An overview on Quantum Machine Learning

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Advanced Topics in Machine Learning and Optimization

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Introduction

Quantum Machine Learning (QML): ML with quantum computers.

First proposals (20 years ago)

Quantum associative memories and pattern recognition.
D. Ventura, T. Martinez, *Information Sciences* ***124*** (2000)
R. Schützhold, *Phys. Rev. A* ***67*** (2003)

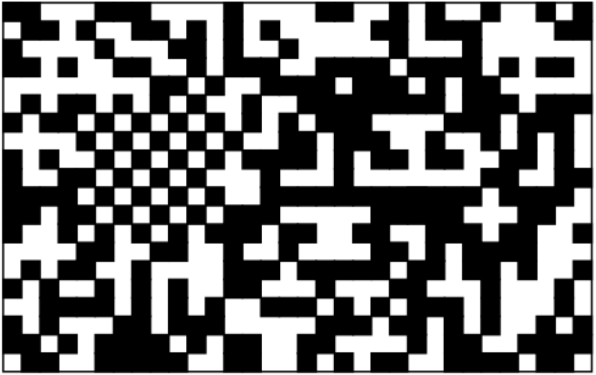
Main results on QML (since 2013)

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	?

Current challenge

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

Introduction



Implementing the Quantum Fourier transform, the chessboard structure can be found **easily** by a quantum computer.

Introduction

Data processing based on quantum effects like *quantum superposition* and *quantum entanglement*.

Examples of quantum advantages

- Calculation of Euclidean distance in $\mathbb{R}^d$:

  Classical time complexity $O(d)$.
  Quantum time complexity $O(\log d)$.

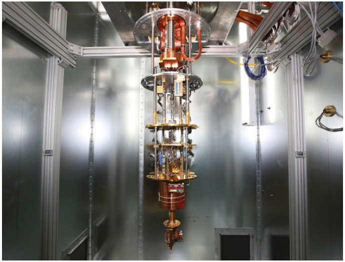
- Search in an unstructured database of N items:

  Query complexity of exhaustive search: $O(N)$.
  Query complexity of Grover's algorithm: $O(\sqrt{N})$.

Qdist and *Grover* are typical subroutine of QML algorithms.

Introduction

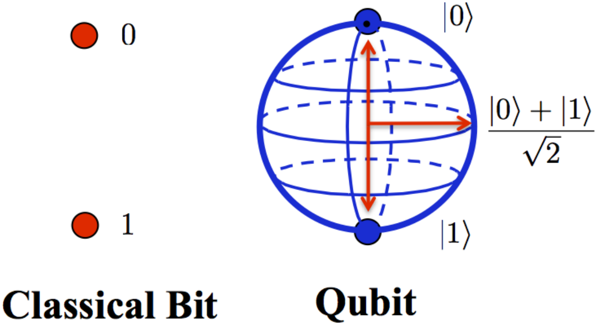
Examples of quantum computers:



D-Wave

IBMQ

Introduction

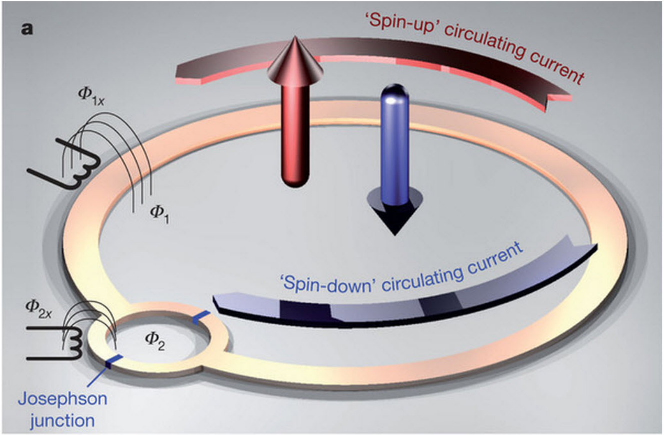


Examples of qubits:

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

Introduction

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:

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

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 processing, telecommunication, data security...

