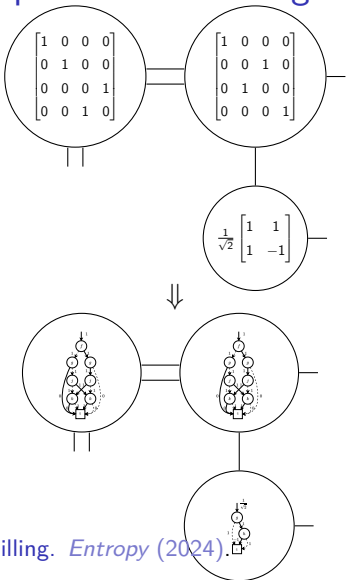
Algorithm combines reverse scheme, tensor networks, and TDDs

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
3. Convert all tensors to TDDs



(TDDs on the right are only exemplary)

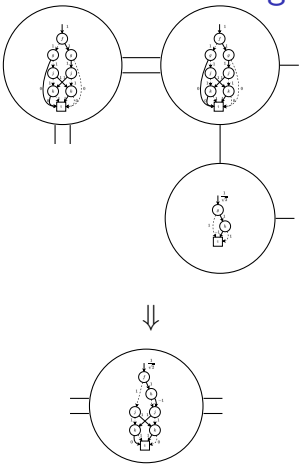
[1] C. B. Larsen, S. B. Olsen, K. G. Larsen, and C. Schilling. *Entropy* (2024).

TDD-based algorithm for equivalence checking[1]

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
3. Convert all tensors to TDDs
4. Contract TDD network



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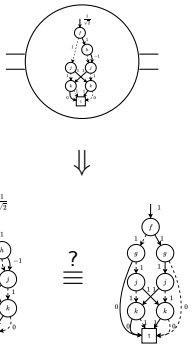
Given: Quantum circuits C_1, C_2

1. Construct circuit $C_1 C_2^{-1}$
2. Convert $C_1 C_2^{-1}$ to tensor network
3. Convert all tensors to TDDs
4. Contract TDD network
5. Compare resulting TDD to identity TDD



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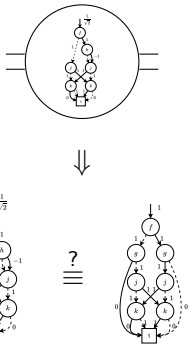
Algorithm combines reverse scheme, tensor networks, and TDDs

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
3. Convert all tensors to TDDs
4. **Contract TDD network** $\leftarrow$ how?
5. Compare resulting TDD to identity TDD



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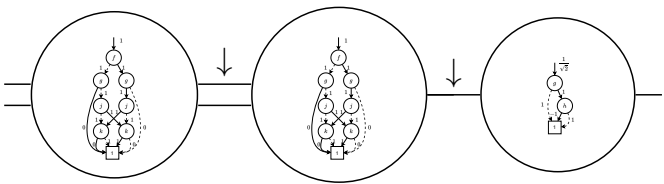
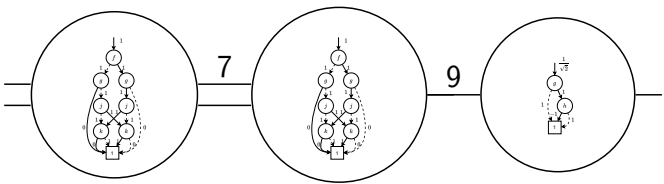
Lookahead heuristic for TDD contraction

- Greedy algorithm
- In each contraction step:
  1. Evaluate all possible contractions



Lookahead heuristic for TDD contraction

- Greedy algorithm
- In each contraction step:
  1. Evaluate all possible contractions
  2. Measure size of resulting TDDs



