IMPROVED SIMULATION OF QUANTUM CIRCUITS DOMINATED BY FREE FERMIONIC OPERATIONS

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Aim

Estimate using a **classical computer**

$$p := |\langle y| U |x\rangle|^2 \quad (1)$$

to precision ϵ with probability greater than $1 - \delta$.
Where

1. x and y are computational basis vectors
2. U consists of
   - many Fermionic linear optical (FLO) unitaries
   - some non-FLO controlled-phase gates.

The Fermionic linear optical subtheory is efficiently classically simulable, while circuits of FLO gates and controlled phase gates are universal for quantum computation (within one parity subspace).

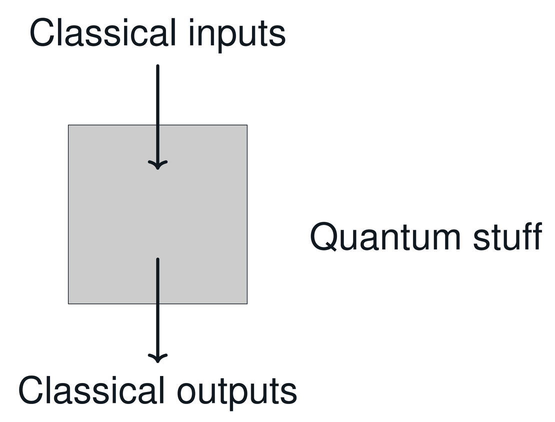

Figure 1: A quantum computer. In our work we do *not* model the internal workings of the computer and only attempt to reproduce the Born rule probabilities of the classical output from the classical input.

Background

Computational resource theories:

Idea: Resource theories where the free subtheory is efficiently classically simulable. Here efficiently means polynomial time, while classically simulable means you can efficiently perform tasks like

1. apply free gates to free states
2. compute inner products of free states
3. Compute Born-rule probabilities of outcomes of free measurements on free states.

Examples:
- Clifford/stabilizer circuits
- FLO/matchgates circuits
- Incoherent circuits
- Log-space universal quantum circuits
- Tensor-product circuits

Using computational resource theories to do universal simulation:

Idea: Write nonfree state as sums of free states and then sample. You can do this in two ways.

Density operator: Write non-free state as linear (not convex) combination of free states

$$\rho = \sum_i q_i \sigma_i. \quad (2)$$

Renormalize to get a probability distribution

$$\rho = ||q||_1 \sum_i \frac{|q_i|}{||q||_1} (-1)^{s_i} \sigma_i. \quad (3)$$

or

Statevector: Write non-free state as superpositions of free states

$$|\psi\rangle = \sum_i \alpha_i |f_i\rangle. \quad (4)$$

Renormalize to get a probability distribution

$$|\psi\rangle = ||\alpha||_1 \sum_i \frac{|\alpha_i|}{||\alpha||_1} e^{i\theta_i} |f_i\rangle \quad (5)$$

What controls the runtime of a classical simulation algorithm?

- $||q||_1$ is called *negativity*
- $||\alpha||_1^2$ is called *extent*
- (Informally) you can either get simulation runtime scaling in the negativity squared or the extent
- In the examples we know the extent is smaller than the negativity squared (usually significantly)

In our algorithm we decompose nonfree states as **statevectors**. This leads to runtime scaling with the *extent* but requires phase-sensitive FLO simulation methods (which we have developed).
Formal definition: Given a resource theory with set of free states S, define the $S-$extent

$$\xi_S(|\psi\rangle) = \inf \left\{ ||a||_1^2 \middle| a \in \mathbb{C}^{|s|}, \sum_{s\in S} a_s |s\rangle = |\psi\rangle \right\} \quad (6)$$

Figure 2(a): Base camp on the Nepalese side of Sagarmāthā. CC licence, Author: Peellden.

Figure 2(b): Base camp on the Tibetan side of Chomolungma. CC licence, Author: Gunther Hagleitner.

Figure 2: Two base camps in the vicinity of the mountain known as ཇོ་མོ་གླང་མ (Chomolungma), सगरमाथा (Sagarmāthā), 珠穆朗玛峰 (Zhūmùlǎngmǎ Fēng) and Everest. Basecamps are relatively easy to get to and make climbing nearby mountains easier. Computational resource theories are easy to simulate and make simulating "nearby" computations easier.

References

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Simulation overview

Rather than directly express our non-free state as a superposition of free states we consider a circuit formed of free (Fermionic linear optical) and non-free (controlled-phase) gates applied to an initial free (computational basis) state. Each non-free gate is then gadgetized - replaced with free gates augmented with additional "magic". The gadgetization we use is similar to that developed in [1, 4] but adapted for our use-case.

