Classical simulation of non-interacting fermion quantum circuits

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References:
- L. Valiant, Quantum Computers that can be simulated classically in polynomial time, STOC ’01.

Power of Quantum Computers

To understand the power of quantum computers, it is useful to understand when, -under what restrictions on the quantum circuit-, a quantum computer can be simulated efficiently by a classical device or is likely to be weaker than universal QC.

- Knill-Gottesman theorem
- Knill-Laflamme 1-qubit quantum computation:1 pure qubit+n completely noise ones, use regular unitary gates and measurement of $\sigma_z^{(1)}$
- Valiant’s class of quantum circuits ! Non-interacting fermion quantum circuits + measurements.

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Knill-Gottesman Theorem

A $n$-qubit quantum circuit consisting of gates which are elements of the Clifford $C_n$ and measurements in the computational basis (and outcomes can determine future gates), can be simulated in polynomial time on a classical device.

$P_n$: Pauli group on $n$ qubits: tensor products of Pauli-matrices $X, Y, Z$ and $I$ (with ±i signs).

$C_n$: Clifford group, generated by 2-qubit CNOT gate, 1-qubit Hadamard gate and 1-qubit $\pi/2$ phasemshift gate.

$$\forall U \in C_n, \forall M \in P_n, \text{ Normalizer}$$

$$\exists M' \in P_n : UMU^{-1} = M'$$

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Simulation

What does it mean to simulate a quantum circuit?

Be able to sample from the probability distribution that would arise as the result of any allowed measurement (after a sequence of allowed gates).

* (Not + in general)

Be able to compute the probabilities of measurement outcomes [conditioned on other outcomes] and then flip coins according to these probabilities.

+ Takes an efficient (polynomial in $n$) representation of the quantum state together with an efficient representation of the measurement.

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Valiant’s class of quantum circuits

Contains nearest-neighbour unitary gates of the form

\[
\begin{pmatrix}
U_{11}^{1} & 0 & 0 \\
0 & U_{21}^{2} & U_{12}^{2} \\
0 & U_{21}^{2} & U_{22}^{2}
\end{pmatrix}
\]

, where \( U^{1} \) and \( U^{2} \) \( \in \text{SU}(2) \).

(Measurements in computational basis)

- Interaction preserves parity of input bit-string.
- Is generated by Hamiltonian which is a linear combination of
  \( X_i \uparrow X_{i+1} \), \( Y_i \uparrow Y_{i+1} \), \( X_i \uparrow Y_{i+1} \), \( Y_i \uparrow X_{i+1} \), \( Z_i \uparrow I_{i+1} \) and \( I_i \uparrow Z_{i+1} \)

Valiant’s simulation via matchgates:
Gate (and circuit) represented by weighted graph. Input/Output of gate determines input/output vertices of graph. Entries in gate-matrix determined by perfect matchings of the graph.

Facts about universal QC

Hamiltonian which is a linear combination of

\( X_i \uparrow X_{i+1} \), \( Y_i \uparrow Y_{i+1} \), \( X_i \uparrow Y_{i+1} \), \( Y_i \uparrow X_{i+1} \), \( Z_i \uparrow I_{i+1} \) and \( I_i \uparrow Z_{i+1} \)

- \( X_i \uparrow X_j + Y_i \uparrow Y_j \) would give universal quantum computation!
- SWAP gate is not part of the Valiant class.
- \( X_i \uparrow X_{i+1} + Y_i \uparrow Y_{i+1} \) and arbitrary 1-qubit gates gives universal QC as well.

Jordan-Wigner transformation to fermion annihilation and creation operators.

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Non-interacting fermion circuits

Hamiltonian is a linear combination of terms that are quadratic in fermion annihilation and creation operators:
\[ a_i \equiv a_j \equiv a_i, \quad a_i a_j \equiv a_i a_j + a_j a_i \]

- Non-nearest neighbour fermion interactions.
- Also include measurements that determine whether a fermion is present or not and gates conditioned on these measurements.

