

# Classical simulation of quantum circuits

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# Motivation (1)

## Simulating quantum computers is useful

### NISQ

Present day & near future technology:

“Noisy, Intermediate Scale Quantum” computers

- ▶ Noisy means you want to compare outputs to theoretical predictions
- ▶ Intermediate scale means you *can* compare outputs to theoretical predictions

### Algorithm design

Can test and benchmark algorithms without having access to a real quantum computer

## Motivation (2)

### Simulating quantum computers is hard



**Figure 1:** Bełchatów Power Station would need to run for roughly 22 years to provide enough energy to simulate Google’s “quantum supremacy” circuits (Google estimate a simulation cost of 1 petawatt hour).

## Motivation (3)

### Simulating quantum computers is interesting!

#### Landscape of computations

- ▶ Quantum computations form a landscape in some high dimensional space
- ▶ For some reason some of these are easy (polynomial) to simulate and some are hard (exponential)
- ▶ Fundamentally we don't really know why

Low qubit number  $\implies$  easy to simulate

Low entanglement  $\implies$  easy to simulate

Low "magic"  $\implies$  easy to simulate

???  $\implies$  hard to simulate

# What is a quantum computer?

For the purposes of this talk:

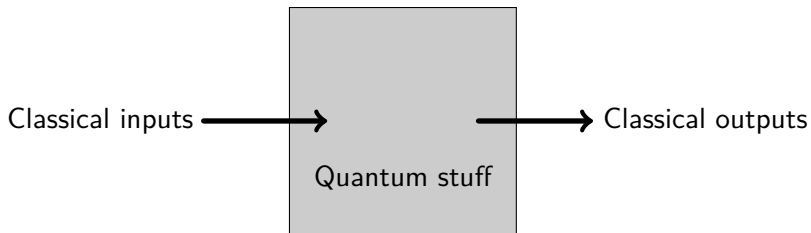
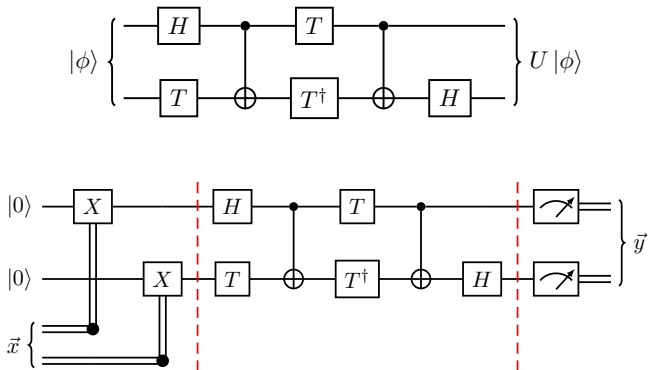


Figure 2: A quantum computer

# What is a quantum computer?

With slightly more detail:



**Figure 3:** The quantum Fourier transform (top) used as a subroutine in a quantum computer (bottom)

## What actually is simulation?

	Weak	Strong
Exact	Draw samples from Born rule distribution	Compute Born rule probabilities
Approximate	Draw samples from a distribution close to the Born distribution	Compute approximations to Born rule probabilities

# Born rule probability estimation

## General problem statement

Given a quantum channel  $\Phi$ , an input state  $\rho$ , an output effect  $E$  and positive real numbers  $\epsilon$  and  $\delta$ , return a real number  $p$  such that

$$\Pr(|\text{tr}(\Phi(\rho)E) - p| > \epsilon) < \delta. \quad (1)$$



# Project overview

## Collaboration with

Hakop Pashayan, Kamil Korzekwa & Stephen Bartlett

## Aims

State of the art algorithms for estimating Born-rule probabilities for quantum circuits consisting of

1. Input computational basis states

2. Clifford gates:  $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ ,  $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$ ,  $CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

3. Non-Clifford  $T_\phi$  “magic” gates:  $T_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$

4. Output computational basis measurements

## Clifford / stabilizer overview (1)

### Pauli operators

These are  $n$  qubit tensor products of

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (2)$$

with a phase  $\omega \in \{1, i, -1, -i\}$ .

### Examples

$$P_1 = X \quad (3)$$

$$P_2 = X \otimes Z \otimes I \otimes Y \quad (4)$$

$$P_3 = -X \otimes X \quad (5)$$

### Notes

- ▶ Form a group (for each fixed qubit number)
- ▶ Each operator takes  $4n + 4$  bits to store on a computer

## Clifford / stabilizer overview (2)

### Clifford operations

These are unitaries which map  $n$  qubit Pauli operators to  $n$  qubit Pauli operators

$$UP_1U^\dagger = P_2, \quad (6)$$

note that these form a (small!) subgroup of the full unitary group on  $n$  qubits.