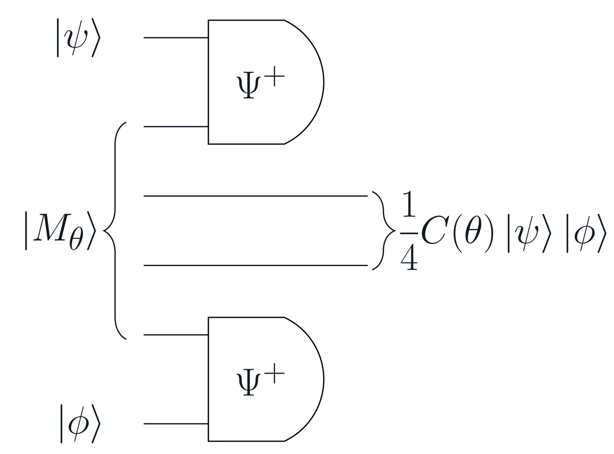

Figure 3(a): Projecting onto the Bell basis state $|\Psi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ for each of the two measurement implements the controlled phase gate.

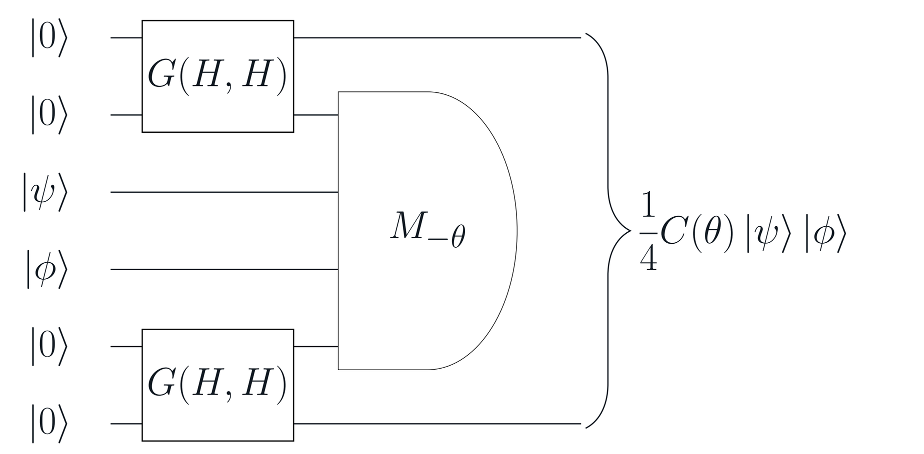

Figure 3(b): The "reverse gadget", the input state is now a FLO state, and magic is injected by the projection onto the non-FLO $M_{-\theta}$ state at the end.

Figure 3: By adapting the gadgetization of refs [1, 4] we are able to replace non-FLO controlled-phase gates with a combination of FLO gates and input (free) vaccum states. The non-FLO "magic" is injected by applying non-FLO projections onto these extra input states.

We then express each of the k projectors onto magic states as a sum of FLO projectors via

$$|M_\theta\rangle = \frac{1}{2}\left(|0000\rangle + |0011\rangle + |1100\rangle + e^{i\theta}|1111\rangle\right) \quad (7)$$

$$= \cos\left(\frac{\theta}{4}\right)|A(\theta)\rangle + i\sin\left(\frac{\theta}{4}\right)|B(\theta)\rangle, \quad (8)$$

where

$$|A(\theta)\rangle = \frac{1}{2}\left(e^{-i\frac{\theta}{4}}|0000\rangle + e^{i\frac{\theta}{4}}|0011\rangle + e^{i\frac{\theta}{4}}|1100\rangle + e^{i\frac{3\theta}{4}}|1111\rangle\right) \quad (9)$$

$$|B(\theta)\rangle = \frac{1}{2}\left(e^{-i\frac{\theta}{4}}|0000\rangle - e^{i\frac{\theta}{4}}|0011\rangle - e^{i\frac{\theta}{4}}|1100\rangle + e^{i\frac{3\theta}{4}}|1111\rangle\right). \quad (10)$$

This allows us to express the probability we are trying to estimate into a sum of 2^k terms, each of which we can compute efficiently. Computing these terms requires novel phase-sensitive FLO simulation routines we have developed, which extend the results of [2]. We can apply FLO unitaries to FLO states and compute inner products of FLO states, in time $O(n^3)$ on a classical computer.

Runtime

We apply equation (8) k times and estimate the value of the resulting sum using a sampling algorithm. Similar to [6] we use Hoeffding's inequality to bound how far the sample mean is from the true probability. This leads to the dominant runtime scaling being due to the extent.