Quantum encoding

Basis encoding

Elements of $X = \{0,1\}^n$ encoded into the states of n qubits

$$\{0,1\}^n \ni (x_1 \cdots x_n) \mapsto |x_1\rangle \otimes \cdots \otimes |x_n\rangle \equiv |x_1 \cdots x_n\rangle \in \mathbb{C}^{2^n}$$

Observation:

The system (n-qubit register) can be prepared in a superposition of data that can be processed in parallel by linearity.

The register can be initialized in a superposition of all data:

$$|\Psi\rangle = \sum_{x=0}^{2^n-1} |x\rangle$$

Quantum encoding

Amplitude encoding

$\mathbf{x} \in \mathbb{C}^d$ with $\| \mathbf{x} \| := \sqrt{\sum_{i=1}^{d} |x_i|^2} = 1$.

Consider a quantum register of $\log d$ qubits.

Components of $\mathbf{x}$ encoded into the amplitudes of a quantum state $|\psi_{\mathbf{x}}\rangle$

Let $\{|i\rangle\}_{i=1,\dots,d}$ be the computational basis:

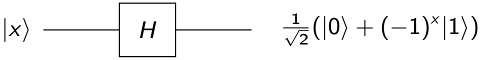
$$|\psi_{\mathbf{x}}\rangle = \sum_{i=1}^{d} x_i |i\rangle.$$

Remark:
Quantum amplitudes cannot be directly observed.
From $|\psi_{\mathbf{x}}\rangle$ we can retrieve only $|x_i|^2$.

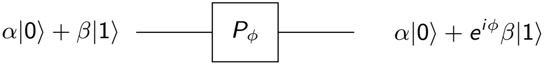
Quantum gates

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

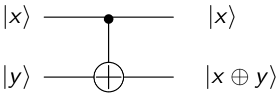
- Hadamard gate:



- Phase gate:



- CNOT gate:



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

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 $i = 0, \dots, N-1$

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

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: $\mathcal{O}(Nd)$
Quantum complexity: $\mathcal{O}(\log(Nd))$

A quantum binary classifier

Training set stored in a n-qubit register within the amplitude encoding.
$\log N$-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 $|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$.

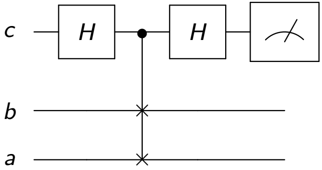
A quantum binary classifier

Add 1 ancillary qubit to the registers and construct:

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

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 $|0\rangle$.

A quantum binary classifier

The probability of measuring 1 on qubit c is:

$$\mathbb{P}(1) = \frac{1}{4}(1 - \langle X|\psi_{\mathbf{x}}\rangle)$$

(Check as an exercise!)

$$\langle X|\psi_{\mathbf{x}}\rangle = \frac{1}{N}\sum_{i,k=0}^{N-1}\langle i|k\rangle\langle \mathbf{x}_i|\mathbf{x}\rangle\langle b_i|-\rangle = \frac{1}{N\sqrt{2}}\sum_{i=0}^{N-1}\langle \mathbf{x}_i|\mathbf{x}\rangle(\langle b_i|0\rangle - \langle b_i|1\rangle)$$

$$= \frac{1}{N\sqrt{2}}\sum_{i=0}^{N-1} y_i \cos(\mathbf{x}_i, \mathbf{x}),$$

$\langle i|k\rangle = \delta_{ik}$ and $\langle b_i|0\rangle - \langle b_i|1\rangle = 1 - 2b_i = y_i$ for any $i = 0, ..., N-1$

The model:

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

Quantum implementation of the model based on:

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

A quantum binary classifier

Input: training set $X = \{\mathbf{x}_i, y_i\}_{i=0,\dots,N-1}$, 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 gate-based quantum computers

