The Approximation of Density Matrices

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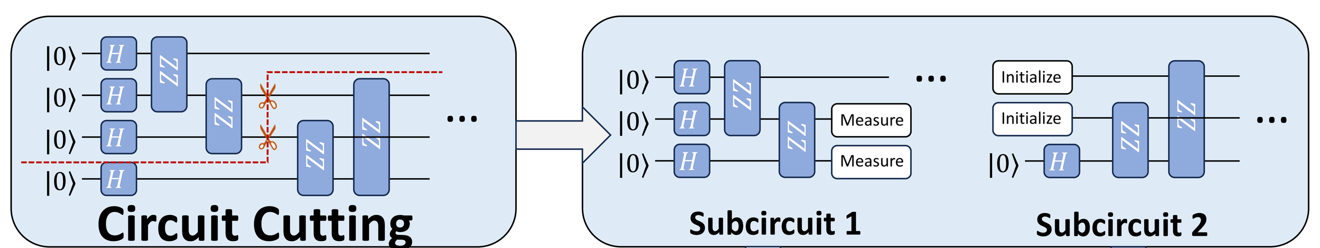
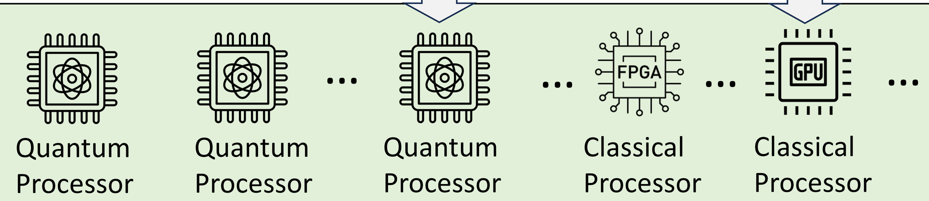
Background

[ASPLOS' 21] CutQC Wei Tang et al.



Circuit Running: Deploy the subcircuit on different devices.



q0	m1	m2	value
I	I	I	0.125
⋮	⋮	⋮	⋮
Z	I	X	0.2
⋮	⋮	⋮	⋮

Tensor 1

m1	m2	q1	q2	q3	value
I	I	I	I	I	0.125
⋮	⋮	⋮	⋮	⋮	⋮
I	X	Z	I	Y	0.12
⋮	⋮	⋮	⋮	⋮	⋮

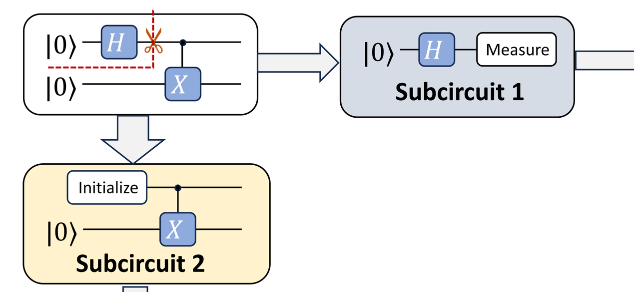
Tensor 2

Postprocessing: contract tensor1 and tensor2

Analysis on Density Matrices:
1) Noise-free density matrices:
· Tensors are sparse!
2) Noisy density matrices:
· Approximate by truncating the small values. Tensors are still sparse.

We can apply sparse tensor contraction to save time and memory!

A Concrete Example of Cutting the Bell Sate Circuit



The density matrix for subcircuit 1 is:

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\frac{1}{\sqrt{2}}(\langle 0| + \langle 1|) = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} = \frac{1}{2}I + \frac{1}{2}X$$

denote the cutting point as m The tensor for subcircuit1 is:

m	value
I	0.5
X	0.5
Y	0
Z	0

Tensor 1

- After cut, we need to initialize 4 different state for m: $|0\rangle, |1\rangle, |+\rangle, |i\rangle$.
- Define $f(m)$ as the density matrix output given initial state m.

① When initial state is $|0\rangle$, $f(m = |0\rangle\langle 0|) = f(m = \frac{1}{2}I + \frac{1}{2}Z) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \frac{1}{4}II + \frac{1}{4}IZ + \frac{1}{4}ZI + \frac{1}{4}ZZ$

② When initial state is $|1\rangle$, $f(m = |1\rangle\langle 1|) = f(m = \frac{1}{2}I - \frac{1}{2}Z) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \frac{1}{4}II - \frac{1}{4}IZ - \frac{1}{4}ZI + \frac{1}{4}ZZ$

③ When initial state is $|+\rangle$, $f(m = |+\rangle\langle +|) = f(m = \frac{1}{2}I + \frac{1}{2}X) = \begin{bmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{bmatrix} = \frac{1}{4}II + \frac{1}{4}XX - \frac{1}{4}YY + \frac{1}{4}ZZ$

