Quantum Machine Learning: When Physics Flirted with Machine Learning, and They Fell in Love

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VNIVERSITAT DE VALÈNCIA

Thematic Semester on Quantum Mathematics

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Institut de Matemàtiques i Aplicacions de Castelló (IMAC)

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Outline

1. IDAL
2. How I got here
3. Machine Learning
4. Quantum computing & quantum technologies
5. Quantum Machine Learning
    5.1. Approaches
    5.2. Current scenario
    5.3. Future research
6. Conclusions

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IDAL

Physicists, computer scientists, data scientists, engineers, a medical doctor (to be), mathematicians

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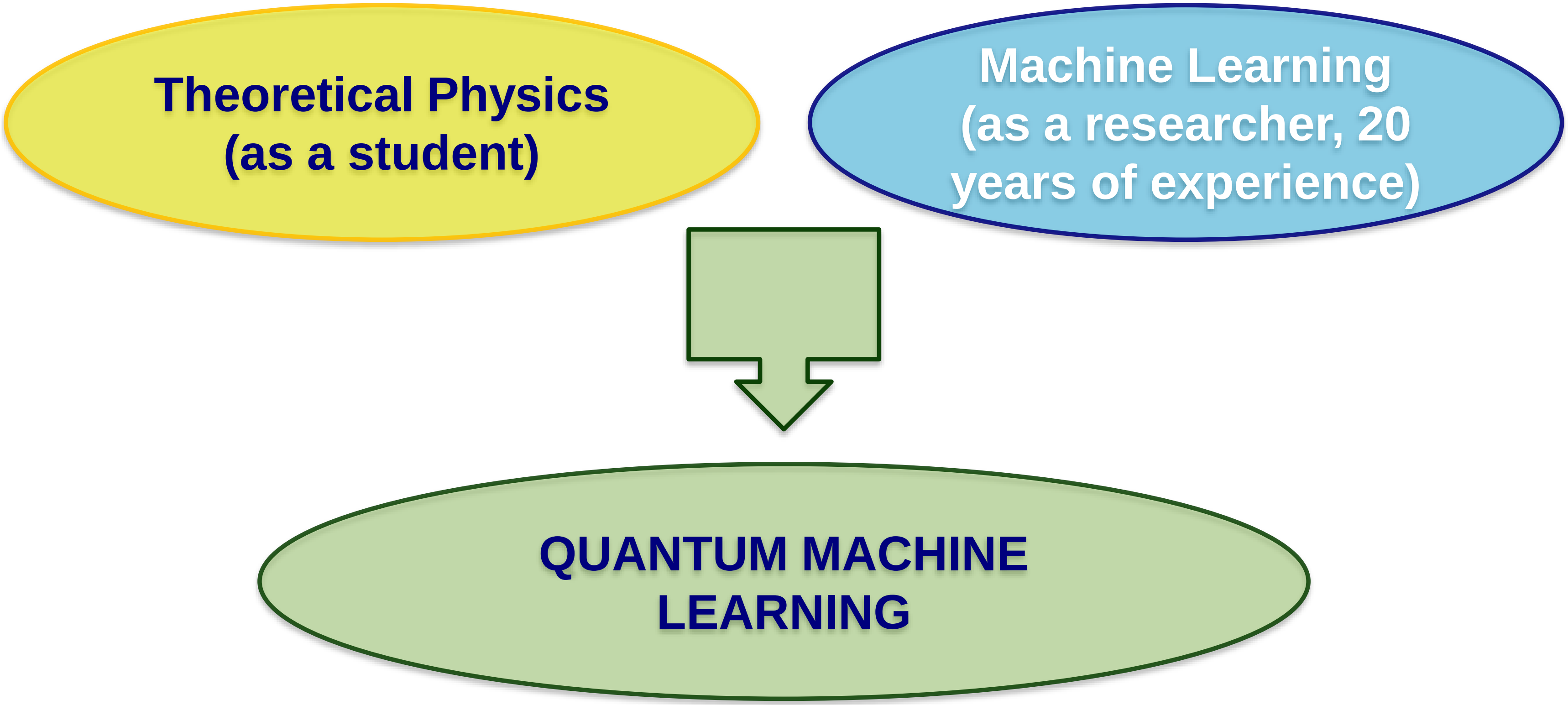
How I got here … and where I want to go



Holistic approaches where not only Physics can be benefited from ML and the other way around ... but enhanced unified approaches