Lookahead heuristic for TDD contraction

- Greedy algorithm
- In each contraction step:
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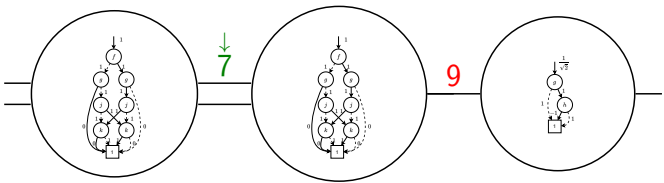
  2. Measure size of resulting TDDs
  3. Execute a contraction with smallest resulting TDD



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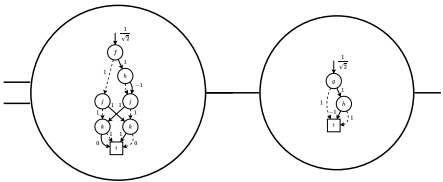

Lookahead heuristic for TDD contraction

- Greedy algorithm
- In each contraction step:
  1. Evaluate all possible contractions
  2. Measure size of resulting TDDs
  3. Execute a contraction with smallest resulting TDD
- 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

Counting heuristic for TDD contraction

- Goal: Imitate lookahead heuristic without expensive step 1
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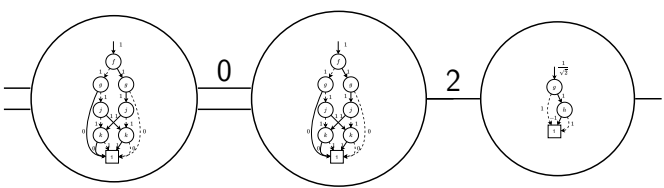
- In each contraction step:
  1. Select nodes with earliest participation in contraction[1]



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

Counting heuristic for TDD contraction

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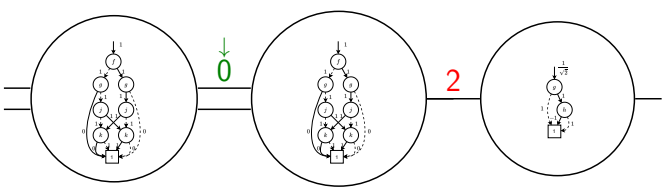

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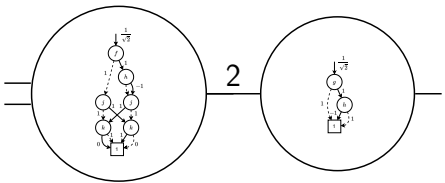

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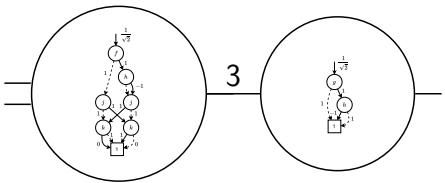
Counting heuristic for TDD contraction

- 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:
  1. Select nodes with earliest participation in contraction[1]
  2. Update usage statistics of neighboring edges



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Overview

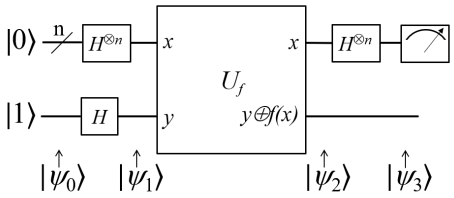
Quantum circuits in evaluation

- 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)

[1] N. Quetschlich, L. Burgholzer, and R. Wille. *Quantum* (2023).

Deutsch-Jozsa algorithm (DJ)[1,2]

- Given $f\colon \{0,1\}^n \to \{0,1\}$ with promise that it is either
  - constant (100% "0" or 100% "1") or
  - balanced (50% "0" and 50% "1")
- Task: Determine which of the two cases it is
- Demonstrates exponential speed-up (requires a single shot)

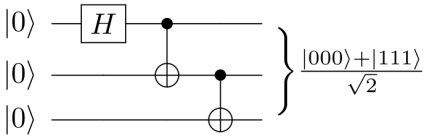


[1] D. Deutsch and R. Jozsa. *Proc. R. Soc. A* (1992).