#### One qubit Examples

$P$	$HPH^\dagger$	$SPS^\dagger$
$I$	$I$	$I$
$X$	$Z$	$Y$
$Y$	$-Y$	$-X$
$Z$	$X$	$Z$

#### Two qubit example

$P$	$CXPCX^\dagger$
$X \otimes I$	$X \otimes X$
$I \otimes X$	$I \otimes X$
$Z \otimes I$	$Z \otimes I$
$I \otimes Z$	$Z \otimes Z$

Storing a Clifford unitary takes  $2n(4n + 4)$  bits.

## Clifford / stabilizer overview (3)

### Stabilizer states

A set of Pauli operators  $S = \{P_1, \dots, P_n\}$  is *independent* if

$$i \neq j \implies P_i P_j \neq I. \quad (7)$$

A quantum state  $|\psi\rangle$  on  $n$  qubits is a *stabilizer state* if there exists a set of  $n$  independent Pauli operators  $\{P_i\}$  such that

$$P_i |\psi\rangle = |\psi\rangle \quad \forall i. \quad (8)$$

### Examples

state	stabilizers	alternative notation
$ 0\rangle$	$\{Z\}$	$\{Z_1\}$
$( 00\rangle +  11\rangle) / \sqrt{2}$	$\{X \otimes X, Z \otimes Z\}$	$\{X_1 X_2, Z_1 Z_2\}$
$ x\rangle$	???	$\{(-1)^{x_j} Z_j \mid j = 1 \dots n\}$

## Clifford / stabilizer overview (4)

### Consequences of $|\psi\rangle$ being an $n$ qubit stabilizer state

- ▶ The set of Pauli operations stabilising  $|\psi\rangle$  form a group written  $\text{Stab}(|\psi\rangle)$
- ▶  $\text{Stab}(|\psi\rangle)$  has  $2^n$  elements
- ▶  $\text{Stab}(|\psi\rangle)$  is Abelian
- ▶ The phases of each Pauli operator in  $\text{Stab}(|\psi\rangle)$  are real
- ▶  $\text{Stab}(|\psi\rangle) \sim \mathbb{Z}_2^n$
- ▶ Storing a stabilizer state requires  $n(4n + 1)$  bits
- ▶ If  $U$  is a Clifford unitary then  $\text{Stab}(U|\psi\rangle) = U\text{Stab}(|\psi\rangle)U^\dagger$

## Clifford / stabilizer overview (5)

### Gottesman-Knill theorem<sup>1</sup>

Circuits consisting of input stabiliser states, Clifford unitaries and computational basis measurements can be simulated (strongly or weakly) in polynomial time on a classical computer.

Moreover the group of Clifford unitaries is generated by the single qubit H and S gates, and the two qubit CX gate for every qubit.

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<sup>1</sup>Gottesman, Daniel (1998). "The Heisenberg Representation of Quantum Computers". arXiv:quant-ph/9807006

## Breaking out of the Clifford/stabilizer subtheory

### Main idea - “gadgetisation”

We replace all the  $T_\phi$  gates using the identity

$$\boxed{T_\phi} = 2^{\frac{1}{2}} \cdot \left( |0\rangle \begin{array}{c} \bullet \\ \oplus \end{array} \langle T_\phi^\dagger | \right)$$

Figure 4: Single gadget

Where

$$|T_\phi^\dagger\rangle = \frac{1}{\sqrt{2}} \left( |0\rangle + e^{-i\phi}|1\rangle \right) \quad (9)$$

This turns our  $n$  qubit universal quantum circuit into an  $n + t$  qubit Clifford circuit with a non-stabilizer measurement at the end.

# Gadgetisation

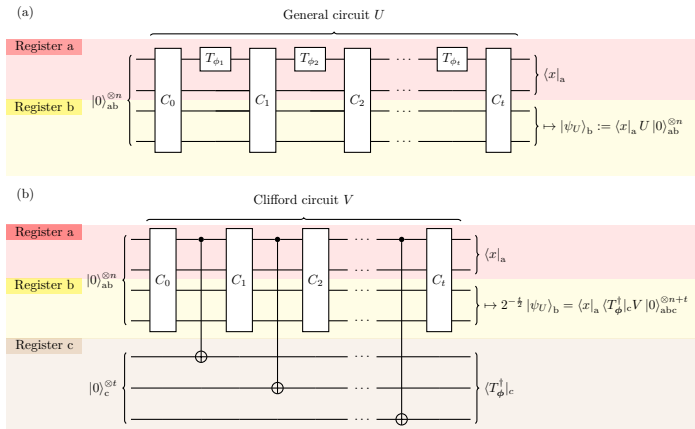


Figure 5: Clifford+T circuit (a) is gadgetised and becomes a Clifford circuit with a non-stabilizer measurement at the end (b).