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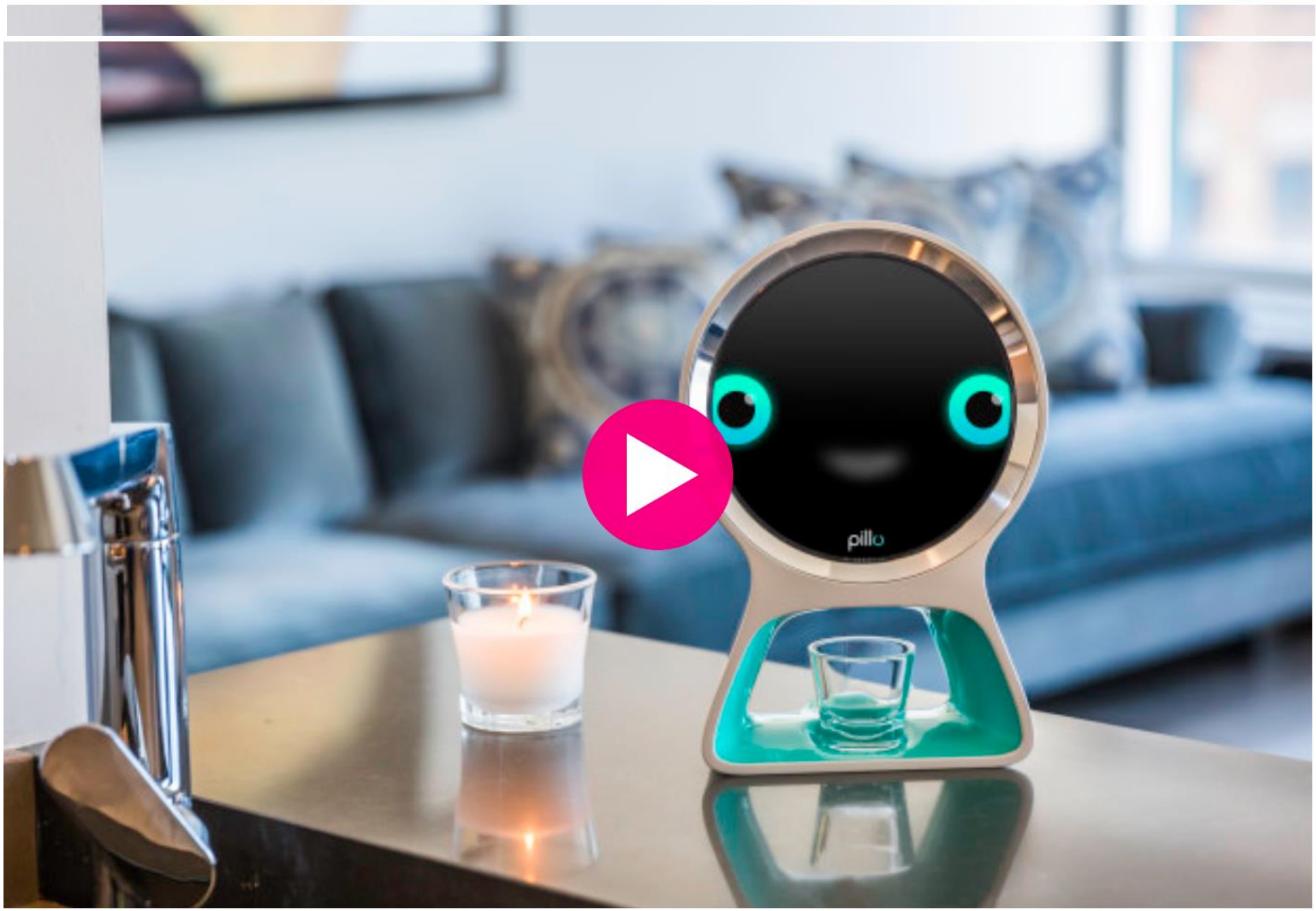
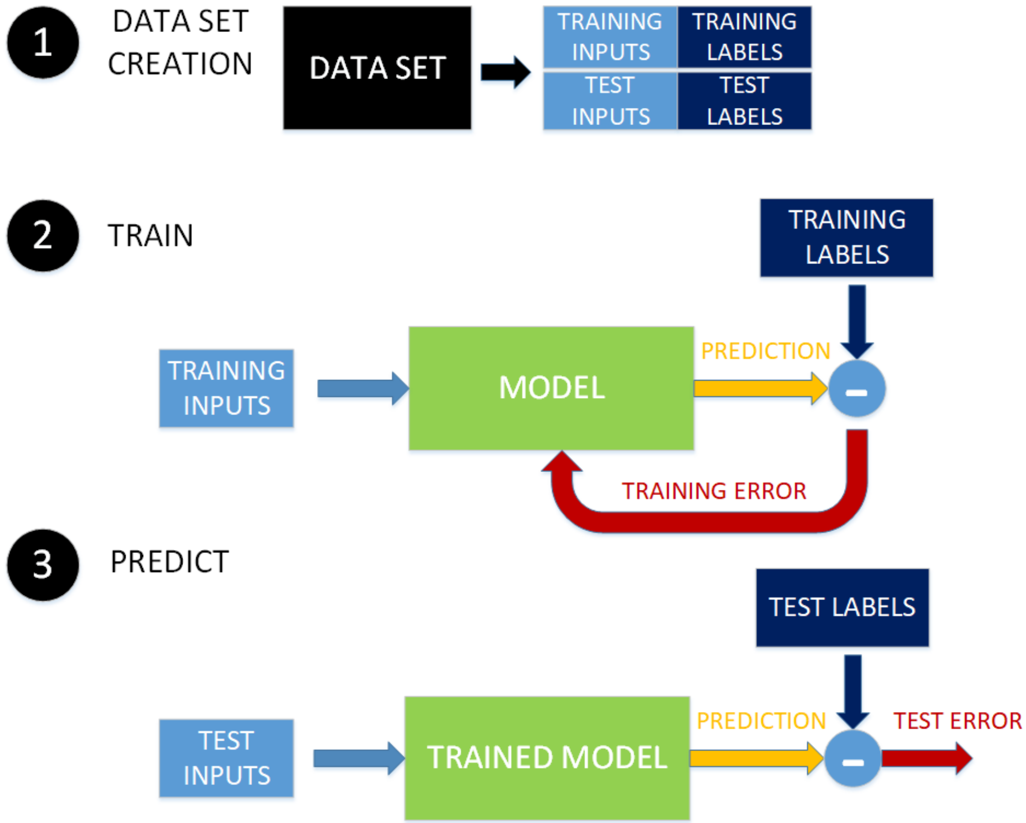
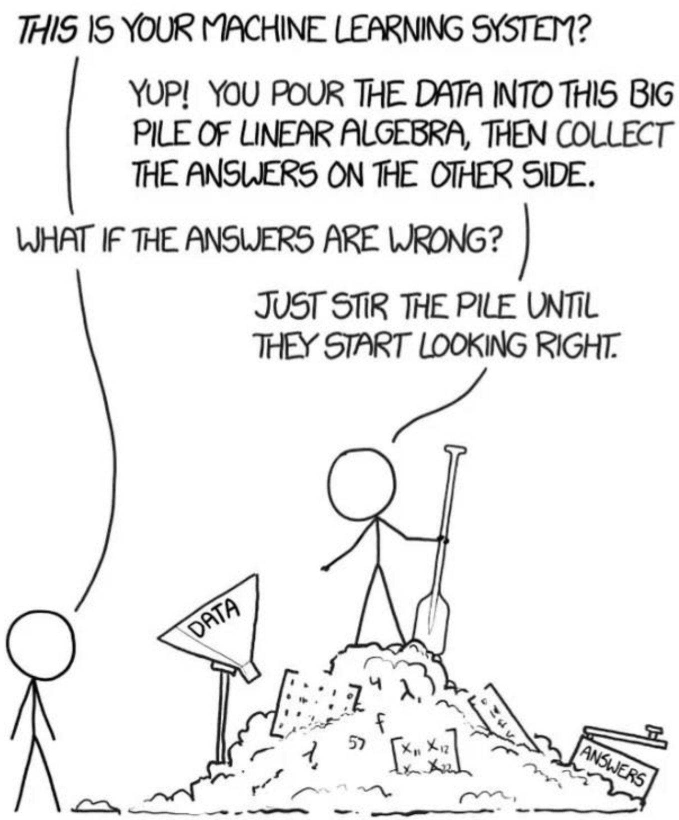
Final ML tools are already here … not just a question of solving a very specific problem



Final ML tools are already here … not just a question of solving a very specific problem

