

INTRODUCTION TO CLASSICAL MACHINE LEARNING AND NEURAL NETWORKS

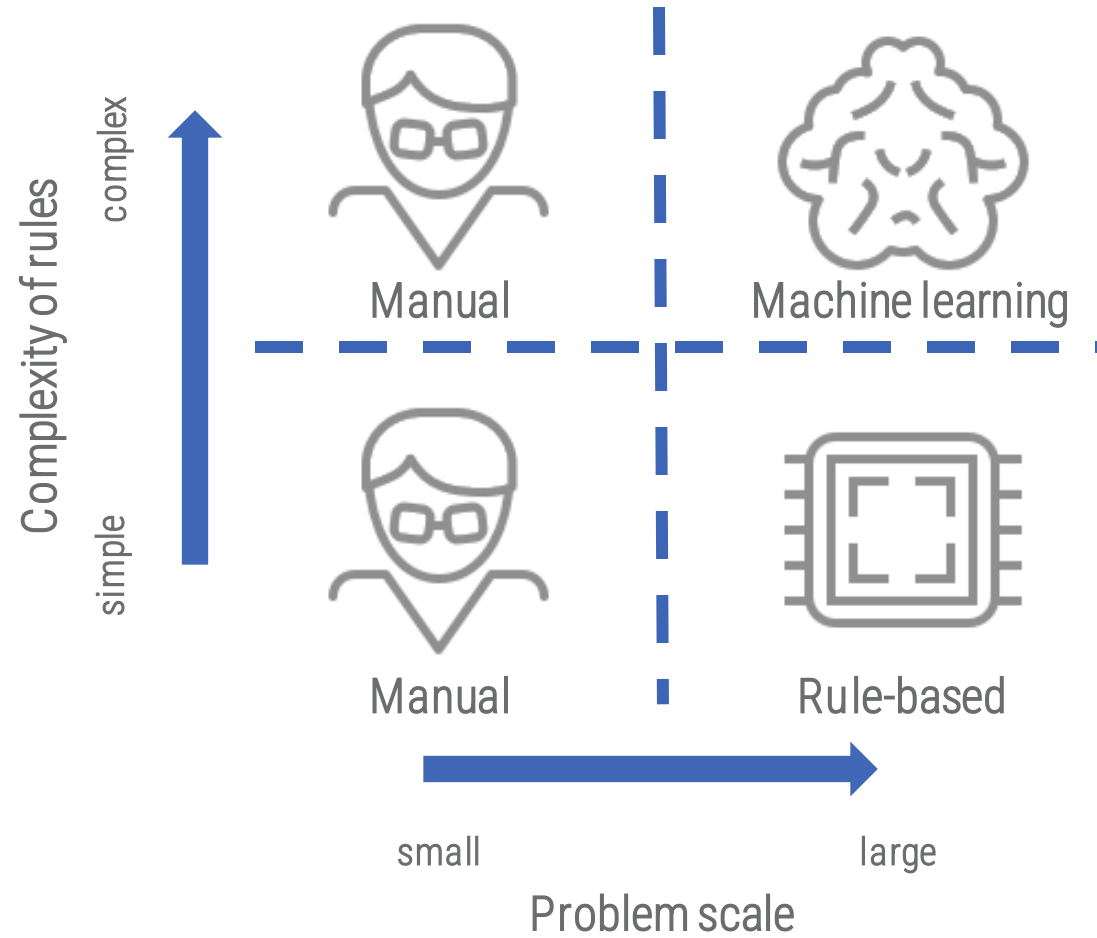
Marco Maronese - PhD student @ University of Bologna

- Machine Learning Introduction
- Classical Support Vector Machine (SVM)
- Neural Networks

Machine Learning Introduction

MACHINE LEARNING

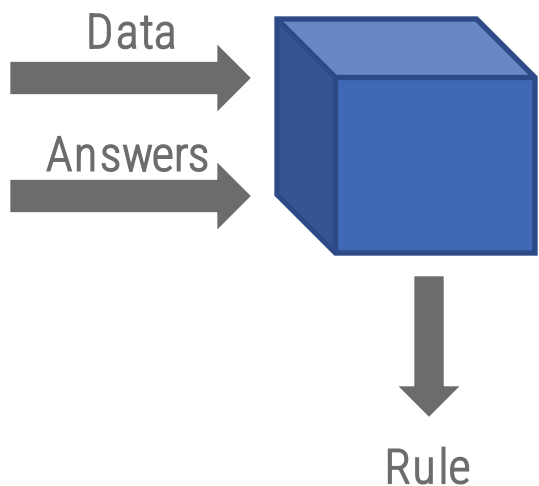
Concept



MACHINE LEARNING

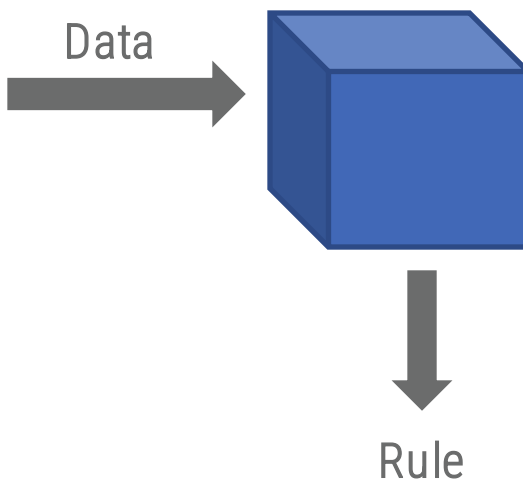
Branches of machine learning

Supervised



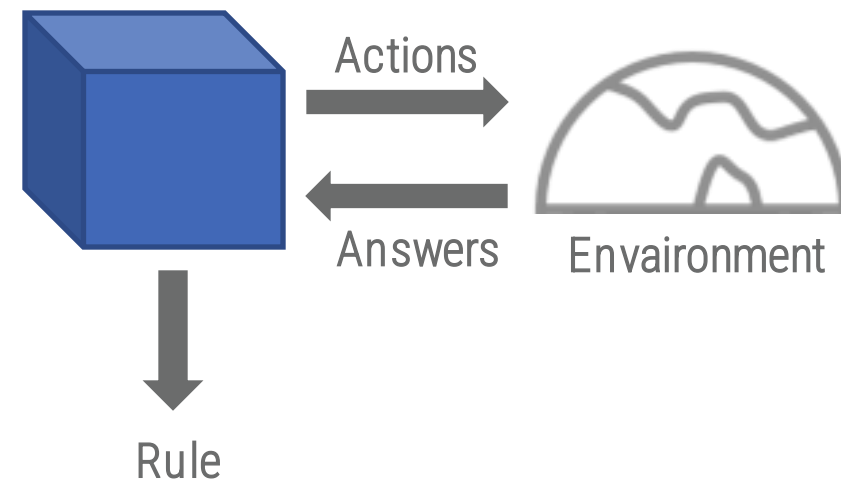
Labeled data

Unsupervised



Correlations

Reinforced



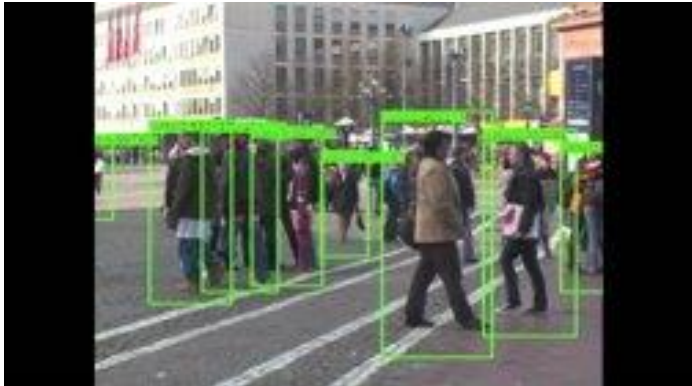
Strategy

MACHINE LEARNING

Branches of machine learning

Supervised

- Classification
- Regression



Unsupervised

- Clustering
- Data Generation



Reinforced

- Game theory
- Robotics



SUPERVISED LEARNING

APPLICATIONS

- Identification of faces in images
- Identification of pedestrian
- Classification of texts
- Bioinformatics research
- Classification of remotely sensed images

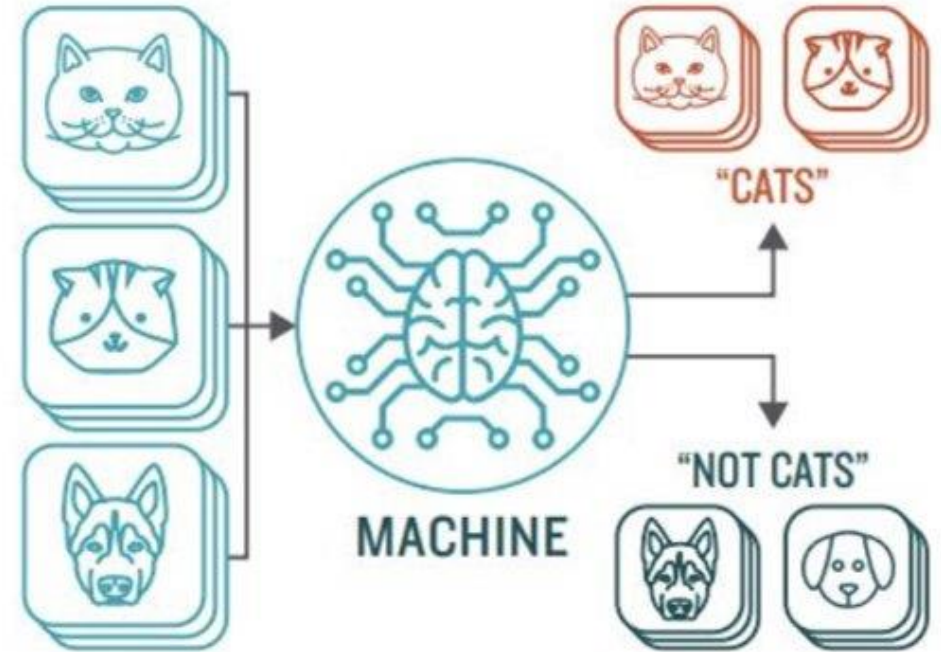


SUPERVISED LEARNING

Classification Problem

Classification Rule

$$y = \begin{cases} 1, & \text{if } f(x, \theta) > \text{threshold} \\ 0, & \text{if } f(x, \theta) \leq \text{threshold} \end{cases}$$



SUPERVISED LEARNING

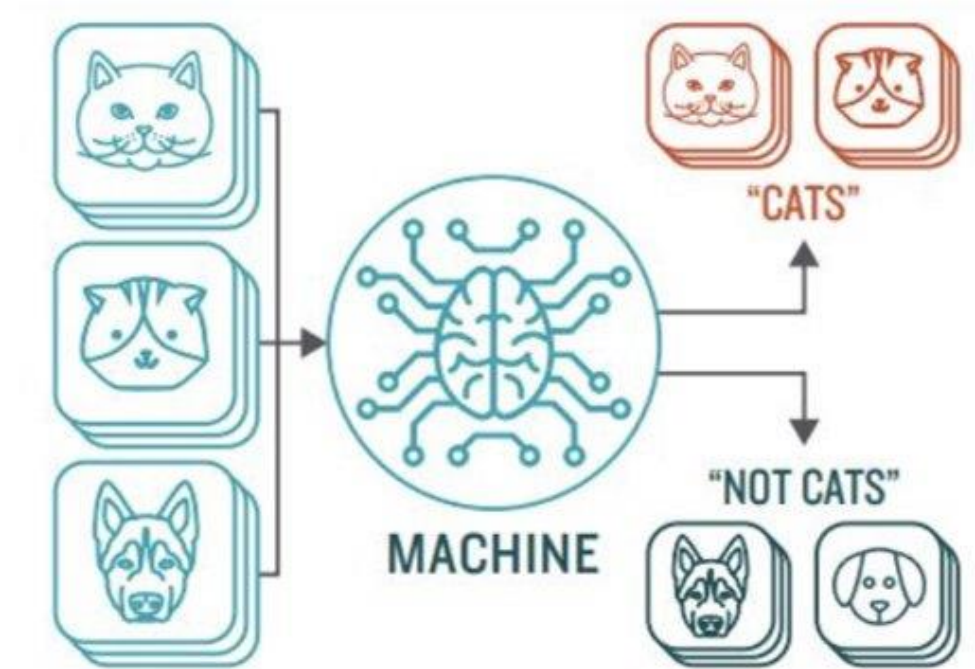
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Model

Learning parameters



SUPERVISED LEARNING

Classification Problem

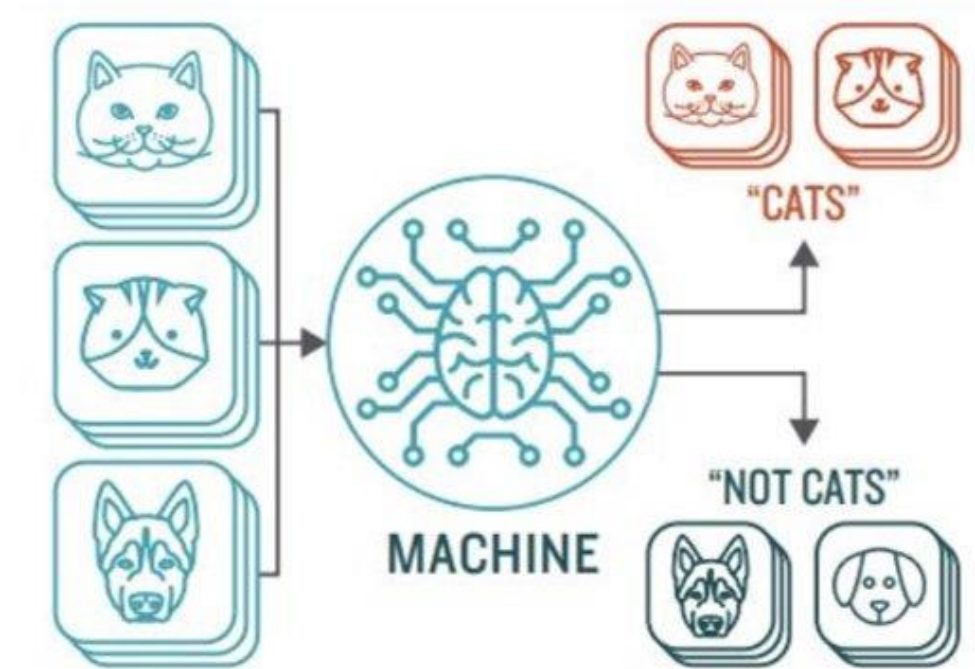
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Model

