# Tensor Networks 

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What makes a quantum circuit difficult to simulate?
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## Long-range class plan

| Date | Class topic | Readings and assignments |
| ---: | :--- | :--- |
| $10 / 20$ | NISQ algorithms: QAOA |  |
| $10 / 25$ | NISQ algorithms: QAOA | QAOA lab out |
| $10 / 27$ | Quantum computing: systems view | New reading assignment release |
| $11 / 1$ | Languages: stabilizers |  |
| $11 / 3$ | Languages: tensor networks |  |
| $11 / 8$ | Languages: density matrices, noise | QAOA lab part 1 due |
| $11 / 10$ | Languages: logical abstractions |  |
| $11 / 15$ | Quantum error correction codes |  |
| $11 / 17$ | NISQ algorithms: quantum chemistry |  |
| $11 / 22$ | NISQ algorithms: VQE | QAOA lab all due, VQE lab out |
| $11 / 29$ | Architecture |  |
| $12 / 1$ | Microarchitecture | VQE lab part 1 due |
| $12 / 6$ | Devices: superconductors |  |
| $12 / 8$ | Devices: ion traps |  |
| $12 / 13$ | Conclusion |  |

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## Representations for Quantum Computing

Different representations useful in different settings

1. Quantum circuits
2. Stabilizers
3. Tensor networks
4. Noisy density matrices and Kraus operator sums
5. Logical formulas

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```


## What makes a quantum circuit difficult to simulate?

## Stabilizers

- Simulation difficulty grows exponentially w.r.t. number of T gates
- A statement about parameters.

Tensor network contraction

- Simulation difficulty grows exponentially w.r.t. maximum treewidth.
- A statement about topology.


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## Tensors

Rank-k generalizations of matrices

- Rank-0 tensor: a scalar
- Rank-1 tensor: a vector
- Rank-2 tensor: a matrix
- Rank-3 tensor: ...


## Rank-0 tensor: a scalar

- In quantum circuits, a single amplitude is a complex scalar and therefore a rank-0 tensor.
- For example, a single qubit state is in general $|\phi\rangle=\alpha|0\rangle+\beta|1\rangle . \alpha$ and $\beta$ are scalars.


## Rank-1 tensor: a vector

- In quantum circuits, a single qubit state is a complex vector and therefore a rank-1 tensor.
- For example, a single qubit state is in general $|\phi\rangle=\alpha|0\rangle+\beta|1\rangle=\left[\begin{array}{l}\alpha \\ \beta\end{array}\right]$, a complex vector.


## Rank-2 tensor: a matrix

Rank-2 tensors appear as single-qubit gates in quantum circuits

- For example, the Hadamard gate has a unitary matrix of $H=\left[\begin{array}{cc}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{array}\right]$.

| - We can view it as a tensor with two ranks, $m 0$ and $m 1$ like so: | $\|0\rangle$ | $\|1\rangle$ | $\frac{1}{\sqrt{2}}$ |
| :--- | :--- | :--- | :--- |
|  | $\|1\rangle$ | $\|0\rangle$ | $\frac{1}{\sqrt{2}}$ |
|  | $\|1\rangle$ | $\|1\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\frac{-1}{\sqrt{2}}$ |  |  |  |

## Rank-2 tensor

Rank-2 tensors also appear as two-qubit states in quantum circuits

- For example, a two-qubit state is in general

$$
|\psi\rangle=\alpha|00\rangle+\beta|01\rangle+\gamma|10\rangle+\delta|11\rangle=\left[\begin{array}{l}
\alpha \\
\beta \\
\gamma \\
\delta
\end{array}\right]
$$

| q0 | q 1 | w |
| :---: | :---: | :---: |
| $\|0\rangle$ | $\|0\rangle$ | $\alpha$ |
| $\|0\rangle$ | $\|1\rangle$ | $\beta$ |
| $\|1\rangle$ | $\|0\rangle$ | $\gamma$ |
| $\|1\rangle$ | $\|1\rangle$ | $\delta$ |

## Rank-4 tensor

Rank- 4 tensors appear as two-qubit gates in quantum circuits
We can view it as a tensor with four ranks, $q 0 m 0, q 0 m 1, q 1 m 0$, and $q 1 m 1$ :

| q 0 m 0 | q 0 m 1 | q 1 m 0 | q 1 m 1 | w |
| ---: | ---: | ---: | ---: | :--- |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 1 |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 1 |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 1 |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 1 |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |

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## Tensor network contraction

- Tensor network contraction is one type of tensor-tensor multiplication.
- It is a generalized form of matrix multiplication.
- Merge two tensors into one. Absorb common edges. If the two tensors share a common index, sum over all possible values of that index.


