Quantum information theory (20110401)
Lecturer: Jens Eisert
Chapter 12: Non-universal quantum computers

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Chapter 12

Non-universal quantum computers

12.1 Quantum simulators

So far, we have discussed universal quantum computers. But then, quantum computers as we have them are not quite universal. They are smallish, have limited control, and are noisy. One speaks of noisy intermediate scale quantum (NISQ) devices. What can such devices do? The answer to this is not quite known, but we have a look at some aspects thereof. The first application is that of a quantum simulation. Quantum simulators come in several flavours. One distinguishes *static quantum simulators* probing static such as ground state properties from *dynamical quantum simulators*. The latter probe dynamical properties that can be probed in a time evolution of the type

$$\langle O(t)\rangle = \mathrm{tr}(e^{-itH}\rho(0)e^{itH}O), \tag{12.1}$$

where

$$H = \sum_{j=1}^{N} h_j \tag{12.2}$$

is typically a *local Hamiltonian* acting on a lattice involving n sites of local dimension d, equipped with a Hilbert space $\mathcal{H} = (\mathbb{C}^d)^{\otimes N}$. Local here means that each of the terms $\{h_j\}$ acts on a small number of sites only, usually nearest neighbours. The observable O is commonly local as well, such as a local Pauli matrix, say, $O = Z$ acting on a single site. We have seen that local Hamiltonian evolution is in principle BQP complete, so one can think of quantum computation in this fashion. But this is not how one usually thinks about such quantum simulators. Instead, one is interested in learning properties of strongly correlated quantum systems, beyond classical capabilities.

12.1.1 Analog quantum simulators

In *analog quantum simulation*, one recreates, mimicks, the exact Hamiltonian of the original system, but under precisely controlled conditions. This is much less of a ridiculous idea than it may first appear. In fact, in systems of cold atoms in optical lattices or with trapped ions one can recreate interacting systems very precisely, and also probe them in the laboratory. The fact that time evolution is BQP complete here comes in as an advantage: One cannot devise universal classical simulation algorithms of quantum dynamics. Therefore, classical simulation algorithms such as quantum Monte Carlo Methods, density functional theory or tensor network methods soon reach their limitations. But analog quantum simulators do not face such restrictions. This is an enormously interesting field of research.

12.1.2 Digital quantum simulators

Digital quantum simulators require basically quantum computers. In the dynamical reading, one slices time evolution into stroboscopic time slices and approximates the continuous time evolution by a number of small time evolution steps approximated by a gate-based quantum computer. The formula at the heart of the matter is here the *Trotter formula*.

Trotter formula: For any two Hermitian operators A and B, one has

$$e^{A+B} = \lim_{n\to\infty} \left(e^{A/n} e^{B/n}\right)^n. \tag{12.3}$$

This can be made a functioning quantum algorithm. For two Hamiltonian terms H_1 and H_2, with $\|H_1\| \leq K$ and $\|H_2\| \leq K$ one has

$$e^{-iH_1} e^{-iH_2)} = e^{-i(H_1+H_2)} + \mathcal{O}(K^2). \tag{12.4}$$

Pushing this idea further, for local terms $h_1, \ldots, h_n$ of a Hamiltonian

$$H = \sum_{j=1}^{N} h_j \tag{12.5}$$

one finds

$$e^{-ih_1} \ldots e^{-ih_n)} = e^{-i(h_1+h_2+\cdots+h_n)} + \mathcal{O}(n^3 K^2), \tag{12.6}$$

if for all j, $\|h_j\| \leq K$. For a constant $C > 0$ such that the number of steps is lower bounded as

$$n > CN^3 (Kt)^2/\epsilon, \tag{12.7}$$

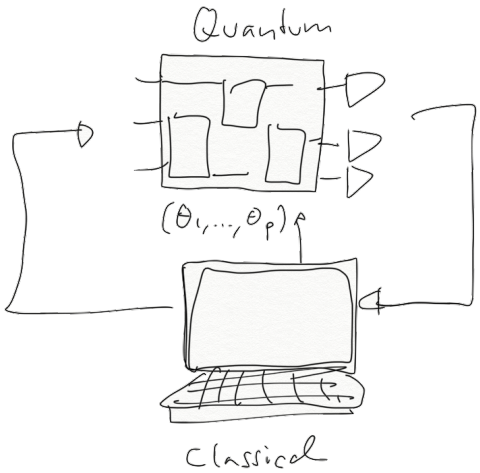
one has

$$\|(e^{-ih_1 t/n} \ldots e^{-ih_N t/n})^2 - e^{-iHt}\| \leq \epsilon. \tag{12.8}$$

This gives rise to an algorithm to approximate continuous time evolution of local Hamiltonians with an effort of $\mathcal{O}(\mathrm{polylog}(N)(\|H\|t)^2/\epsilon)$: The time evolution is slices

into pieces that can be gate decomposed on a quantum computer. This is the most basic of all digital quantum simulation schemes. It has been further developed into higher order schemes that have a favourable error scaling, linear combination of unitaries approaches, an idea called qubitization and randomized schemes. It is a flourishing topic of research still.