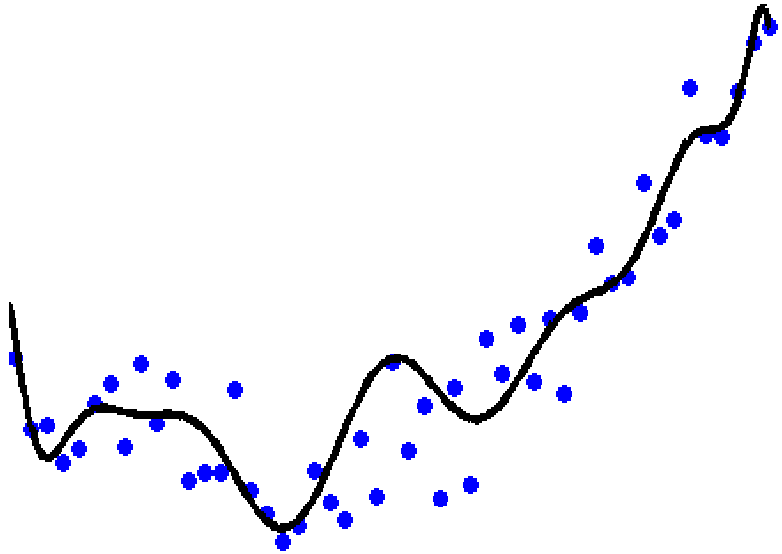
ML in a nutshell

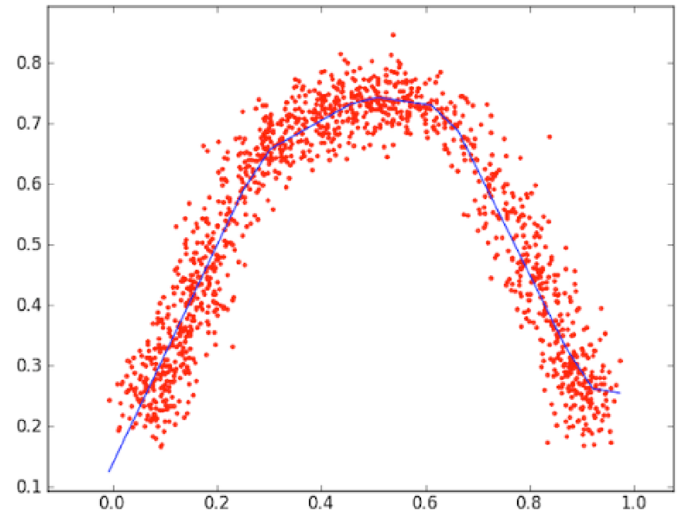


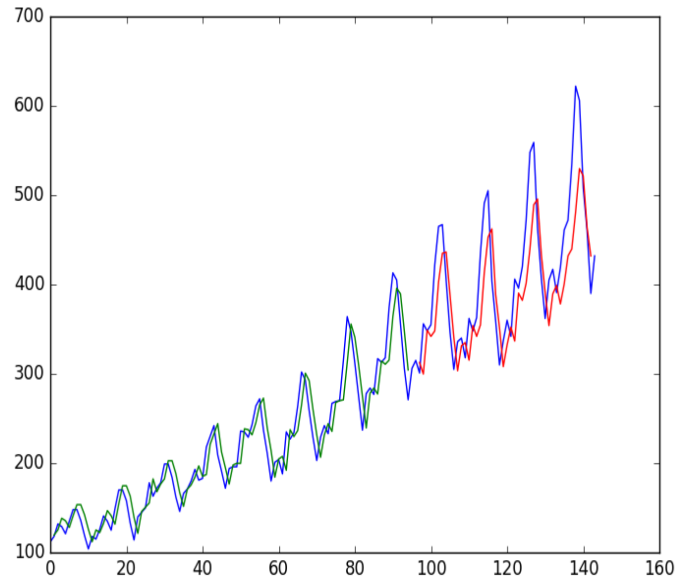


Building **models** that automatically **extract knowledge from data** using **learning algorithms**

Regression (supervised learning)

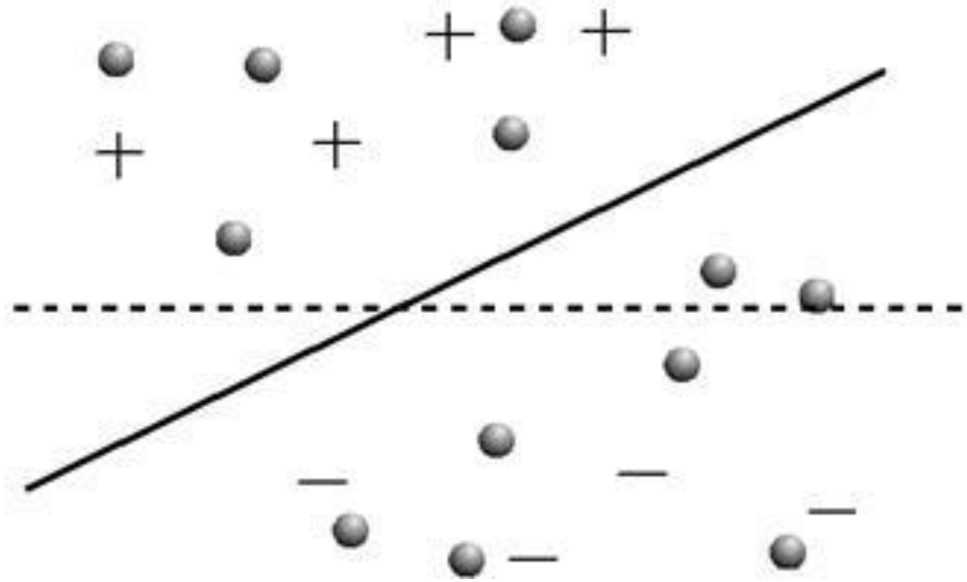


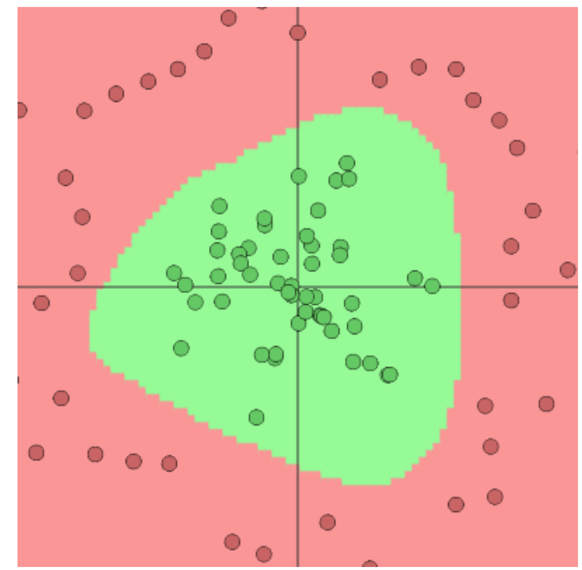


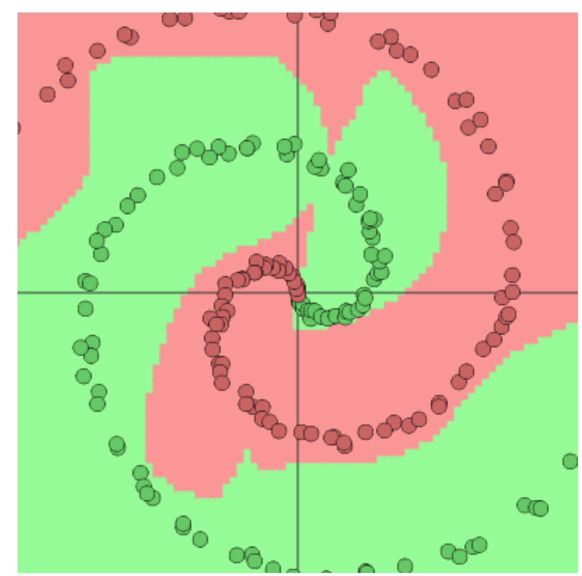


Classification (supervised learning)