Support Vector Machine Rule

$$y = \text{sign}(\vec{\varphi}(\vec{x}) \cdot \vec{w} + b)$$



SUPERVISED LEARNING

Classification Problem

Classification Rule

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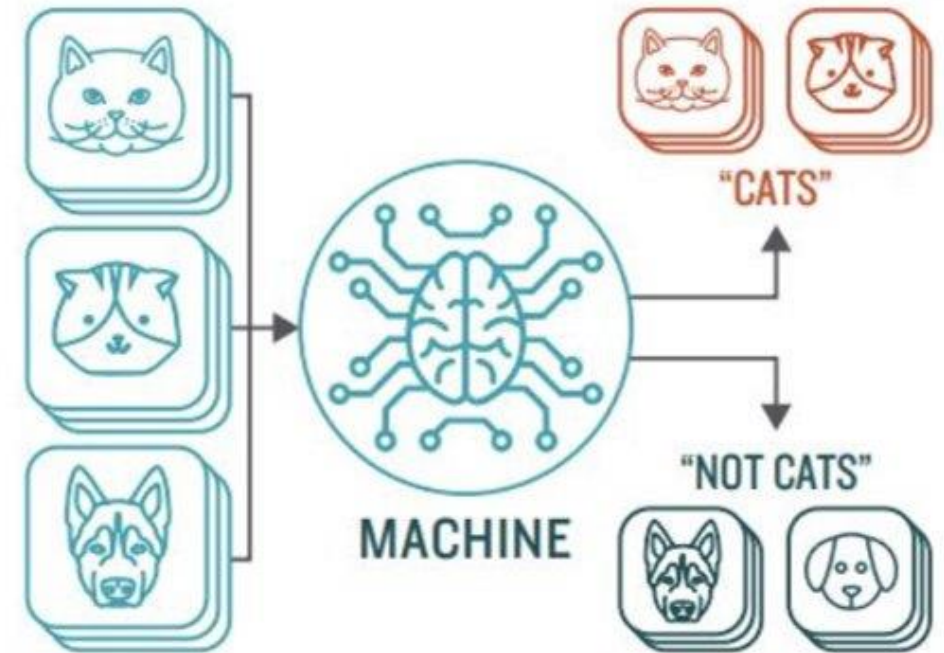
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$$y = \text{sign}(\underline{\vec{\varphi}}(\vec{x}) \cdot \vec{w} + b)$$

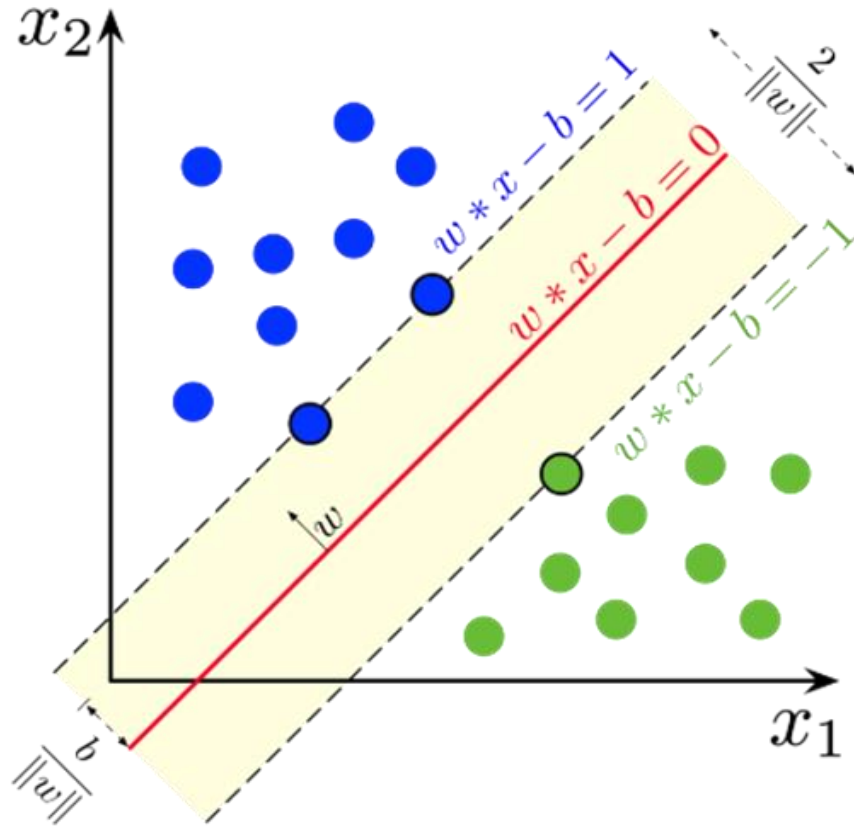
Non linear
feature map



Classical Support Vector Machine (SVM)

SUPPORT VECTOR MACHINE

Overview



Margin width

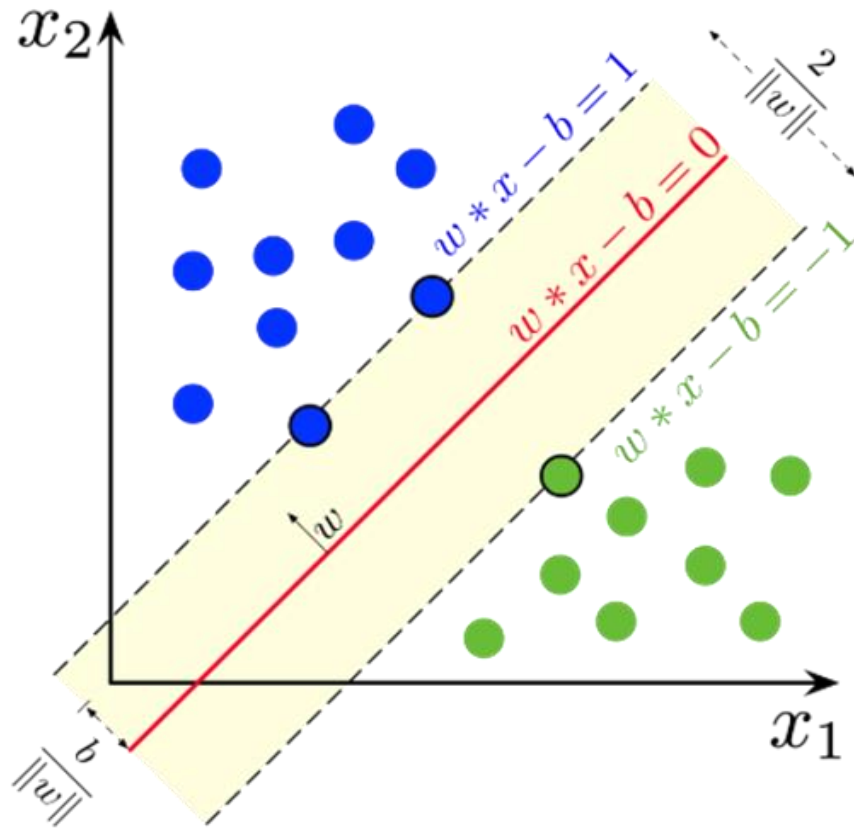
$$\frac{b + 1}{\|\mathbf{w}\|} - \frac{b - 1}{\|\mathbf{w}\|} = \frac{2}{\|\mathbf{w}\|}$$

Support vector

$$\mathbf{x}_i \text{ Such that } y_i(\mathbf{x}_i \cdot \mathbf{w} - b) = 1$$

SUPPORT VECTOR MACHINE

Overview



Objective:

minimize $\|w\|$

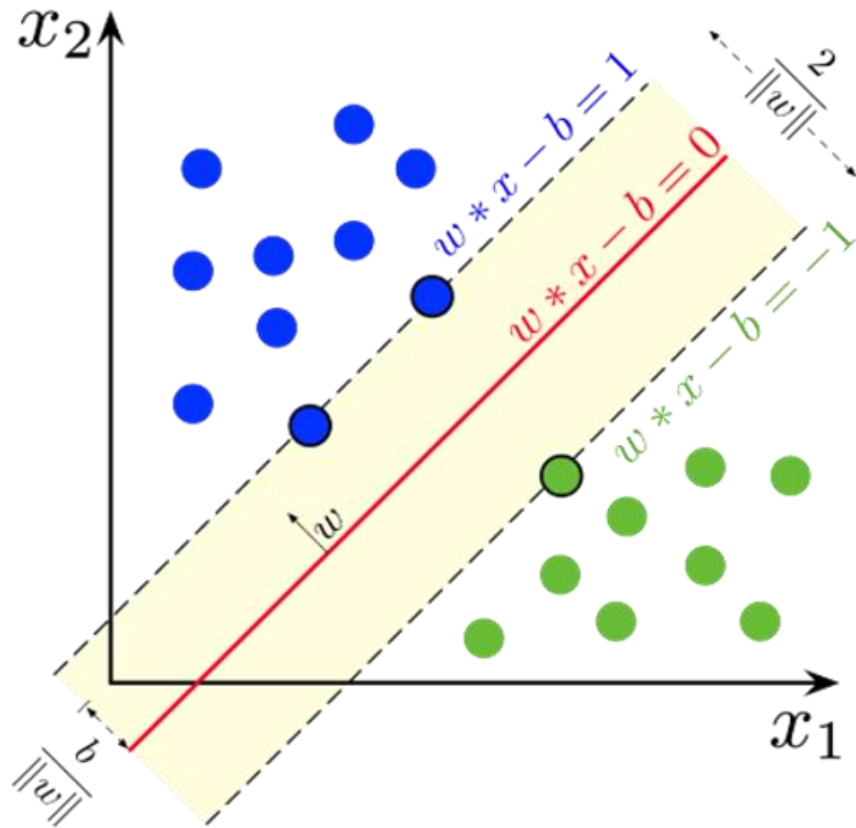
Constraints

$$x_i \cdot w - b \leq -1 \quad \text{for } y_i = -1$$

$$x_i \cdot w - b \geq 1 \quad \text{for } y_i = 1$$

SUPPORT VECTOR MACHINE

Overview



Objective:

minimize $\|w\|$

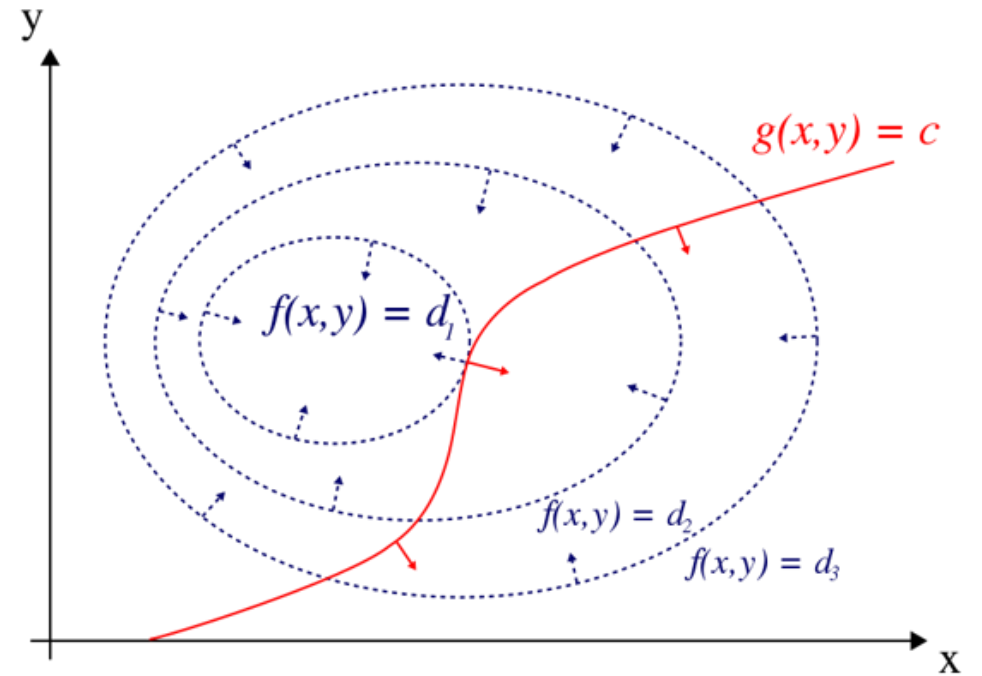
Constraints

$$y_i(x_i \cdot w - b) - 1 \geq 0 \quad \forall i$$

SUPPORT VECTOR MACHINE

Optimization

$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i \left[y_i (\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \right]$$

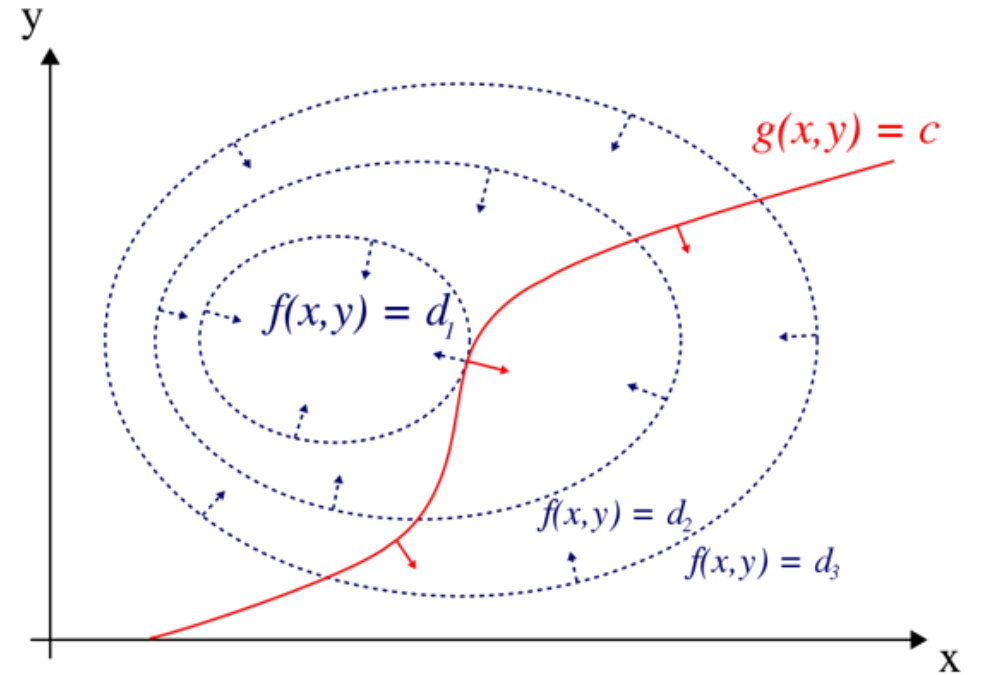


SUPPORT VECTOR MACHINE

Optimization

$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i [y_i (\mathbf{x}_i \cdot \mathbf{w} + b) - 1]$$