12.2 Variational quantum computers



12.2.1 Variational quantum eigensolvers

Quantum computers exist, with system sizes up to $N = 72$ qubits. This is too little to perform the Shor algorithm for reasonable system sizes including quantum error correction. But is still good enough to tackle interesting problem. One such approach is to use quantum computers in *hybrid algorithms* in which a quantum computer is only a part of a larger classical algorithm. This classical algorithm takes data from measurements from the quantum circuits, alters the control parameters and accordingly prepares states and alters the variational quantum circuits along the way. The quantum part at the heart of the algorithm is a short quantum circuit

$$(\theta) := (\theta_1, \ldots, \theta_p) \mapsto U(\theta_1, \ldots, \theta_p) \tag{12.9}$$

defined by real variational parameters $(\theta_1, \ldots, \theta_p)$. In variational quantum eigensolvers, one hence basically solves the following problem.

Variational quantum eigensolvers: They aim at approximately finding a solution to

$$E_{\min} = \min\langle\psi(\theta)|H|\psi(\theta)\rangle, \tag{12.10}$$

where

$$|\psi(\theta)\rangle := U(\theta_1, \ldots, \theta_p)|0, \ldots, 0\rangle. \tag{12.11}$$

This may look like a simpler an enterprise that it actually is in practice. After all, one has to find good variational sets so that one can expect a good approximation in the first place. This is not obvious, and one has to find a good compromise between expressivity and depth of the involved circuits. This applies, e.g., to problems in quantum chemistry where one has to find good representations to start with. Then, one has to find strategies of finding good updates

$$(\theta_1, \ldots, \theta_p) \mapsto (\theta_1', \ldots, \theta_p'). \tag{12.12}$$

Indeed, one can estimate gradients by taking measurements and performing updates based on that. Using ideas such as *parameter shift rules* help reducing the number of expectation values one needs to measure to find good updates.

12.2.2 Quantum approximate optimization algorithm

Quantum approximate optimization goes a step further. It aims at finding good approximations to combinatorical optimization problems, such as `MaxCUT`. Such problems are often `NP`-hard in worst case complexity. Still, one hopes to find good approximations with quantum algorithms. The goal is to find an approximate solution to a cost function

$$f : \{0,1\}^n \to \mathbb{R}_0^+. \tag{12.13}$$

Such a cost function can be encoded in a Hamiltonian H_f , so that finding the maximum of f amounts to finding the ground state energy

$$E_{\min} := \min\langle\psi|H_f|\psi\rangle, \tag{12.14}$$

of H_f over all quantum states. One aims at finding a binary string that achieves an approximation ratio r for

$$\frac{f(z)}{f_{\max}} \geq r \tag{12.15}$$

for all $z \in \{0,1\}^n$, for the optimal solution being

$$f_{\max} := \max_{z\in\{0,1\}^n} f(z). \tag{12.16}$$

One does not expect to get an exact solution: The problem being `NP`-hard in worst case complexity means that an exact solution is also out of reach for a quantum computer.

But one aims at realizing an approximate solution. This is achieved by initially preparing a product state described by a state vector $|+\rangle^{\otimes N}$ and by applying a sequence of steps

$$e^{-i\gamma_j H_f} \tag{12.17}$$

for $j = 1, \ldots, p$, implementing the encoding Hamiltonian, followed by products of local Pauli X rotations

$$(e^{-i\beta_j X})^{\otimes N}, \tag{12.18}$$

that "kick the state out of the Pauli-Z basis". At the end of the day, after p steps, this sequence is followed by an estimation of the expectation value $\langle H_f \rangle$ by virtue of repeated measurements. The variational parameters $(\gamma_1, \ldots, \gamma_p, \beta_1, \ldots, \beta_p)$ are optimized to minimize $\langle H_f \rangle$. The entire state vector before the measurement is hence

$$(e^{-i\beta_p X})^{\otimes N} e^{-i\gamma_p H_f} \ldots (e^{-i\beta_1 X})^{\otimes N} e^{-i\gamma_1 H_f} |+\rangle^{\otimes N}. \tag{12.19}$$

The variational parameters are again chosen using similar strategies as above. Similar issues of expressivity and classical control appear as well. This algorithm is called *quantum approximate optimization algorithm*. It is much studied, for good reason. At the same time, there is evidence that with too short circuits, no quantum speedup can be attained. Since one cannot expect an exact solution, people are also deeply concerned with what improvements one can precisely expect over classical algorithms. One has to be aware of the fact that one can also find good classical efficient approximations, for example, by so-called convex relaxations of the original combinatorical problem.

12.2.3 Closing remarks

These are highly interesting and exploratory fields that receive a lot of attention. Similar ideas are being considered in *quantum-assisted machine learning*. At the end of the day, the key question is to what extent one can realize a quantum advantage, so in what way such near-term algorithms can achieve computational tasks outperforming classical algorithms for the same task.