[2] R. Cleve, A. Ekert, C. Macchiavello, and M. Mosca. *Proc. R. Soc. A* (1998).

Greenberger-Horne-Zeilinger state preparation (GHZ)[1]

- The **GHZ state** generalizes the Bell state
- For 3 qubits: $\frac{|000\rangle + |111\rangle}{\sqrt{2}}$
- For k qubits: $\frac{|0\rangle^{\otimes k} + |1\rangle^{\otimes k}}{\sqrt{2}}$
- Used in quantum communication and cryptography protocols



[1] D. M. Greenberger, M. A. Horne, and A. Zeilinger. *Bell's theorem, quantum theory and conceptions of the universe*. 1989.

Graph state preparation (GS)[1]

- A **graph state** is a state that can be represented by a graph
- Each vertex corresponds to a qubit
- $|G\rangle = \prod_{(u,v)\in E} CZ^{(u,v)} |+\rangle^{\otimes |V|}$

  where $CZ^{(u,v)}$ is the corresponding controlled-Z gate
- Used, e.g., in quantum error-correcting codes

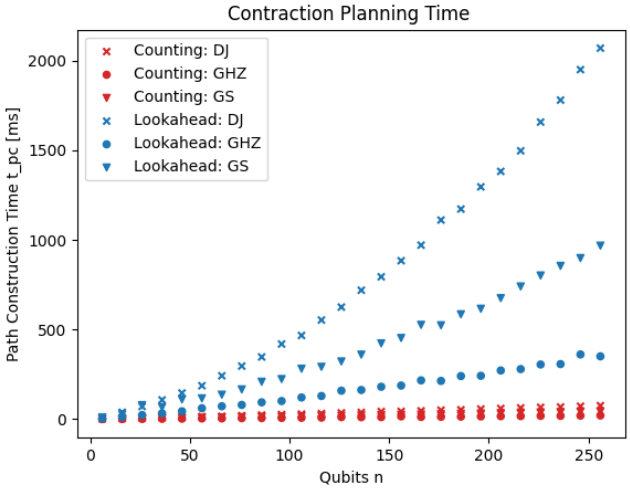
[1] M. Hein, J. Eisert, and H. J. Briegel. *Physical Review A—Atomic, Molecular, and Optical Physics* (2004).

Types of experiments

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

[1] J. Gray and S. Kourtis. *Quantum* (2021).
[2] L. Burgholzer and R. Wille. *Softw. Impacts* (2021).

Comparison of proposed heuristics



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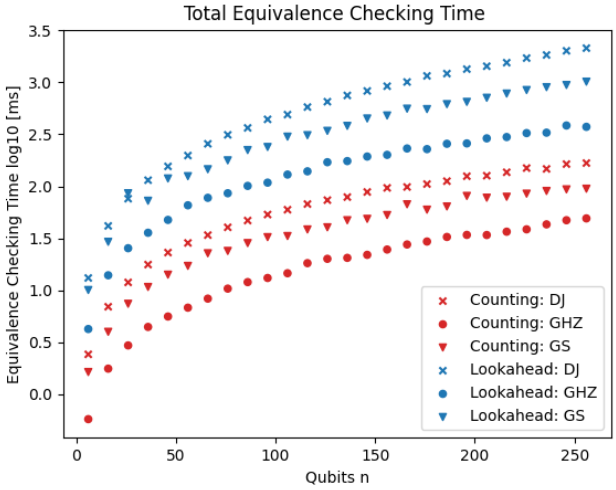
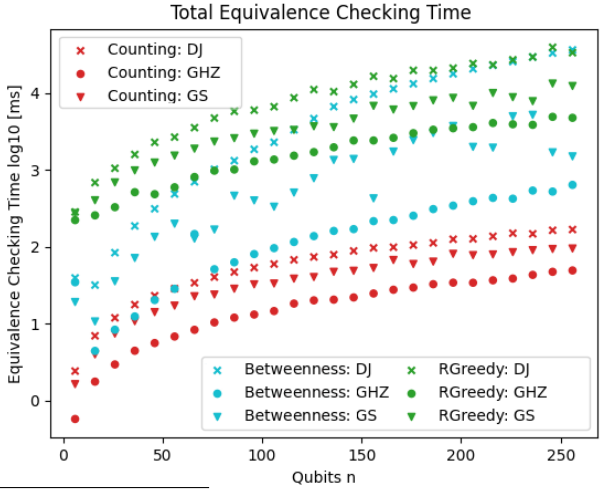


