Embedding classical into quantum computation

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Abstract

We describe a simple formalism for generating classes of quantum circuits that are classically efficiently simulatable and show that the efficient simulation of Clifford circuits (Gottesman-Knill theorem) and of matchgate circuits (Valiant’s theorem) appear as two special cases. Viewing these simulatable classes as subsets of the space of all quantum computations, we may consider minimal extensions that suffice to regain full quantum computational power, which provides an approach to exploring the efficacy of quantum over classical computation.

1 Introduction

The characterisation of the possibilities and limitations of quantum computational power is one of the most interesting issues in quantum information science. All of the early and best known quantum algorithms [1] that exhibit an exponential time speed-up over any known classical algorithm for the task, utilize properties of the quantum Fourier transform modulo $N$. One may then develop generalisations of these insights, studying Fourier transforms over further abelian and non-abelian groups and invent associated computational tasks such as the hidden subgroup problem and various kinds of hidden shift problems. Around the years of 1997 and 1998 Thomas Beth, with memorable characteristic exuberance, was one of the earliest workers in the subject to recognise the potential possibilities of the abstract formalism of Fourier transforms for novel quantum algorithms, and take up this line of development which has now become an important cornerstone in our understanding.

Despite this seminal development it is probably fair to say that apart from the Fourier transform formalism, no other similarly fruitful quantum algorithmic primitive for exponential speed-up has been identified. This motivates a need for alternative approaches to exploring the efficacy of quantum vs. classical algorithms. One interesting such approach is the identification...
and study of classes of quantum computations that are classically efficiently simulatable i.e. processes which although quantum, do not offer computational benefit. Indeed the relation of classical to quantum computation that emerges is intriguingly rich and multi-faceted – (sub-) classical computation can be embedded into quantum computation in many inequivalent ways. Given any such class of simulatable quantum computations we may ask: what kind of added (minimal) ingredient suffices to restore full quantum computational power? In a sense, any such ingredient may be viewed as an “essence” of quantum computational power, albeit relative to a given substrate of simulatable processes. In this talk we will outline a formalism for providing simulatable classes of quantum circuits and discuss two examples – the Gottesman-Knill theorem for Clifford circuits and Valiant’s theorem for simulation of matchgate circuits. These examples will show that the added ingredient above can be strikingly trivial, especially if thought of as a competitor to the oft-quoted blanket attribution of quantum computational power to the enigmatic phenomenon of entanglement.

2 Classically simulatable quantum computations

We focus on comparing and contrasting two theorems of classical simulation viz. the Gottesman-Knill theorem for Clifford circuits [1, 9] and Valiant’s theorem [4, 2] for simulation of matchgate circuits. At first sight these appear to be very different in their content and provenance but we will outline a proof method that reveals a formal similarity between the two results.

The Gottesman-Knill (GK) theorem arose out of the development of the so-called stabiliser formalism for the theory of quantum error correction [1]. Let \( H \) denote the 1-qubit Hadamard gate, \( P \) the 1-qubit phase gate \( P = \text{diag}(1, i) \) and \( CZ \) the 2-qubit controlled-\( Z \) gate \( CZ = \text{diag}(1, 1, 1, -1) \). These gates and arbitrary circuits of them on \( n \) qubits are called Clifford operations on \( n \) qubits. Our adopted version (slightly modified from the original, c.f. also [3]) of the GK theorem is the following.

**Theorem 1** Consider any uniform (hence poly sized) quantum circuit family comprising the gates \( H, P \) and \( CZ \) (i.e. a Clifford circuit) such that:

(i) the input state is any product state;
(ii) the output is a final \( Z \) measurement on any single qubit line.

Then the output may be classically efficiently simulated.

More formally our notion of efficient classical simulation is the following:
given a description of the circuit on \( n \) qubit lines, the output probabilities may be classically computed to \( k \) digits in poly\((n, k)\) time.

Next we introduce the notion of “matchgate” and Valiant’s classical simulation theorem \[4\], which arose originally from considerations of counting perfect matchings in graphs.

A matchgate \[4, 2\] is defined to be any 2-qubit gate \( G(A, B) \) of the form (in the computational basis):

\[
G(A, B) = \begin{pmatrix}
p & 0 & 0 & q \\
0 & w & x & 0 \\
0 & y & z & 0 \\
r & 0 & 0 & s
\end{pmatrix}
\]

\[
A = \begin{pmatrix}
p & q \\
r & s
\end{pmatrix}
\]

\[
B = \begin{pmatrix}
w & x \\
y & z
\end{pmatrix}
\]

(1)

where \( A \) and \( B \) are both in \( SU(2) \) or both in \( U(2) \) with the same determinant. Thus the action of \( G(A, B) \) amounts to \( A \) acting in the even parity subspace (spanned by \( |00⟩ \) and \( |11⟩ \)) and \( B \) acting in the odd parity subspace (spanned by \( |01⟩ \) and \( |10⟩ \)).

