Classical simulability and the significance of modular exponentiation in Shor’s algorithm

Nadav Yoran\(^1\) and Anthony J. Short\(^1\)

\(^1\)H.H.Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

We show that a classical algorithm efficiently simulating the modular exponentiation circuit, for certain product state input and with measurements in a general product state basis at the output, can efficiently simulate Shor’s factoring algorithm. This is done by using the notion of the semi-classical Fourier transform due to Griffith and Niu, and further discussed in the context of Shor’s algorithm by Browne.

The most celebrated quantum algorithm to date is undoubtedly Shor’s factoring algorithm. Distilling the crucial elements in this algorithm which allow for the (assumed) speed-up it exhibits, may lead to a better understanding of the power of quantum computation in general. Shor’s algorithm has two main components: modular exponentiation, and the quantum Fourier transform (QFT). Of the two the first is basically a classical circuit employing classical gates (manipulating computational basis states). The only quantum aspect of this circuit is that it maintains quantum coherence, i.e. it can act on a superposition of classical inputs and yields the corresponding superposition of classical outputs. The QFT on the other hand uses gates that have no classical equivalents, such as conditional phase and Hadamard gates, and is considered as the truly quantum component of the algorithm. The QFT is a key component not only in Shor’s algorithm but also in several related quantum algorithms such as phase estimation and discrete logarithm.

Yet, it was recently demonstrated\(^1\)\(^2\) that an approximate quantum fourier transform (which can be used in Shor’s algorithm\(^3\)) can be efficiently classically simulated using tensor contraction methods. This was shown for any product input state and product state measurements on the output, and furthermore for a class of entangled states\(^2\) (as input or as basis for output measurements). This seems to indicate that the computational power of Shor’s algorithm lies with the modular exponentiation circuit. Here, we demonstrate that this is indeed the case by the following simple observation: Any classical algorithm that can efficiently simulate the circuit implementing modular exponentiation for general product input states and product state measurements on the output, allows for an efficient simulation of the entire Shor algorithm on a classical computer. In other words the power of Shor’s algorithm lies in the ability to implement the classical modular exponentiation operation on a certain product state input and with measurements in a general product state basis.

The above result is also true for any circuit that can replace the modular exponentiation in the overall quantum circuit for Shor’s algorithm (Fig. 1). For instance, the multiplication operations used in the log-depth version of the (quantum part of) Shor’s algorithm due to Cleve and Watrous\(^4\).

A particular method for classically simulating quantum circuits, in which general product input and output states are automatically taken into account, is tensor contraction\(^5\)\(^6\). Therefore, Our observation implies that any tensor contraction scheme that efficiently simulates modular exponentiation would be able to simulate Shor’s factoring algorithm efficiently.

Let us first describe in exact terms what we consider as a simulation of a quantum circuit for product input states and product state measurements. For a given quantum circuit let us denote a set of (general) single qubit measurements on the output by \(M_1, \ldots, M_n\), their corresponding sets of possible outcomes by \((m_1, \ldots, m_n)\) and some specific outcomes of these measurements by \((r_1, \ldots, r_n)\). We say that a quantum circuit can be efficiently simulated by a classical computer for product state input and product state measurements if for any such set of single qubit measurements and any product state input there is an efficient classical algorithm for calculating the conditional probabilities:

\[
P(m_i | r_{j_1}, \ldots, r_{j_k})
\]

where the indices \(j_1, \ldots, j_k\) correspond to any subset of the measurements \((M_1, \ldots, M_n)\) including the empty set. (Of course, there are exponentially many such conditional probabilities, one for each value of the bit-string \(r_{j_1}, \ldots, r_{j_k}\), therefore there is no way to efficiently calculate all of them; however, we only require that each particular conditional probability can be calculated efficiently.) Sampling from these conditional probabilities qubit by qubit one is able, using the classical algorithm, to obtain a final outcome with the same probability as it would have been obtained by the quantum computer.

Our definition above for a simulation of a quantum circuit is similar to the ‘density computation of quantum circuit’ given by Terhal and DiVincenzo\(^7\). The difference being the fact that here we allow general product state input and product state measurements at the output, whereas in the weaker density computation only computational basis input and measurements in the computational basis at the output are permitted.

The quantum part of Shor’s algorithm, where we wish to factor an \(n\) qubit integer \(N\), is composed of the fol-
FIG. 1: The quantum circuit for Shor’s algorithm. The empty triangles on the left side represent the computational basis input state the shaded triangles on the right represent measurements in the computational basis and the boxes denoted by H stand for Hadamard gates. The QFT together with the output measurements can be replaced by the semi-classical circuit in Fig. 2.

The following steps (Fig. 1).