Lagrange multipliers



SUPPORT VECTOR MACHINE

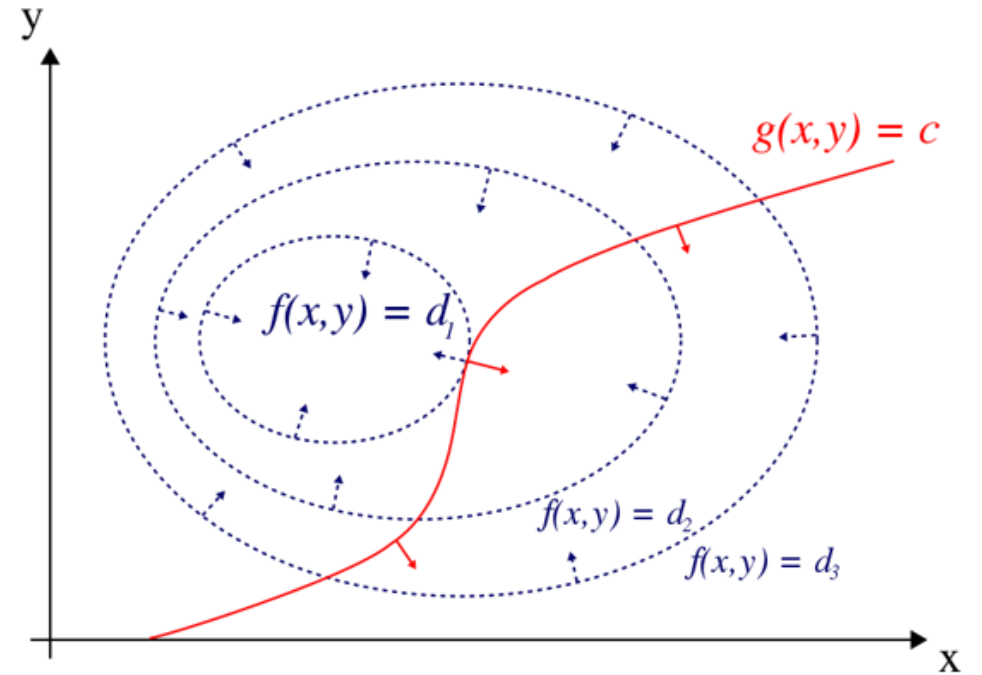
Optimization

$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i \left[y_i (\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \right]$$

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^l \alpha_i y_i \mathbf{x}_i$$

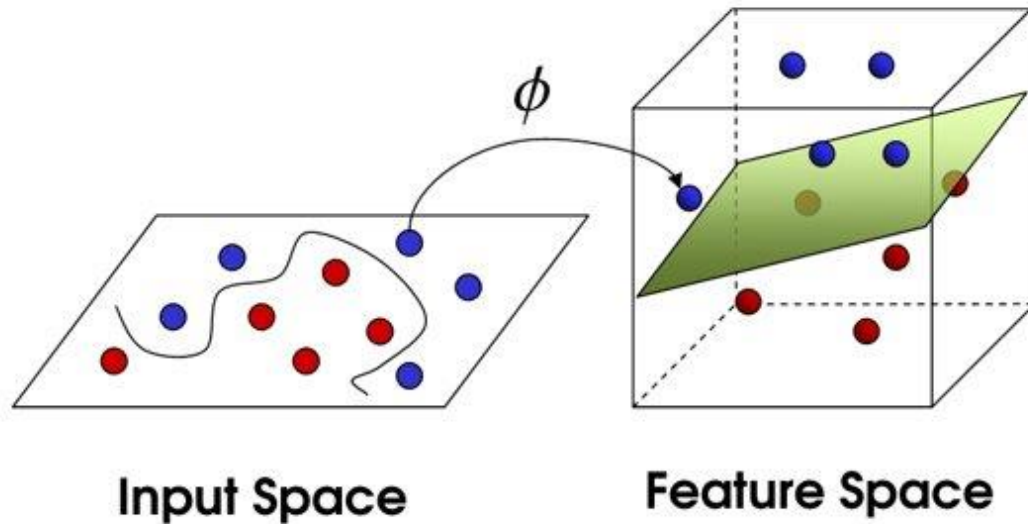
$$\frac{\partial L_P}{\partial b} = 0 \quad \Rightarrow \quad \sum_{i=1}^l \alpha_i y_i = 0$$

$$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$



SUPPORT VECTOR MACHINE

Non-linear case



Input space

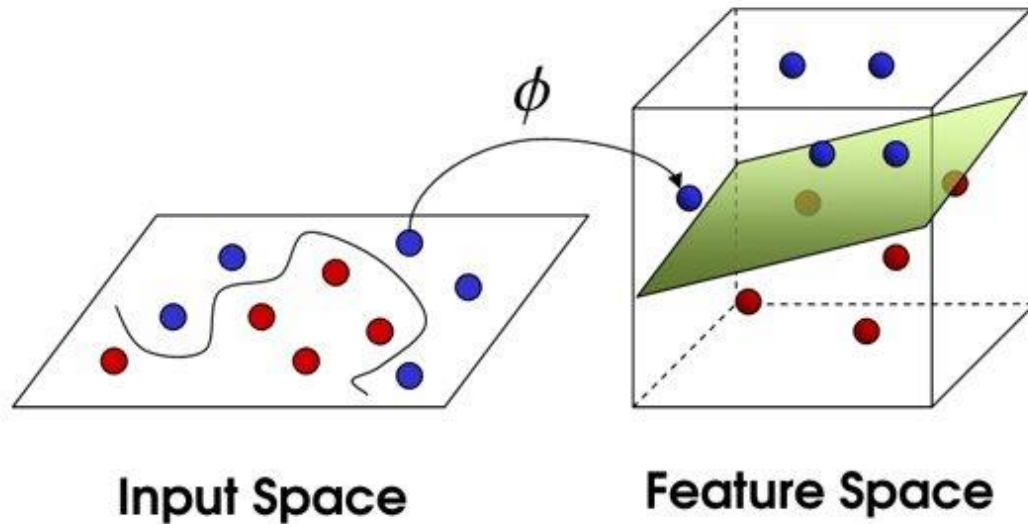
$$\mathbf{x}_i = (x_{0,i}, x_{1,i}, \dots)$$

Feature space

$$\varphi(\mathbf{x}_i) = (x_{0,i}, x_{1,i}, \dots, \phi(x_{0,i}, x_{1,i}, \dots))$$

SUPPORT VECTOR MACHINE

Non-linear case



Input space

$$\mathbf{x}_i = (x_{0,i}, x_{1,i}, \dots)$$

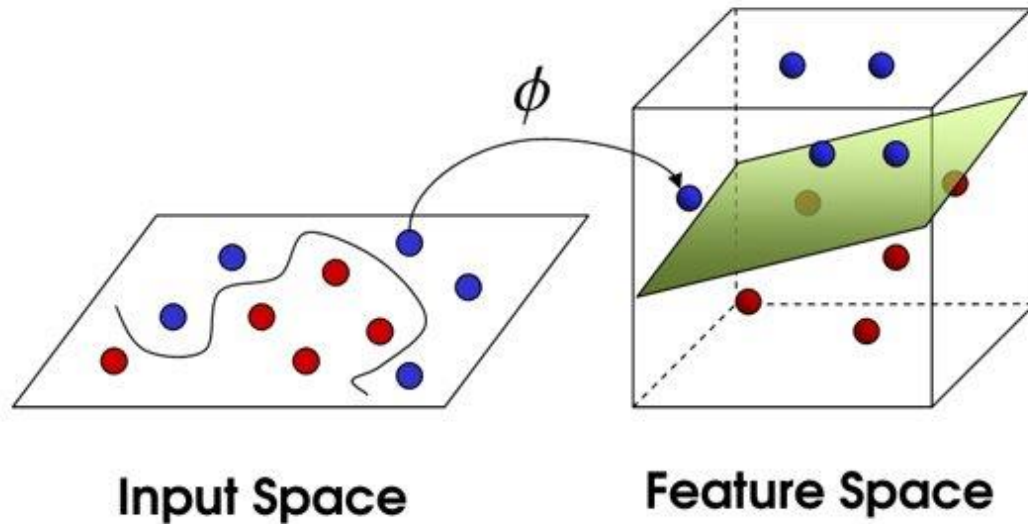
Feature space

$$\underline{\varphi(\mathbf{x}_i)} = (x_{0,i}, x_{1,i}, \dots, \phi(x_{0,i}, x_{1,i}, \dots))$$

Feature map

SUPPORT VECTOR MACHINE

Non-linear case



$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i \left[y_i (\boldsymbol{\varphi}(\mathbf{x}_i) \cdot \mathbf{w} + b) - 1 \right]$$

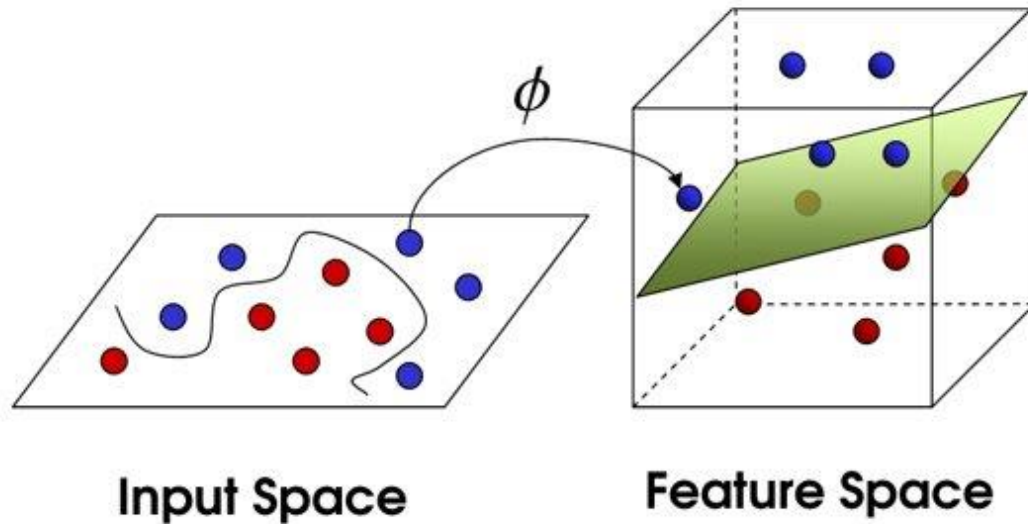
$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^l \alpha_i y_i \boldsymbol{\varphi}(\mathbf{x}_i)$$

$$\frac{\partial L_P}{\partial b} = 0 \quad \Rightarrow \quad \sum_{i=1}^l \alpha_i y_i = 0$$

$$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$$

SUPPORT VECTOR MACHINE

Non-linear case



$$L_P \equiv \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^l \alpha_i \left[y_i (\boldsymbol{\varphi}(\mathbf{x}_i) \cdot \mathbf{w} + b) - 1 \right]$$

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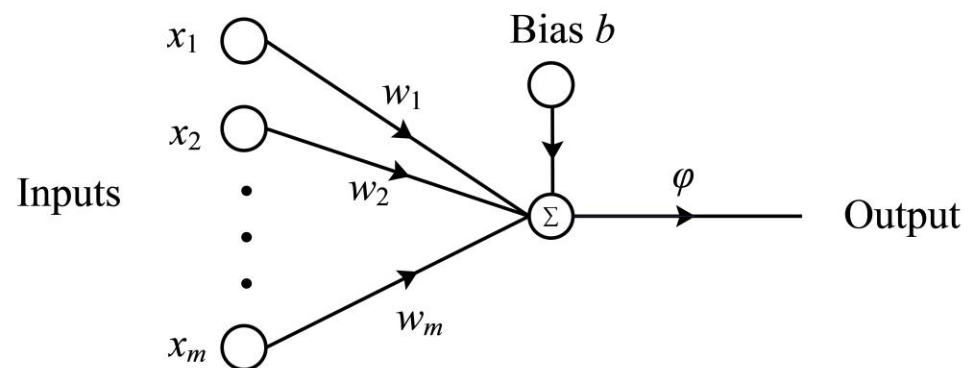
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$$L_D = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{\boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)}$$

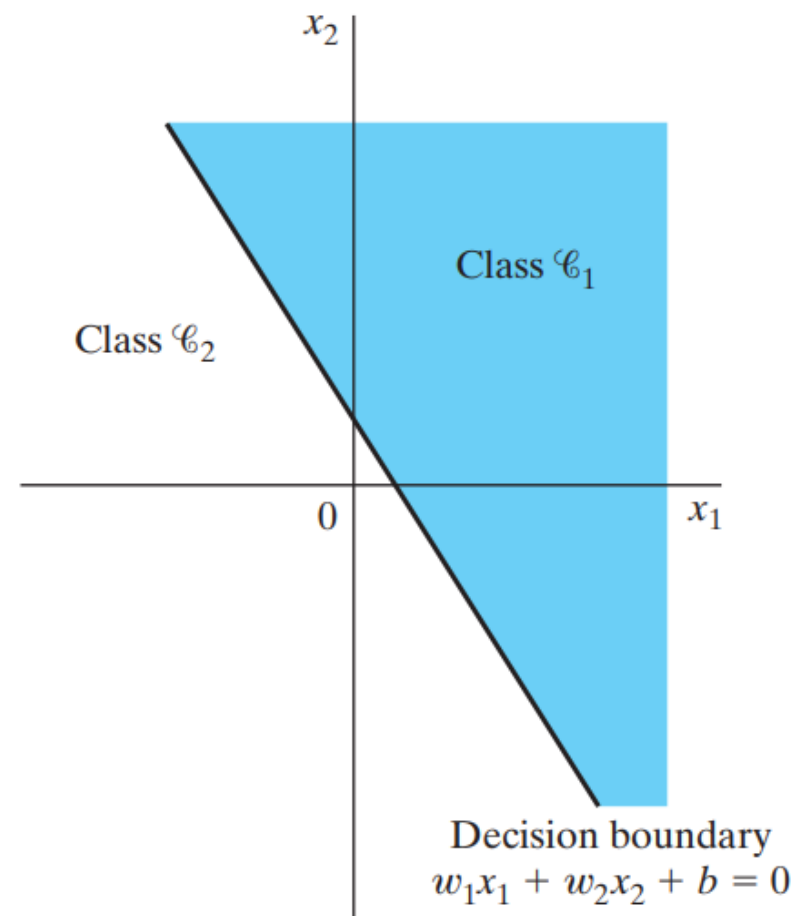
Kernel matrix $K(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$