Our version of Valiant’s theorem (again slightly different from the original version) is the following.

**Theorem 2** Consider any uniform (hence poly-sized) quantum circuit family comprising only \( G(A, B) \) gates such that:

(i) the \( G(A, B) \) gates act on nearest neighbour (n.n.) lines only;

(ii) the input state is any product state;

(iii) the output is a final measurement in the computational basis on any single line.

Then the output may be classically efficiently simulated.
having outputs 0,1 with probabilities \( p_0, p_1 \) respectively. Then the difference \( p_0 - p_1 \) is given by the expectation value of \( Z_1 = Z \otimes I \otimes \ldots \otimes I \) in the final state \( C |\psi_0\rangle \):

\[
p_0 - p_1 = \langle \psi_0 | C^\dagger Z_1 C |\psi_0\rangle
\]  

(2)

This computation suffices to simulate the output (as also \( p_0 + p_1 = 1 \)). Now \( Z_1 \) is clearly a product of Pauli operations so \( C^\dagger Z_1 C \) also has the product form \( P_1 \otimes \ldots \otimes P_n \) for Pauli operations \( P_i \) (whose identity can be determined in linear time by an update rule for successive conjugations by the elementary gates in the circuit). Hence if \( |\psi_0\rangle = |a_1\rangle \ldots |a_n\rangle \) is any product state we get

\[
p_0 - p_1 = \prod_{k=1}^{n} \langle a_k | P_k | a_k \rangle
\]  

(3)

which can clearly be calculated in time \( O(n) \) (as a product of \( n \) terms of fixed size) giving an efficient (linear time) simulation of the Clifford circuit.

The essential ingredients of the above proof are the following.

(SIM1): we have a set \( S_n \) of \( n \)-qubit operations such that \( \langle \psi_0 | S |\psi_0\rangle \) can be computed in \( \text{poly}(n) \) time for any \( S \in S_n \) and any allowed input state \( |\psi_0\rangle \);

(For the GK theorem \( S_n \) is the \( n \)-qubit Pauli group \( P_n \).)

(SIM2): we have a class \( K_n \) of unitary operations such that \( K^\dagger SK \in S_n \) for all \( S \in S_n \) and \( K \in K_n \).

(For the GK theorem \( K_n \) is the Clifford group \( C_n \).)

Then if \( Z_1 \) is in \( S_n \) for all \( n \) (or can be expressed in suitably simple terms using elements of \( S_n \), c.f. later) then it follows (just as in the above outlined proof) that circuits of gates from \( K_n \), with input state \( |\psi_0\rangle \) and output measurement of \( Z \) on the first line, can be classically efficiently simulated.

Note that this simulation result, resting on (SIM1) and (SIM2) does not actually require any special group (or other algebraic) structure on \( S_n \) or \( K_n \). For example, the fact that \( P_n \) is a group is not needed at all in our proof of the GK theorem in contrast to the usual proof resting on the stabiliser formalism, depending heavily on the subgroup structure of \( P_n \).

Turning now to matchgates we will show that Valiant’s theorem can be understood as just another example of the above formalism with a suitably clever choice of \( S_n \) and \( K_n \). For \( n \) qubits we introduce the \( 2n \) Pauli product operators (omitting tensor product symbols \( \otimes \) throughout):

\[
c_1 = XI \ldots I \quad c_3 = ZXI \ldots I \quad \cdots \quad c_{2k-1} = Z \ldots ZXI \ldots I \\
c_2 = Y I \ldots I \quad c_4 = ZYI \ldots I \quad \cdots \quad c_{2k} = Z \ldots ZYI \ldots I
\]  

(4)
where $X$ and $Y$ are in the $k^{\text{th}}$ slot for $c_{2k-1}$ and $c_{2k}$, and $k$ ranges from 1 to $n$. For $\mathcal{S}_n$, we take the linear span of $c_1, \ldots, c_{2n}$, which is a $2n$-dimensional vector space (in contrast to the group $\mathcal{P}_n$). Since each $c_j$ is a product operator and a general vector $v \in \mathcal{S}_n$ is a linear combination of only $2n$ of them, it is clear that $\langle \psi_0 | v | \psi_0 \rangle$ is poly($n$)-time computable if $| \psi_0 \rangle$ is a product state i.e. (SIM1) is satisfied.

