Università del Salento
CdLM in Fisica

An Introduction to Quantum Machine Learning

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Outline

Basic references


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Quantum Physics-Informed Neural Networks.
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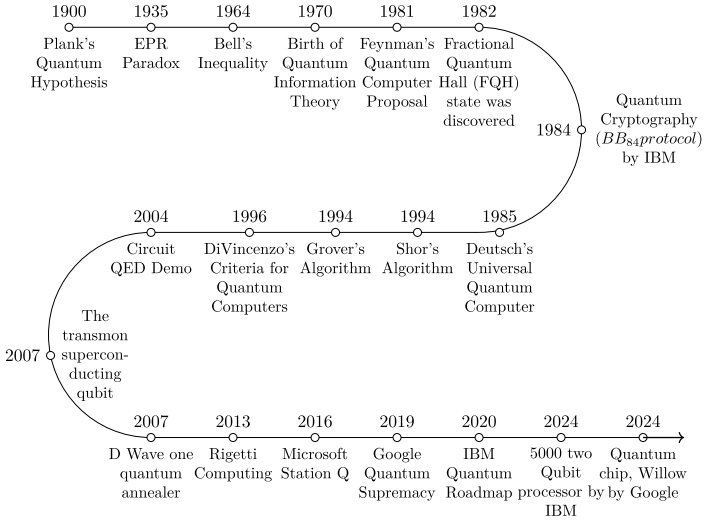
The Quantum Computing Era

Timeline of Quantum Computing



What Are Quantum Computers Good For?

- **Quantum computers** exploit **quantum coherence** and **entanglement** to perform certain computations beyond the capabilities of classical machines.
- They promise significant advantages in problems involving:
  - Quantum simulation (e.g., molecules, materials)
  - Combinatorial and global optimization
  - Factoring and cryptography
  - High-dimensional data processing
- **Quantum Machine Learning (QML)** combines quantum computing with machine learning to:
  - Speed up learning algorithms by leveraging quantum parallelism
  - Represent data and models more compactly via quantum states
  - Potentially solve learning tasks more efficiently
- While still in early stages, QML could lead to breakthroughs in areas such as drug discovery, finance, pattern recognition, and AI.

Elements of Machine Learning

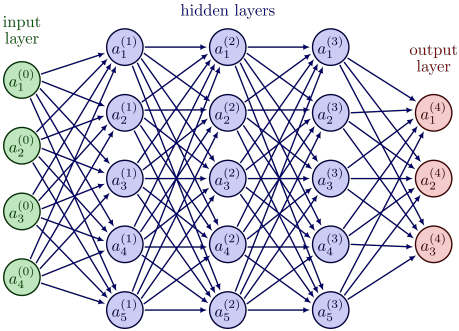
Definition (Tom Mitchell)

A computer program is said to ***learn*** *from experience E with respect to some class of tasks T, and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.*

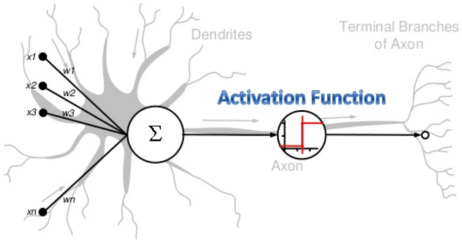
One distinguish many different kinds of learning tasks:

- **Supervised learning**
- **Unsupervised learning**
- **Reinforcement learning**.

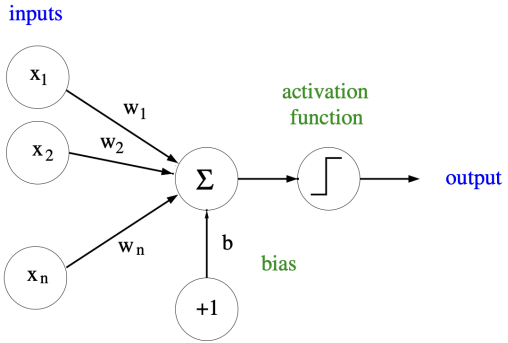
- The task T is to learn a mapping f from inputs $\boldsymbol{x} \in X$ to outputs $\boldsymbol{y} \in Y$.
- The inputs $\boldsymbol{x}$ are also called the **features**, **covariates**, or **predictors**.
- In this case, $X = \mathbb{R}^D$, where D is the number of input features. The output $\boldsymbol{y}$ is also known as the **label**, **target**, or **response**.
- The experience E is given as a set of N input-output pairs $\mathcal{D} = \{(\boldsymbol{x}_n, \boldsymbol{y}_n)\}_{n=1}^N$, known as the **training set**. (N is called the **sample size**).
- The performance measure P depends on the type of output we are predicting.
- Use cases: classification, regression, object detection, natural language processing, image and video analysis, speech recognition, ...