## Tensor network contraction

For example, we can contract the tensor network for a Bell state circuit
CNOT gate rank-4 tensor:

| q 0 m 1 | q 0 m 2 | q 1 m 1 | q 1 m 2 | w |
| ---: | ---: | ---: | ---: | :--- |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 1 |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 1 |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 1 |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 1 |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |

## Tensor network contraction

Contract tensors by summing over q0m1:

| q 0 m 0 | q 0 m 2 | q 1 m 1 | q 1 m 2 | w |
| ---: | ---: | ---: | ---: | :--- |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | $\|1\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\frac{1}{\sqrt{2}}$ |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|0\rangle$ | 0 |
| $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\|1\rangle$ | $\frac{-1}{\sqrt{2}}$ |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|0\rangle$ | $\frac{-1}{\sqrt{2}}$ |
| $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle$ | 0 |

Compare this with unitary matrix:

CNOT $(H \otimes I)$
$=\left[\begin{array}{llll}1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0\end{array}\right]\left[\begin{array}{cccc}\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}}\end{array}\right]$
$=\left[\begin{array}{cccc}\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0\end{array}\right]$

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## Tensor network contraction order

Contraction ordering says the order in which edges are contracted.

- To minimize computation and memory requirements, best to avoid forming large intermediate tensors.
- Akin to the classic dynamic programming problem of optimal chain matrix multiplication.


## Tensor network contraction order



Figure 9.4: Part of a generic tensor network, consisting of ten rank-4 tensors and four rank-1 tensors.

Figure: Source: [Ding and Chong, 2020]


Figure 9.5: First strategy of contraction that results in two rank-12 tensors and four rank-1 tensors. Then contracting the two rank- 12 tensors involves contracting 5 edges at once, by summing over $2^{5}$ terms.

Figure: Source: [Ding and Chong, 2020]


Figure 9.6: Second strategy of contraction that results in five rank-6 tensors and four rank-1 tensors. Then contracting the five rank- 6 tensors involves contracting from left to right 2 edges at a time, by summing over $2^{2}$ terms four times.

## Tensor network contraction order



Figure 1: Tensor network contraction of a quantum circuit from the random circuit family [7], visualized as a binary contraction tree. Each node in the tree represents a step in the contraction. Larger, darker nodes indicate more expensive steps. The central stem dominates the overall contraction cost.

Figure: Source:Cupjin Huang et al., Classical Simulation of Quantum Supremacy Circuits, 2020. [Huang et al., 2020]

Cost of simulating the quantum circuit is via tensor network contraction is O(exp(treewidth)) [Markov and Shi, 2008]

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## Unification of stabilizers and tensors

- If you feed a Clifford circuit to a tensor network contraction based simulator, it will not see Clifford symmetry
- Need some way to enable Clifford simplification of tensor networks.


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## Example: inverting a CNOT

## What is this circuit: $(H \otimes H) \operatorname{CNOT}_{0,1}(H \otimes H)$ ?

$$
\begin{aligned}
& (H \otimes H) \mathrm{CNOT}_{0,1}(H \otimes H) \\
& =\frac{1}{2}\left[\begin{array}{cccc}
1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1
\end{array}\right]\left[\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right] \frac{1}{2}\left[\begin{array}{cccc}
1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 \\
1 & -1 & -1 & 1
\end{array}\right] \\
& =\left[\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0
\end{array}\right] \\
& =\mathrm{CNOT}_{1,0}
\end{aligned}
$$

All gates here $(H, C N O T)$ in Clifford gate set. Automatic simplification method?

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## Splitting a CNOT into network of two rank-3 tensors

| "Copy" rank-3 tensor |  | "XOR" rank-3 <br> tensor |  |
| :---: | :---: | :---: | :---: |
| a b c | W | c d e | W |
| 0000 | 1 | 000 | 1 |
| $0 \quad 0$ | 0 | 000 | 0 |
| $0 \quad 10$ | 0 | $0 \quad 10$ | 0 |
| $0 \begin{array}{lll}0 & 1 & 1\end{array}$ | 0 | $0 \begin{array}{lll}0 & 1 & 1\end{array}$ | 1 |
| 100 | 0 | 100 | 0 |
| $1 \begin{array}{lll}1 & 0 & 1\end{array}$ | 0 | 1001 | 1 |
| 110 | 0 | 110 | 1 |
| $1 \begin{array}{lll}1 & 1\end{array}$ | 1 | 111 | 0 |