1. Initialize two registers, the first with 2n qubits and the second with n qubits, in the state $|0\rangle_1|0\rangle_2$.

2. Apply a Hadamard gate on each of the qubits of register 1. the state of the computer would now be:

$$|+\rangle\cdots|+\rangle|0\rangle_2 = \sum_{x=0}^{2^n-1} |x\rangle_1|0\rangle_2,$$  

where $|+\rangle = 1/\sqrt{2}(|0\rangle + |1\rangle)$.

3. Apply modular exponentiation. Namely, apply the unitary operation:

$$|x\rangle_1|0\rangle_2 \rightarrow |x\rangle_1|a^x \mod N\rangle_2,$$  

where $a$ is a randomly chosen number ($a < N$) co-prime with $N$.

4. Apply a QFT on the first register.

5. Measure the first register in the computational basis.

In order to prove our result above we make use of the following fact, first demonstrated by Griffith and Niu [8]: The QFT circuit followed by measurements in the computational basis can always be replaced by a ‘semi-classical’ QFT circuit which includes only single qubit gates, measurements in the computational basis, and feed-forward (without any two qubit gates). Griffith and Niu observed that when a controlled unitary is immediately followed by a measurement in the computational basis on the control qubit, the gate operation can be implemented by first measuring the control qubit and then applying a gate on the second qubit according to the outcome (that is, the gate would only be applied if the control is measured in the required state). In Shor’s algorithm the QFT is immediately followed by measurements in the computational basis (see [10] for example) therefore it can be replaced by the semi-classical circuit (shown in Fig. 2).

Browne [9] used the semi-classical QFT to show that in the case where the modular exponentiation circuit together with Hadamard gates at the input does not produce much entanglement, and therefore can be simulated classically [11, 12]. Shor’s algorithm can be efficiently simulated as well (typically modular exponentiation does produce highly entangled states [11], however there may be special cases for which it does not).

Let us now assume that the modular exponentiation circuit can be simulated efficiently when the input is a direct product and the output is subjected to single qubit measurements. Our simulation of Shor’s algorithm proceeds via an iterative procedure as follows:

1. First, we calculate the probabilities $P_{Shor}(m_1)$ for a measurement on the first qubit (in the first register) in Shor’s algorithm. From our assumption it follows that these probabilities can be efficiently calculated. Indeed, in the Shor circuit with the semi-classical QFT (which obviously produces the same output as the original Shor algorithm) the measurement of the first qubit in the computational basis at the output of the semi-classical QFT is nothing else than a single qubit measurement of the output of the modular exponentiation. (More precisely, it is the measurement of the first qubit of the output of the modular exponentiation in the Hadamard transformed basis.) Furthermore, the input state into the modular exponentiation is a direct product state (the state $(|+\rangle\cdots|+\rangle)|0\rangle_2$) so the conditions in our assumption apply.

2. We sample from the distribution $P_{Shor}(m_1)$. Let $r_1$ be the result of this sampling.
3. We calculate the conditional probabilities 
\[ P_{\text{Shor}}(m_2|r_1) \]
for the measurement on the second 
qubit in Shor’s algorithm, given the outcome \( r_1 \) for the first qubit.

Again, from our assumption it follows that these 
probabilities can be efficiently calculated. Once
the output \( r_1 \) of the first qubit is fixed, we know
what is the feed-forward from the first qubit in the
semi-classical QFT. With this knowledge, the mea-
surement in the computational basis of the second
qubit in the circuit for Shor’s algorithm becomes
a well-defined measurement on the second qubit of
the output of the modular exponentiation circuit.

4. We repeat steps (2) and (3) for \( i = 2, \ldots, 2n \). That
is in the next step we sample from the conditional
probability distribution 
\[ P_{\text{Shor}}(m_2|r_1) \]
and obtain 
outcome \( r_2 \), and in general we calculate and then
sample from
\[ P_{\text{Shor}}(m_i|r_1, \ldots, r_{i-1}) \] for \( 2 \leq i \leq 2n \),
where the basis for the measurement \( m_i \) is set ac-
cording to the outcomes of previous measurements
\( r_1, \ldots, r_{i-1} \).

At the end of the process an outcome \( (r_1, \ldots, r_{2n}) \) is ob-
tained with the same probability it would have been ob-
tained by measuring the output of the quantum circuit
implementing Shor’s algorithm.

Clearly, for the purpose of simulating the Shor al-
gorithm it is enough to consider only one input state
(Eq. 2). (Note that we could not simply redefine this as
a new computational basis state \( |0'\rangle \) if we do not want
to change the modular exponentiation circuit.) For
the output measurements, however, we need to take into ac-
count every possible phase gate. It was noted by Browne
that if we consider the above input state but allow out-
put measurements only in the computational basis, then
the modular exponentiation circuit can be simulated ef-
ficiently. In the same way it is not hard to see that if one
considers only computational basis input states and al-
 lows any product state measurement at the output, then
the circuit would be simulable as well. Thus, in some
sense, our requirements are the minimal ones with which
quantum advantage is achieved.