Neural Networks

PERCEPTRON

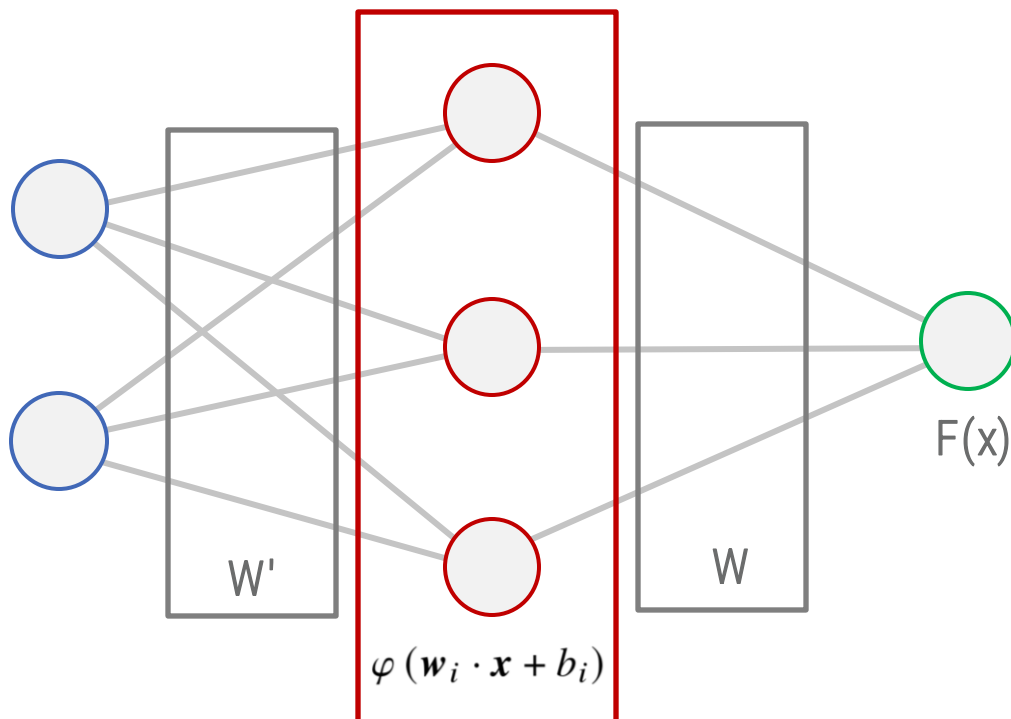


$$F(\mathbf{x}) = \phi \left(\sum_{i=0}^m x_i w_i + b \right) = \begin{cases} 1, & \text{if } \sum_{i=0}^m x_i w_i + b > 0 \\ 0, & \text{otherwise} \end{cases}$$



NEURAL NETWORKS

From Perceptron to Hornik theorem



Hornik theorem

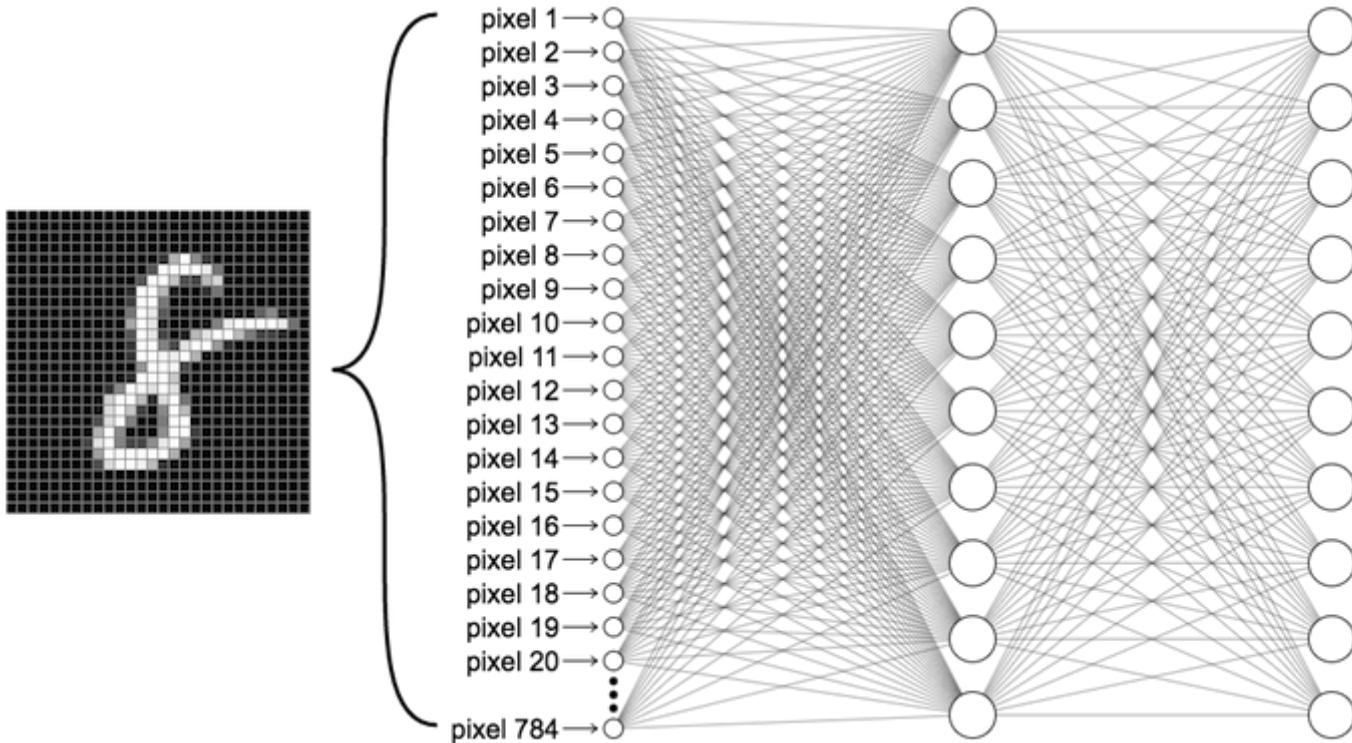
$$F(\mathbf{x}) = \sum_{i=1}^N \mathbf{w}'_i \varphi(\mathbf{w}_i \cdot \mathbf{x} + b_i)$$

- 1 output
- 1 hidden layer
- N hidden neurons

NEURAL NETWORKS

Deep supervised learning

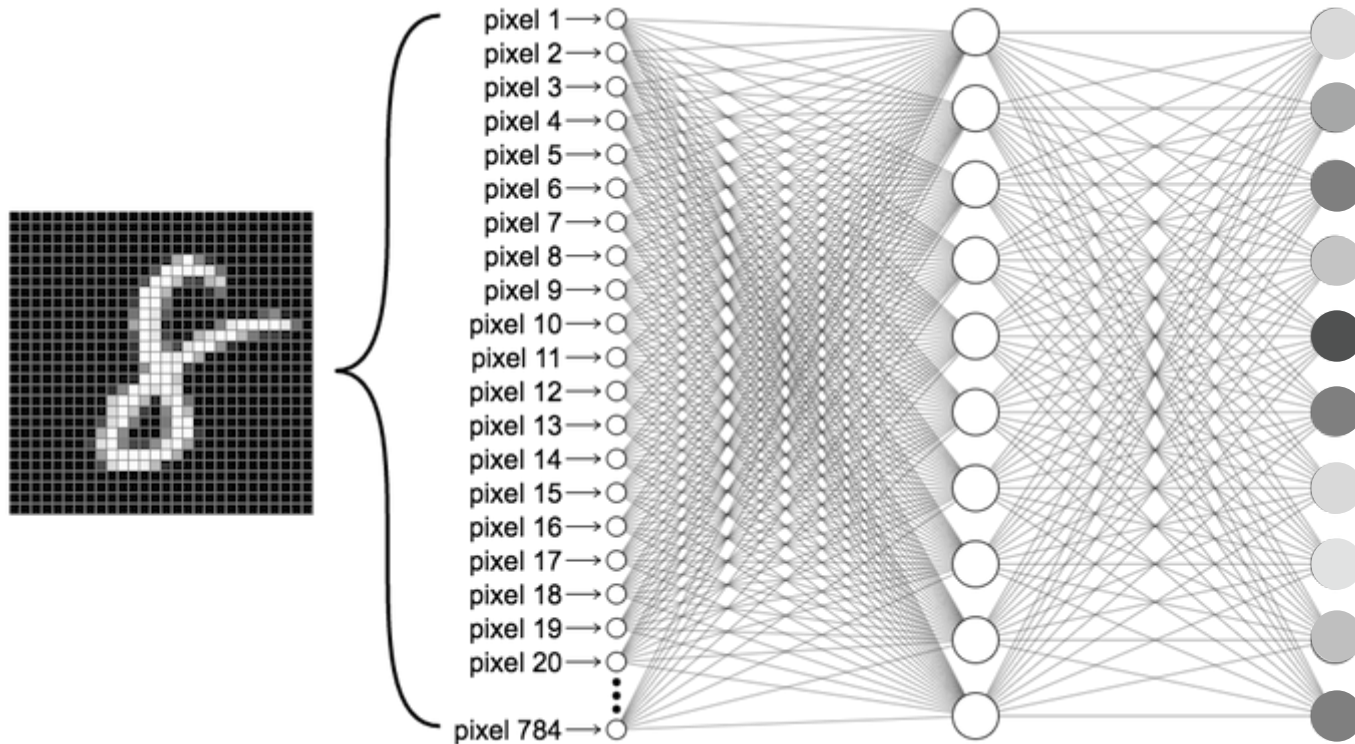
Before Training: Random parameters



NEURAL NETWORKS

Deep supervised learning

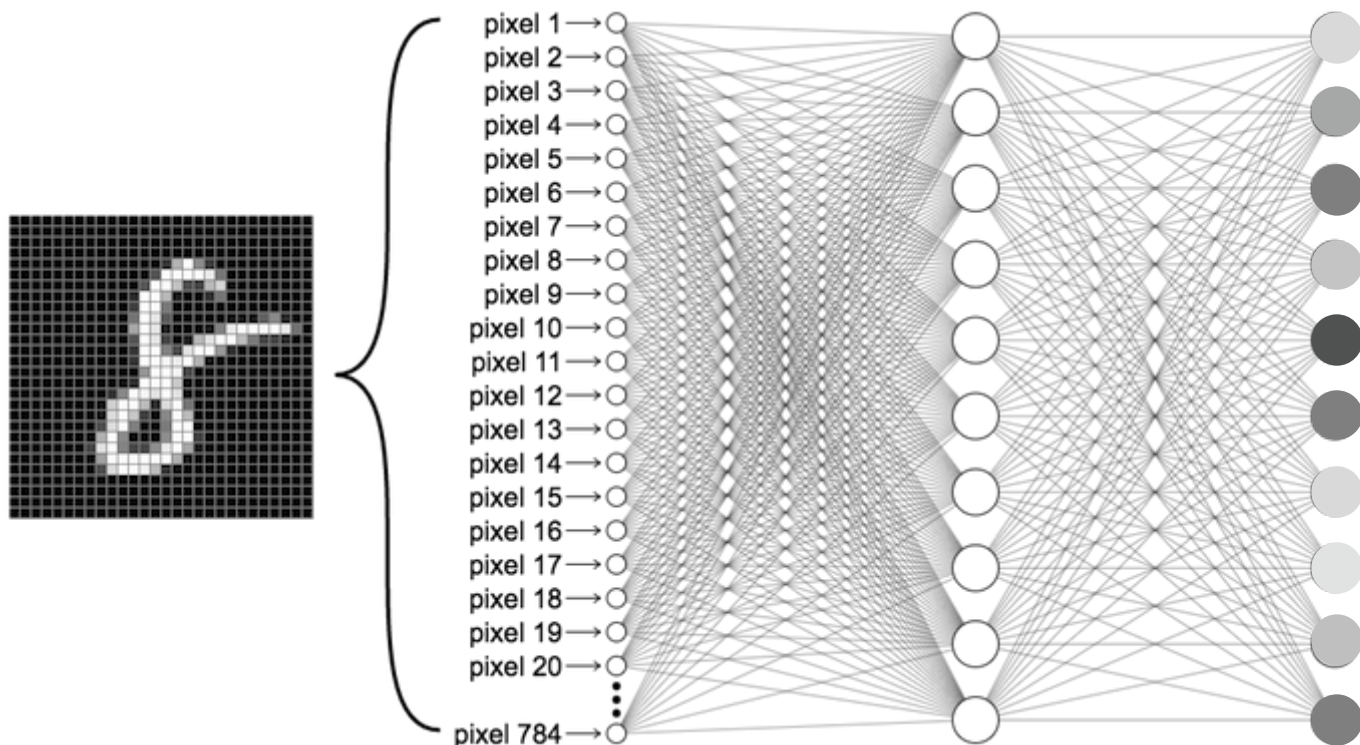
Before Training: Random parameters



NEURAL NETWORKS

Deep supervised learning

Before Training: Random parameters



LOSS function

The distance between the neural network predictions and the labels of the training set