- Nodes are connected only from one layer to the next and all possible connections are present.
- Size of input and output layers are fixed by the problem.
- The parameters to learn are the weights of the connection.



Neuron



Artificial Neuron

- How do you get the right weights? By **training** your network.
- The goal of training is to minimize a **loss function**, as a function of the weights

$$\mathcal{L}(\boldsymbol{w}, \boldsymbol{b}) = \frac{1}{2} \sum_i ||\boldsymbol{y}(\boldsymbol{x}_i) - \hat{\boldsymbol{y}}(\boldsymbol{x}_i)||^2$$

- The loss function measures how well the neural network is performing on a given dataset.

For a MLP:

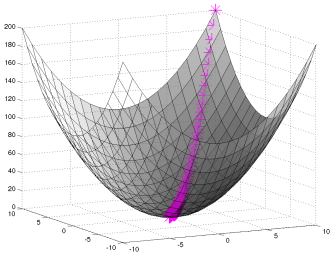
1. Start with random weights
2. Compute the prediction for a given input $\boldsymbol{x}$ and check the difference with target $\boldsymbol{y}$ and the loss.
3. Estimate an update for the weights that reduce the loss
4. Iterate from (2), repeating for all samples of the training dataset.

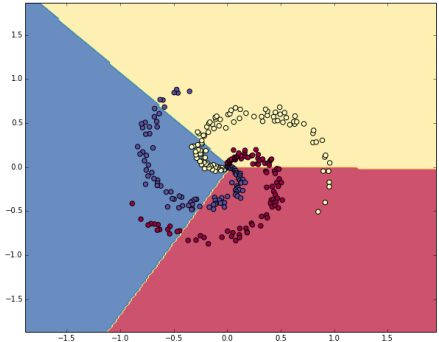
Gradient Descent

- One minimizes the loss function as a function of weights by using the **Gradient Descent method**.
- The gradient of the loss function $\mathcal{L}(\boldsymbol{w}, \boldsymbol{b})$ with respect to the parameters indicates the direction of steepest descent.
- By taking small steps in the opposite direction of the gradient, the algorithm converges towards the optimal set of parameters that minimize the loss function:

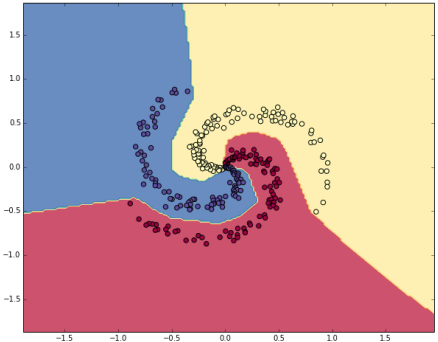
$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, \boldsymbol{b}),$$

  where η is the **learning rate**.
- The gradient is computed by the **backpropagation algorithm**.
- Variants: Stochastic Gradient Descent, Mini-batch Gradient Descent, ...





Linear Classifier



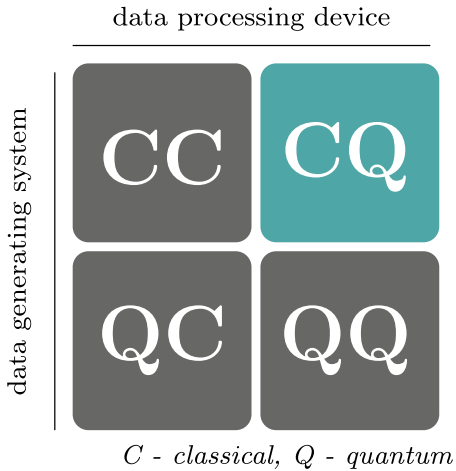
Neural Network Classifier

From `https://cs231n.github.io/neural-networks-case-study/`.

Quantum Machine Learning

Classical vs Quantum Machine Learning

- Classical ML models are able to recognise the statistical patterns in the data and produce the data that possess the same statistical patterns.
- If a small quantum processor can produce some statistical patterns that are difficult for a classical computer to perform computationally, they can perhaps also recognise patterns that are computationally difficult for a classical computer to find.
- This whole observation is the basis for the hope of answering whether an efficient quantum algorithm can be found for ML.
- ML relies heavily on probabilities. This is also what makes quantum systems a good candidate for ML applications.
- Due their strength in handling vast quantities of data and parallel processing, QC can aid in ML tasks.


data processing device
data generating system
CC
CQ
QC
QQ
C - classical, Q - quantum

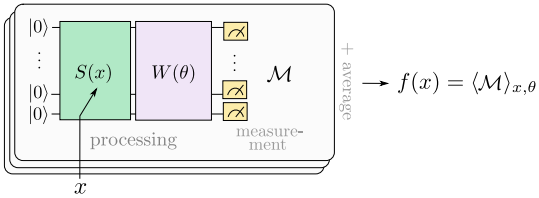
Variational Circuits as Machine Learning Models

- Quantum computing is in the **NISQ era**.
- To perform even the smallest of empirical benchmarks on simulators and early-stage quantum hardware, QML algorithms underlie strict design limitations.
- Large routines are not simulable on classical hardware, and quickly become drowned in noise on real quantum devices.
- Instead of outsourcing the entire ML pipeline to a QC, **hybrid quantum-classical algorithms** consider brief quantum computations as parts of more complex classical ones.
- A second strategy is to investigate generic **quantum models** as alternatives to classical ones.
- A perfect candidate for these requirements are **variational quantum circuits** (VQC), or **quantum neural networks** (QNN).