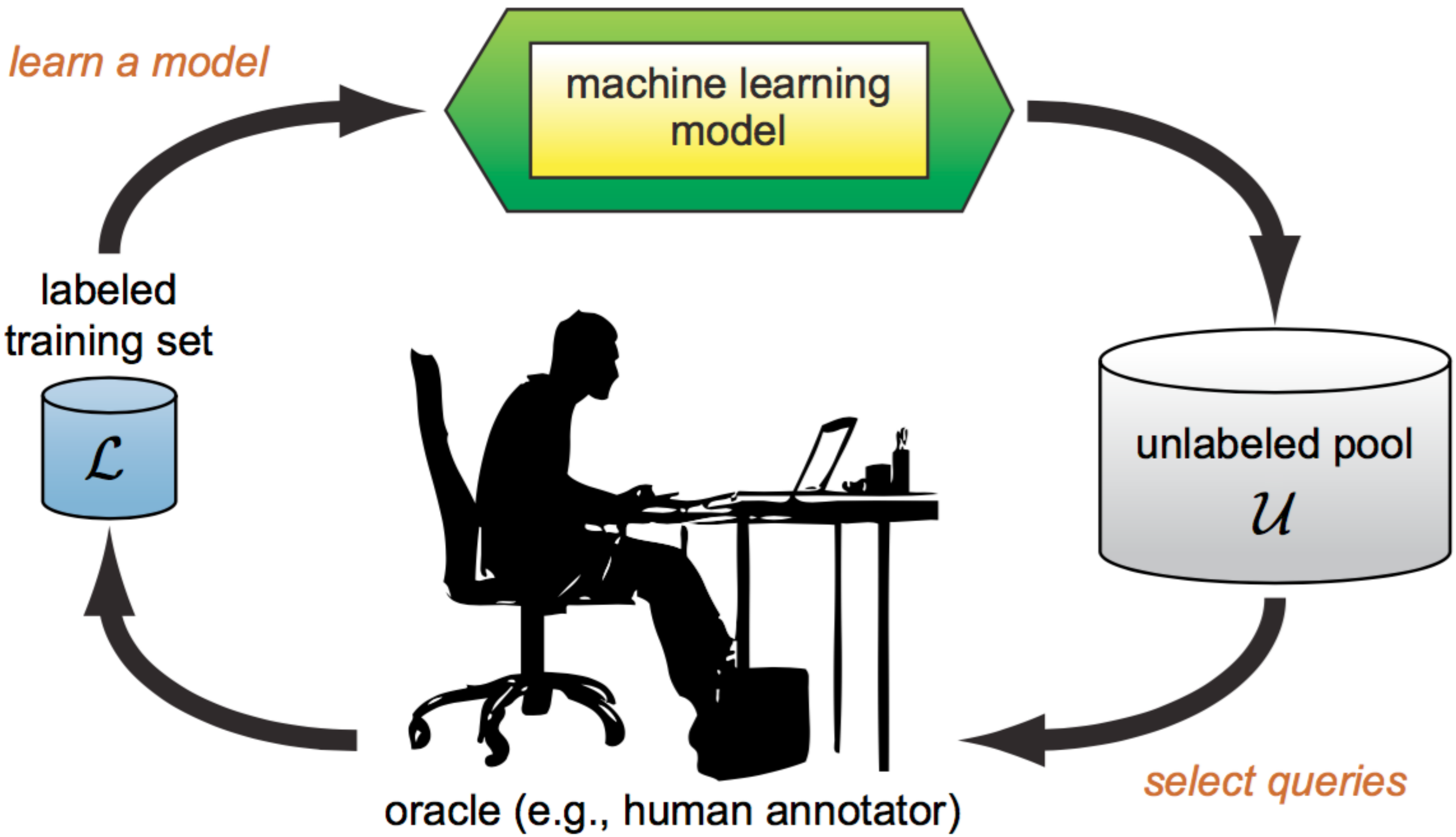
Determine optimal separation boundary between classes



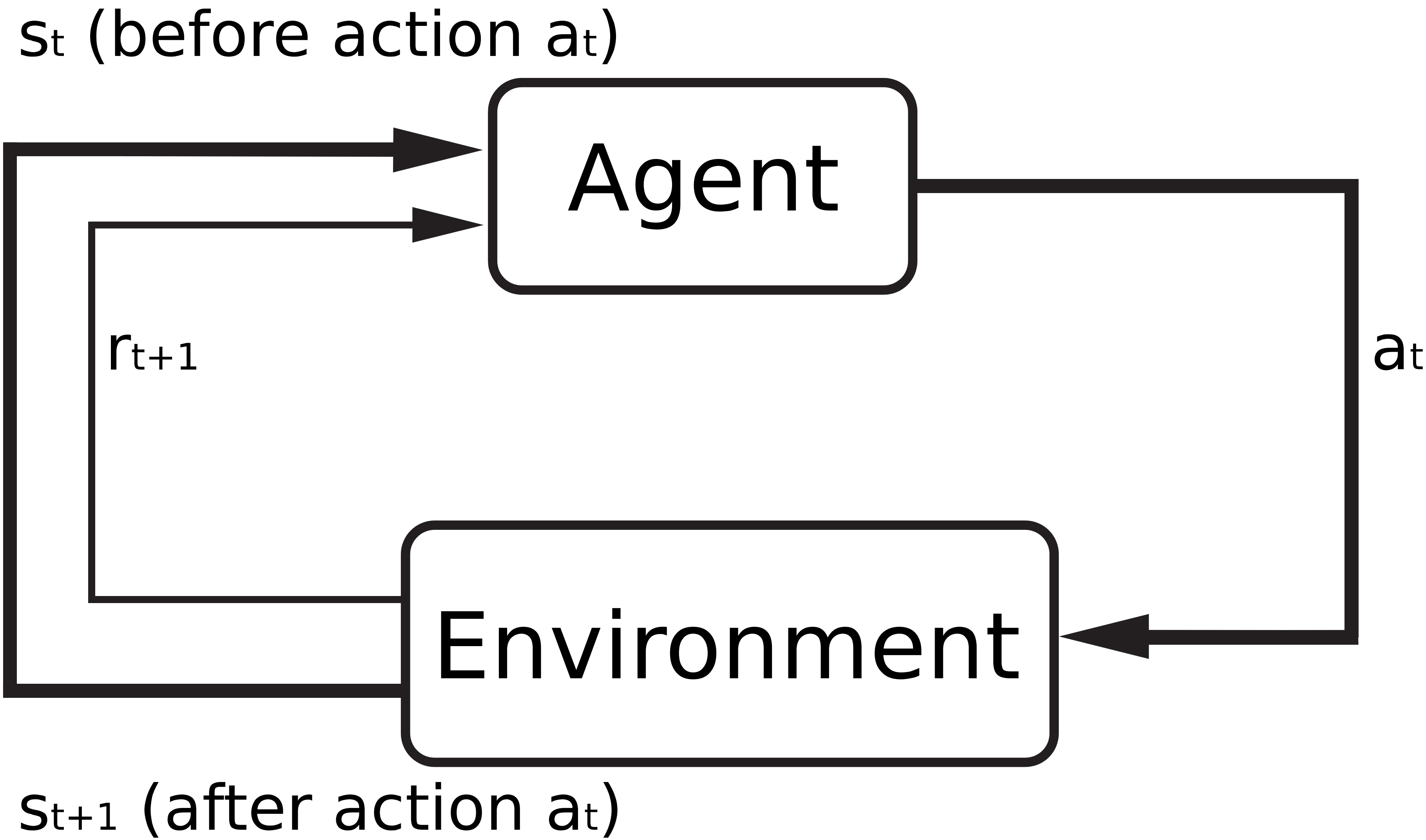




Semisupervised and active learning



Reinforcement learning



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Quantum computing

Classical bit: {0,1}

Qubit: $|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ (State superposition)

