Simulation of quantum circuits by ZX-diagram contraction

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Holy Trinity of quantum circuits

Optimization

Verification
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Optimization

PyZX

Simulation  Verification
Quantum circuit simulation

The Problem: Given quantum circuit \( C \), and input state \( |\psi\rangle \), answer some question about \( C |\psi\rangle \).

Why do we care?

§ Verification of correctness of circuits.
§ Modelling physical systems.
§ Understand when quantum supremacy has been reached.
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All these methods in a sense rely on tensor contraction. They are all exponential in number of qubits.
Stabilizer decompositions 1

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Any Clifford computation can be efficiently simulated.

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2. Write input state + ancillae as linear combination of Cliffords:
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3. Note: Each $C |\phi_i\rangle$ can be efficiently simulated!
Given Clifford circuit $C$ and input $|\psi\rangle = \sum_i^n \lambda_i |\phi_i\rangle$
where the $|\phi_i\rangle$ are Clifford. How do we approximate $C |\psi\rangle$?

Two methods:

1. Monte-Carlo over the $|\phi_i\rangle$ weighted by $|\lambda_i\rangle$.
   Polynomial in the negativity $\lambda^\dagger^\lambda$.

2. Compute $\lambda_i \rho_i C |\phi_i\rangle$.
   Polynomial in the stabilizer rank $R |\psi_q\rangle$.

Benefit of first: can deal with density matrices and noise.
Benefit of second: better constants and thus scaling.
We will only use the second approach.
Stabilizer decompositions 2

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2. Compute $\sum_i^n \lambda_i C |\phi_i\rangle$. Polynomial in the stabilizer rank: $R(|\psi\rangle) = n$. 

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e.g. $|T\rangle^\otimes |T\rangle = |00\rangle + e^{i\pi/4}|01\rangle + e^{i\pi/4}|10\rangle + e^{i\pi/2}|11\rangle$
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$$R(|T\rangle^{\otimes n}) = R((|T\rangle \otimes |T\rangle)^{n/2}) \leq 2^{n/2}$$
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$$R(|T\rangle^\otimes n) = R((|T\rangle \otimes |T\rangle)^{n/2}) \leq 2^{n/2}$$

Can also show that $R(|T\rangle^\otimes 6) = 7$, and hence:

$$R(|T\rangle^\otimes n) \leq 2^{\alpha n} \quad \text{where } \alpha = \log_2(7)/6 \approx 0.468$$
The goal: combine tensor contraction & stabilizer decompositions using the ZX-calculus.
ZX-diagrams

What gates are to circuits, *spiders* are to ZX-diagrams.
ZX-diagrams

What gates are to circuits, spiders are to ZX-diagrams.

Z-spider
\[ |0 \cdots 0\rangle \langle 0 \cdots 0| + e^{i\alpha} |1 \cdots 1\rangle \langle 1 \cdots 1| \]

X-spider
\[ |+ \cdots +\rangle \langle + \cdots +| + e^{i\alpha} |\cdots -\rangle \langle \cdots -| \]
ZX-diagrams

What gates are to circuits, *spiders* are to ZX-diagrams.

\[
\begin{align*}
\text{Z-spider} & \\
|0 \cdots 0\rangle \langle 0 \cdots 0| & + e^{i \alpha} |1 \cdots 1\rangle \langle 1 \cdots 1| \\
\end{align*}
\]

\[
\begin{align*}
\text{X-spider} & \\
|+ \cdots +\rangle \langle + \cdots +| & + e^{i \alpha} |- \cdots -\rangle \langle - \cdots -| \\
\end{align*}
\]

Spiders can be wired in any way:
Quantum gates as ZX-diagrams

Every quantum gate can be written as a ZX-diagram:

\[
\begin{align*}
S &= \phantom{=} \bigoplus x_1 = \frac{\pi}{2} \\
T &= \phantom{=} \bigoplus x_2 = \frac{\pi}{4} \\
H &= \phantom{=} \bigoplus x_1 = \bigotimes x_2 = \frac{\pi}{2} \bigotimes \frac{\pi}{2} \bigotimes \frac{\pi}{2} \\
CNOT &= \phantom{=} x_1 \bigotimes x_2 \\
CZ &= \phantom{=} \bigotimes x_1 = \phantom{=} \bigotimes x_2
Quantum gates as ZX-diagrams

Every quantum gate can be written as a ZX-diagram:

\[ S = \begin{array}{c}
\text{\rotatebox{90}{$\pi$}}
\end{array} \quad T = \begin{array}{c}
\text{\rotatebox{90}{$\pi/4$}}
\end{array} \quad H = \begin{array}{c}
\text{\rotatebox{90}{$\pi/2$}}
\end{array} \quad := \begin{array}{c}
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\text{\rotatebox{90}{$\pi/2$}}
\end{array} \]