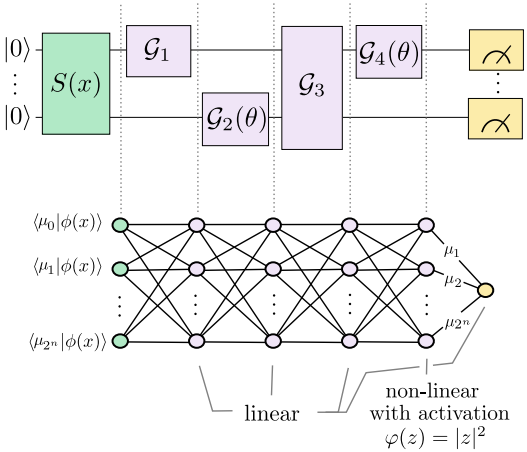
- Let $U(\boldsymbol{x}, \theta)$, with $\boldsymbol{x} \in X$, $\theta \in \mathbb{R}^K$ be a parametrized quantum circuit, and $\mathcal{M}$ a quantum observable.
- Let $|\psi(\boldsymbol{x}, \theta)\rangle \equiv U(\boldsymbol{x}, \theta)\,|0\rangle$. The function

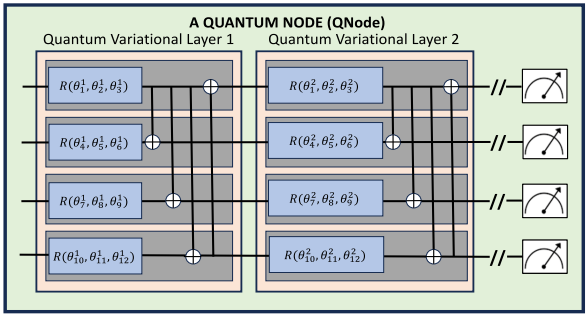
$$f_\theta(\boldsymbol{x}) := \langle\psi(\boldsymbol{x}, \theta)|\,\mathcal{M}\,|\psi(\boldsymbol{x}, \theta)\rangle\,,$$

defines a **deterministic variational quantum model**.



- Both VQCs and NNs can be thought of as layers of connected computational units controlled by adjustable parameters.
- This has led some authors to refer to VQCs as **quantum neural networks** but...
- First, quantum circuit operations are unitary and therefore linear; classical NNs use nonlinear activation functions.
- Second, it is impossible to access the quantum state at intermediate points during computation.
- This implies that executing the VQC cannot be seen as performing the forward pass of a neural network.
- Moreover, it is difficult to conceive a circuit learning algorithm that truly resembles backpropagation.


$|0\rangle$
$|0\rangle$
$S(x)$
$\mathcal{G}_1$
$\mathcal{G}_2(\theta)$
$\mathcal{G}_3$
$\mathcal{G}_4(\theta)$
$\langle\mu_0|\phi(x)\rangle$
$\langle\mu_1|\phi(x)\rangle$
$\langle\mu_{2^n}|\phi(x)\rangle$
μ_1
μ_2
μ_{2^n}
linear
non-linear
with activation
$\varphi(z) = |z|^2$



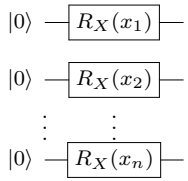
Hardware-efficient circuits alternate layers of native entangling gates and single-qubit rotations.

Angle (Rotation) Encoding

Goal: Encode classical data $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ into a quantum state using single-qubit rotations.

Idea: Use the data values as rotation angles for quantum gates acting on qubits.