# The Compress algorithm (1)

## Representation

Gadgetisation gives us a powerful representation of a quantum state, in terms of a stabilizer state and a non-stabilizer measurement at the end (which just gets stored as a list of one  $\phi$  angle for each  $T_\phi$  gate).

## Compression

Playing with this representation lets our algorithm prove stuff about the state being represented

- ▶ Reduce number of qubits (measured/unmeasured/magic)
- ▶ Reduce number of stabilizers
- ▶ Output “compression number”  $r$
- ▶ Runs in polynomial time (in all relevant parameters)

## The Compress algorithm (2)

### Input/Output

**Input:** Initial computational basis state, Clifford unitary and computational basis measurement outcome.

**Output:** Integers  $v$  and  $w$  and a set of  $t - r$  qubit Pauli operators on  $t$  qubits,  $g_i$  such that

$$p = 2^{v-w} \langle T_\phi^\dagger | \prod_{i=1}^{t-r} (I + g_i) | T_\phi^\dagger \rangle, \quad (10)$$

the  $g_i$  generate a group isomorphic to  $\mathbb{Z}_2^{t-r}$

$$p = 2^{v-w} \sum_{g \in \langle G \rangle} \langle T_\phi^\dagger | g | T_\phi^\dagger \rangle. \quad (11)$$

# The Compute algorithm (1)

## Naive runtime for compute

We want to compute

$$p = 2^{v-w} \sum_{g \in \langle G \rangle} \langle T_\phi^\dagger | g | T_\phi^\dagger \rangle. \quad (12)$$

The elements of the runtime are

1. Computing each  $g$  involves multiplying (on average)  $\frac{t-r}{2}$  product operators on  $t$  qubits -  $O(t(t-r))$
2. Each inner product takes  $O(t)$  since the states and operators are tensor products
3. Total runtime  $O(2^{t-r}t(t-r))$

## The Compute algorithm (2)

### Better runtime for compute

There are efficiently computable functions

$f: [0, 1 \dots, 2^n - 1] \rightarrow \langle G \rangle$  and  $g: [0, 1 \dots, 2^n - 1] \rightarrow G$  such that

$$f(x+1) = g(x)f(x), \quad (13)$$

and moreover  $f$  is a bijection.

## The Compute algorithm (3)

### Better runtime for compute

We want to compute

$$p = 2^{v-w} \sum_{g \in \langle G \rangle} \langle T_\phi^\dagger | g | T_\phi^\dagger \rangle. \quad (14)$$

The elements of the runtime are

1. Computing each  $g$  involves multiplying (on average)  ~~$\frac{t-r}{2}$~~   $2$  product operators on  $t$  qubits -  ~~$O(t(t-r))$~~   $O(t)$
2. Each inner product takes  $O(t)$  since the states and operators are tensor products
3. Total runtime  ~~$O(2^{t-r} t(t-r))$~~   $O(2^{t-r} t)$

## Better runtime in detail

### How does this actually work?

- ▶ Recall we have a set of  $t - r$  generators  $G$  generating a group  $\langle G \rangle \sim \mathbb{Z}_2^{t-r}$
- ▶ This group corresponds to the set of vertices of a  $t - r$  dimensional hypercube where each generator in  $G$  corresponds to moving unit distance in an orthogonal direction
- ▶  $f$  represents a path that visits each vertex of the hypercube exactly once,  $g$  tells you which direction to walk to get to the next node in the path

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

1. Take an  $n - 1$  dimensional cube and clone it
2. Translate the clone 1 unit in the  $n^{\text{th}}$  dimension
3. Join each vertex in the original with its corresponding vertex in the clone



Figure 6:  $n = 0$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

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Figure 6:  $n = 1$



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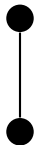


Figure 6:  $n = 1$

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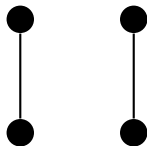


Figure 6:  $n = 2$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

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2. Translate the clone 1 unit in the  $n^{\text{th}}$  dimension
3. Join each vertex in the original with its corresponding vertex in the clone

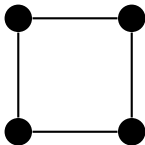


Figure 6:  $n = 2$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

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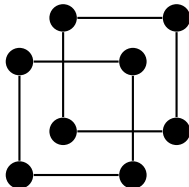


Figure 6:  $n = 3$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

1. Take an  $n - 1$  dimensional cube and clone it
2. Translate the clone 1 unit in the  $n^{\text{th}}$  dimension
3. Join each vertex in the original with its corresponding vertex in the clone

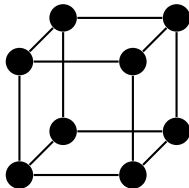


Figure 6:  $n = 3$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

1. Take an  $n - 1$  dimensional cube and clone it
2. Translate the clone 1 unit in the  $n^{\text{th}}$  dimension
3. Join each vertex in the original with its corresponding vertex in the clone

