Improved Graph Formalism for Quantum Circuit Simulation

Alex Hu
Mentor: Andrey Khesin

October 16-17, 2021
MIT PRIMES Conference

Motivation

- Quantum mechanics is the theory of physics governing everything on very small scales such as atoms.
- **Quantum computers can be exponentially faster than classical computers.**
- Simulating quantum computation on classical computers can be used for testing large quantum circuits without having to build them physically. Also, we can better understand why, how, and in what situations quantum computers are faster than classical computers.

Quantum mechanical postulates

- The state of a quantum system can be represented by a normalized complex vector, $|\psi\rangle$ ("ket" psi), and $|\psi\rangle \in \mathcal{H}$, where $\mathcal{H}$ is a complex inner product space called the state space.
- If quantum system A has state space $\mathcal{H}_A$ and quantum system B has state space $\mathcal{H}_B$, then the quantum system consisting of A and B together has state space $\mathcal{H}_A \otimes \mathcal{H}_B$.
- The evolution of a closed quantum system over time can be described by a unitary linear operator on $\mathcal{H}$, U.

$$\left|\psi'\right\rangle = U\left|\psi\right\rangle.$$

Qubits

- A qubit is a quantum system with $\dim \mathcal{H} = 2$. The two basis vectors are $|0\rangle$ and $|1\rangle$.

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix},$$

  where $\alpha, \beta \in \mathbb{C}$, $|\alpha|^2 + |\beta|^2 = 1$.

- n-qubits has state space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$, and $\mathcal{H}$ has 2^n orthonormal basis vectors of the form $|x\rangle$, where $x \in \{0,1\}^n$.

$$|\psi\rangle = \sum_{x \in \{0,1\}^n} c_x |x\rangle,$$

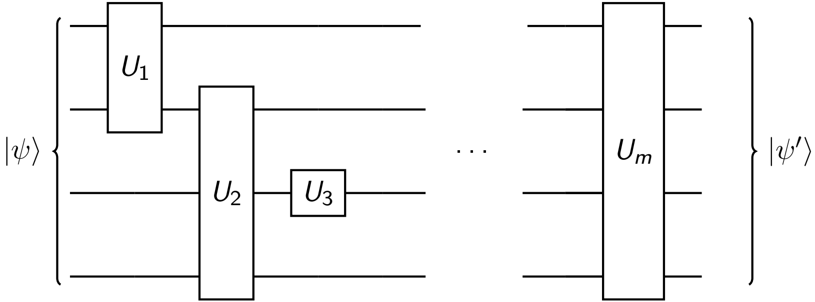
  where $c_x \in \mathbb{C}$ and $\sum_x |c_x|^2 = 1$.

- A quantum circuit performs computations on qubits through a series of quantum logic gates.

Quantum logic gates

- n-qubits travel through quantum logic gates along n wires. Quantum logic gates are equivalent to unitary linear operators.
- Classical simulation of quantum computers is, in general, slow, since state vectors have 2^n components.

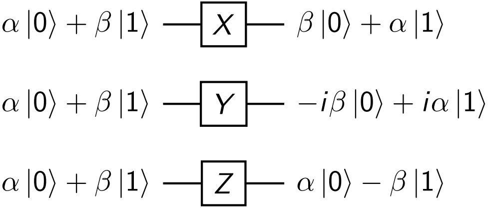
$$\left|\psi'\right\rangle = U_m U_{m-1} \dots U_3 U_2 U_1 \left|\psi\right\rangle .$$



Pauli group

The Pauli matrices are defined as

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$



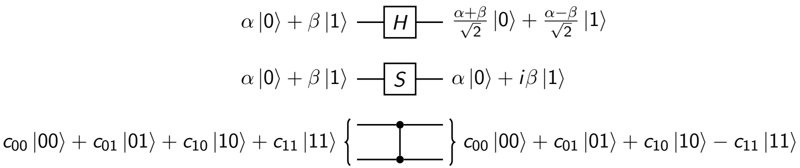
$\mathcal{P} = \{\pm I, \pm X, \pm Y, \pm Z, \pm iI, \pm iX, \pm iY, \pm iZ\}$ is the Pauli group.
$\mathcal{P}^{\otimes n}$ is the Pauli group on n qubits or the Pauli group.

- $iX \otimes Y \otimes Z = iX_1 Y_2 Z_3 \in \mathcal{P}^{\otimes 3}$.

Clifford group

The Clifford group on n qubits, $\mathcal{C}_2$, is the normalizer of $\mathcal{P}^{\otimes n}$. They are the set of operators C such that $C\mathcal{P}^{\otimes n}C^{-1} \subseteq \mathcal{P}^{\otimes n}$. Examples include the Hadamard, Phase, and Controlled-Z ("Zed") operators.