The measurement of a qubit in superposition state involves that it will collapse to one of its basic states, but there is no way to determine in advance which one; the unique available information is that the probability of $|0\rangle$ is $|\alpha|^2$ and the probability of $|1\rangle$ is $|\beta|^2$

Unitary transformations of superposition states result in another superposition state obtained by superposing all basis vectors (quantum parallelism)

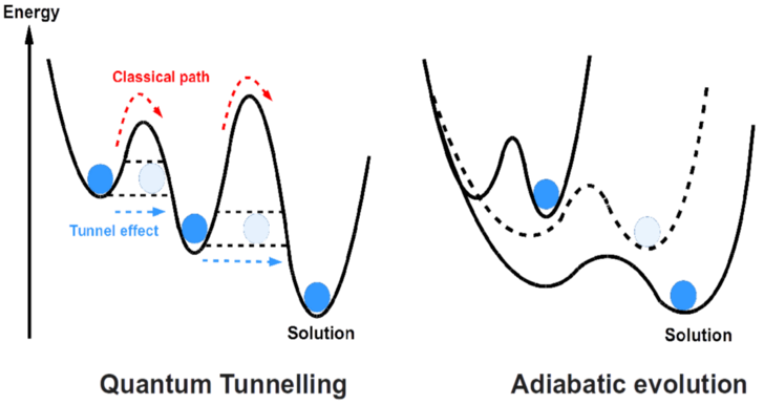
Number of atoms in the Earth ~ 10^{50}
Number of atoms in the Universe ~ 10^{80}
Number of simultaneous operations with N qubits= 2^N
(N<300 will be able to produce as many states as atoms)

Generalization to qudits: more than two states

- Encryption outperforms any classical communication
- No-cloning theorem (no way of copying encoded data): spies will be detected

Quantum technologies: quantum annealing

- Superconductors (temperatures close to absolute zero)
- Up to 2,000 qubits (speedup classical computing)
- Purchase: ~$15M
- Licenses: ~$1M /year
- D-Wave Systems

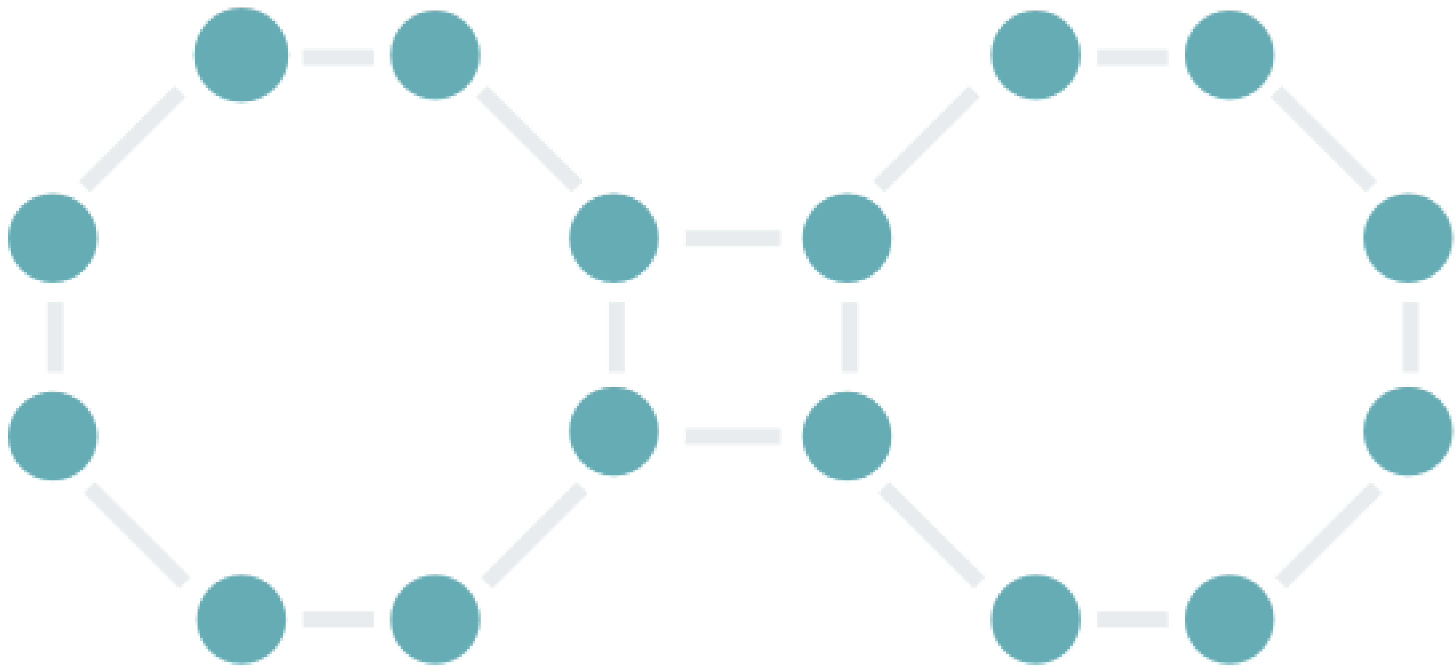


Quantum technologies: superconducting wires

- Superconductors (temperatures close to absolute zero)
- ~20 real qubits for computation
- Issue with scalability: as the number of qubits grows, the more likely they are to interact with the outside world, losing their quantum state (coherence)
- IBM, Google

Quantum cloud: Rigetti

A smart way to produce scalability



Quantum technologies: trapped ions, quantum dots

- Electromagnetic fields to trap ions
- Low temperature to isolate the ions
- ~20 real qubits for computation
- Scalability is also an issue

- Pairs electron-holes
- Temperatures close to absolute zero to prevent quantum states to decohere
- A few qubits (purely quantum)
- Current research focused on scalability
- Microsoft

Quantum technologies: photons, nanodiamonds

- Photons do not interact with the environment (no problem with short coherence time)
- Information transmitted at the speed of light
- Current research focused on coming up with an idea to produce many identical and entangled photons in a chip