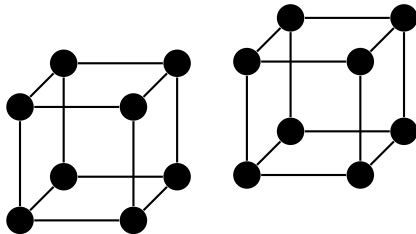


Figure 6:  $n = 4$

## (Aside) How do you build an $n$ dimensional cube?

### Recipe

1. Take an  $n - 1$  dimensional cube and clone it
2. Translate the clone 1 unit in the  $n^{\text{th}}$  dimension
3. Join each vertex in the original with its corresponding vertex in the clone

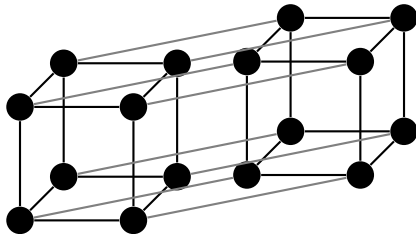


Figure 6:  $n = 4$

## Binary reflected “Gray” code

### A path through every node of the hypercube

This recursive structure is what we exploit to build a path through the  $n$  dimensional cube

1. Follow a path that visits every node in an  $n - 1$  dimensional cube once
2. Now move one unit in the direction orthogonal to every edge in this path
3. Now follow the path *backwards* in the second  $n - 1$  dimensional cube that makes up the  $n$  dimensional cube

This path forms a bijection from the natural numbers  $\{0, 1, \dots, 2^n - 1\}$  to themselves known as the *binary reflected Gray code* after Robert Gray who patented it in 1947.

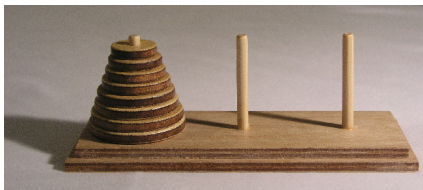




(a) Édouard Lucas



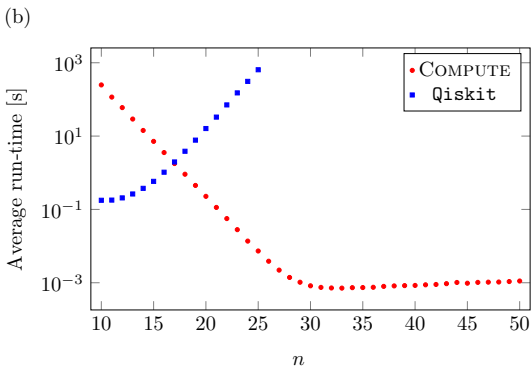
(b) Baguenaudier (time waster)



(c) Towers of Hanoi

**Figure 7:** Édouard Lucas invented the Baguenaudier (1872) and invented the Towers of Hanoi puzzle (1883), both employing the binary reflected code we employ in our algorithm.

## Compute vs Statevector simulator



**Figure 8:** Performance of the Compute algorithm for random circuits. Random circuits with  $c = 10^3$  Clifford gates,  $t = 30$   $T$  gates and  $w = 10$  measured qubits with average taken over 100 random circuits for each  $n$ .

# RawEstim (1)

## Compress

In addition to the stuff for the Compute algorithm Compress gives us a  $t$ -qubit unitary  $W$  as a circuit of  $O(t^2)$  Clifford gates including  $O(t)$  Hadamards such that

$$p = \left\| \langle 0 |^{\otimes (t-r)} W | T_{\phi}^{\dagger} \rangle \right\|^2, \quad (15)$$

where

$$|T_{\phi}^{\dagger}\rangle = \prod_{j=1}^t |T_{\phi_j}^{\dagger}\rangle = 2^{-\frac{t}{2}} \prod_{j=1}^t \left( |0\rangle + e^{-i\phi_j} |1\rangle \right) = \prod_{j=1}^t \left( \alpha_{\phi_j} |+\rangle + \alpha'_{\phi_j} |-\rangle \right). \quad (16)$$

## RawEstim (2)

### Expanding the magic state

Define  $|\tilde{0}\rangle := |+\rangle$ ,  $|\tilde{1}\rangle := |-\rangle$  and  $|\tilde{y}\rangle := \prod_j |\tilde{y}_j\rangle$  then,

$$|\mathcal{T}_\phi^\dagger\rangle = \prod_{j=1} \left( \alpha_{\phi_j} |\tilde{0}\rangle + \alpha'_{\phi_j} |\tilde{1}\rangle \right) \quad (17)$$

$$= \sum_{y=0}^{2^t-1} \left( \prod_j \alpha_{\phi_j}^{1-y_j} (\alpha'_{\phi_j})^{y_j} \right) |\tilde{y}\rangle \quad (18)$$

$$= \sqrt{\xi^*} \sum_{y=0}^{2^t-1} p(y) \left( \prod_j e^{i\psi_j(1-y_j)} e^{i\psi'_j y_j} \right) |\tilde{y}\rangle, \quad (19)$$

where  $p(y)$  is a normalized product probability distribution the  $\psi_j$  and  $\psi'_j$  are real numbers and  $\xi^*$  is the *stabilizer extent*.