For bosons such a circuit gives rise to full QC!

\[ a_i | x \rangle = 0, \quad \text{when } x_i = 0 \]
\[ a_i | x \rangle = (-1) \oplus x_i^l x_k | x_1 \ldots x_{i-1}, \bar{x}_i, x_{i+1} \ldots x_n \rangle \quad \text{when } x_i = 1 \]

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Fermion number preserving operations

Efficient representation of dynamics:
\[ U a_i U^{-1} = \sum_{k=1}^{n} V_{ik} a_k \]

Example:
Compute \( \langle y | U | x \rangle \) where \( x, y \) are bit-strings and \( U \) is a circuit corresponding to fermion number preserving operations

\[ | x \rangle = a_{i_1} \equiv a_{i_2} \equiv \ldots \equiv a_{i_k} \equiv | 0 \rangle \text{ etc.} \]
Use \( U | 0 \rangle = | 0 \rangle \), \( x \) and \( y \) same Hamming weight.

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Example continued

\[
\langle y | U | x \rangle = \sum_{m_1, m_2, \ldots, m_k} V_{m_1 \ldots m_k} 
\]

\[
\langle 0 | a_{j_k} \ldots a_{j_1} a_{m_1}^+ \ldots a_{m_k}^+ | 0 \rangle = 
\]

\[
\sum_{\pi} \text{sign}(\pi) V_{\pi(j_1)} \ldots V_{\pi(j_k)} = \det(V')
\]

Compute determinant of an, at most, \( n \times n \) matrix in time < \( n^3 \)

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Measurements

Simulate measurement on subset of qubits.

Evaluate the probability that some subset of the qubits is in a particular state, \( y^* = 10...0 \), given a starting state \( x = 0110.. \)

\[
p(y^* | x) = \langle x | U^{-1} a_{j_1} a_{j_1}^+ \ldots a_{j_k} a_{j_k}^+ U | x \rangle
\]

Write \( |x\rangle = a_{i_1}^+ a_{i_2}^+ \ldots \ldots a_{i_l}^+ |0\rangle \), use conjugation relation and use \( U|0\rangle = |0\rangle \).

Use Wick’s theorem to evaluate vacuum expectation value of sequence of annihilation and creation operators.

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The Pfaffian

$M$ is an anti-symmetric $2n \times 2n$ matrix. (If the dimension of $M$ is odd, Pf(M)=0).

$$Pf( M ) = \frac{1}{n!2^n} \sum_{\pi \in S_{2n}} \text{sign}(\pi)M_{\pi(1),\pi(2)} \cdots M_{\pi(2n-1),\pi(2n)}$$

$$Pf( M )^2 = \det(M)$$ Can be efficiently computed.

Graph with $2n$ vertices. Edges between vertex $i$ and $j$ ($i < j$) have weight $M_{ij}$. Pfaffian is sum of products of weights corresponding to perfect matchings of the graph. Each matching comes with a sign which is 1 if the number of crossings is even and $-1$ otherwise.

Example of odd # crossings: 1 2 3 4 9 10

Wick’s Theorem for fermions

$$\langle 0 | A_1 A_2 \cdots A_n | 0 \rangle = Pf( M )$$

$A_1 \ldots A_n$ fermion creation and annihilation operators.

$M$ is anti-symmetric. For $i < j$:

$$M_{ij} = A_i A_j \equiv A_i A_j - :A_i A_j:$$

contraction Normal ordered form

$$\langle 0 | : A_i A_j : | 0 \rangle = 0 \quad \text{Only non-zero contraction:}$$

$$a_i^+ a_j^+ = a_i a_j + a_j^+ a_i = \delta_{ij}$$
Putting things together

\[ p(y^* \mid x) = \langle x \mid U^{-1} a_i^+ a_{j_1}^+ \cdots a_{j_k}^+ a_j U \mid x \rangle = Pf(T) \]

\(|x\rangle = a_{i_1} a_{i_2}^* \cdots a_{i_j} \mid 0 \rangle\). Rewrite using conjugation relation and Wick's theorem. \(T\) is an anti-symmetric 2(k+1) x 2(k+1) matrix whose entries are determined by \(U\).