- Room temperature
- Alternative for trapped ions but many are statistically needed to create a qubit
- Quantum sensing

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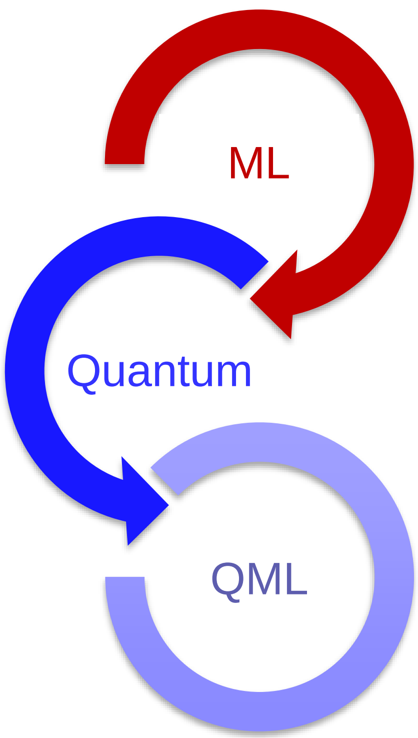
A natural evolution of ML?

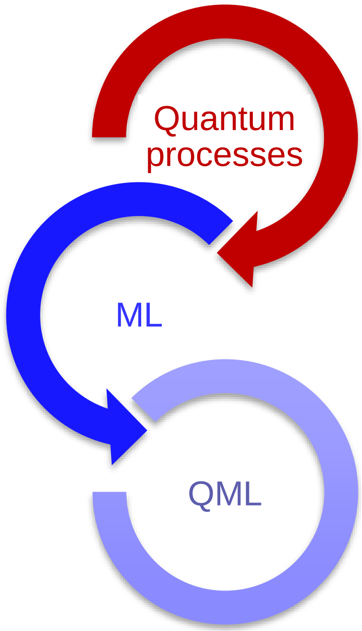
Quantum computers ... More robustness to noise and outliers …
Need of error correction

FIRST APPROACH



- Linearization involves quadratic or even exponential speedups (Quantum SVMs, Quantum KNNs, Quantum RL, Quantum NNs, …)
- Quantum concepts come up with alternative approaches (e. g., quantum clustering) that may involve a higher (or different, at least) learning capability
- Quantum generalization of causal networks (superposition and entanglement)
- Adiabatic quantum evolution (quantum annealing) to improve ML applications
- Grover’s search. Faster (in a quadratic term) than any classical version

SECOND APPROACH



- RL to control aspects of quantum processes
- **Active learning**
- Particle detection
- Prediction of given phenomena

SYNERGIC APPROACH

- Learning in quantum environments
- Digital-Analog quantum simulations

Additional considerations

1. The generalization capability of QML models has been scarcely studied

2. How different types of learning are mapped onto quantum processes is still a (very) open problem

3. Even what learning means in a quantum environment is not trivial and needs new proposals and thorough research, e.g. what happens when an agent is entangled with its environment

4. Are quantum oracles really necessary? What the hell means a quantum oracle?

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Recent works

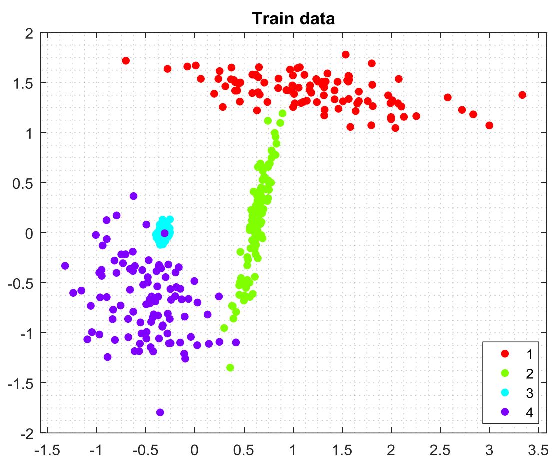
- **Quantum clustering**
- **Quantum learning**
- **Quantum autoencoders**

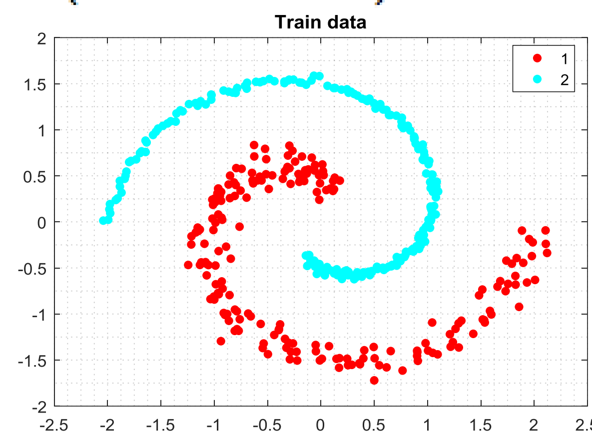
Quantum clustering (I)

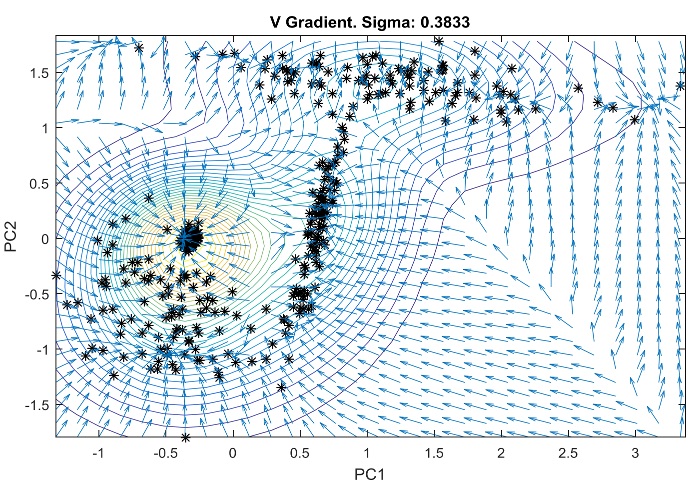
Inspired in Schrödinger equation (data encoded in wave functions; potential wells corresponding with the cluster prototypes)

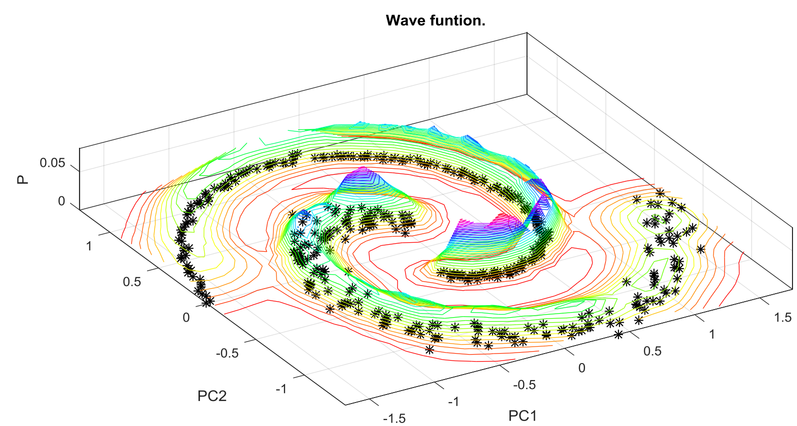
$$\Psi(\mathbf{x}) = \sum_i \exp\left(-\frac{(\mathbf{x}-\mathbf{x}_i)^2}{2\cdot\sigma^2}\right)$$

$$H\Psi \equiv \left(-\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x})\right)\Psi(\mathbf{x}) = E\Psi(\mathbf{x})$$