Contract "Copy" with "XOR":

- Sum over $c$.
- Gives the CNOT rank-4 tensor.

| a | b | d | e | w |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | 0 | 1 |
| 0 | 0 | 0 | 1 | 0 |
| 0 | 0 | 1 | 0 | 0 |
| 0 | 0 | 1 | 1 | 1 |
| 0 | 1 | 0 | 0 | 0 |
| 0 | 1 | 0 | 1 | 0 |
| 0 | 1 | 1 | 0 | 0 |
| 0 | 1 | 1 | 1 | 0 |
| 1 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 1 | 0 |
| 1 | 0 | 1 | 0 | 0 |
| 1 | 0 | 1 | 1 | 0 |
| 1 | 1 | 0 | 0 | 0 |
| 1 | 1 | 0 | 1 | 1 |
| 1 | 1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 1 | 0 |

[Biamonte and Bergholm, 2017], [Biamonte, 2019]

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## Tensor simplification rules: Duality of Copy and XOR tensors.

| Hadamard rank-2tensor: |  | b c e w |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | 0 | 0 |  | 1 |
| a b | w | 0 | 0 | 1 | 0 |
| 00 | $\frac{1}{\sqrt{2}}$ | 0 | 1 |  | 0 |
| 01 | $\frac{1}{\sqrt{2}}$ | 0 | 1 | 1 | 0 |
| 10 | $\frac{1}{\sqrt{2}}$ | 1 | 0 | 0 | 0 |
| 11 | $\frac{\sqrt{2}}{\frac{1}{2}}$ | 1 | 0 | 1 | 0 |
|  |  |  | 1 | 1 | 1 |

Contraction of $H$ with
"Copy" rank-3 tensor: Copy summing over b :

| a | c | e | w |
| :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | $\frac{1}{\sqrt{2}}$ |
| 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | $\frac{1}{\sqrt{2}}$ |
| 1 | 0 | 0 | $\frac{1}{\sqrt{2}}$ |
| 1 | 0 | 1 | 0 |
| 1 | 1 | 0 | 0 |
| 1 | 1 | 1 | $\frac{-1}{\sqrt{2}}$ |

## Tensor simplification rules: Duality of Copy and XOR tensors.

Contraction of $H$ with
Copy summing over b :

|  | nso |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | d |  |  |  |
|  | 0 |  |  | $\frac{1}{\sqrt{2}}$ |
|  | 1 |  |  | $\frac{1}{1}$ |
|  |  |  |  | 1 |
|  |  |  |  |  |

Contraction of $H$ with \{contraction of $H$ with Copy summing over b\} summing over c:

| a | d | e | w |
| :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | $\frac{1}{2}$ |
| 0 | 0 | 1 | $\frac{1}{2}$ |
| 0 | 1 | 0 | $\frac{1}{2}$ |
| 0 | 1 | 1 | $\frac{-1}{2}$ |
| 1 | 0 | 0 | $\frac{1}{2}$ |
| 1 | 0 | 1 | $\frac{-1}{2}$ |
| 1 | 1 | 0 | $\frac{1}{2}$ |
| 1 | 1 | 1 | $\frac{1}{2}$ |

Tensor simplification rules: Duality of Copy and XOR tensors.

Contraction of $H$ with \{contraction of $H$ with Copy summing over b \} summing over c:

| a | d | e | w |
| :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | $\frac{1}{2}$ |
| 0 | 0 | 1 | $\frac{1}{2}$ |
| 0 | 1 | 0 | $\frac{1}{2}$ |
| 0 | 1 | 1 | $\frac{-1}{2}$ |
| 1 | 0 | 0 | $\frac{1}{2}$ |
| 1 | 0 | 1 | $\frac{-1}{2}$ |
| 1 | 1 | 0 | $\frac{1}{2}$ |
| 1 | 1 | 1 | $\frac{1}{2}$ |

Contraction of $H$ with \{contraction of H with \{contraction of H with Copy summing over b \} summing over c\} summing over e:

| a | d | f | w |
| :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | $\frac{1}{\sqrt{2}}$ |
| 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 0 |
| 0 | 1 | 1 | $\frac{1}{\sqrt{2}}$ |
| 1 | 0 | 0 | 0 |
| 1 | 0 | 1 | $\frac{1}{\sqrt{2}}$ |
| 1 | 1 | 0 | $\frac{1}{\sqrt{2}}$ |
| 1 | 1 | 1 | 0 |

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## Automatic simplification of circuits

What is this circuit: $(H \otimes H) \operatorname{CNOT}_{0,1}(H \otimes H)$ ?

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