Consider now a tensor contraction method for simula-
tion. In these methods one associates tensors to
circuit elements – one and two qubit gates, single-qubit
input and output states. The latter may correspond to
outcomes of single qubit measurements or to unmeasured
output qubits. The rank of the tensors is determined by
the number of (input and output) qubits on which the
circuit element operates. That is, the tensor has an in-
dex for each input or output wire connected to the circuit
element. Thus, for an input state or an output measure-
ment correspond to tensors of rank one, single-qubit gates
correspond to rank two tensors and two-qubit gates are
represented by rank four tensors. Two circuit elements
connected by a qubit wire (the output of one is the input
of the other) share a joint index. A probability for obtaining
a certain outcome at one or more output qubits can be
calculated by contracting (summing over all indices of)
all tensors representing the circuit with the appropriate
configuration at the outputs (tensors corresponding to
the required outcomes for the measured qubits and ten-
sors corresponding to unmeasured qubits for the rest).
The problem with such a contraction process is that the
number of terms is exponentially large. To avoid this, the
tensors are contracted one at a time breaking the overall
sum to a series of separate sums, where in each step two
existing tensors are replaced with a new tensor obtained
by summing over joint indices. For instance, summing
over a joint index of a pair of two qubit gates connected
by a single qubit wire one obtains a tensor of rank six
(e.g. \( T_{ij}^{kl}T_{lm} \rightarrow T_{ij}^{kno} \)). A tensor contraction simulation
is efficient (i.e. can be implemented in polynomial time)
if the tensors generated in the procedure have at most
\[ O(\log n) \] indices.

The only factor which determines the complexity of
a contraction process of a given quantum circuit is its
topology. The type of gates or their actual operation
on the input (beyond the fact that it is linear) is irre-
levant. furthermore rank one tensors, representing the
input and output elements, and rank two tensors corre-
sponding to single-qubit gates, do not affect the topology
of the circuit and therefore do not affect the efficiency of
the simulation. For example, these tensors can be in-
corporated into tensors of neighbouring elements by con-
tracting them together at the first stage of the simulation.
This produces new tensors with the same number of in-
dices as the original neighbouring tensor (in the case of
one-qubit gates) or less (in the case of input or output
elements) without changing the graph of connections of
the circuit.

From our discussion above it is clear that a tensor con-
traction simulation for a given quantum circuit with a
certain set of input and output elements would also work
for any other set of input states and output measure-
ments as long as these are single qubit states and mea-
surements. Thus, a tensor contraction algorithm simu-
lating the modular exponentiation would also be able to
simulate Shor’s factoring algorithm. Note that this im-
plies that it is unlikely that a tensor contraction scheme
would be able to efficiently compute modular exponenti-
ation even for ‘classical’ computational basis input and
output states, a task which obviously can be done by
other classical algorithms.

So far we have discussed only modular exponentiation.
However from our method of simulation it is clear that
any quantum circuit with the same structure (as in Fig. 1),
where the modular exponentiation is replaced by some
other unitary operation \( U \), can be simulated efficiently on
a classical computer if $U$ is efficiently simulable for product state input states and measurements, and in particular if $U$ has an efficient tensor contraction scheme.

The authors wish to thank S. Popescu, D. E. Browne and D. J. Shepherd for fruitful discussions. The work of N. Y. was supported by UK EPSRC grant (GR/527405/01), and A.J.S. was supported by the UK EPSRC’s “QIP IRC” project.

---

* Electronic address: N.Yoran@bristol.ac.uk

[1] D. Aharonov, Z. Landau, J. Makowsky, quant-ph/0611156

[2] N. Yoran and A. J. Short, quant-ph/0611241

[3] D. Coppersmith, IBM research report RC 19642 (1994).
[4] R. Cleve and J. Watrous, 41st Annual Symposium on Foundations of Computer Science 526 (2000).
[5] I. Markov and Y. Shi, quant-ph/0511069
[6] M. Van den Nest, W. Dr, G. Vidal, H. J. Briegel, quant-ph/0608060
[7] B. Terhal and D. DiVincenzo, quant-ph/0205133
[8] R. B. Griffith and C. -S. Niu, Phys. Rev. Lett. 76, 3228 (1996).
[9] D. E. Browne, quant-ph/0612021.
[10] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000).
[11] R. Jozsa and N. Linden, Proc. Royal Soc. A 459, 2011 (2003).
[12] G. Vidal, Phys. Rev. Lett. 91, 14062 (2003).