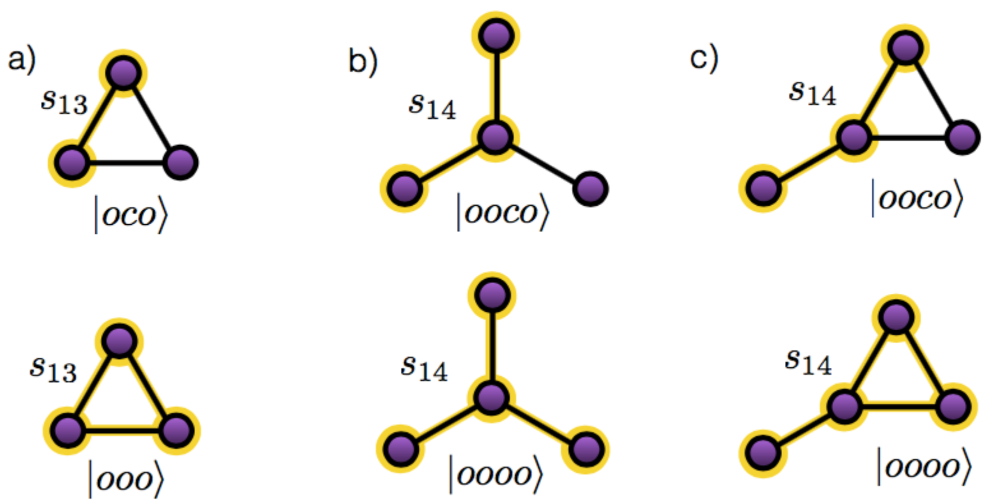
Quantum clustering (II)

- Collaboration with Data Science Research Centre, LJMU
  - ✓ Best poster award at INIT-AERFAI Summer School on Machine Learning 2017
  - ✓ First version already published in Neurocomputing (2017)
  - ✓ Probabilistic version under review in Neural Networks
- Optimization of the number of groups
- Probabilistic interpretation
- Basis for an objective assessment of unsupervised classification (high correlation with Jaccard index)

Quantum supervised learning without measurements (I)

GOAL → Finding the optimal control state in a quantum multitask

- Analysis of the feasibility of ML to remove the necessity of intermediate measures
- Network made up of nodes, each one with a control qubit (superposition of open and close states), and a goal qubit (states corresponding with the classes)
- The most efficient solution is that that sends the excitation thorough the minimum number of open nodes
- Extensions to qudits tested

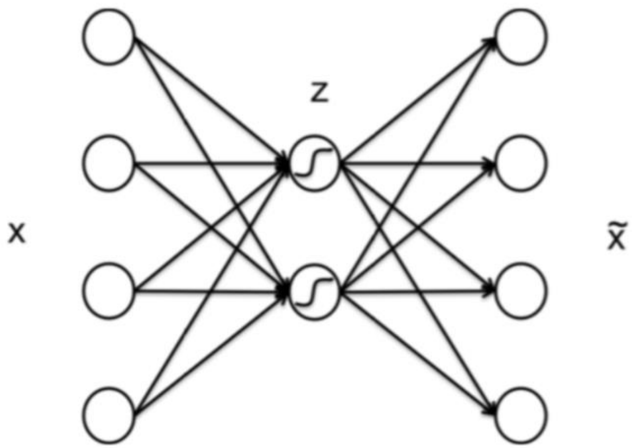


Setups: triangular (a), bell-shaped (b) and radiation (c)

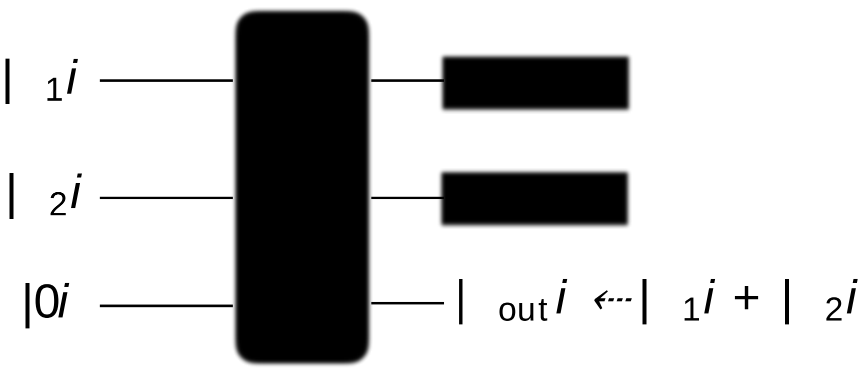
Quantum supervised learning without measurements (II)

- Collaboration with Quantum Technologies for Information Science (UPV-EHU) and Physics Department of Shanghai University
  - ✓ Keynote at QML-BQT 2018
  - ✓ Scientific Reports: 26th most downloaded paper in 2017 (Q1 2017, Multidisciplinary Sciences)
- QML gives a satisfactory efficiency without the need of intermediate measurements
- Independent of the basis

Quantum autoencoder (I)



- ✓ Classical autoencoder
- ✓ Information compression: high-level features
- ✓ Pre-training of deep neural networks



- ✓ Quantum autoencoder
- ✓ Efficient compression of quantum data (fewer measurements)
- ✓ Implementation: quantum adders

Quantum autoencoder (II)

- Collaboration with Quantum Technologies for Information Science (UPV-EHU) and Physics Department of Shanghai University
  - ✓ Firstly presented at American Physical Society March 2018 Meeting
  - ✓ Published in Quantum Science and Technology (2019)

- Optimization: genetic algorithms
  - ✓ Crossover and mutation operators
  - ✓ The goal to be optimized by the new offspring is to maximize the fidelity with respect to the original state

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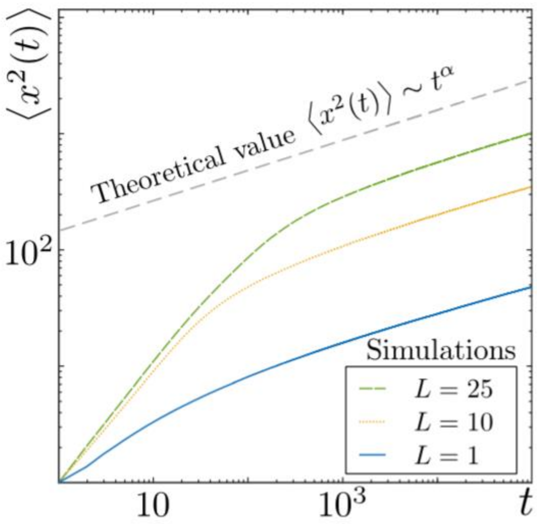
Particle diffusion