General quadratic interactions?

Majorana Fermions

For general quadratic interactions preserving the parity of fermion number we introduce Hermitian operators \(c_{2i} = a_i + a_i^+\), \(c_{2i+1} = -i(a_i - a_i^+)\). It can be shown that

\[ UC_i U^{-1} = \sum_{k=1}^{2n} R_{ik} c_k \]

\[ p(y^* \mid x) = \langle x \mid U^{-1} a_i^+ a_{j_1}^+ \cdots a_{j_k}^+ a_j U \mid x \rangle = Pf(T') \]

Use \(|x\rangle = c_{2i_1} c_{2i_2} \cdots c_{2i_l} \mid 0 \rangle\). Wick's theorem still applies by defining \(\bigotimes_{i} c_i c_j\).
Conditional Dynamics

Simulate non-interacting fermion circuit where the choice of gates can depend on outcomes of previous measurements in the computational basis. (Measured qubits are discarded.) Say, the first measurement has outcome $y_1^*$ and now we would like to simulate the next measurement, so we compute

$$p(y_2^*, y_1^*|x) = \text{Tr} \left( P(y_2^*) U_2(y_1^*) \rho U_2(y_1^*)^{-1} \right)$$

where $P()$ is a projector, $U_2()$ a conditional unitary evolution and $\rho$ is the (unnormalized) state after the first measurement:

$$\rho = P(y_1^*) U_1 |x><x| U_1^{-1} P(y_1^*)$$

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CD Continued...

Thus

$$p(y_2^*, y_1^*|x) = <x| U_1^{-1} P(y_1^*) U_2^{-1} P(y_2^*) U_2(y_1^*) P(y_1^*) U_1 |x>$$

- $P()$ is a sequence of annihilation and creation operators.
- Now, different sets of annihilation and creation operators will be conjugated by different unitary operators.
- The conditional probability can be expressed as a Pfaffian again.

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Discussion about Knill's results

Valiant's class of gates includes
(1) non-unitary gates on adjacent qubits (decoupled $|00>$, $|11>$ and $|01>$, $|10>$ block with determinant condition).
(2) more general gate on first 2 qubits obeying some identities.

Knill:
$\mathcal{L}_1$: set of linear combinations of annihilation/creation operators plus identity.
$\mathcal{G}_1$: Invertible matrices that preserve $\mathcal{L}_1$ by conjugation.
$\dagger$. Closure of $\mathcal{G}_1$ includes (1) gates of Valiant.

Take $\mathcal{L}_2 = \mathcal{L}_1 \mathcal{L}_1$. $\mathcal{G}_2$ is group of invertible matrices preserving $\mathcal{L}_2$ by conjugation.
$\mathcal{G}_2$ includes (unphysical) gates generated by terms linear in $a_i$ and $a_i^\dagger$.
$\dagger$. Closure of $\mathcal{G}_2$ includes (2) gates.

In fact, he shows that Closure of $\mathcal{G}_2 \sim$ Valiant's class \sim

Non-interacting Fermions + fermion number measurements

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A few comments about bosons

What is different for noninteracting bosons?

We still have an efficient representation of the dynamics

$$ Ua_iU^{-1} = \sum_{k=1}^{n} V_{ik} a_k $$

A quantity such as $\langle y | U | x \rangle$ will be the permanent of some matrix, due to the commutation relations for bosons. Is hard to compute efficiently.

No efficient representation of measurement: projector onto state with 0 or 1 boson (equals $aa^\dagger$ and $a^\dagger a$ for fermions) involves many terms with creation/annihiliation operators.

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