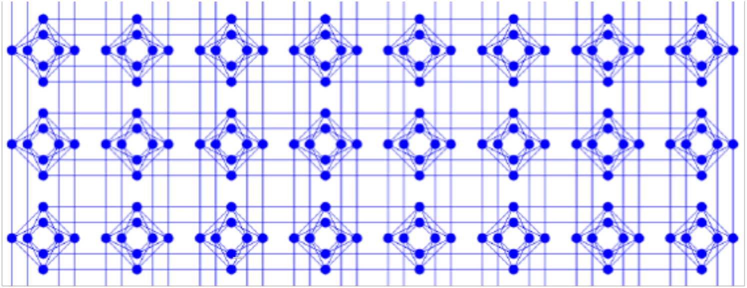
- **Quantum divisive clustering**
  W. Aïmeur et al. *Quantum clustering algorithms* ICML '07: Proceedings of the 24th international conference on Machine learning (2007)
- **Quantum principal component analysis**
  S. Lloyd, et al. *Quantum principal component analysis* Nature Physics 10, 631 (2014)
- **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 $20\mu s$)

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 Annealer task

Minimization (w.r.t. $\mathbf{z}$) of the cost function (Ising model):

$$E(\theta, \mathbf{z}) = \theta_0 + \sum_{i \in V} \theta_i z_i + \sum_{(i,j) \in E} \theta_{ij} z_i z_j \qquad \mathbf{z} \in \{-1, 1\}^{|V|}\ ,\ \theta_0, \theta_i, \theta_{ij} \in \mathbb{R}$$

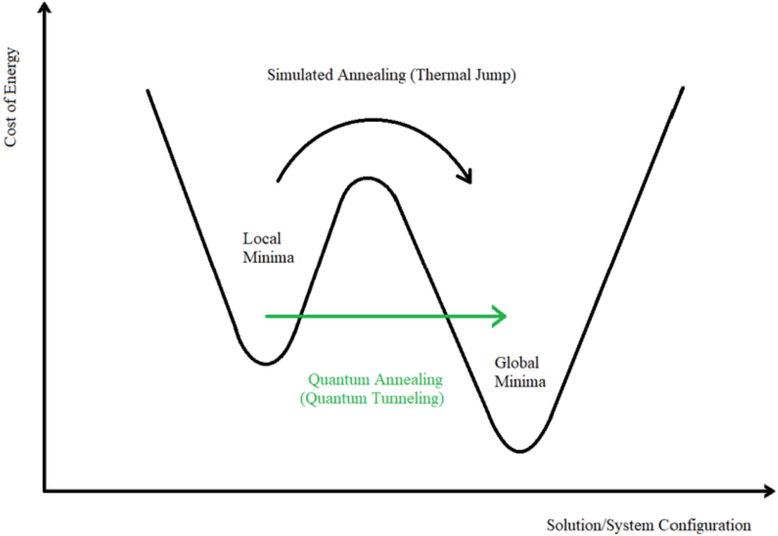
Initialization of the machine

- Assignment of the weights θ;
- Mapping the binary variables into the qubits.

QA vs Simulated Annealing

QA employs the tunnel effect to escape from local minima.
SA employs thermal hill-climbing.

Quantum Annealing



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)

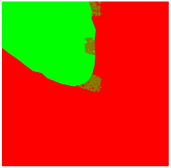
Quantum-inspired ML

Using quantum formalism to devise classical ML algorithms

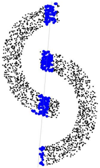
Quantum-inspired classifiers:

- 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)

Conclusions

Goals of the scientific research on QML:

- Exploiting exponential improvements in time and space of quantum techniques to find new strategies to deal with big data.
- Finding promising commercial applications of quantum computing. (Nowadays attraction of investments has strong impact also on research in the academy... like it or not!)
- Increasing our knowledge about the connection between the abstract concept of *learning* and the quantum nature of the World.
- Devising *learning mechanisms* of new quantum algorithms, since providing efficient quantum algorithms is an extremely difficult task.

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