Comparison to cotengra[1]



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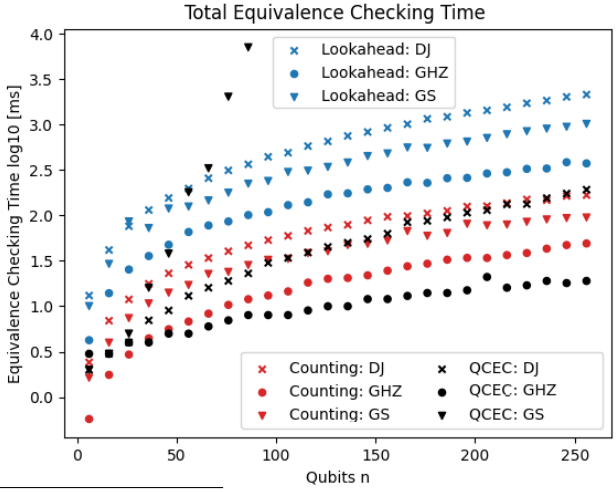


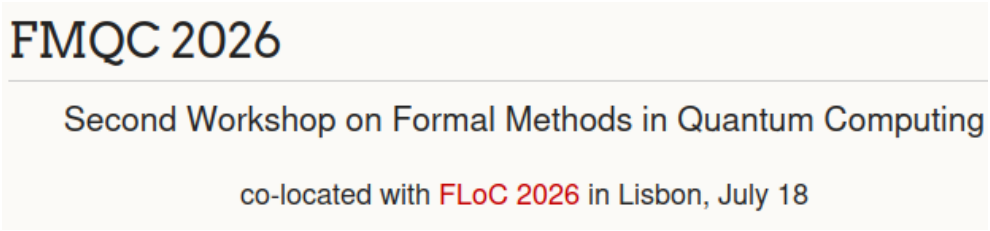
[1] L. Burgholzer and R. Wille. *Softw. Impacts* (2021).

Overview

Conclusion

- Algorithm for equivalence checking of quantum circuits:
  - Integration of "reverse scheme" and TDD networks
  - Lookahead heuristic (greedy)
  - Counting heuristic (cheap approximation)

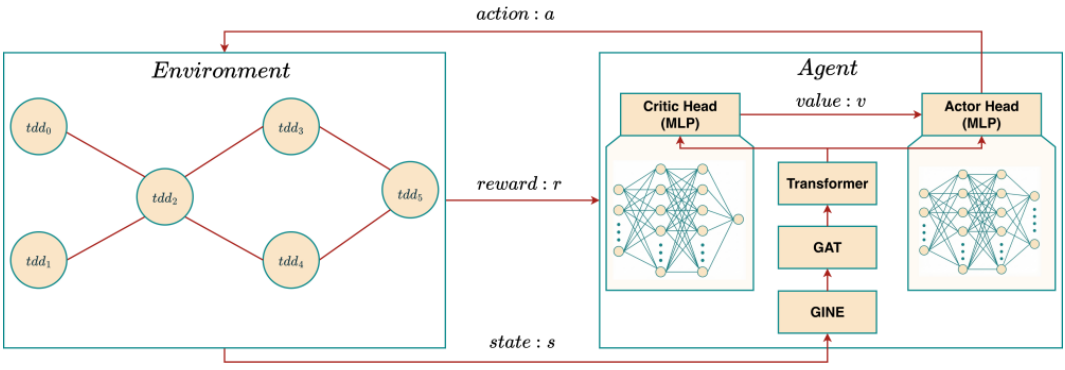
Upcoming events



We are hiring

- 1 PhD student and 4 postdoc positions
  - Basic Research Center on quantum communication
  - Grand Solutions project on quantum software stack
  - EU Quantum Center of Excellence
- Open call for 2 postdoc positions (deadline May 25)