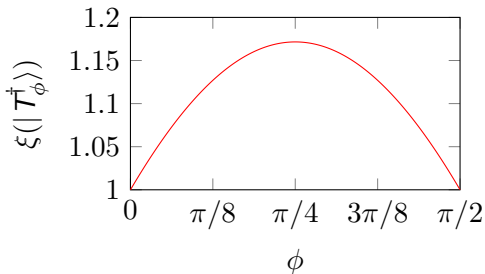
## RawEstim (3)

### Quantifying “magic”

- ▶ The stabilizer extent  $\xi^*$  will be an important factor in the runtime of our algorithm
- ▶ Intuition - think of  $\log \xi^*$  as a measure of how far your state is from a stabilizer state

Explicitly we have

$$\begin{aligned} \xi(|T_{\phi_j}^\dagger\rangle) &= (|\alpha_{\phi_j}| + |\alpha'_{\phi_j}|)^2 \\ &= \left(\sqrt{1 - \sin \phi_j} + \sqrt{1 - \cos \phi_j}\right)^2 \\ \xi^* &= \prod_j \xi(|T_{\phi_j}^\dagger\rangle) \end{aligned}$$



# Sampling

## Basic idea

Substitute in the decomposition of the magic state from before

$$\rho = \xi^* \left\| \sum_{y=0}^{2^t-1} \rho(y) \left( \prod_j e^{i\psi_j(1-y_j)} e^{i\psi'_j y_j} \right) \langle 0|^{\otimes(t-r)} W |\tilde{y}\rangle \right\|^2 \quad (20)$$

- ▶ The thing inside the norm is an (unnormalised) state written as the mean of a (stabiliser state-valued) probability distribution
- ▶ Take  $s$  samples from this distribution and approximate the true mean with the sample mean

## Sampling (2)

### Theorem: Hayes<sup>2</sup>

Let  $X$  be a very-weak martingale taking values in  $\mathbb{R}^N$  such that  $X_0 = 0$  and for every  $j$ ,  $\|X_j - X_{j-1}\|_2 \leq 1$ . Then for every  $a > 0$ :

$$\Pr(\|X_s\| \geq a) \leq 2e^{1-(a-1)^2/2s} < 2e^2 \exp(-a^2/2s). \quad (21)$$

**Intuitively:** Take enough samples and the sample mean vector will be close to the expected value.

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<sup>2</sup>Thomas P Hayes, "A large-deviation inequality for vector-valued martingales," *Combinatorics, Probability and Computing*(2005)

# Norm estimation

## Fast norm estimation<sup>3</sup>

Given real numbers  $\epsilon$  and  $\delta$  and an  $n$  qubit state of the form

$$|\psi\rangle = \sum_{j=1}^k b_j |\phi_j\rangle, \quad (22)$$

the fast norm estimation algorithm returns a number  $\eta$  such that

$$\Pr (|\eta - \|\psi\|| > \epsilon \|\psi\|) < \delta, \quad (23)$$

with runtime  $O(kn^3\epsilon^{-2} \log \delta^{-1})$ .

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<sup>3</sup>Sergey Bravyi, Dan Browne, Padraic Calpin, Earl Campbell, David Gosset, and Mark Howard, "Simulation of quantum circuits by low-rank stabilizer decompositions," Quantum 3, 181 (2)



## Putting it together

### RawEstim

Given the output of the Compress algorithm and two positive integers  $s$  and  $L$ , RawEstim outputs an estimate  $\hat{p}$  of the outcome probability  $p$  such that for all  $\epsilon_{\text{tot}} > 0$  and  $\epsilon \in (0, \epsilon_{\text{tot}})$ :

$$\Pr (|\hat{p} - p| \geq \epsilon_{\text{tot}}) \leq 2e^2 \exp \left( \frac{-s(\sqrt{p+\epsilon} - \sqrt{p})^2}{2(\sqrt{\xi^*} + \sqrt{p})^2} \right) \quad (24)$$

$$+ \exp \left( - \left( \frac{\epsilon_{\text{tot}} - \epsilon}{p + \epsilon} \right)^2 L \right) =: \delta_{\text{tot}}. \quad (25)$$

