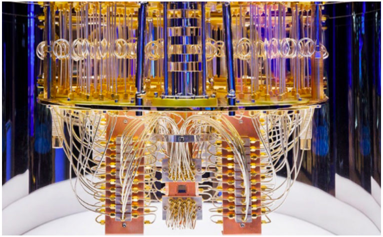
Machine Learning with Quantum Computers

Overview and basic ideas



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Advanced topics in Machine Learning and Optimization

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Premise: The World is quantum...

At microscopic length scales (molecules, atoms, electrons,...):

Newton's laws of dynamics and electromagnetism based on **Maxwell's equations** do not work.

We need **quantum mechanics** to describe physical phenomena.

Quantum things:

- Superposition of states
  (is the electron either "here" or "there"? In both places!).
- Observations alters the state of the observed system.
  (We observe the electron "here" with some probability)
- Entanglement ("spooky action at distance" as Einstein said)

Using physical phenomena to process information is a good and old idea...
What if are we able to use quantum phenomena?

A bit of history...

1981. At the *First Conference of Physics of Computation* (MIT), R. Feynman observed that quantum systems cannot be efficiently simulated by classical computers and proposed a model of quantum computer.

1985. D. Deutsch described the *universal quantum computer* in terms of the *quantum Turing machine*.

1994. P. Shor proposed an algorithm for a quantum computer to factor large integers in polynomial time.

1995. L. Grover presents the *quantum search algorithm* in an unsorted database.

2000s. First prototypes of working quantum computers.

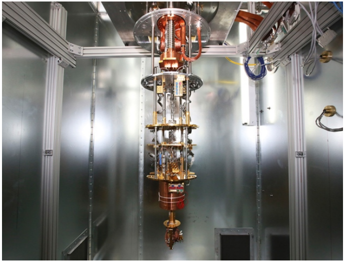
2010s. Quantum computers on the market (D-Wave, IBM Q System 1).

Present days (2022)

- Anyone can run his/her quantum algorithms on available quantum machines (a basic access is usually free).
- Real-life problems are tackled by quantum computers.
- The interest by industry and non academic institutions is dramatically increasing.
- Availability of fault-tolerant, error-corrected, universal quantum computers?
  Not yet, we are in the Noisy Intermediate-Scale Quantum (NISQ) era (few hundred qubits).
- Quantum supremacy? *Not yet.*
- Hot topics: **quantum optimization** and **quantum machine learning**...

Quantum computers exist

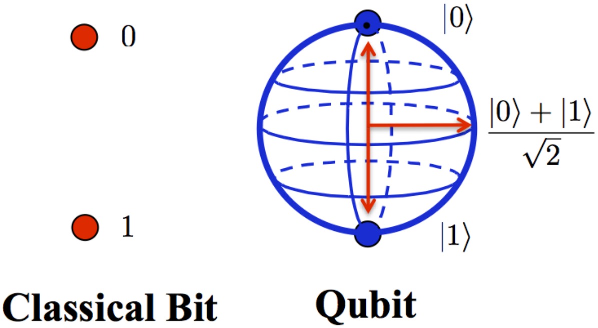
Examples of quantum computers:



D-Wave

IBMQ

Quantum bits

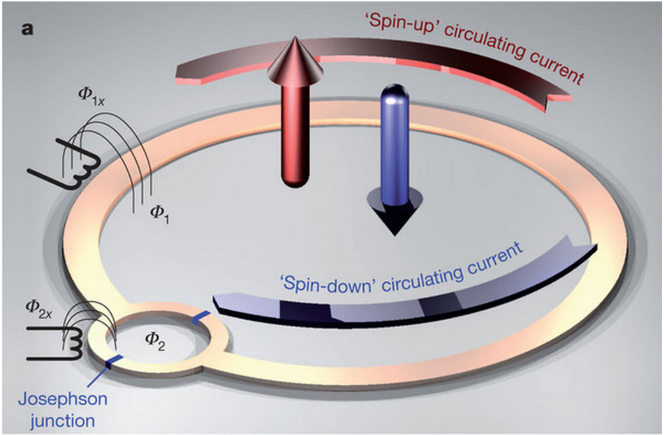


Examples of qubits:

- Particle with spin 1/2;
- Polarized Photons;
- Controlled superconducting circuits.

Quantum bits

Qubit as a superconducting circuit:



Qubits

Quantum state superposition

The state of a qubit is a unit vector in $\mathbb{C}^2$:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \qquad \alpha, \beta \in \mathbb{C}\ , \quad |\alpha|^2 + |\beta|^2 = 1$$

$\{|0\rangle, |1\rangle\}$ computational basis.