④ When initial state is $|i\rangle$, $f(m = |i\rangle\langle i|) = f(m = \frac{1}{2}I + \frac{1}{2}Y) = \begin{bmatrix} 1/2 & 0 & 0 & -1/2\,i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2\,i & 0 & 0 & 1/2 \end{bmatrix} = \frac{1}{4}II + \frac{1}{4}YX + \frac{1}{4}XY + \frac{1}{4}ZZ$

- As $f(m)$ is a linear function, we can deduce the following:

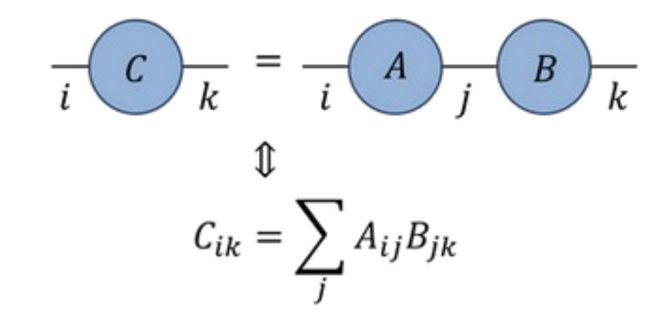
⑤ $f(m = I) = f(m = \frac{1}{2}I + \frac{1}{2}Z) + f(m = \frac{1}{2}I - \frac{1}{2}Z) = \frac{1}{2}II + \frac{1}{2}ZZ$;
⑥ $f(m = X) = 2f(m = \frac{1}{2}I + \frac{1}{2}X) - f(m = I) = \frac{1}{2}XX - \frac{1}{2}YY$;
⑦ $f(m = Y) = 2f(m = \frac{1}{2}I + \frac{1}{2}Y) - f(m = I) = \frac{1}{2}YX + \frac{1}{2}XY$;
⑧ $f(m = Z) = f(m = \frac{1}{2}I + \frac{1}{2}Z) - f(m = \frac{1}{2}I - \frac{1}{2}Z) = \frac{1}{2}IZ + \frac{1}{2}ZI$;

- With ⑤⑥⑦⑧, we can build the tensor for subcircuit2 as Tensor 2.

m	q0	q1	value
I	I	I	0.5
I	Z	Z	0.5
X	X	X	0.5
X	Y	Y	-0.5
Y	Y	X	0.5
Y	X	Y	0.5
Z	I	Z	0.5
Z	Z	I	0.5
otherwise			0

Tensor 2

Tensor contraction example:
- Tensor A has variables i, j;
- Tensor B has variables j, k;
- Contract A and B, we eliminate the common variable j and get C with variables I, k;



$$C_{ik} = \sum_j A_{ij} B_{jk}$$

Let's contract Tensor 1 and Tensor 2:
- Eliminate the common variable m.
- We get the tensor of the Bell state.

q0	q1	value
I	I	0.25
X	X	0.25
Y	Y	-0.25
Z	Z	0.25
Otherwise		0

Tensor of the Bell state

match!

Density matrix of the Bell state:

