Quantum Computation, Quantum Algorithms and Implications on Data Science

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Abstract
Quantum computing is a new revolutionary computing paradigm, first theorized in 1981. It is based on quantum physics and quantum mechanics, which are fundamentally stochastic in nature with inherent randomness and uncertainty. The power of quantum computing relies on three properties of a quantum bit: superposition, entanglement, and interference. Quantum algorithms are described by the quantum circuits, and they are expected to solve decision problems, functional problems, oracular problems, sampling tasks and optimization problems so much faster than the classical silicon-based computers. They are expected to have a tremendous impact on the current Big Data technology, machine learning and artificial intelligence. Despite the theoretical and physical advancements, there are still several technological barriers for successful applications of quantum computation. In this work, we review the current state of quantum computation and quantum algorithms, and discuss their implications on the practice of Data Science in the near future. There is no doubt that quantum computing will accelerate the process of scientific discoveries and industrial advancements, having a transformative impact on our society.

Key Words: artificial intelligence, data science, machine learning, quantum algorithms, quantum computation, quantum information

1. Quantum Computing

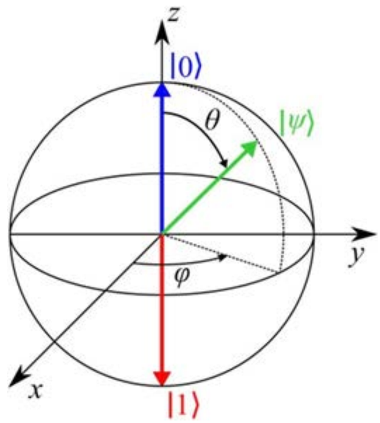
Quantum computing is a new revolutionary computing paradigm. The quantum Turing machine was first theorized at Argonne National Laboratory in 1981, opening the era of post Moore's Law beyond silicon-based computer. The basic building block of quantum computing is quantum bit (**qubit**), which has inherent randomness and uncertainty due to the fundamental *stochastics*; see Wang (2012). Based on the quantum physics and the quantum mechanics, a pure state of a quantum system is given by a unit vector $|\psi\rangle$ in a complex Hilbert space, and the time evolution of a state is generated by Hamiltonian H according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \quad \leftrightarrow \quad |\psi(t)\rangle = e^{-iH/\hbar}|\psi(0)\rangle$$

with the Planck constant $\hbar$ and the imaginary number $i = \sqrt{-1}$. It is noted that the structure of composite systems is given by tensor products, and the projective measurements (*observables*) are according to non-degenerate Hermitian operators. Importantly, the measurement process changes the observed system from state $|\psi\rangle$ to eigenstate $|\phi(t)\rangle$ with probability $p(\phi) = |\langle\psi|\phi\rangle|^2$ by the Born rule; see Nielsen and Chuang (2010).

2. Three Aspects of Quantum Computing

The power of quantum computing relies on the following three properties of a quantum bit.



- **Superposition:** Any state can be represented by $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$ where $|\alpha_0|^2 + |\alpha_1|^2 = 1,\ \alpha_i \in C$; see Figure 1. This enables a natural *parallelism* in computing.
- **Entanglement:** This property enables the *indirect measurement* preserving the system's integrity.
- **Interference:** The quantum inference can be constructive or destructive. It enables speedy processing of Big Data.

Figure 1: Bloch sphere representation of a qubit

3. Quantum Algorithms

The quantum algorithms are described by the quantum *circuits*, and they are solving or expected to solve many crucial problems such as

- *genuine* random number generation;
- quantum random walks to speed up stochastic diffusion processes;
- quantum Fourier transformation, quantum phase estimation;
- Shor's factoring algorithm; see Shor (1997);
- Grover's search/sort algorithm; see Grover (1997);
- quantum state tomography (density matrix); see Gross et al. (2010);
- quantum Monte Carlo integration, Monte Carlo simulation, quantum MCMC; see Wang et al. (2016).

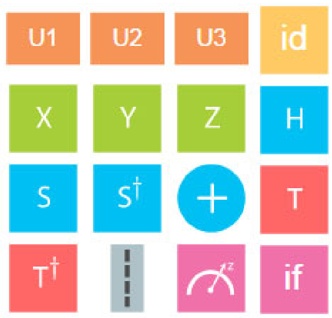
Quantum algorithms speed up solving decision problems, functional problems, *oracular* problems, sampling tasks and optimization problems so much faster than the classical silicon-based computers; see Wang et al. (2016). They are expected to have a tremendous impact on the current Big Data technology, machine learning and artificial intelligence.

- Quantum algorithms speed up **Machine Learning (ML)** with **Big Data**.
  - They often rely on quantum annealers for learning-type problems.
  - Quantum *Simulated Annealing* (SA) for the NP-hard problems has been developed; for example, Ising model to minimize (Hamiltonian) energy, given coupling and local field; see Wang et al. (2016).
  - Quantum *Principal Component Analysis* (qPCA)
  - Quantum *Support Vector Machines* (qSVM)
- Quantum algorithms speed up **Artificial Intelligence (AI)**.

  - They can search all possible solutions at the same time, and then collapse the output to the most probable solution.
  - They provide faster training and update of *neural networks* by estimating the weights instantly; see Dunjko and Briegel (2018).
  - Quantum *Reinforcement Learning* (qRL) based on PO-MDP
  - They can assist in the design and evaluation of the agents and environments interactions; see Dunjko and Briegel (2018).