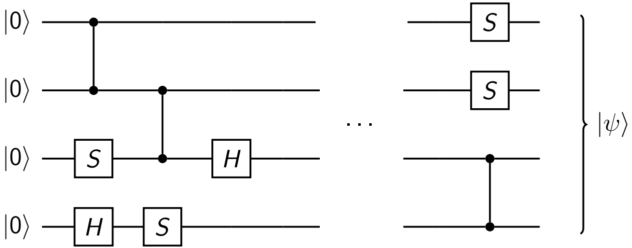
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \quad S = \begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix} \quad CZ = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}.$$



Theorem (Gottesman)

Up to a global constant factor, $\mathcal{C}_2$ is generated by products of H, S, and CZ operators applied to various qubits.

Stabilizer states



- Let $|\psi\rangle$ be a stabilizer state iff $|\psi\rangle = U|0\rangle^{\otimes n}$ for some $U \in \mathcal{C}_2$. Let a circuit consisting of Clifford gates be a Clifford circuit.
- Clifford circuits have many applications, including quantum error-correction.
- (Gottesman-Knill) Clifford circuits can be classically simulated in $O(n^2 m)$, where n is the number of qubits and m is the number of gates, because stabilizer states have efficient representations on classical computers enabling $O(n^2)$ Clifford gate updates.

Efficient representation of stabilizer states

- A stabilizer state is the unique eigenvector of n commuting Pauli operators $g_1, g_2, \ldots g_n \in \mathcal{P}^{\otimes n}$.
- Examples of stabilizer states:

$$|\psi\rangle = \frac{|00\rangle + |01\rangle + |10\rangle - |11\rangle}{2} \sim \begin{bmatrix} X & Z \\ Z & X \end{bmatrix}$$

because $X_1 Z_2 |\psi\rangle = |\psi\rangle$ and $Z_1 X_2 |\psi\rangle = |\psi\rangle$.

$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \sim \begin{bmatrix} X & X \\ -Y & Y \end{bmatrix}$$

because $X_1 X_2 |\psi\rangle = |\psi\rangle$ and $-Y_1 Y_2 |\psi\rangle = |\psi\rangle$.

- Example of non-stabilizer state:

$$|\psi\rangle = \frac{|0\rangle + e^{i\frac{\pi}{4}} |1\rangle}{\sqrt{2}}$$

- The generators are stored in matrix. Row multiplication and swapping not change state. Need unique representation of stabilizer states.

Extended graph state representation

- A graph state is a stabilizer state with generators $g_i = X_i \prod_{j \in N(i)} Z_j$. Let $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$.

$$|G\rangle = \prod_{(i,j)\in E(G)} CZ_{i,j} \, |+\rangle^{\otimes n}$$

- Can get any stabilizer state by applying H and S to graph states (Van de Nest, 2004).

$$|\psi\rangle = C\,|G\rangle\,,$$

  where C is a tensor product of local Clifford operators ($\langle H, S\rangle$). $C\,|G\rangle$ is the extended graph state representation.
- Let G be the complete graph on two vertices. If $|\psi\rangle = \frac{|00\rangle+|11\rangle}{\sqrt{2}}$, $H_1\,|G\rangle = |\psi\rangle$.
- From the above example, $H_1\,|G\rangle = H_2\,|G\rangle$. It would be nice to represent each stabilizer state in terms of a graph *uniquely*.

Unique canonical form

Definition

Let an extended graph state $C|G\rangle$ be in *canonical form* if there exist n-tuples $c \equiv (c_1, \ldots c_n)$ and $z \equiv (z_1, \ldots z_n)$ with $c_i \in \{I, S, H\}$ and $z_i \in \{I, Z\}$ such that $C = \bigotimes_{i=1}^{n} c_i z_i$, and for all $(i,j) \in E(G)$ such that $c_i = H$, we have $j > i$.

Theorem (Hu, Khesin)

Any stabilizer state $|\psi\rangle$ can be expressed uniquely in canonical form up to a constant factor.

Visualizing the canonical form

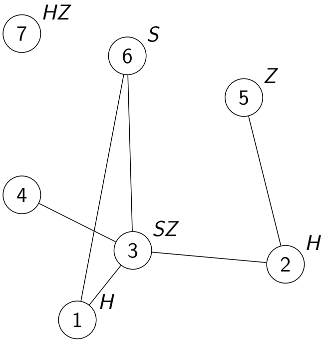


Figure: An illustration of $|\psi\rangle = H_1 H_2 S_3 Z_3 Z_5 S_6 H_7 Z_7 |G\rangle$.

- Each H cannot be slid down further.
- Can explore the connection between stabilizer states and graphs.

Graph state stabilizer simulation

	S	H	CZ	CNOT	X	Z	Tens. prod.	Measure	Global phase
Tableau	n	n	$\min(kn, n^\omega)$	n	n	n	mn	$n^2k^{\omega-2}$	✗
Affine form	1	n^2	1	$\min(kn^2, n^\omega)$	1	1	mn	$n^2k^{\omega-2}$	✓
Graph states	1	1	n^2	n^2	1	1	mn	n^2	✓
CH form	1	n^2	1	1	n^2	1	mn	n^2	✓

Figure: Kerzner 2021. Best runtimes for various methods of stabilizer simulation. They all improve the original Gottesman-Knill algorithm.