Circuit Representation:



- Each classical input x_i controls a rotation gate.
- Common choices: $R_X(x_i)$, $R_Y(x_i)$, or $R_Z(x_i)$.
- Transforms each qubit into:
  $|\psi_i\rangle = \cos(x_i/2)\,|0\rangle + \sin(x_i/2)\,|1\rangle$
- Resulting quantum state: $|\psi(\boldsymbol{x})\rangle = \bigotimes_{i=1}^{n} |\psi_i\rangle$

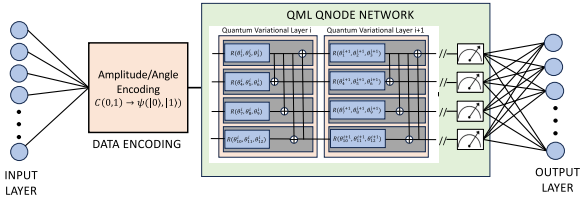
Pros:

- Simple and hardware-efficient
- Maintains normalization

- We want to optimize the parameters of a VQC in order to minimize a classical loss function.
- Quantum circuits do not allow direct computation of derivatives as in classical software.
- The **parameter-shift rule** provides an analytical method to estimate gradients using finite shifts.
- For a single parameter θ_i, the rule is:

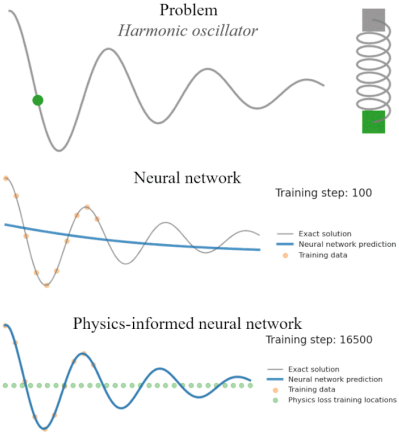
$$\frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \theta_i} = \frac{1}{2}\left[\mathcal{L}(\boldsymbol{\theta}_i^+) - \mathcal{L}(\boldsymbol{\theta}_i^-)\right], \qquad \boldsymbol{\theta}_i^{\pm} = \boldsymbol{\theta} \pm \frac{\pi}{2}\boldsymbol{e}_i.$$

- This means we must evaluate the quantum circuit twice per parameter, with positive and negative shifts.
- In **hybrid quantum-classical models** automatic differentiation can still be used.
- This allows training QNNs similarly to classical NNs.


QML QNODE NETWORK
Quantum Variational Layer i
Quantum Variational Layer i+1
Amplitude/Angle Encoding
$C(0,1) \rightarrow \psi(|0\rangle, |1\rangle)$
DATA ENCODING
INPUT LAYER
OUTPUT LAYER
Amplitude/Angle Encoding
$C(0,1) \rightarrow \psi(|0\rangle, |1\rangle)$
DATA ENCODING 1
QNN 1
Amplitude/Angle Encoding
$C(0,1) \rightarrow \psi(|0\rangle, |1\rangle)$
DATA ENCODING 2
QNN 2
INPUT LAYER
OUTPUT LAYER

Example: Quantum Physics-Informed Neural Networks I

- **Quantum Physics-Informed Neural Networks** (QPINNs) are a class of NNs that leverage QC principles to solve PDEs.
- While NN function approximation/regression has shown to be a valuable tool for data-rich scenarios, data-only models are not constrained by physics and can perform poorly in sparse- or no-data regions.
- To build reliable physical models in these regions, **Physics-Informed NNs** (PINNs) can be used.



Example: Quantum Physics-Informed Neural Networks II

- PINNs supplement the data-driven loss with **PDE residuals** representing physical conservation principles.
- Consider a time-dependent PDE of the form

$$u_t + \mathcal{N}[u] = 0, \qquad t \in [0, T], \quad x \in \Omega$$

subject to initial and boundary conditions

$$u(0, x) = g(x), \quad x \in \Omega, \qquad \mathcal{B}[u] = u_0, \quad t \in [0, T], \quad x \in \partial\Omega$$

where $\mathcal{B}[\cdot]$ is a boundary operator corresponding to the equation's boundary conditions (Dirichlet, Neumann, etc.).

Example: Quantum Physics-Informed Neural Networks III

- If the NN solution is given by $u_\theta(t, x)$, where θ denotes the tunable parameters of the network, then the parameterized solution of the PDE in residual form is given by

$$\mathcal{R}_\theta(t, x) \coloneqq \frac{\partial u_\theta}{\partial t} + \mathcal{N}[u_\theta],$$

and the PINN is trained on the composite loss function

$$\mathcal{L}_\theta \coloneqq \mathcal{L}_{\text{IC}}(\theta) + \mathcal{L}_{\text{BC}}(\theta) + \mathcal{L}_r(\theta),$$

where $\mathcal{L}_{\text{IC}}$ and $\mathcal{L}_{\text{BC}}$ are the losses associated with the ICs and BCs, respectively, and $\mathcal{L}_r$ is the residual loss given by

$$\mathcal{L}_r(\theta) \coloneqq \frac{1}{N_r} \sum_{i=1}^{N_r} ||\mathcal{R}_\theta(t_i, x_i)||^2,$$

- Recently, QPINNs have been shown capable of increasing model accuracy when compared to purely classical NNs in computational fluid dynamics.