The run-time  $\tau_{\text{RAWESTIM}}$  of the algorithm scales as

$$\tau_{\text{RAWESTIM}} = O(st^3 + sLr^3). \quad (26)$$

## RawEstim summary

### Good

- ▶ Runtime linear in  $\xi^*$  (since you need  $S = O(\xi^*)$ )
- ▶ Takes advantage of Compress -  $r$  appears in runtime instead of  $t$
- ▶ Complementary to Compute - good for small  $r$
- ▶ Very good constants in the  $O(\cdot)$  statements
- ▶ Polynomial memory use

### Bad

- ▶ The  $s$  and  $L$  you need depend on the unknown probability  $p$
- ▶ Unclear how to divide error/runtime between norm estimation and vector estimation
- ▶ Doesn't actually solve the problem I gave at the start

# The Estimate algorithm (1)

## Recall

$$\delta_{\text{tot}} = 2e^2 \exp\left(\frac{-s(\sqrt{p+\epsilon} - \sqrt{p})^2}{2(\sqrt{\xi^*} + \sqrt{p})^2}\right) + \exp\left(-\left(\frac{\epsilon_{\text{tot}} - \epsilon}{p + \epsilon}\right)^2 L\right)$$

## Note

- ▶ Each exponential is increasing in  $p$
- ▶ The first exponential is decreasing in  $s$
- ▶ The second exponential is decreasing in  $L$
- ▶ The  $\epsilon$  lets you choose how the error is allocated between the magic sampling and the norm estimation

Taking the obvious upper bound  $p \leq 1$  will give us a correct estimation algorithm but lose a lot of performance.

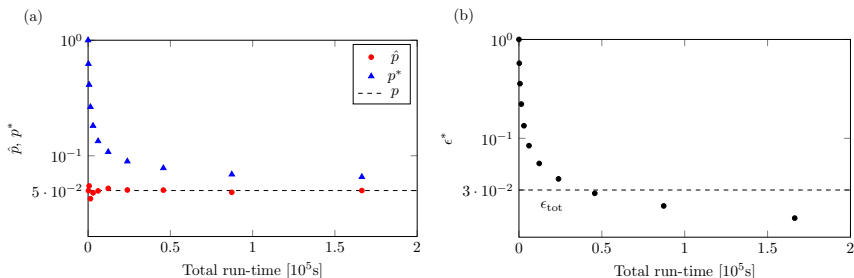
## The Estimate algorithm (2)

### Solution!

Roughly speaking:

1. Use the obvious upper bound  $p_0 \leq 1$  but take a very large allowed error  $\epsilon_0$
2. Since  $\epsilon_0$  is large the RawEstim doesn't take very long even though we're choosing  $s$  and  $L$  based on  $p_0 = 1$
3. RawEstim returns an estimate  $p_0^*$  such that (with high probability)  $p \leq p_0^* + \epsilon_0$
4. Now choose  $p_1 = p_0^* + \epsilon_0$  and run RawEstim with  $\epsilon_1 < \epsilon_0$

## The Estimate algorithm (3)



**Figure 10: Performance of the Estimate algorithm.** An  $n = 50$  qubit,  $r = 10$ ,  $t = 60$  non-Clifford gate circuit designed to have  $p = 0.05$ . The circuit consists of approximately 2000 Clifford. The parameters are chosen such that the total circuit has stabiliser extent  $\xi^* \approx 3767$ , equivalent to 52  $T_{\pi/4}$  gates. The total run-time of approximately  $1.6 \times 10^5$ s includes approximately 34s of overhead from the Estimate algorithm.

## Estimate summary

### Good

- ▶ All of the “good” column from RawEstim
- ▶ Works out the  $s$  and  $L$  you need for you
- ▶ “Relatively small” overhead over calling RawEstim with the optimal parameters
- ▶ Does actually solve the problem I gave at the start

### Bad

- ▶ The runtime is probabilistic
- ▶ The runtime depends on the initially unknown parameter  $p$

# Qiskit

## Overview

- ▶ A pretty popular library - 52380 downloads in the 30 days preceding 23.09.2021
- ▶ Useful for all sorts of things
  1. Quantum algorithms development
  2. Wide variety of classical simulation algorithms
  3. Access to (IBM) quantum hardware
  4. Noise mitigation research
  5. Circuit optimisation
- ▶ Started and largely developed by IBM research, technically in the hands of a community team
- ▶ By far the biggest computer library for quantum computing & information work (that I know of)

# Implementation

## What I'm doing

- ▶ I already wrote an implementation of our algorithms in C
- ▶ Qiskit is a python library but the guts are written in C++
- ▶ In addition to writing it I'm talking to the qiskit people about
  1. The user interface
  2. Which bits should/shouldn't be parallelised
  3. Various improvements
  4. Testing & documentation
- ▶ So far I have contributed code representing roughly half our paper
- ▶ I also fixed some issues in other simulation algorithms for them



# Matchgate overview

## Matchgates

Matchgate circuits are generated by two qubit gates of the form

$$G(A, B) = \begin{pmatrix} A_{11} & 0 & 0 & A_{21} \\ 0 & B_{11} & B_{21} & 0 \\ 0 & B_{12} & B_{22} & 0 \\ A_{12} & 0 & 0 & A_{22} \end{pmatrix},$$

where  $A$  and  $B$  are single qubit unitaries with  $\det(A) = \det B$ , and the two qubit gates act on adjacent qubits.