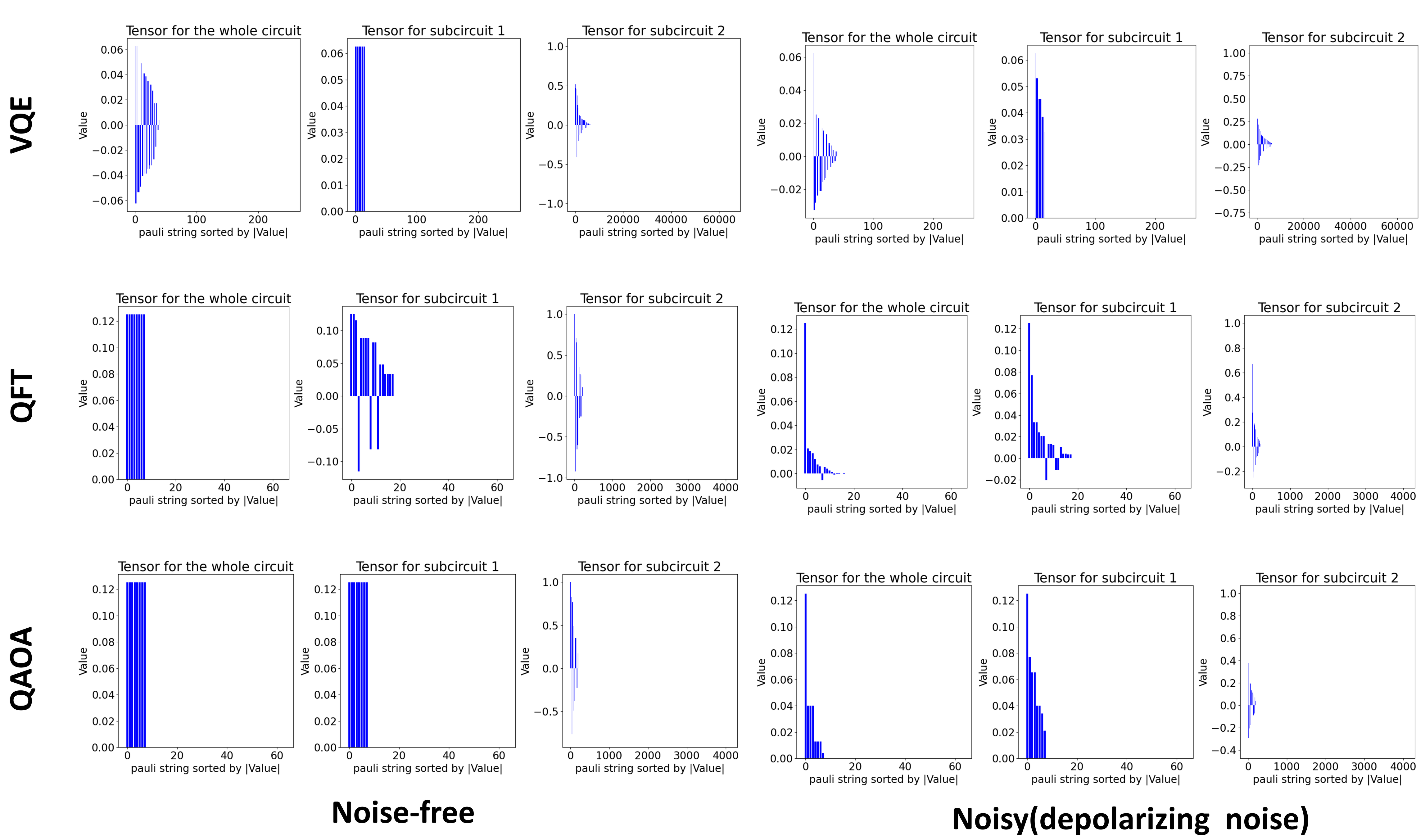
$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)\frac{1}{\sqrt{2}}(\langle 00| + \langle 11|) = \begin{bmatrix} 0.5 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0.5 \end{bmatrix} = \frac{1}{4}II + \frac{1}{4}XX - \frac{1}{4}YY + \frac{1}{4}ZZ$$

How to decompose density matrix to tensor?
- Paulistrings: $\{PS_1, PS_2, \cdots, PS_{4^n}\} = \{I, X, Y, Z\}^{\otimes n}$
- Density matrix ρ is a $2^n \times 2^n$ Hermitian Matrix.
- Decomposition of density matrix ρ:

$\rho = \sum_{i=1}^{4^n}(a_i * PS_i),\ a_i \in [-1, 1],\ \ a_i = tr(\rho \cdot PS_i)$.

Tensor Sparsity Analysis

- We plot the tensor's sorted value for 3 different types of circuits under noise-free and noisy environment.



Sparse Tensor Performance Analysis

- Assume we have a density matrix ρ representing an N qubit state below are some common quantum operations:
- unitary gate: $\rho^* = U\rho U^\dagger$;
- measure: $\langle A\rangle = tr(A\rho)$;
- tensor product: $\rho^* = \rho \otimes \rho'$, also called Kronecker product. ρ is a matrix of $2^N \times 2^N$ and ρ' is a matrix of $2^M \times 2^M$, ρ^* is a matrix of $2^{N+M} \times 2^{N+M}$;
- partial trace: $tr_{\rho_4}(\rho_3 \otimes \rho_4) = \rho_3$, Partial trace is like the inverse of tensor product. In quantum computing, it means disentanglement brought by measurement.

- For tensor of size K, the sparsity is usually $\frac{\sqrt{K}}{K}$. The time complexity for each operation are listed below:

	unitary gate	measure	tensor product	partial trace
normal tensor	2^{2N}	2^{2N}	2^{2N+2M}	2^{2N+M}
sparse tensor	2^N	$2^N N$	2^{N+M}	2^{N+M}

Future Direction

(1) Apply a sparse tensor contraction framework to show the performance gap in real experiments.
(2) Analyze the tensor sparsity on a more complex noisy environment, like introducing crosstalk noise or test it on real quantum computer.
(3) Compare the approximation idea with other approximation methods such as SVD, QR decomposition from Nvidia cuQuantum.

References

M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition.* Cambridge University Press, 2010.
D. Gottesman, "*The heisenberg representation of quantum computers*,"1998.
Tang, W., Tomesh, T., Suchara, M., Larson, J., & Martonosi, M. (2021, March 19). *CUTQC: Using small quantum computers for large quantum circuit evaluations*. arXiv.org. https://arxiv.org/abs/2012.02333

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