Next we can verify by straightforward direct calculation that if $U$ is any n.n. $G(A,B)$ gate then $U^\dagger c_j U \in \mathcal{S}_n$ for all $j$ so $U^\dagger v U \in \mathcal{S}_n$ for any $v \in \mathcal{S}_n$ i.e. property (SIM2) is satisfied. More explicitly note that if $U$ is a n.n. $G(A,B)$ gate, it applies to two consecutive qubit lines so (from eq. (4)) the part of $c_j$ that it “sees” can only be one of

$$\alpha_1 = ZZ \quad \alpha_2 = ZX \quad \alpha_3 = ZY \quad \alpha_4 = XI \quad \alpha_5 = YI \quad \text{or} \quad \alpha_6 = II.$$ \hspace{1cm} (5)

Then a straightforward calculation with 4 by 4 matrices shows that for each $i$, $G(A,B)^\dagger \alpha_i G(A,B)$ always returns a linear combination of allowable $\alpha_i$’s and property (SIM2) follows immediately.

It is instructive to note that if we attempt to apply a $G(A,B)$ gate on not nearest-neighbour qubit lines then in addition to the six terms in eq. (5) we can get a further possibility, namely $\alpha_7 = ZI$ on the chosen two lines. But now we can check that $G(A,B)^\dagger \alpha_7 G(A,B)$ does not generally lie in the span of the allowed Pauli products at those lines, and property (SIM2) is violated. This gives a way of understanding the curious n.n. requirement for $G(A,B)$ actions in theorem 2 which has no analogue in the GK theorem (as $\mathcal{P}_n$ is defined by a uniformly local product requirement).

With properties (SIM1) and (SIM2) we can say that if $M$ is the total operation of any n.n. matchgate circuit on $n$ lines then $\langle \psi_0 | M^\dagger D M | \psi_0 \rangle$ is poly($n$)-time computable for any $D \in \mathcal{S}_n$. To complete our simulation theorem we want to set $D = Z_k = I \ldots I ZI \ldots I$ (i.e. $Z$ on the $k^{\text{th}}$ line) to obtain $p_0 - p_1$ for a measurement on the $k^{\text{th}}$ line. In the GK theorem with $\mathcal{S}_n = \mathcal{P}_n$ we had $Z_k \in \mathcal{P}_n$ directly. In the present case we do not have $Z_k \in \mathcal{S}_n$ but looking at eq. (4) we see that $Z_1 = -ic_1 c_2$ and generally $Z_k = -ic_{2k-1} c_{2k}$. Then, for example,

$$M^\dagger Z_1 M = -iM^\dagger c_1 c_2 M = -i(M^\dagger c_1 M)(M^\dagger c_2 M) \hspace{1cm} (6)$$

and each bracket in the last expression is a linear combination of $c_j$’s. Thus $p_0 - p_1 = \langle \psi_0 | M^\dagger Z_1 M | \psi_0 \rangle$ has the form $-i \sum_{i,j} a_i b_j \langle \psi_0 | c_i c_j | \psi_0 \rangle$. Since the $c_i$’s are product operators, so are the $O(n^2)$ product terms $c_i c_j$ in the final sum. Hence $p_0 - p_1$ is again poly($n$)-time computable but now we have $O(n^2)$ terms instead of the previous $O(n)$ terms in the sum. This completes a proof outline of Valiant’s theorem 2.
3 Extensions of simulatable circuits

We may now view Clifford circuits and matchgate circuits as two “islands” of quantum processes in the space of all quantum computations, that offer no computational time benefit over classical computations. As such, it is interesting to try to characterise their relationship to the whole and one approach is to consider what (minimal) extra ingredient suffices to expand their computational power to regain full universal efficient quantum computation.

In the case of Clifford circuits it is well known (e.g. see [1]) that the inclusion of the phase gate \( \sqrt{P} = \text{diag}(1, e^{i\pi/4}) \) suffices, and more generally, (using a result of Shi [10], noting that \( \text{CNOT} \) is a Clifford operation), the inclusion of essentially any single extra non-trivial 1-qubit gate will suffice.

For the case of matchgate circuits we have the following intriguing result.

**Theorem 3** Let \( C_n \) be any uniform family of quantum circuits with output given by a Z basis measurement on the first line. Then \( C_n \) may be simulated by a circuit of \( G(A,B) \) gates acting on n.n. or next n.n. lines only (i.e. on line pairs at most distance 2 apart) with at most a constant factor increase in the size of the circuit.