Universality

Any linear map between qubits can be represented as a ZX-diagram.
Rules for ZX-diagrams: The ZX-calculus

\[ \alpha, \beta \in [0, 2\pi], \ a \in \{0, 1\} \]
Completeness of the ZX-calculus

Theorem
ZX-diagrams representing same linear map, can be transformed into one another using previous rules (and some additional ones).
Circuit simulation with ZX-calculus

1. Write circuit+state as ZX-diagram.
2. Simplify using ZX-calculus rules.
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1. Write circuit+state as ZX-diagram.
2. Simplify using ZX-calculus rules.
3. Replace magic states by stabilizer decomposition.
4. Repeat.
5. ...
6. Profit!
Simplifying ZX-diagrams

Same as in previous talk
(local complementation, pivoting, gadgetization)
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But:
  ▶ All rewrites now need to be scalar accurate.
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But:

- All rewrites now need to be scalar accurate.
- We no longer care about circuit extraction, so we can do more stuff!
Scalar-accurate local complementation and pivot

\[ e^{\pm i\pi/4} \sqrt{2^{\frac{(n-1)(n-2)}{2}}} \]

These variations kill all internal Clifford spiders.
Scalar-accurate local complementation and pivot

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Further optimization

From previous talk:

\[
\alpha \beta \ldots = \alpha \beta \ldots = \alpha + \beta \\
\alpha_1 \beta \ldots \alpha_n \beta = (\frac{1}{\sqrt{2}})^{n-1} \alpha_1 \alpha_n \ldots
\]
New rule: Supplementarity

Rule used in ZX for completeness:

\[ \alpha \quad \alpha + \pi \quad 2\alpha + \pi \]

\[ = \quad \frac{1}{2} \]

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New rule: Supplementarity

Rule used in ZX for completeness:

\[ \alpha = \frac{1}{2} \]

Can be generalised to following four cases:

\[ \alpha + \pi = \frac{1}{2^n} \]

\[ -\alpha + \pi = -\frac{e^{-i\alpha}}{2^n} \]

\[ e^{-i\alpha} = \frac{1}{2^{n+1}} \]
Example

Consider benchmark circuit hw6: 7 qubits, and 105 T-gates. After PyZX simplification: 75 T-gates.
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This has 33 T-gates.
Consider benchmark circuit hw6: 7 qubits, and 105 T-gates. After PyZX simplification: 75 T-gates. Inputting the state $|+ + - - - + -\rangle$ and effect $\langle +011 - 1- |$, and further simplifying gives (up to scalar):

This has 33 T-gates.
Now we should apply the stabilizer decomposition to these states.
Stabilizer decompositions in ZX

\[ \frac{\pi}{4} + \frac{\pi}{4} = \frac{\pi}{2} + \pi \]

But what about the 6 T-gate rank 7 decomposition?
FIG. 3. Graphs $G'$ and $G''$ used in the definition of stabilizer states $\phi'$ and $\phi''$; see Eq. (11).

$$|H^{\otimes 6}\rangle = (-16 + 12\sqrt{2})|B_{6,0}\rangle + (96 - 68\sqrt{2})|B_{6,6}\rangle + (10 - 7\sqrt{2})|E_6\rangle + (-14 + 10\sqrt{2})|O_6\rangle + (7 - 5\sqrt{2})Z^{\otimes 6}|K_6\rangle + (10 - 7\sqrt{2})|\phi'\rangle + (10 - 7\sqrt{2})|\phi''\rangle,$$

where

$$|\phi'\rangle = \prod_{(i,j) \in E'} \Lambda(Z)_{i,j}|O_6\rangle \quad \text{and} \quad |\phi''\rangle = \prod_{(i,j) \in E''} \Lambda(Z)_{i,j}|O_6\rangle.$$

$e^{i\pi/4} = +2e^{i\pi/4}$

$-\frac{1+\sqrt{2}}{4} + \frac{1-\sqrt{2}}{4}$

$-2\sqrt{2}i - 2i + 8\sqrt{2}i + 8\sqrt{2}i$
Demo time
Conclusions

- With ZX-calculus we can combine tensor contraction with stabilizer decomposition.
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- With ZX-calculus we can combine tensor contraction with stabilizer decomposition.
- With rewriting we can further reduce amount of non-Cliffords in each sub-diagram.
- Even removing just 1 extra spider in every diagram would allow \( \approx 15\% \) bigger circuits.
Future work

- Investigate which groups of spiders should be replaced.
- Find right trade-off in using more computation early on.
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- Make high-performance implementation of the algorithm.
- Marginal probabilities possible with CPM construction. Is there a better way?
Thank you for your attention!

[Image of an airplane with the text F-PYZX]

github.com/Quantomatic/pyzx  zxcalculus.com/pyzx