Learning contraction orders (WIP)



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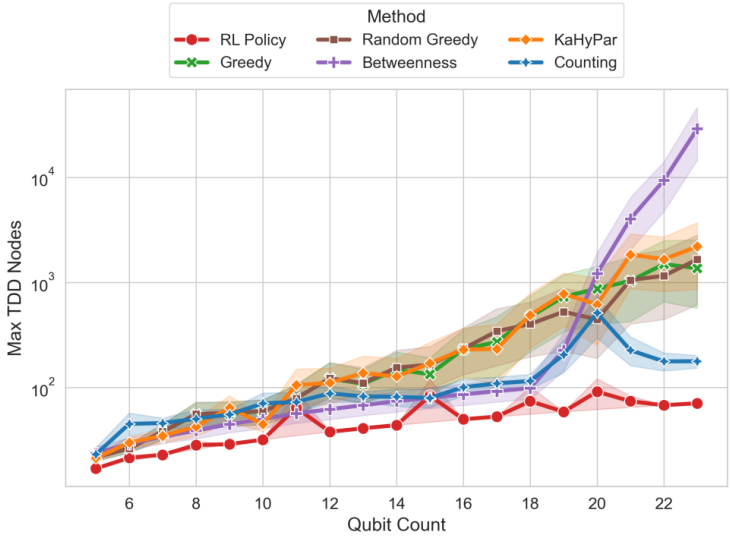

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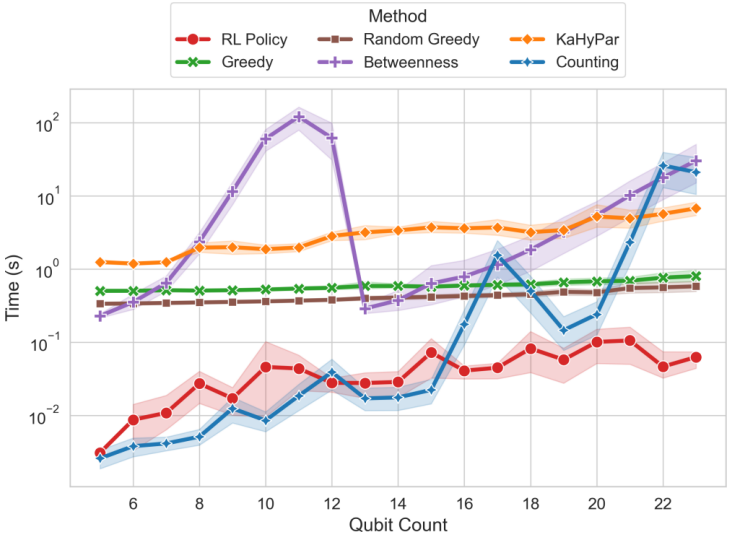

Learning contraction orders (WIP)

Qubits	Method	Peak Size	Time (s)	Status
30	Hybrid heuristic/RL (Ours)	**220**	**0.221**	Success
	KaHyPar	32,748	3.996	Success
	Greedy	33,249	24.571	Success
	Random Greedy	165,373	25.828	Success
	Counting / Betweenness	–	–	TO
38	Hybrid heuristic/RL (Ours)	**127**	**0.243**	Success
	KaHyPar	2,204,566	99.321	Success
	Greedy / Random Greedy / Counting	–	–	TO
50	Hybrid heuristic/RL (Ours)	**15,289**	**8.200**	Success
	All Baselines	–	–	TO