- MSE

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=0}^N (y_i - \hat{y}_i)^2$$

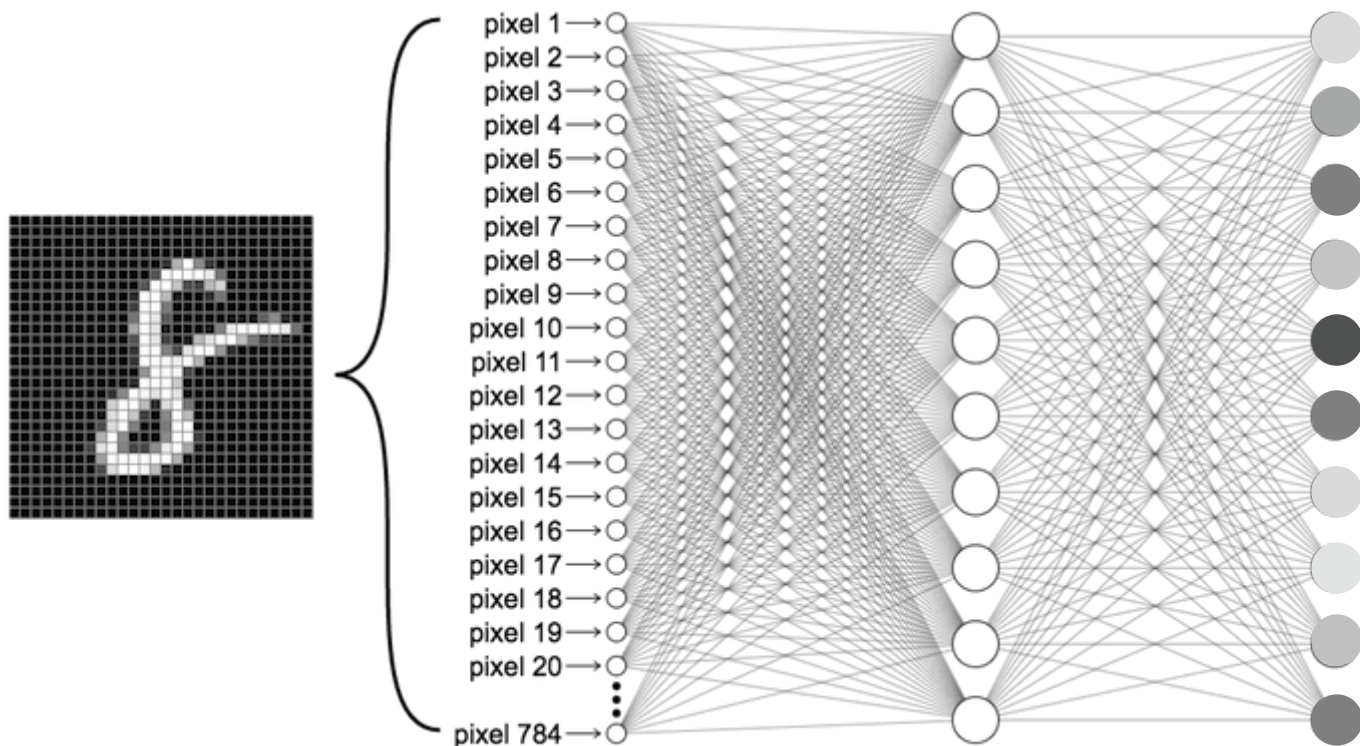
- Cross-Entropy

$$\mathcal{L}(\theta) = - \sum_{i=0}^N \hat{y}_i \cdot \log(y_i)$$

NEURAL NETWORKS

Deep supervised learning

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LOSS function

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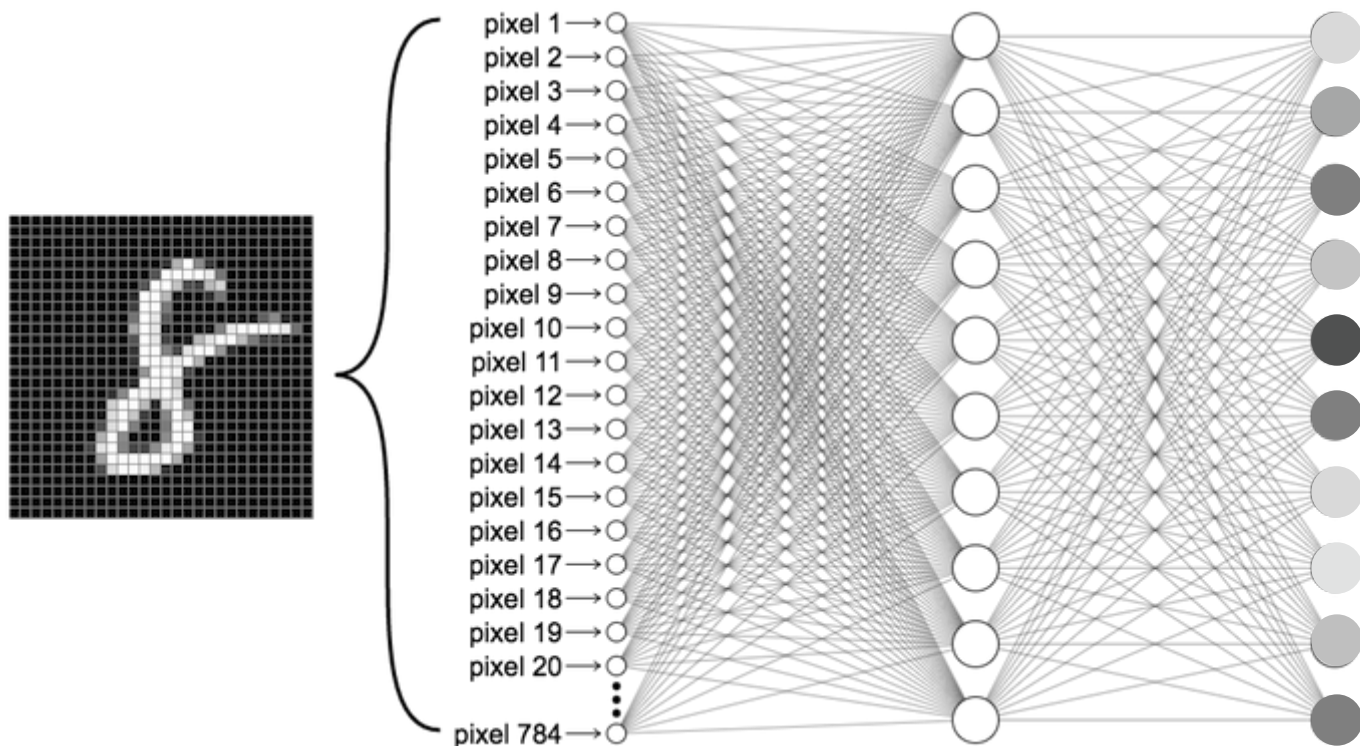
Truth label

Neural network prediction

NEURAL NETWORKS

Deep supervised learning

Before Training: Random parameters



Loss function optimization

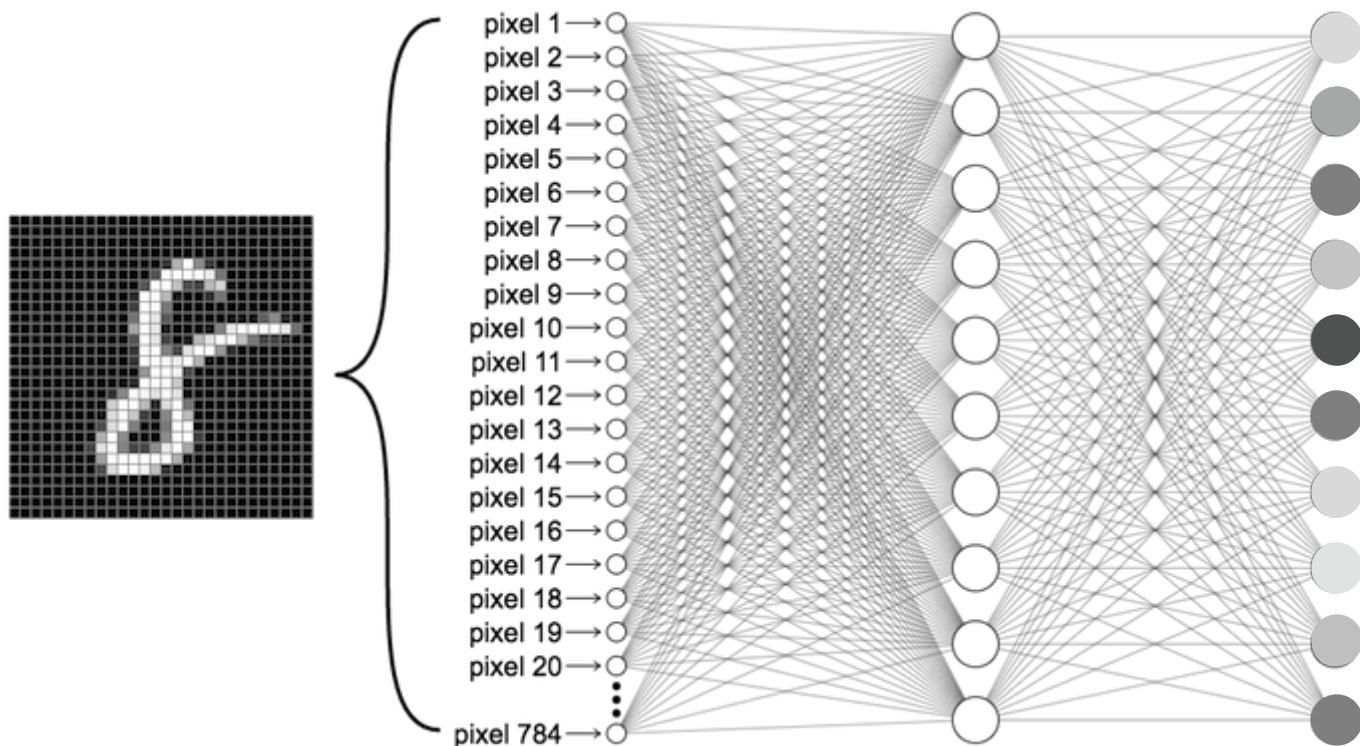
Gradient descent

$$\theta \leftarrow \theta - \alpha \nabla \mathcal{L}(\theta)$$

NEURAL NETWORKS

Deep supervised learning

Before Training: Random parameters



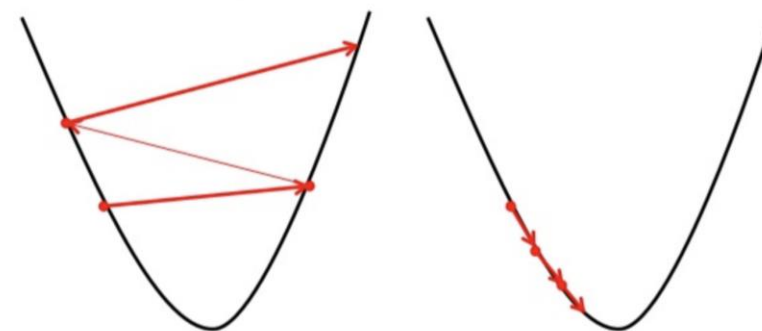
Loss function optimization

Gradient descent

$$\theta \leftarrow \theta - \alpha \nabla \mathcal{L}(\theta)$$

Learning rate

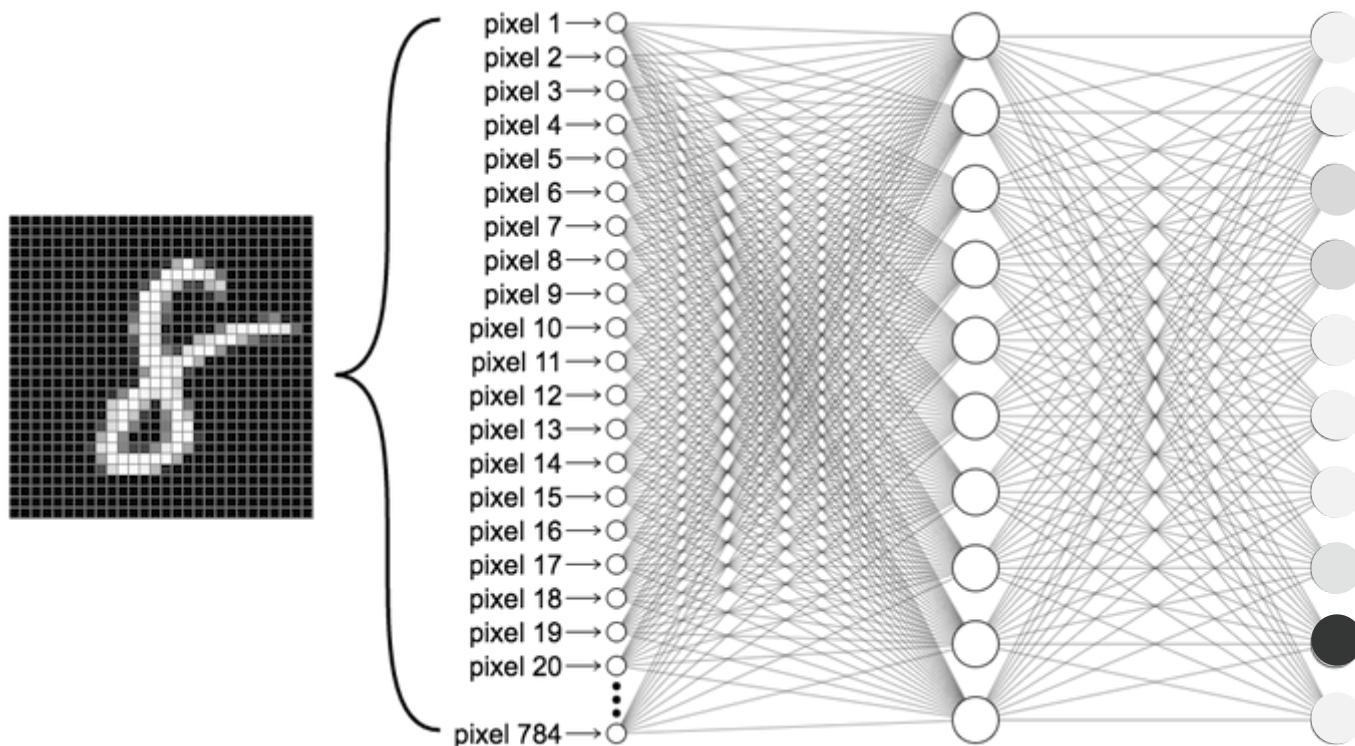
Backpropagation:
Compute the gradient by
chain rule