## Fermionic linear optics overview (1)

### Creation and annihilation operators

Define Fermionic creation ( $a_i^\dagger$ ) and annihilation ( $a_i$ ) operators for  $i = 1 \dots n$  with

$$\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0 \qquad \{a_i, a_j^\dagger\} = \delta_{ij}, \quad (27)$$

Note that if (for any given qubit)

$$\sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad (28)$$

then

$$a_i^\dagger = (-1)^{\sum_{j=1}^{i-1} N_j} \sigma_i^+ \qquad a_i = (-1)^{\sum_{j=1}^{i-1} N_j} \sigma_i^-, \quad (29)$$

where  $N_j|0\rangle_j = 0$ ,  $N_j|1\rangle_j = |1\rangle_j$ .

## Fermionic linear optics overview (2)

### Fermionic linear optics

Now define the *Majorana Fermion* operators

$$c_{2i} = a_i + a_i^\dagger \quad (30)$$

$$c_{2i+1} = i(a_i - ia_i^\dagger), \quad (31)$$

Note

$$\{c_i, c_j\} = 2\delta_{ij} \quad (32)$$

A unitary  $U$  is *Fermionic* if (and only if)

$$Uc_iU^\dagger = \sum_j R_{ij}c_j, \quad (33)$$

for a real, special orthogonal,  $2n \times 2n$  matrix  $R$ .

# Terhal and DiVincenzo

## Theorem (1)

Matchgate circuits = Fermionic Linear optic circuits

## Theorem (2)

Given a Fermionic linear optic circuit  $U$  and states

$$|x\rangle = (a_1^\dagger)^{x_1} (a_2^\dagger)^{x_2} \dots (a_n^\dagger)^{x_n} |0\rangle \quad (34)$$

$$|y\rangle = (a_1^\dagger)^{y_1} (a_2^\dagger)^{y_2} \dots (a_n^\dagger)^{y_n} |0\rangle, \quad (35)$$

there is a polynomial-time classical algorithm which computes

$$p = |\langle y|U|x\rangle|^2. \quad (36)$$

# Hebenstreit, Jozsa, Kraus, Strelchuk and Yoganathan

## Theorem

Matchgate circuits supplemented by single qubit measurements and magic states of the form

$$|\psi_\phi\rangle = |0000\rangle + |1100\rangle + |0011\rangle + e^{i\phi}|1111\rangle, \quad (37)$$

are universal for quantum computation.

## Decomposition

### Lemma (ORS)

The magic state  $|\psi_\phi\rangle$  admits the decomposition

$$|\psi_\phi\rangle = \frac{e^{iz}N_{-z}}{1 + e^{iz}} \left( \frac{1}{N_{-z}} (|0000\rangle + e^{-iz}|1100\rangle + e^{-iz}|0011\rangle + e^{-2iz}|1111\rangle) \right) \\ + \frac{N_z}{1 + e^{iz}} \left( \frac{1}{N_z} (|0000\rangle + e^{iz}|1100\rangle + e^{iz}|0011\rangle + e^{2iz}|1111\rangle) \right),$$

where  $\cos(z) = \frac{1}{2} (1 + e^{i\phi})$ ,  $N_z = 2e^{-2\text{Im}(z)} \cosh(\text{Im}(z))^2$ .

The two highlighted terms are each Fermionic Gaussian states (states obtainable by the action of matchgate circuits on an initial  $|0\rangle$  vacuum state).

## Decomposition (2)

### Lemma (ORS)

The projector  $|\psi_\pi\rangle\langle\psi_\pi|$  admits the decomposition

$$\begin{aligned}
 |\psi_\pi\rangle\langle\psi_\pi| = & \frac{1}{16} (I + c_0 c_1 c_2 c_3 c_4 c_5 c_6 c_7 + c_0 c_1 c_5 c_6 + c_2 c_3 c_4 c_7 \\
 & + c_0 c_3 c_4 c_5 + c_1 c_2 c_6 c_7 + c_0 c_1 c_4 c_7 + c_2 c_3 c_5 c_6 \\
 & + c_0 c_3 c_6 c_7 + c_1 c_2 c_4 c_5 + c_0 c_2 c_5 c_7 + c_1 c_3 c_4 c_6 \\
 & - c_0 c_1 c_2 c_3 - c_4 c_5 c_6 c_7 - c_0 c_2 c_4 c_6 - c_1 c_3 c_5 c_7)
 \end{aligned}$$

There are similar decompositions for  $\phi \in (0, 2\pi)$ , this state is magic except as long as  $\phi \neq 2k\pi$  for some  $k \in \mathbb{Z}$ .