ICFO
The Institute of Photonic Sciences

- Normal diffusion: variance proportional to diffusion time
- Anomalous diffusion: $\langle x^2(t)\rangle \sim t^\alpha$ $(0<\alpha<1)$
- Goal 1: Classify between normal and anomalous diffusions ✓
- Goal 2: Find out the exact value of α in simulated environments ✓
- Final goal: Find out the exact value of α in real environments **(under development)**



✓ **Promising** results (with **simulated** diffusions)

✓ Real experiments involve additional difficulties:

1. The asymptotic limit is reached after a long time or with many diffusion compartments
2. The trace of some particles might be lost

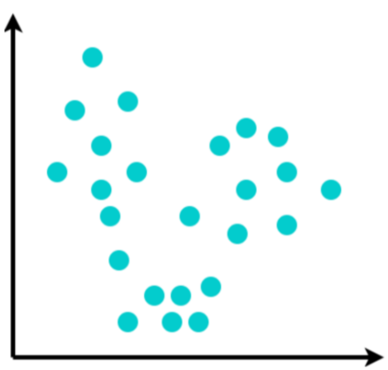
Quantum learning

- Copy of a a quantum data set (states): two quantum Turing machines: master with the original data set, and slave to perform the copy
- Perfect copy: complete(?) learning
- Learning should be more than making a copy: abstraction capability
- Classical oracle to assess the goodness of the copy

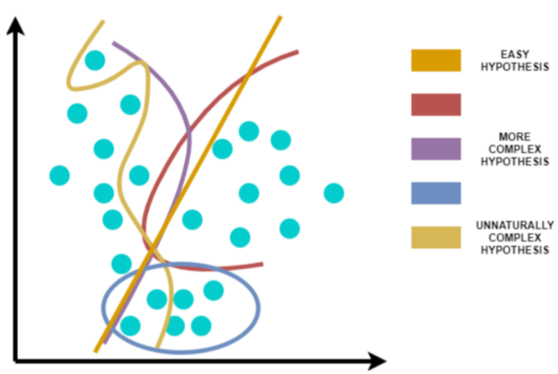
Active learning for quantum experimentation

- Choice of the most informative samples to be labeled
- Measurement destroys the information of superposition states
- AL to make a decision about when to measure

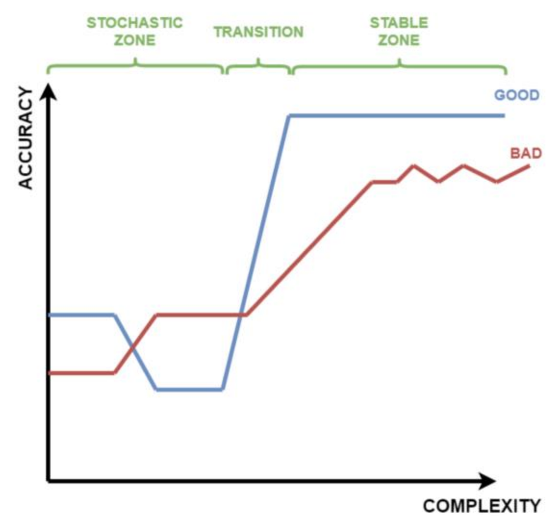
HYPOTHETICAL LEARNING



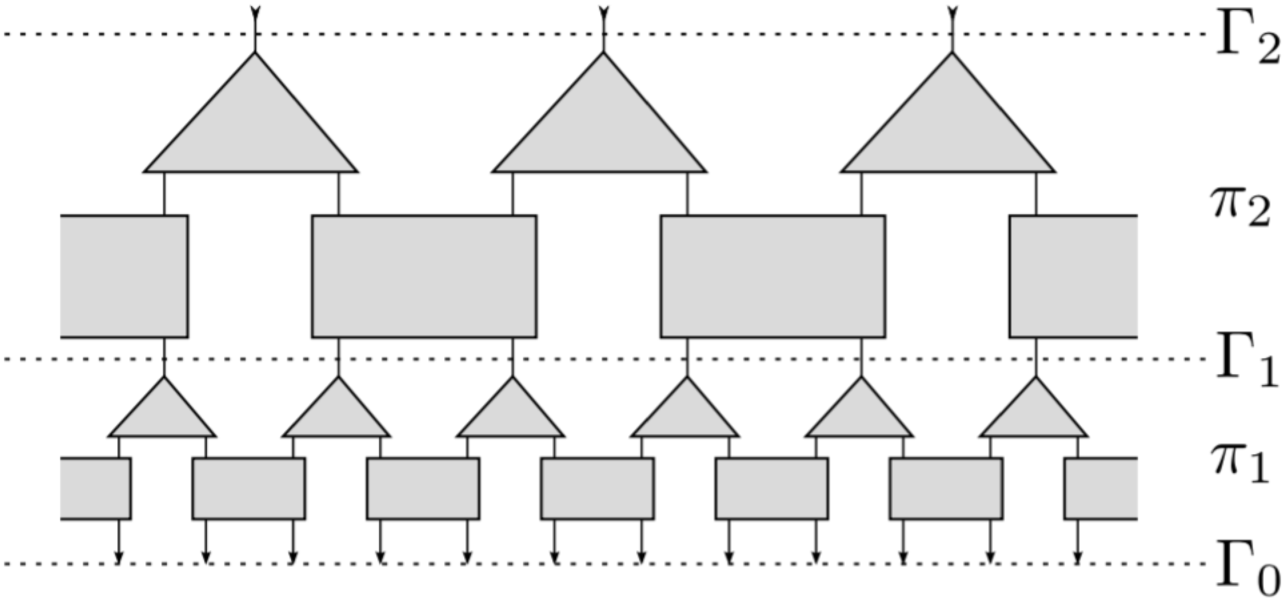
(a) Random points with no labels



(b) Some possible hypothesis



Connections with the renormalization group



- ✓ It recalls autoencoder processing
- ✓ ML may model renormalization groups
- ✓ Learning behaviors and relationships

Quantum linguistics and quantum economics

Quantum linguistics

- ✓ Natural Language Processing (NLP) to be implemented in quantum computers
- ✓ Fast way to implement NLP tasks
- ✓ Named-Entity Recognition, **Merge**, Part-of-Speech, Parsing, Sentiment Analysis, Translation

Quantum economics

- ✓ Forecasting financial events (ML)
- ✓ Immediacy may be crucial
- ✓ Behavioral economics: economic behaviors sometimes difficult to be modeled with classical approaches (several simultaneous and changing sub-behaviors, intrinsic to human beings)

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Conclusions

- **QML: ambitious and novel field of research**

- **Alternative and complementary point of view**

- **Promising results already**

- **Many work to do, and there is for everyone: quantum computers, QML algorithms, learning from quantum processes**

Thank you very much for your attention

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