A measurement process affects the qubit state

Measurement of a qubit (e.g. we measure the polarization of a photon)

$$\mathbb{P}(0) = |\alpha|^2 \qquad \mathbb{P}(1) = |\beta|^2$$

The qubit state after the measurement is $|i\rangle$ if the outcome is $i = 0, 1$.

Remark:
The vectors $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ with $\theta \in \mathbb{R}$ represent the same *physical state*.

Qubits

Tensor product

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{C}^2 \qquad |\varphi\rangle = \begin{pmatrix} \gamma \\ \delta \end{pmatrix} \in \mathbb{C}^2$$

$$|\psi\rangle \otimes |\varphi\rangle = \begin{pmatrix} \alpha\gamma \\ \alpha\delta \\ \beta\gamma \\ \beta\delta \end{pmatrix} \in \mathbb{C}^4$$

2 qubits (as a composite system) are described in:

$$\mathbb{C}^2 \otimes \mathbb{C}^2 := \mathrm{span}\{|\psi\rangle \otimes |\varphi\rangle \ : \ |\psi\rangle, |\varphi\rangle \in \mathbb{C}^2\} = \mathbb{C}^4.$$

n qubits (as a composite system) are described in:

$$(\mathbb{C}^2)^{\otimes n} = \mathbb{C}^{2^n}.$$

Entangled qubits

Let $|\Psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be the state of a qubit pair.

$|\Psi\rangle$ is said to be:

- **separable** if it has form $|\Psi\rangle = |\psi\rangle \otimes |\varphi\rangle \equiv |\psi\varphi\rangle$;
- **entangled** otherwise.

Example

Entangled state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Measure the **first qubit**:

- The probability of measuring 0 is $\frac{1}{2}$.
- If the outcome is 0 then the post-measurement state is $|\Psi_0\rangle = |00\rangle$.
- Non-local action on the **second qubit** (quantum correlation).

EPR paradox: inconsistency with QM and Einstein's locality.

A new kind of information

Empirical evidence:
Quantum randomness, state superpositions, entanglement are **physical phenomena** not simply *theoretical interpretations*.

$$\Downarrow$$

Encoding information into qubits (or more general quantum objects) allows completely new kinds of:

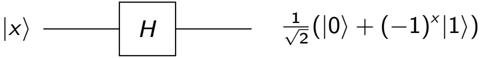
- information storing and processing
- data representation
- telecommunication
- cybersecurity
- ...

In particular we are interested in machine learning!

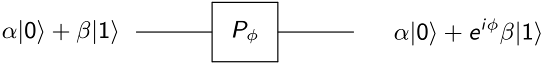
Quantum gates

Let $\{|0\rangle, |1\rangle\}$ be the computational basis

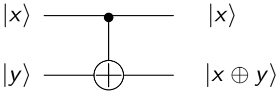
- Hadamard gate:



- Phase gate:



- CNOT gate:



Theorem: $\{H, P_{\pi/4}, CNOT\}$ is a universal set for quantum computation.

Machine learning with quantum computers?

Achievements in Quantum Machine Learning (since 2013)

Algorithm	**Quantum speedup**
K-medians	Quadratic/Exponential
Hierarchical clustering	Quadratic
K-means	Exponential
Principal component analysis	Exponential
Support vector machines	Exponential
Nearest neighbors	Quadratic / Exponential
Neural networks	?

General observation

Quantum architectures enable new paradigms of data representation and information processing.

Current challenge

Devising *quantum learning mechanisms* for available or near-term quantum machines.

A quantum binary classifier

The model

Let $\{(\mathbf{x}_i, y_i)\}_{i=0,\dots,N-1}$ be a training set where:
$x_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$ for any $i = 0, ..., N-1$

$$y(\mathbf{x}) := \operatorname{sgn}\left(\sum_{i=0}^{N-1} y_i \cos(\mathbf{x}_i, \mathbf{x})\right) \qquad \cos(\mathbf{x}, \mathbf{z}) := \frac{\mathbf{x} \cdot \mathbf{z}}{\| \mathbf{x} \| \| \mathbf{z} \|} \qquad \mathbf{x}, \mathbf{z} \in \mathbb{R}^d.$$

Quantum implementation on the IBM ibmq_melbourne

- Quantum superposition of training vectors;
- Test instance in quantum superposition of the two classes;
- Cosine similarities computed by SWAP test.

Classical complexity: $O(Nd)$
Quantum complexity: $O(\log(Nd))$

A quantum binary classifier

Training set stored in a n-qubit register ($n = \log d$).
$\log N$-qubit register, with Hilbert space $\mathcal{H}_{index} \simeq (\mathbb{C}^2)^{\otimes \log N}$, to encode the indexes of training data vectors.