NEURAL NETWORKS

Deep supervised learning

After Training: Optimal parameters



<https://playground.tensorflow.org/>

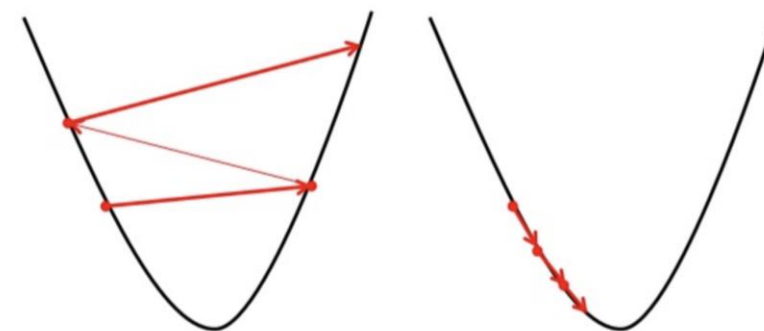
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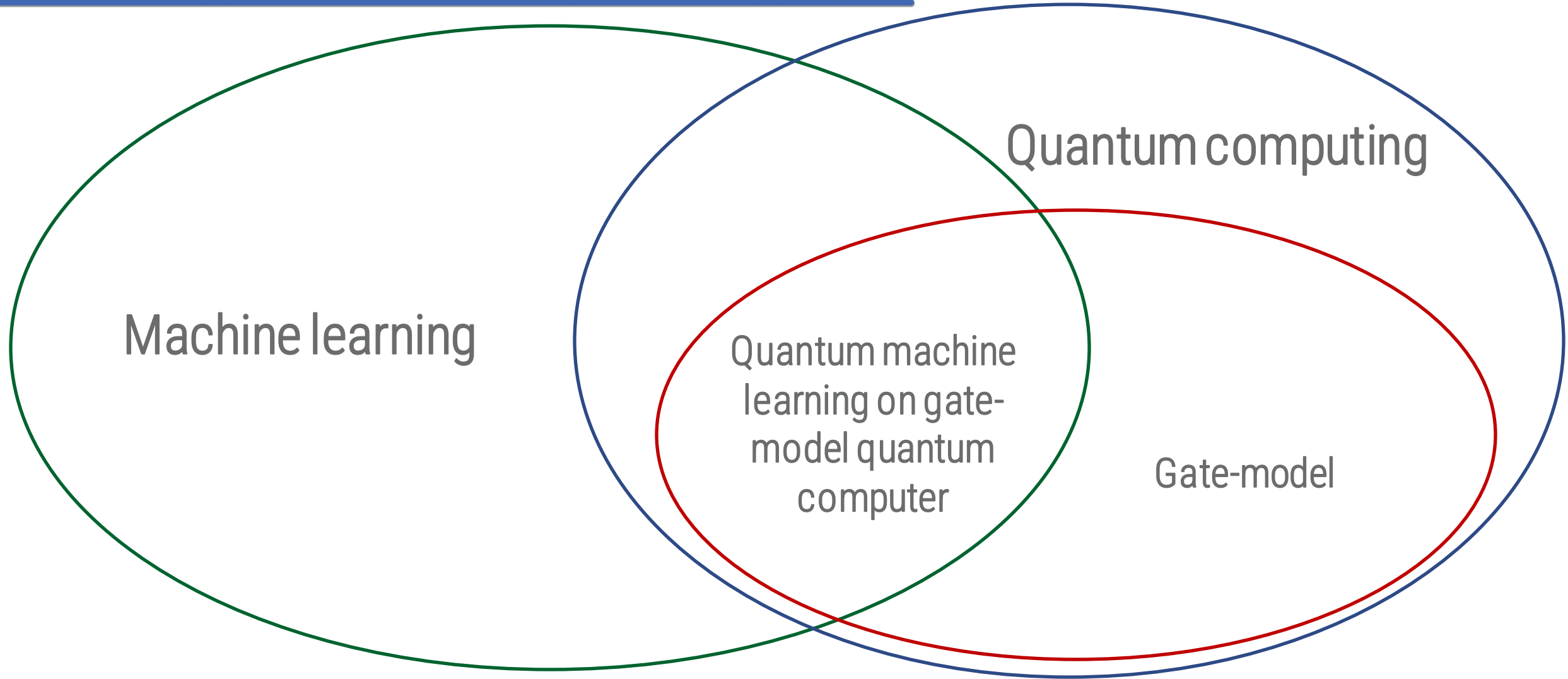
QUANTUM MACHINE LEARNING ON NISQ DEVICES

Marco Maronese - PhD student @ University of Bologna

- Quantum Machine Learning on NISQ devices
- Quantum Support Vector Machine (QSVM)
- Quantum Neural Networks (QNN)

Quantum Machine Learning on NISQ devices

QUANTUM MACHINE LEARNING



APPLICATIONS

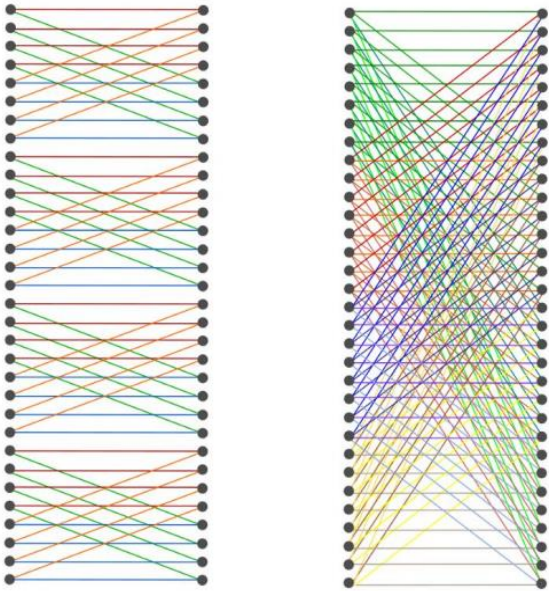


- Drug discovery
- Finance
- Space
- Cybersecurity

QUANTUM MACHINE LEARNING

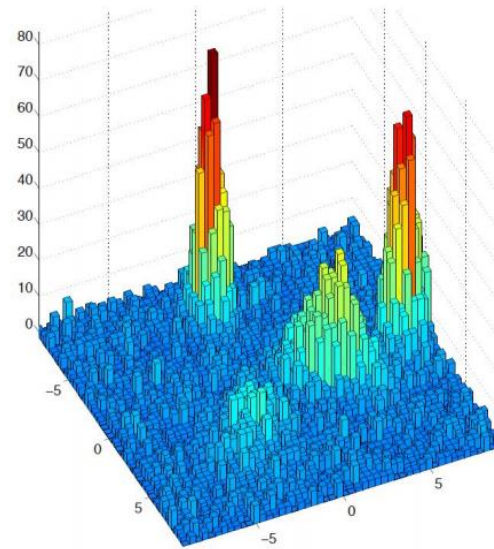
Possible advantage

Linear algebra



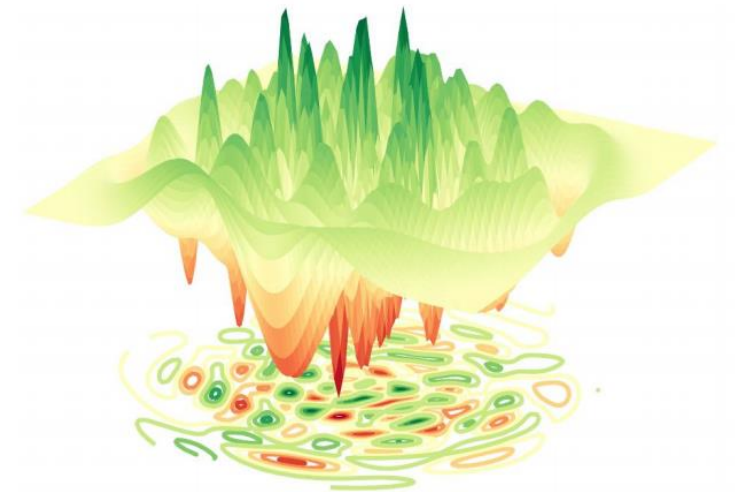
Operations on gate-model quantum computers follow the linear algebra rules

Sampling



Quantum mechanics is intrinsically probabilistic

Optimization



Explore more paths with quantum phenomena

QUANTUM MACHINE LEARNING

Overview

- First generation of QML
 - Accelerated linear algebra on quantum computers
 - Only applies to fault-tolerant quantum computers

QUANTUM MACHINE LEARNING

Overview

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- Second generation of QML
 - Low-depth quantum circuit learning (QNN)
 - Applicable to noisy-intermediate quantum (NISQ) devices

QUANTUM MACHINE LEARNING

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- First generation of QML
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QUANTUM MACHINE LEARNING

Frameworks

QISKIT



Most used quantum SDK
with access of quantum
devices

Machine learning modules

PENNYLANE

P E N N Y L A N E

For hybrid quantum-
classical computation

Integration of pytorch and
tensorflow with different
quantum SDK

TF QUANTUM



For hybrid quantum-
classical computation

Equivalence between
quantum and tensor
operations

QUANTUM MACHINE LEARNING

NISQ application

Supervised learning with quantum enhanced feature spaces

Vojtech Havlicek^{1,*}, Antonio D. Córcoles¹, Kristan Temme¹, Aram W. Harrow²,
Abhinav Kandala¹, Jerry M. Chow¹, and Jay M. Gambetta¹
¹IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA and
²Center for Theoretical Physics, Massachusetts Institute of Technology, USA
(Dated: June 7, 2018)

Supervised learning:

Quantum Support Vector Machine (QSVM)
for regression and classification

Unsupervised learning:

Quantum Generative Adversal Network (QGAN)
hybrid quantum-classical generative model

Quantum Generative Adversarial Networks for Learning and Loading Random Distributions

Christa Zoufal,^{1,2,*} Aurélien Lucchi,² and Stefan Woerner¹
¹IBM Research - Zurich
²ETH Zurich
(Dated: April 2, 2019)

REINFORCEMENT LEARNING WITH QUANTUM VARIATIONAL CIRCUITS

Owen Lockwood¹ and Mei Si²

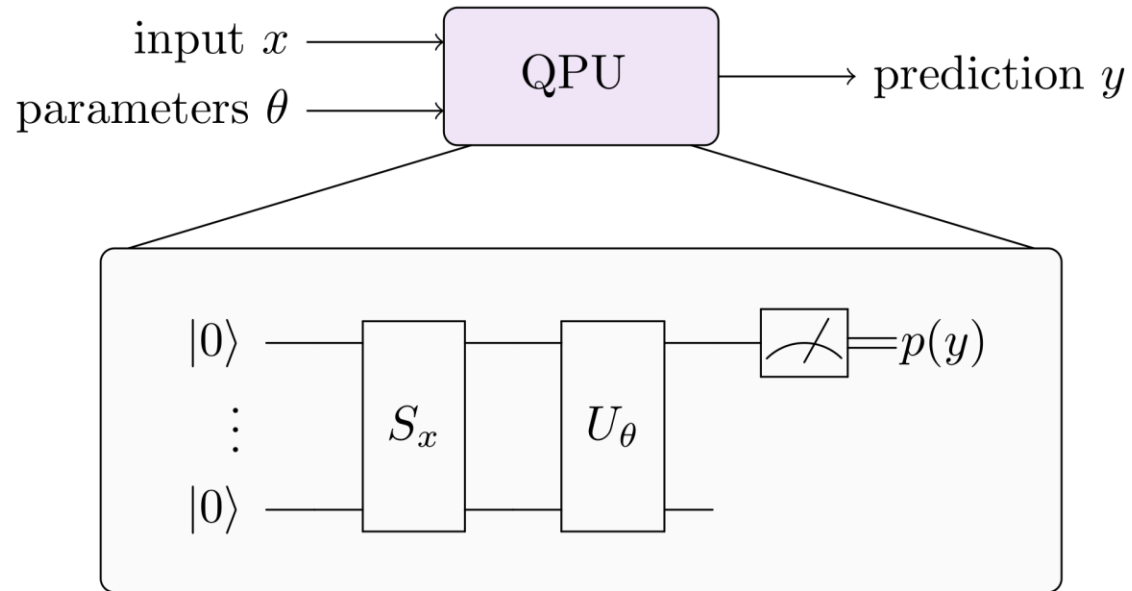
¹Department of Computer Science, Rensselaer Polytechnic Institute
²Department of Cognitive Science, Rensselaer Polytechnic Institute

Reinforcement learning:

Reinforcement learning with QVC
hybrid reinforcement learning algorithm

QUANTUM MACHINE LEARNING

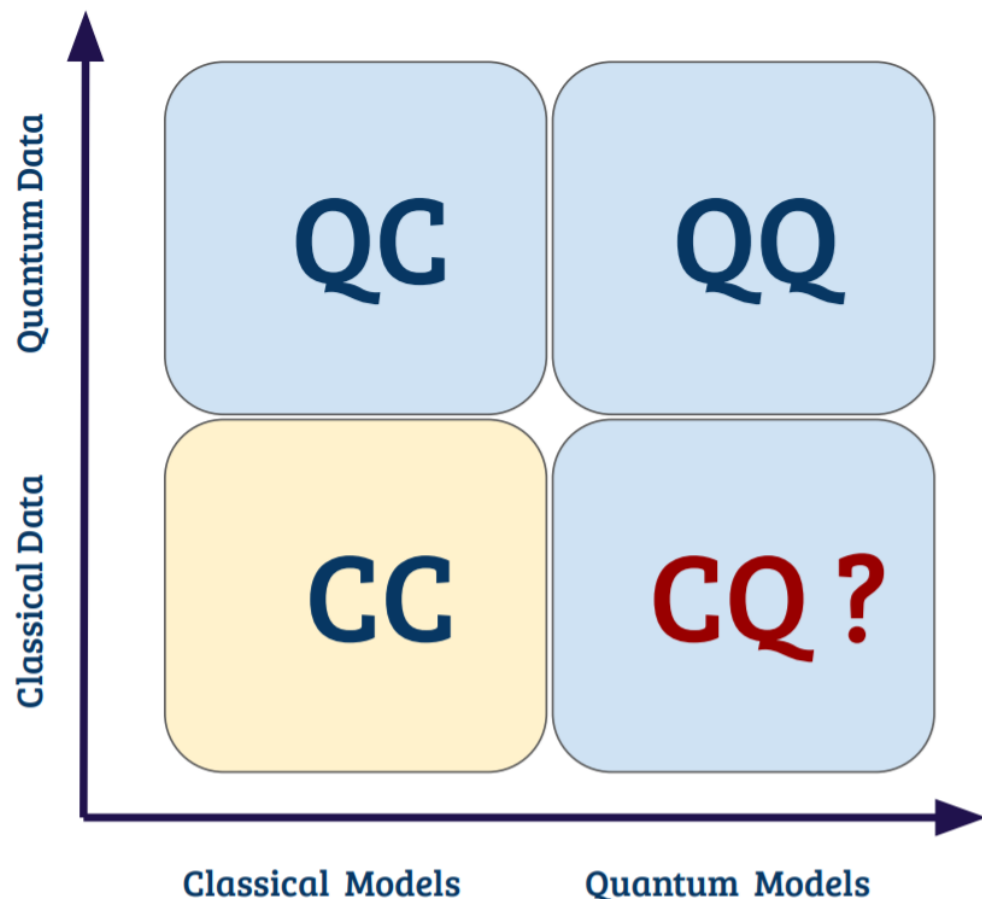
Ideal blocks



- **Feature map:** Store the inputs in a quantum state
- **Variational circuit:** Learnable parameter circuit
- **Expectation value:** Measurements introducing non-linearity

