Tensor Network Simplification

Yipeng Huang

Rutgers University

November 16, 2022

Table of contents

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

Table of contents

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.

Table of contents

Table of contents

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 $|\phi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$. α and β 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 $|\phi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix}\alpha \\ \beta\end{bmatrix}$, 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 $H = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$.
- We can view it as a tensor with two ranks, $m0$ and $m1$ like so:

m0	m1	w
$\|0\rangle$	$\|0\rangle$	$\frac{1}{\sqrt{2}}$
$\|0\rangle$	$\|1\rangle$	$\frac{1}{\sqrt{2}}$
$\|1\rangle$	$\|0\rangle$	$\frac{1}{\sqrt{2}}$
$\|1\rangle$	$\|1\rangle$	$\frac{-1}{\sqrt{2}}$

Rank-2 tensor

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

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

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle = \begin{bmatrix}\alpha\\ \beta\\ \gamma\\ \delta\end{bmatrix}$$

- We can view it as a tensor with two ranks, $q0$ and $q1$ like so:

q0	q1	w
$\|0\rangle$	$\|0\rangle$	α
$\|0\rangle$	$\|1\rangle$	β
$\|1\rangle$	$\|0\rangle$	γ
$\|1\rangle$	$\|1\rangle$	δ

Rank-4 tensor

Rank-4 tensors appear as two-qubit gates in quantum circuits

For example, the *CNOT* gate has a unitary matrix of

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

We can view it as a tensor with four ranks, $q0m0$, $q0m1$, $q1m0$, and $q1m1$:

q0m0	q0m1	q1m0	q1m1	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

Table of contents

Table of contents

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

Hadamard gate rank-2 tensor:

q0m0	q0m1	w
$\|0\rangle$	$\|0\rangle$	$\frac{1}{\sqrt{2}}$
$\|0\rangle$	$\|1\rangle$	$\frac{1}{\sqrt{2}}$
$\|1\rangle$	$\|0\rangle$	$\frac{1}{\sqrt{2}}$
$\|1\rangle$	$\|1\rangle$	$\frac{-1}{\sqrt{2}}$

CNOT gate rank-4 tensor:

q0m1	q0m2	q1m1	q1m2	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 $q0m1$:

q0m0	q0m2	q1m1	q1m2	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:

$$CNOT(H \otimes I)$$

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

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

Table of contents

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

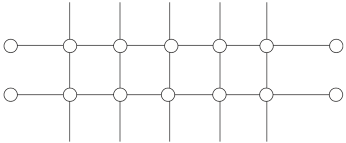

Figure 9.4: Part of a generic tensor network, consisting of ten rank-4 tensors and four rank-1 tensors.

Figure: Source: [Ding and Chong, 2020]

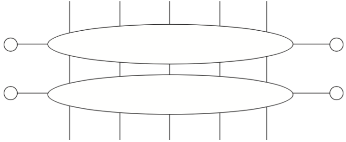

Figure 9.5: First strategy of contraction that results in two rank-12 tensors and four rank-1 tensors. Then contracting the two rank-12 tensors involves contracting 5 edges at once, by summing over 2^5 terms.

Figure: Source: [Ding and Chong, 2020]

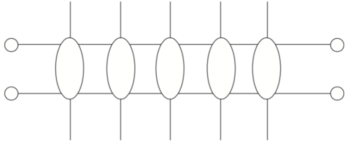

Figure 9.6: Second strategy of contraction that results in five rank-6 tensors and four rank-1 tensors. Then contracting the five rank-6 tensors involves contracting from left to right 2 edges at a time, by summing over 2^2 terms four times.

Figure: Source: [Ding and Chong, 2020]

Tensor network contraction order

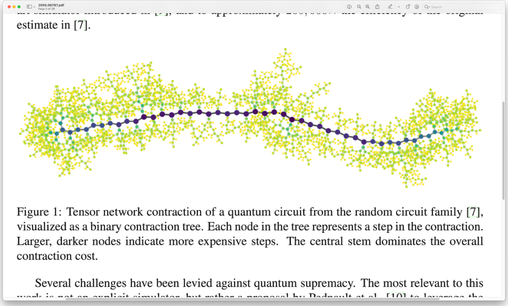
estimate in [7].

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.

Several challenges have been levied against quantum supremacy. The most relevant to this

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]

Table of contents

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.

Table of contents

Example: inverting a CNOT

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

$$
\begin{aligned}
&(H \otimes H)CNOT_{0,1}(H \otimes H) \\
&= \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \\
&= CNOT_{1,0}
\end{aligned}
$$

All gates here (H, $CNOT$) in Clifford gate set. Automatic simplification method?

Table of contents

Splitting a CNOT into network of two rank-3 tensors

"Copy" rank-3 tensor

a	b	c	w
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	0
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

"XOR" rank-3 tensor

c	d	e	w
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	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]

Table of contents

Tensor simplification rules: Duality of Copy and XOR tensors.

Hadamard rank-2 tensor:

a	b	w
0	0	$\frac{1}{\sqrt{2}}$
0	1	$\frac{1}{\sqrt{2}}$
1	0	$\frac{1}{\sqrt{2}}$
1	1	$\frac{-1}{\sqrt{2}}$

"Copy" rank-3 tensor:

b	c	e	w
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	0
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

Contraction of H with 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.

Hadamard rank-2 tensor:

c	d	w
0	0	$\frac{1}{\sqrt{2}}$
0	1	$\frac{1}{\sqrt{2}}$
1	0	$\frac{1}{\sqrt{2}}$
1	1	$\frac{-1}{\sqrt{2}}$

Contraction of H with 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	$\frac{-1}{\sqrt{2}}$

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.

Hadamard rank-2 tensor:

e	f	w
0	0	$\frac{1}{\sqrt{2}}$
0	1	$\frac{1}{\sqrt{2}}$
1	0	$\frac{1}{\sqrt{2}}$
1	1	$\frac{-1}{\sqrt{2}}$

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

Table of contents

Automatic simplification of circuits

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

Biamonte, J. (2019).
Lectures on quantum tensor networks.
arXiv preprint arXiv:1912.10049.

Biamonte, J. and Bergholm, V. (2017).
Tensor networks in a nutshell.
arXiv preprint arXiv:1708.00006.

Ding, Y. and Chong, F. (2020).
Quantum Computer Systems: Research for Noisy Intermediate-Scale Quantum Computers.
Synthesis Lectures on Computer Architecture. Morgan & Claypool Publishers.

Huang, C., Zhang, F., Newman, M., Cai, J., Gao, X., Tian, Z., Wu, J., Xu, H., Yu, H., Yuan, B., et al. (2020).
Classical simulation of quantum supremacy circuits.
arXiv preprint arXiv:2005.06787.

Markov, I. L. and Shi, Y. (2008).
Simulating quantum computation by contracting tensor networks.
SIAM Journal on Computing, 38(3):963–981.