Estimation algorithm. *Let $\epsilon, \delta > 0$ be real numbers, and p be the Born-rule probability for a computational basis measurement outcome applied to an n qubit state constructed by applying a circuit of f FLO and c controlled-phase gates to an initial FLO state. Our algorithm returns a number $\hat{p}$ drawn from a probability distribution such that*

$$\Pr(|p - \hat{p}| > \epsilon) < \delta, \quad (11)$$

with the leading-order of the runtime given by

$$\tau = O\left(2\frac{(\sqrt{\xi^*} + \sqrt{p})^2}{(\sqrt{p+\epsilon} - \sqrt{p})^2}\log\left(\frac{2e^2}{\delta}\right)c(n+4c)^3\right) \le O\left(\frac{\xi^*}{\epsilon^2}\log\left(\frac{1}{\delta}\right)c(n+4c)^3\right), \quad (12)$$

where in the last expression we have used the upper bound $p \le 1$ and the series expansion for the denominator when ϵ is small.

In equation (12) the quantity ξ^* is the only super-polynomial contribution to the run-time. It is given by the product of the extents for all of the non-FLO gates. In figure 4 we compare the the contribution to the runtime (i.e. the extent) for our method, with the corresponding factor (the Fermionic negativity) from prior works [5, 3]. For us the worst-case CZ gate multiplies the runtime by 2, that of the prior work is multiplied by 9.

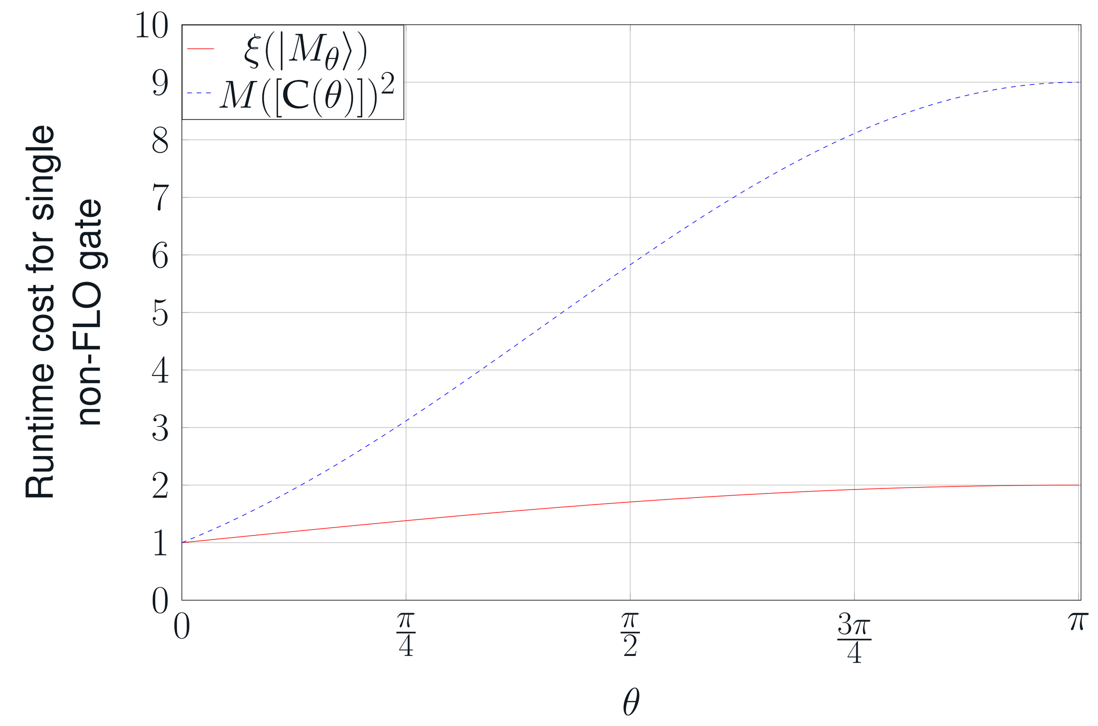

Figure 4: A comparison of the runtime cost of adding non-FLO controlled phase to a quantum circuit for our simulation method, and the algorithm of Ref. [3]. The notation $M([C(\theta)])$ indicates the Fermionic nonlinearity defined in that paper, computed for the channel $[C(\theta)] : \rho \mapsto C(\theta)\rho C(\theta)^\dagger$. The runtime reported Ref. [3] increases by a factor $M([C(\theta)])^2$ for each controlled-phase gate added while ours increases by a factor of $\xi(|M_\theta\rangle)$.

Conclusions & Outlook

We have developed phase sensitive classical simulation routines for the Fermionic linear optical subtheory. These allow us to estimate Born-rule probabilities for universal quantum circuits by decomposing states at the level of statevectors (rather than density operators) leading to an algorithm which is significantly faster than the prior state-of-the-art for this problem. In addition to exploring improvements, we are implementing our algorithm and seek to apply it to interesting (and useful!) simulation tasks.