## Issues with these decompositions

### Vector decomposition

We don't have a phase sensitive (i.e. vector) matchgate simulation algorithm.

Maybe if we're smart we can invent one.

### Projector decomposition

Decomposition consists of 16 terms - leading to an algorithm with runtime like  $O(t^{16})$  - this is very, very slow!

Maybe if we're smart we can optimize this.



# Phase sensitive Fermionic linear optics simulator

## Basic issue

Efficient simulation is based on “adjoint action”

$$Uc_iU^\dagger = \sum_j R_{ij}c_j. \quad (38)$$

Any phase information is lost in this representation.

## Basic solution

Fix the phase of  $U$  by fixing the action on some vector

$$U|0\rangle = |0\rangle. \quad (39)$$

## Preserving the vacuum (1)

### Task 1

Characterise the FLO unitaries  $U$  for which

$$U|0\rangle = |0\rangle. \quad (40)$$

Solution: If  $Uc_iU^\dagger = \sum_j R_{ij}c_j$  and  $U|0\rangle = |0\rangle$  then

$$RJR^T = J, \quad (41)$$

where  $J$  is the *symplectic form*

$$J = \bigoplus_{q=0}^{n-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (42)$$

In other terms -  $R \in \text{SP}(2n, \mathbb{R})$

## Preserving the vacuum (2)

### Question:

What can we say about the real, orthogonal matrices  $2n \times 2n$  matrices which are also symplectic?

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Concretely we have, for any  $R \in O(2n, \mathbb{R}) \cap SP(2n, \mathbb{R})$ ,

$$R = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}, \quad I = cc^T + ss^T, \quad 0 = cs^T - sc^T, \quad (44)$$

and these conditions are exactly equivalent to

$$c + is \in U(n, \mathbb{C}). \quad (45)$$

## What is left over? (1)

### Generating set

The FLO unitaries on  $n$  qubits are generated by a set of  $6n$  one-parameter unitary groups  $\exp(itH)$  where  $H$  is one of

$$a_i^\dagger a_i \qquad a_{i+1}^\dagger a_{i+1} \qquad (46)$$

$$a_i^\dagger a_{i+1} - a_i a_{i+1}^\dagger \qquad i(a_i^\dagger a_{i+1} + a_i a_{i+1}^\dagger) \qquad (47)$$

$$a_i^\dagger a_{i+1}^\dagger - a_i a_{i+1} \qquad i(a_i^\dagger a_{i+1}^\dagger + a_i a_{i+1}) \qquad (48)$$

Each can be written in terms of the Majorana Fermion operators

$$H = \frac{i}{4} \sum_{jk} \alpha_{jk} c_j c_k, \qquad (49)$$

where  $\alpha$  is a real, antisymmetric  $2n \times 2n$  matrix.

## What is left over? (2)

### Type 1

- ▶ Preserve the vacuum
- ▶  $[\alpha, \mathcal{J}] = 0$

### Type 2

- ▶ Do not preserve the vacuum
- ▶  $\{\alpha, \mathcal{J}\} = 0$

### Lemma (ORS)

If  $\alpha$  is a real antisymmetric matrix and  $\{\alpha, \mathcal{J}\} = 0$  then there exists a zero-preserving FLO unitary  $U$  such that

$$U \exp \left( \sum_{jk} \alpha_{jk} c_j c_k \right) U^\dagger = \prod_i \exp (\lambda_i (c_{4i} c_{4i+2} - c_{4i+1} c_{4i+3})). \quad (50)$$

# FLO CH-form?

## Conjecture

Any Gaussian Fermionic state  $|\psi\rangle$  may be written in the form

$$|\psi\rangle = \omega U_0 \left[ \prod_j \exp(\lambda_j (c_{4j} c_{4j+2} - c_{4j+1} c_{4j+3})) \right] |0\rangle \quad (51)$$

$$= \omega U_0 \left[ \prod_j \left( \cos(2\lambda_j) I + \sin(2\lambda_j) a_{2j}^\dagger a_{2j+1}^\dagger \right) \right] |0\rangle, \quad (52)$$

for  $\omega \in \mathbb{C}$ ,  $\lambda_j \in \mathbb{R}$  and  $U_0|0\rangle = |0\rangle$ .



## Other projects

### In progress

- ▶ Verification, validation & characterisation of NISQ computers
- ▶ Quantum machine learning
- ▶ Improvements to Clifford+T algorithm

### Not really in progress

Other efficiently simulable subtheories

- ▶ Low entanglement - Schrödinger-Feynmann simulators
- ▶ Low qubit number - Statevector simulators

# Thank you for your time