We can construct the state:

$$|X\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle |\mathbf{x}_i\rangle |b_i\rangle \in \mathcal{H}_{index} \otimes \mathcal{H}_n \otimes \mathcal{H}_l,$$

where $\mathcal{H}_l$ is a 1-qubit register encoding the labels with $b_i = \frac{1-y_i}{2} \in \{0, 1\}$.

We can construct also:

$$|\psi_{\mathbf{x}}\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle |\mathbf{x}\rangle |-\rangle \in \mathcal{H}_{index} \otimes \mathcal{H}_n \otimes \mathcal{H}_l,$$

where $|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$.

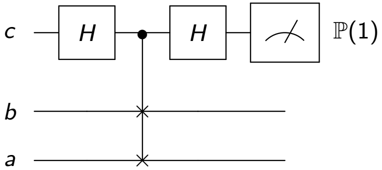
A quantum binary classifier

Add 1 ancillary qubit to the registers and construct:

$$|\Psi\rangle \frac{1}{\sqrt{2}} (|X\rangle|0\rangle + |\psi_{\mathbf{x}}\rangle|1\rangle) \in \mathcal{H}_{index} \otimes \mathcal{H}_n \otimes \mathcal{H}_l \otimes \mathcal{H}_a,$$

that can be retrieved from the QRAM in time $O(log(Nd))$.

Perform the SWAP test:



where qubit b is prepared in $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and qubit c is prepared in $|0\rangle$.
The model:

$$y(\mathbf{x}) := \text{sgn}\left(\sum_{i=0}^{N-1} y_i \cos(\mathbf{x}_i, \mathbf{x})\right),$$

Quantum implementation of the model based on:

$$y(\mathbf{x}) = \text{sgn}\left[1 - 4\,\mathbb{P}(1)\right].$$

A quantum binary classifier

Input: training set $X = \{\mathbf{x}_i, y_i\}_{i=0,\ldots,N-1}$, unclassified instance $\mathbf{x}$.
Result: label y of $\mathbf{x}$.

repeat
    initialize the register $\mathcal{H}_{index} \otimes \mathcal{H}_n \otimes \mathcal{H}_l$ and an ancillary qubit a in the state $|\Psi\rangle$;
    initialize a qubit b in the state $|-\rangle$;
    perform the SWAP test on a and b with control qubit c prepared in $|0\rangle$;
    measure qubit c;
until *desired accuracy on the estimation of* $\mathbb{P}(1)$;
Estimate $\mathbb{P}(1)$ as the relative frequency $\hat{\mathbb{P}}$ of outcome 1;
if $\hat{\mathbb{P}} > 0.25$ **then**
    return $y = -1$
else
    return $y = 1$
end

Overall complexity within an error ϵ in the estimation of $\mathbb{P}(1)$: $O(\epsilon^{-2} \log(Nd))$

Quantum clustering

Qdist is a quantum algorithm based on the SWAP test to calculate Euclidean distance in logarithmic time.

Grover is a quantum search algorithm with quadratic speedup.

Example: K-medians clustering

Input: Data set $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$, number of clusters K
Result: Partition of $\{\mathbf{x}_1, \cdots, \mathbf{x}_N\}$ into K clusters

initialize K centroids $C_1, ..., C_K$ from the elements of the dataset V;
repeat
    foreach $i \leftarrow 1, ..., N$ **do**
        Qdist $(\mathbf{x}_i, C_j)\ \forall j = 1, ..., K$;
        find $\text{argmin}_j \parallel \mathbf{x}_i - C_j \parallel$ with **Grover**;
    end
    construct the cluster $P_j = \{\mathbf{x}_i : C_j \text{ is the nearest centroid}\}$ for all $j = 1, ..., K$;
    foreach $j \leftarrow 1, ..., K$ **do**
        use **Qdist** and **Grover** for centroid calculation;
    end
until *convergence*;
return $P_1, ..., P_K$

Some QML schemes designed for universal quantum computers

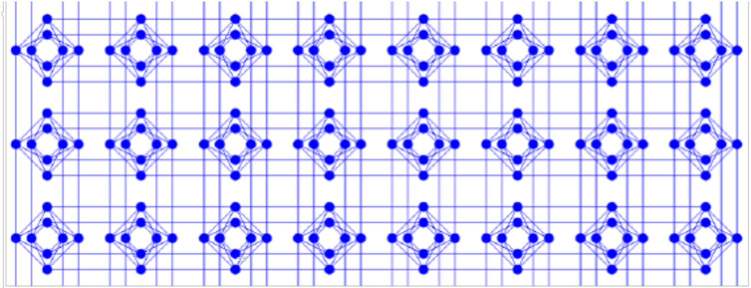
- **Quantum divisive clustering**
  W. Aïmeur et al. *Quantum clustering algorithms* ICML '07: Proceedings of the 24th international conference on Machine learning (2007)
- **Quantum principal component analysis**
  S. Lloyd, et al. *Quantum principal component analysis* Nature Physics 10, 631 (2014)
- **Quantum support vector machine**
  P. Rebentrost et al. *Quantum support vector machine for big data classification* Phys. Rev. Lett. 113, 130503 (2014)
- **Quantum nearest neighbor**
  N. Wiebe et al. *Quantum Algorithms for Nearest-Neighbor Methods for Supervised and Unsupervised Learning* Quantum Information and Computation 15(3,4): 0318- 0358 (2015)
- **Quantum perceptron** M. Schuld *Simulating a perceptron on a quantum computer* Physics Letters A, 379, pp. 660-663 (2015)
- **Quantum meta-learning** M. Wilson et al. *Optimizing quantum heuristic with meta-learning* Quantum Machine Intelligence 3 (2021)