A proof of this theorem may be found in [2] and here we just make a few remarks. Comparing theorems 2 and 3 we see that the gap between classical and full quantum computational power can be bridged by a very modest use of a seemingly innocuous resource viz. the ability of matchgates to act on next n.n. – instead of just n.n. – qubit lines. Equivalently this may be characterised by use of the \( \text{SWAP} \) operation (on n.n. lines) in a very constrained context where ladders of consecutive \( \text{SWAPs} \) (which would allow 2-qubit gates to act on arbitrarily distant lines) are not even allowed. From this perspective, the power of quantum (over classical) computation is attributable to the mere inclusion of such isolated single \( \text{SWAP} \) gates. The result becomes perhaps even more striking if we note that \( \text{SWAP} \) itself is very close to being expressible in the allowed \( G(A,B) \) form. Indeed \( \text{SWAP} = G(I,X) \) and fails only through a mere minus sign in \( \det X = -\det I \). Thus if we drop the \( \det A = \det B \) condition in eq. [1], then the resulting \( G(A,B) \) gates acting on n.n. lines become efficiently universal for quantum computation.

Is it conceivable that the passage from n.n. to next-n.n. use of \( G(A,B) \) gates may be achieved while maintaining classical simulatability? We may argue on formal complexity theoretic grounds that this is highly implausible.
Indeed it is shown in [2] that the classical complexity classes NP and PP (cf. [7]) would then become classically poly-time decidable i.e. we would get $P=NP=PP$ (as well as $P=BQP$). Thus an extra supra-classical computational power must be associated to the single distance extension of the range of n.n. 2-qubit $G(A,B)$ gates in general matchgate circuits, if these classical computational complexity classes are to be unequal.

4 Concluding remarks

From the viewpoint of (SIM1) and (SIM2) we see a formal similarity between the GK theorem and Valiant’s theorem although these results arose historically from very different considerations. This suggests that we might be able to construct further interesting classes of classically simulatable circuits by simply taking other choices of $S_n$ and identifying a suitable associated $K_n$. However “interesting” pairs $(S_n, K_n)$ appear to be difficult to invent – the known examples arising as outcomes of some prior elaborate underlying mathematical structures. In the GK case we have the identification of the Clifford group via a lengthy argument with group theoretic ingredients (see e.g. appendix in [11]) applied to the Pauli group $P_n$ which is a well known structure in the subject.

However in the case of Valiant’s theorem, how might we initially come upon this result, and guess the choice for $S_n$ that we used (i.e. eq. (4) and its linear span)!? Actually the operators in eq. (4) are well known in physics – they comprise the so-called Jordan-Wigner representation [8] that appears in the theory of non-interacting fermions. The connection between Valiant’s theorem and simulation of free fermions was recognised by Knill [5] and Terhal and DiVincenzo [6] and our proof of Valiant’s theorem above is a re-writing of this connection. A more formal mathematical treatment (albeit without reference to fermions) based on abstract properties of the mathematical structure of Clifford algebras is given in [2] which also clarifies the appearance of matchgates as normalisers of the linear part of the Clifford algebra, leading to property (SIM2). We will not elaborate here on these further ingredients (detailed in [2]) except to point out that again here, we have a significant underlying theory leading to the choice of $S_n$ and the identification of its associated normalisers $K_n$. Perhaps an intuitive signal feature of such an underlying theory is some construction that could potentially produce an exponentially large structure but surprisingly remains only polynomially complex. In the case of the Pauli group $P_n$, conjugation by arbitrary $V \in U(2^n)$ can generate general $n$-qubit matrices for which
the calculation of the expectation value in eq. (2) becomes exponentially inefficient. But the special case of \( V \) being Clifford guarantees a polynomial simplicity via the preserved product structure. In the case of the \( c_i \)'s of eq. (4), conjugation by an arbitrary \( V \in U(2^n) \) leads to a general element of the full Clifford algebra generated by the the \( c_i \)'s – a space of exponential dimension \( 2^{2n} \) – but again the special case of n.n. matchgates (associated to a theory of quadratic hamiltonians \([2]\)) guarantees that the conjugates remain in the polynomially small subspace of linear elements of the full Clifford algebra. It is an interesting open problem to exhibit further examples of such simplifications and of our formalism (SIM1), (SIM2), that may already exist within the literature of the theory of some yet more general kind of algebraic structure.

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