QUANTUM MACHINE LEARNING

Encoding problems



No QRAM to store data



Encoding data generally hard



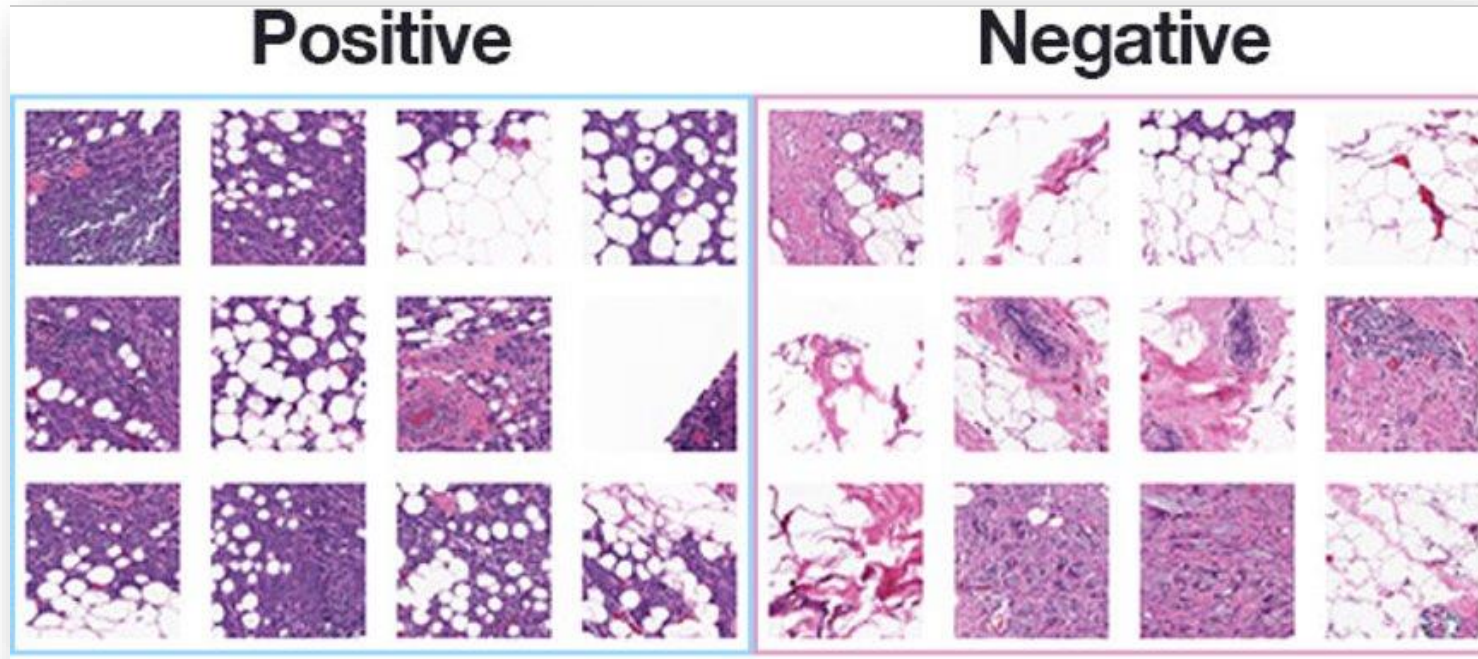
Better if are intrinsically quantum such as quantum states of a system

Quantum Support Vector Machine (QSVM)

QUANTUM SUPPORT VECTOR MACHINE

Use case

Breast cancer Wisconsin

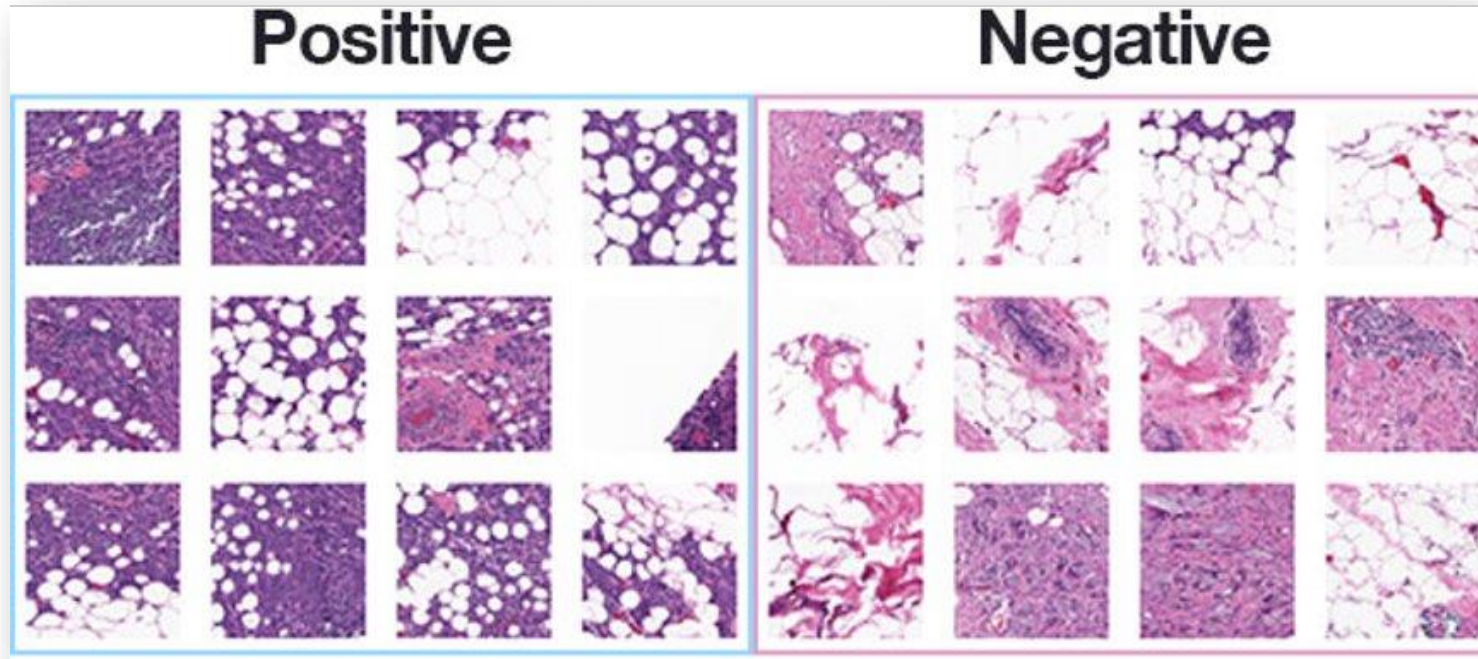


<https://www.kaggle.com/uciml/breast-cancer-wisconsin-data/version/2>

QUANTUM SUPPORT VECTOR MACHINE

Use case

Breast cancer Wisconsin



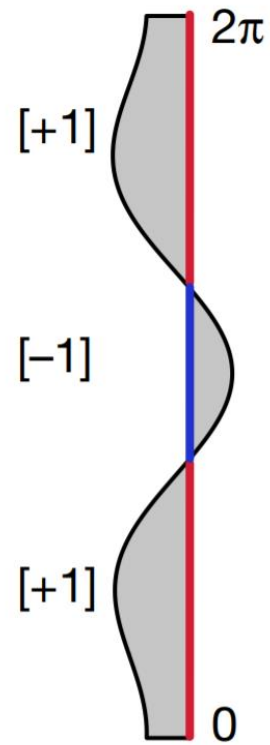
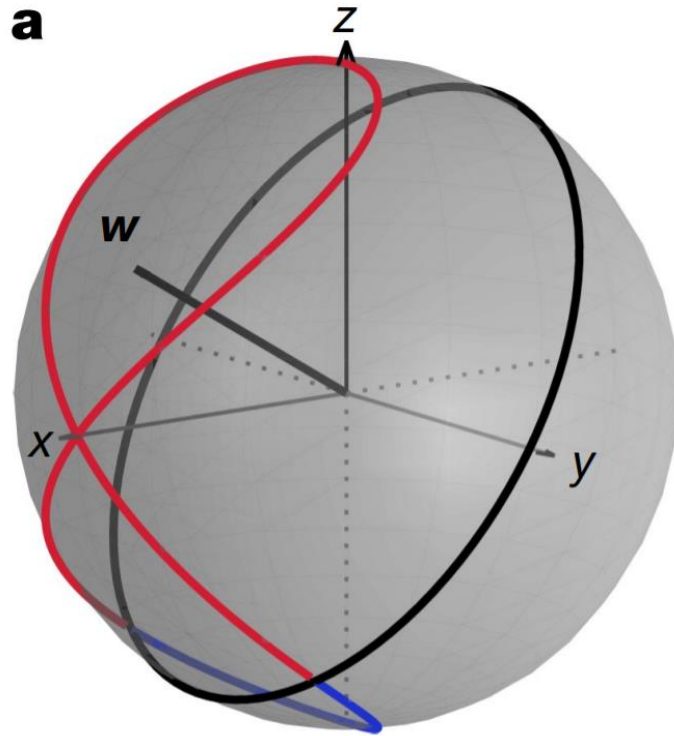
Dataset with 2 feature

2 qubits to performe QSVM

<https://www.kaggle.com/uciml/breast-cancer-wisconsin-data/version/2>

QUANTUM SUPPORT VECTOR MACHINE

Intuition



Quantum advantage:

More complex feature map at low computational cost

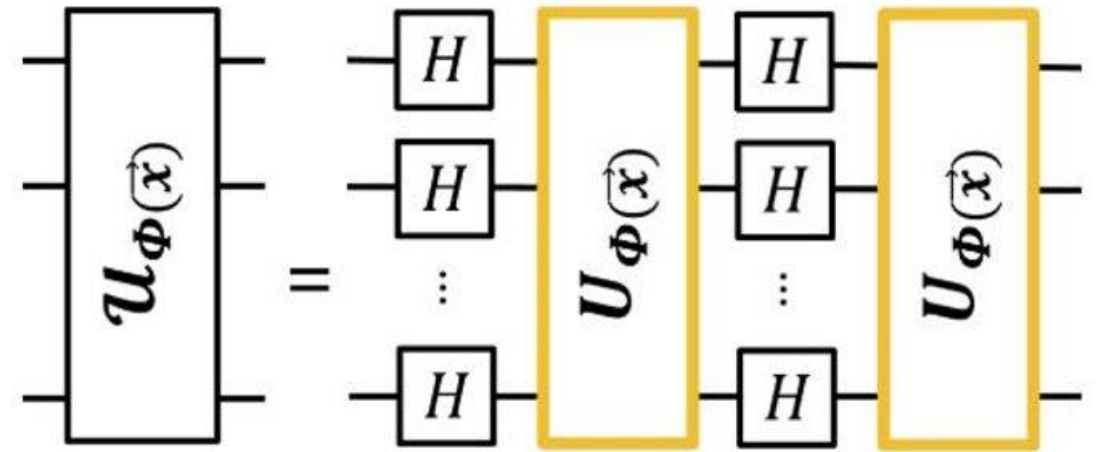
QUANTUM SUPPORT VECTOR MACHINE

Intuition

Non-linear feature map

$$\vec{x} \mapsto |\Phi(\vec{x})\rangle = \mathcal{U}_{\Phi(\vec{x})} |0\rangle^{\otimes n}$$

$$U_{\Phi(\vec{x})} = \exp\left(i \sum_{S \subseteq [n]} \phi_S(\vec{x}) \prod_{j \in S} Z_j\right)$$



QUANTUM SUPPORT VECTOR MACHINE

Feature map

$$U_{\Phi(\vec{x})} = \exp \left(i \sum_{S \subseteq [n]} \phi_S(\vec{x}) \prod_{j \in S} Z_j \right)$$

- First order expansion (1 or more qubits, no entanglement)

$$S \in \{0, 1, \dots, n-1\}$$

$$\phi_i(\mathbf{x}) = x_i$$

- Second order expansion (2 or more qubits, entanglement)

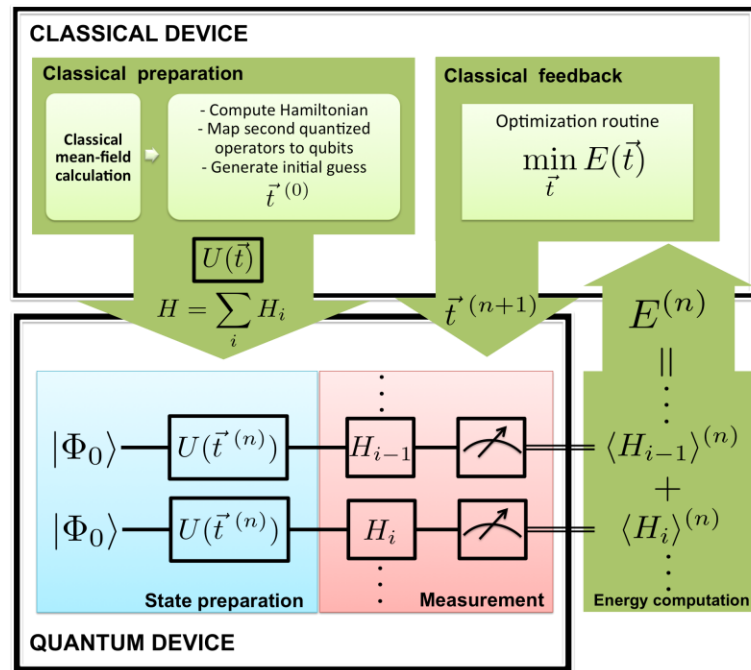
$$S \in \{0, 1, \dots, n-1, (0, 1), (1, 2), \dots, (n-2, n-1)\}$$

$$\phi_{(i,j)}(\mathbf{x}) = (\pi - x_i) (\pi - x_j)$$

$$e^{i\phi_{\{l,m\}}(\vec{x})Z_l Z_m} = \begin{array}{c} \text{---} \\ | \\ \oplus \text{---} \boxed{Z_\phi} \text{---} \oplus \\ | \\ \text{---} \end{array}$$