- Each method of stabilizer simulation works best for certain types of circuits. Can runtime of applying CZ to extended graph states be improved from $O(n^2)$ to $O(n)$ (Kerzner)?
- We improve the runtime in some cases by deriving multi-case formulas to directly compute the updated state upon CZ gate application

Theorem (Hu, Khesin)

There exists a family of extended graph states such that applying a CZ gate requires $\Omega(n^2)$ edges of G to be toggled.

Working with linear combinations of stabilizer states

Extended work of Elliot et. al 2010 and Garcia et al. 2014.

Theorem (Hu, Khesin)

Let $k = 2m + 1$. Let $A \subseteq \{1, 2 \ldots n\}$ be an arbitrary set. Then

$$(I + i^{2m+1} \prod_{p \in A} Z_p) \left| G \right\rangle = (1 + i^{2m+1}) \prod_{p \in A} Z_p^{m+1} \prod_{p,q \in A} CS_{p,q} \left| G \right\rangle .$$

Theorem (Hu, Khesin)

Let $\mathcal{S} \equiv \{ \left|\psi_1\right\rangle, \left|\psi_2\right\rangle, \left|\psi_3\right\rangle \}$ be a set of linearly dependent stabilizer states that are not all parallel. Then, either $\mathcal{S} = \{ \left|\phi\right\rangle, P\left|\phi\right\rangle, \frac{I+P}{\sqrt{2}} \left|\phi\right\rangle \}$ for some Pauli operator P or by adjusting each stabilizer state by constant factors, $\left|\psi_1\right\rangle + \left|\psi_2\right\rangle + \left|\psi_3\right\rangle = 0$ and $\left\langle \psi_2 \middle| \psi_3 \right\rangle = \left\langle \psi_3 \middle| \psi_1 \right\rangle = \left\langle \psi_1 \middle| \psi_2 \right\rangle \in \{ \frac{i-1}{2}, -\frac{1}{2} \}$.

Stabilizer rank of magic states

- A *n-qubit magic state* $|T_n\rangle$ is the state $(T\,|+\rangle)^{\otimes n}$, where $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$. The *stabilizer rank* $\chi(|\psi\rangle)$ is the smallest integer χ such that there exists a set of χ stabilizer states S such that $|\psi\rangle \in \text{span}(S)$.
- The upper bound for the time complexity of simulating universal quantum computation scales with $\chi(|T_m\rangle)$.

m	2	3	4	5	6	7	8
$\chi(T^{\otimes m})$	2	3	≤ 4	≤ 6	≤ 6	≤ 12	≤ 12

Figure: From Qassim et al. 2021. These are the best known upper bounds for $m \leq 8$. Not much is known about the stabilizer rank of magic states even for small number of qubits.

Improving upper bounds on $\chi(|T_n\rangle)$

- Number of stabilizer states is $2^{\frac{n^2}{2}+o(n)}$, so brute force search is infeasible for $n \geq 7$.
- Possible approach:
  - Start with $|+\rangle^{\otimes n}$ and apply $T_1, T_2, \ldots T_n$. Applying T_i will split each stabilizer state into two stabilizer states.
  - Teach computer how to combine and split stabilizer states.
- Characterizing linear dependence of stabilizer states is useful

Small case stabilizer decompositions

- Difficult to find structure even in small cases
- Even for $n = 3$, many possible stabilizer decompositions. Can all orbits of stabilizer decompositions be characterized up to swapping of qubits?
- For $n = 3$, all stabilizer decompositions have complete graph, star graph, and empty graph.

$$(T\left|+\right\rangle)^{\otimes 3} = \frac{i - e^{i\frac{\pi}{4}}}{2} Z_1 Z_2 Z_3 \left|I_3\right\rangle$$

$$- \frac{i + e^{\frac{\pi i}{4}}}{2} Z_1 Z_2 Z_3 \left|K_3\right\rangle + \frac{1 + e^{i\frac{\pi}{4}}}{2} H_1 H_2 S_3 \left|S_{3,3}\right\rangle$$

Research journey and lessons learned

- Worked on improving upper bounds on stabilizer rank of magic states for 3 months and didn't work— don't give up
- After discovering canonical form, found another paper written in 2007 that did very similar work— do good literature review early on
- Overall, doing math research felt rewarding

Acknowledgements

I would like to thank

- My mentor, Andrey Boris Khesin, for valuable guidance and mentorship.
- Professor Pavel Etingof, Dr. Tanya Khovanova, and Dr. Slava Gerovitch for organizing MIT PRIMES.
- The MIT Math Department.
- Professor David Gosset and Dr. Hammam Qassim for advice regarding the stabilizer rank of magic states.