As aforementioned, the quantum computation and quantum technologies are expected to have a tremendous impact on the current practice of Data Science, leading to the super-duper-exponential learning*!!*

4. Quantum Information



With the principle of quantum information, it is aimed to design the target quantum evolutions, including the quantum gate design, as it is necessary to find the optimal control functions or the extended system parameters; see Figure 2. This problem is non-convex and very difficult to do. Perhaps one could utilize the online learning and reinforcement learning (RL).

Figure 2: Quantum gates of IBM Q

5. Current Development

Currently, researchers are working on to develop quantum computers with more qubits. The *quantum volume* has been increasing (more than doubling) each year; see Figure 3 below. At the present, Google 72 qubit processor is the chip with most qubits while D-Wave with 2,000 qubits ($15 million) is the computer with most qubits. Researchers are also developing a broad library of functions (*circuits*) for various research problems; see Bravyi et al. (2018). This has been considered particularly important as IBM started providing a public cloud service for quantum computing.

6. Technical Barriers

Despite the theoretical and physical advancements, there still remain several technological barriers for successful applications of quantum computation. They include

- the operatability of quantum computers at temperatures far above 0 K, preferably at room temperature;
  - The current operation of quantum computers requires near 0 K with the use of liquid nitrogen or helium. This severely limits its broad usage.
- better error correction to put more qubits in superposition;
  - The current state of quantum computation is notorious for very high error rate (*e.g.*, millions of errors per hour). Thus, most qubits are being used for the error correction rather than for the actual computing.

- better stability to hold the superposition states longer for running more sophisticated algorithms;
    - Currently, the superposition state is being held only for fractions of a second.
- better techniques for setting and holding the quantum states.
    - Currently, the quantum states are being controlled by ion traps using *magnetic fields*, optical traps by light waves, quantum dots, semiconductor impurities, or superconducting circuits.

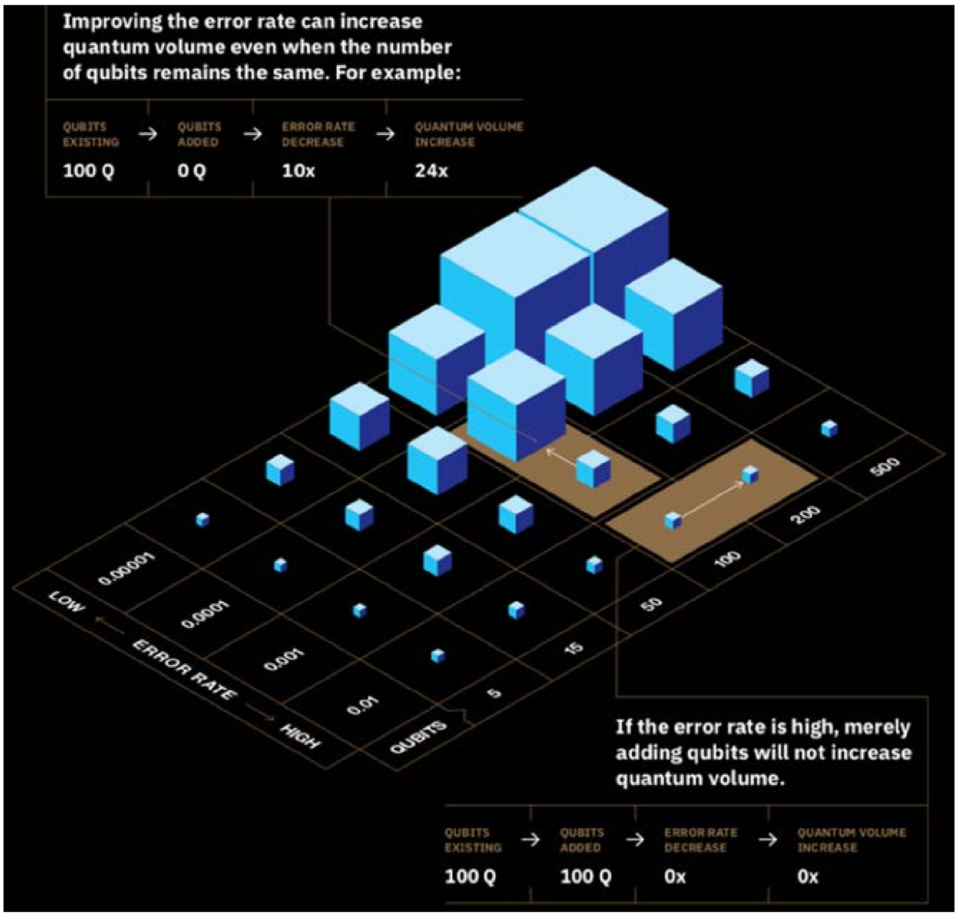


Figure 3: The quantum volume in relation to the error rate and the number of qubits (*source*: IBM Research)

7. Concluding Remarks

It is expected that the recent advancements in ML and AI could help with some critical steps in building better quantum computers; see Dunjko and Briegel (2018). As a result, the ML and AI applications can benefit tremendously by quantum computers. There is no doubt that quantum computing will accelerate the process of scientific discoveries and technological innovations, having a transformative impact on our society (*e.g.*, computation, communication, cryptography); see Wang (2012).

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