Quantum Annealing

Quantum Annealers

The hardware is a *quantum spin glass*, i.e. a collection of qubits arranged in the vertices of a graph (V, E) where edges represent the interactions between neighbors.

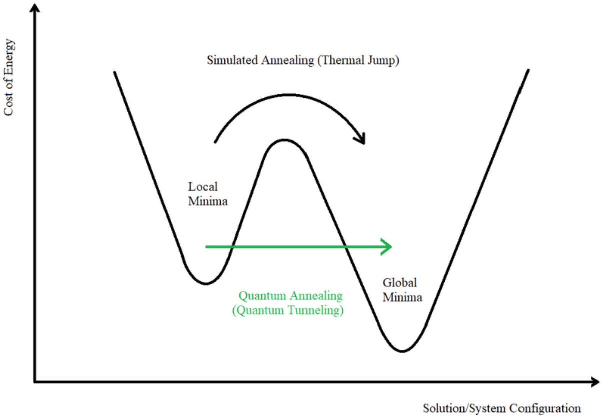
Example: *D-Wave Chimera topology*



Quantum Annealing

Annealing process (annealing time 20μs)

By energy dissipation the quantum system evolves in the **ground state** (the less energetic state) corresponding to the **solution** of a given optimization problem.



Quantum Annealing

Shortcoming

Representing a given problem into the quantum hardware architecture is difficult in general and can destroy the efficiency of the quantum computation.

Proposed solution

Quantum Annealing Learning Search (QALS):

A hybrid quantum-classical algorithm enabling a learning mechanism so that the quantum machine learns the representation of the problem on its own without an expensive classical pre-processing.

References:

-) D.P., E. Blanzieri. **Quantum Annealing Learning Search for solving QUBO problems**. Quantum Information Processing 18: 303 (2019)

-) A. Bonomi, T. De Min, E. Zardini, E. Blanzieri, Valter Cavecchia, D. P. **Quantum annealing learning search implementations** in Quantum Information and Computation, v. 22, n. 3&4 (2022)

ML with quantum annealers

- **Boltzmann machine implementation**
  M.H. Amin *Quantum Boltzmann machine* Phys. Rev. X 8, 021050 (2018)
- **Classification**
  N. T. Nguyen et al. *Image classification using quantum inference on the D-wave 2X*. In: 2018 IEEE International Conference on Rebooting Computing (ICRC), pp. 1-7. IEEE (2018)
- **Clustering**
  V. Kumar et al. *Quantum Annealing for Combinatorial Clustering* Quantum Inf Process (2018) 17: 39
- **Training of a SVM**
  D. Willsch et al. *Support vector machines on the D-wave quantum annealer* Computer Physics Communications 248, 107006 (2020)

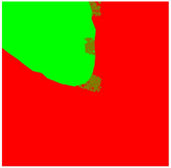
Quantum-inspired ML

Using quantum formalism to devise classical ML algorithms

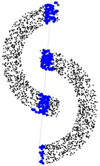
Quantum-inspired classifiers:

- Data encoding into density operators (quantum states);
- Construction of the centroids in the space of quantum states;
- Application of *discrimination of quantum states* to attach a new data instance to the *most similar* centroid.

Example:



Quantum-inspired classifier



SVM with linear kernel

Ref.: R. Leporini and D. P.. *Support vector machines with quantum state discrimination*. Quantum Reports vol. 3, n. 3 (2021)

Some concluding remarks

- Quantum architectures enable new kinds of data processing.
- There is a bottleneck about the efficient data representation into quantum hardware (QRAM are not feasible yet).
- The era of quantum machine learning is just started but it is maybe the most promising road for putting forward the frontiers of quantum computing.
- The quantum-classical hybrid approach is the best way to use the existing quantum machines.
- Providing efficient quantum algorithms is a very difficult task. So we have to devise learning mechanisms of new quantum algorithms towards a "quantum meta-learning"...

In other words, quantum computers must learn how to solve problems on their own...

Thanks for your attention!

Credit: IBM