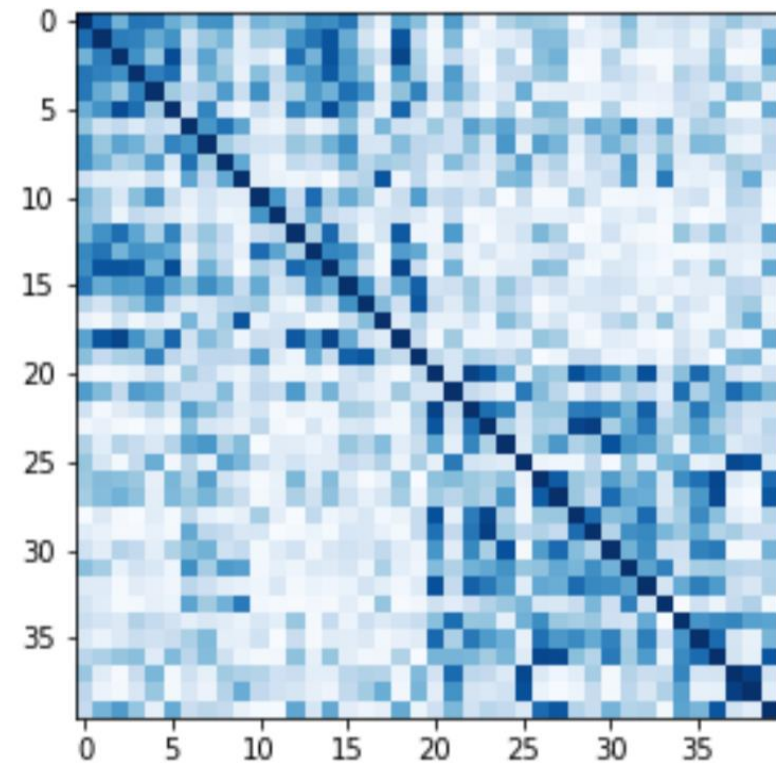
QUANTUM SUPPORT VECTOR MACHINE

- Variational quantum circuit



Using variational quantum eigensolver (VQE)

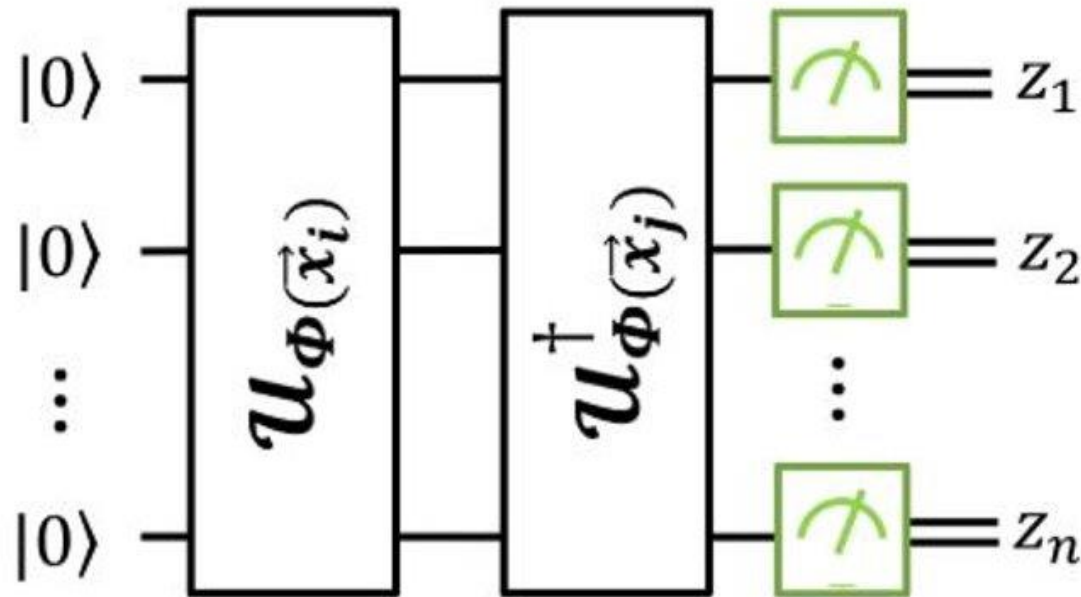
- Kernel matrix estimation



QUANTUM SUPPORT VECTOR MACHINE

Kernel estimation

$$K(\vec{x}_i, \vec{x}_j) = |\langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle|^2 = \left| \langle 0 | \mathcal{U}_{\Phi(\vec{x}_j)}^\dagger \mathcal{U}_{\Phi(\vec{x}_i)} | 0 \rangle^{\otimes n} \right|^2$$



$$p_{0\dots 0} \sim K(\vec{x}_i, \vec{x}_j)$$

QUANTUM SUPPORT VECTOR MACHINE

Quantum variational circuit

$$p_y(\mathbf{x}) = \langle \Phi(\mathbf{x}) | W^\dagger(\boldsymbol{\theta}) M_y W(\boldsymbol{\theta}) | \Phi(\mathbf{x}) \rangle$$

$$\text{If } \hat{p}_y(\mathbf{x}) > \hat{p}_{-y}(\mathbf{x}) - yb$$

$$\tilde{m}(\mathbf{x}) = y$$

Cost function

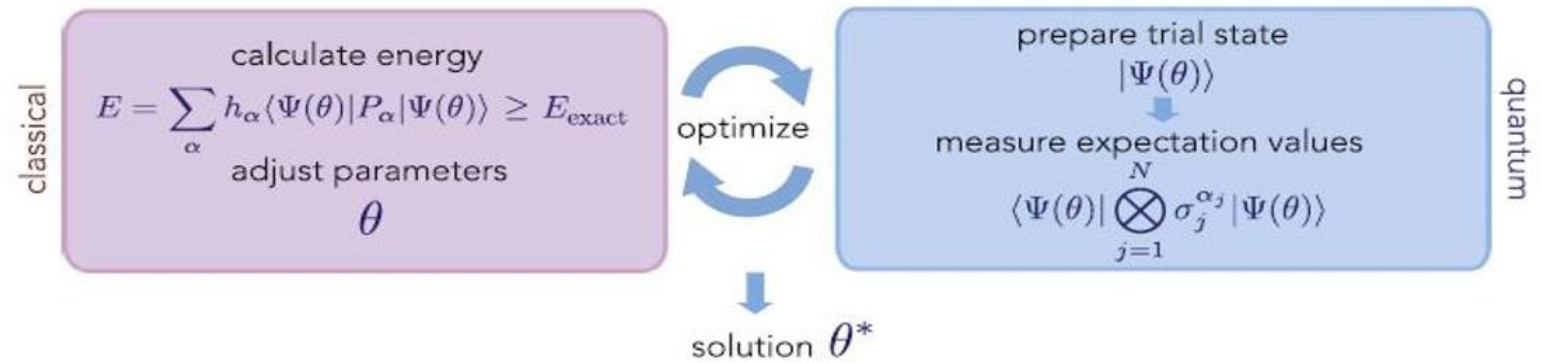
$$\Pr(\tilde{m}(\mathbf{x}) \neq m(\mathbf{x}))$$

Learnable parameters

$$(\boldsymbol{\theta}, b)$$

qubit Hamiltonian

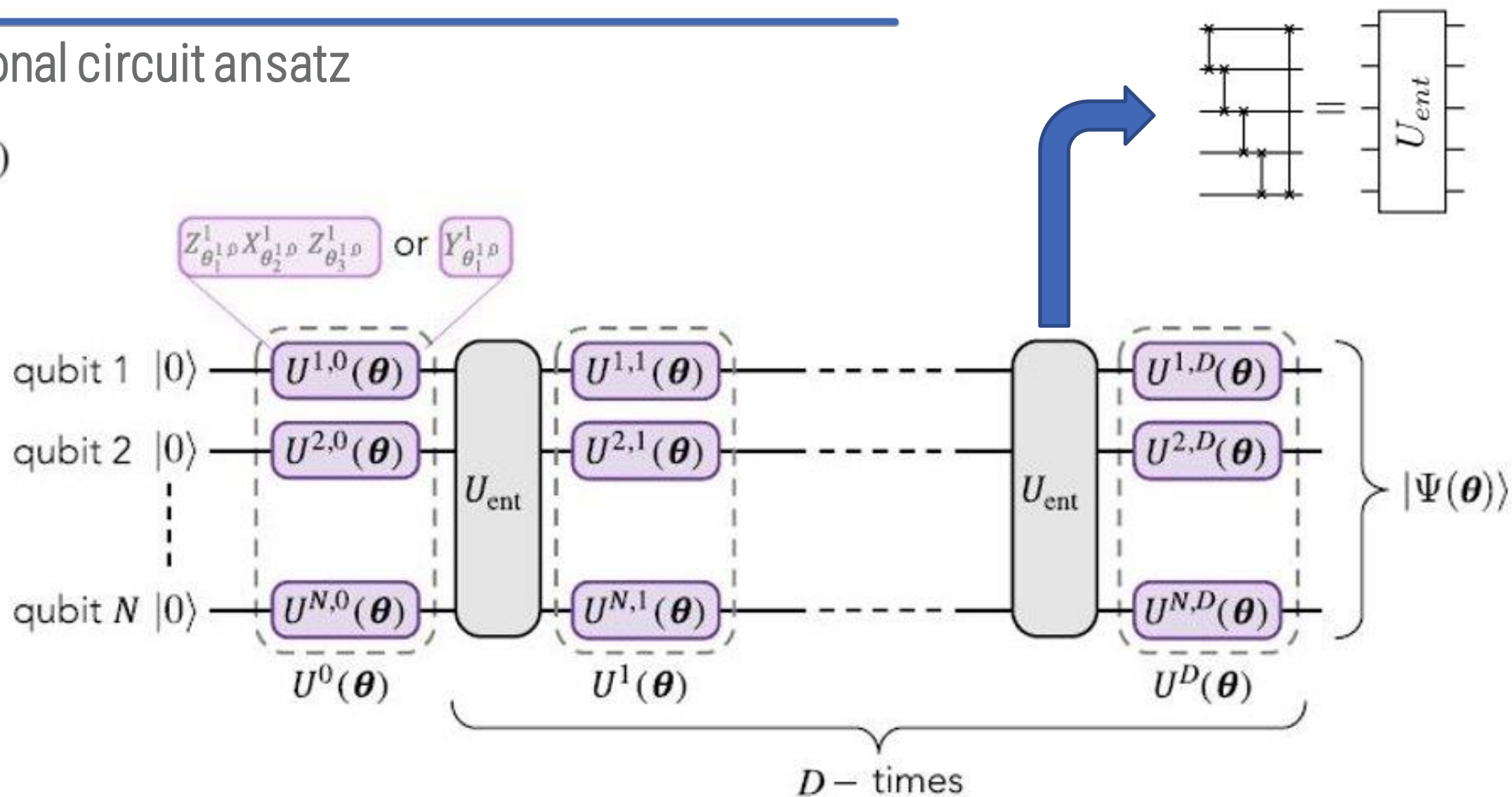
$$H_q = \sum_{\alpha} h_{\alpha} P_{\alpha} = \sum_{\alpha} h_{\alpha} \bigotimes_{j=1}^N \sigma_j^{\alpha_j}$$



QUANTUM SUPPORT VECTOR MACHINE

Variational circuit ansatz

$W(\theta)$



QUANTUM SUPPORT VECTOR MACHINE

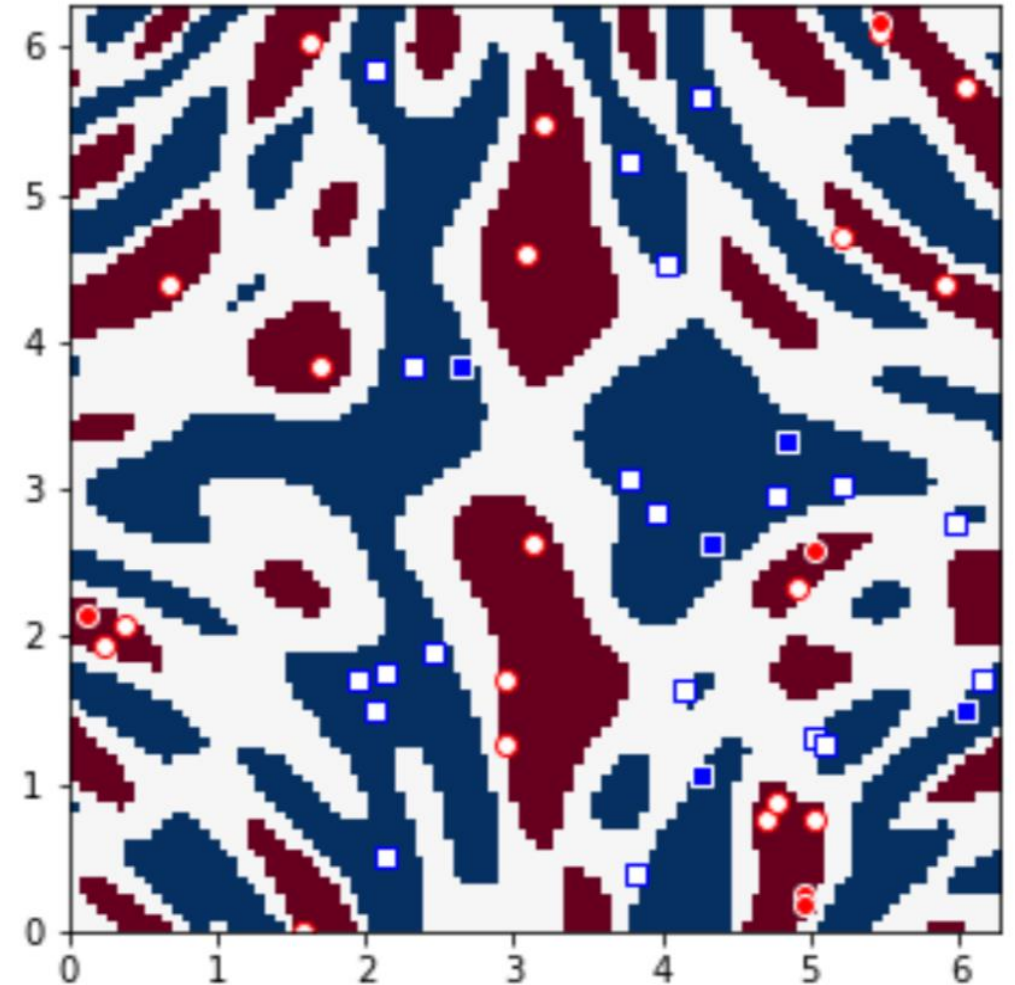
Quantum variational circuit

- Expectation value of an operator f

$$\langle \Phi(\vec{x}) | W^\dagger(\theta) \mathbf{f} W(\theta) | \Phi(\vec{x}) \rangle = \frac{1}{2^n} \sum_{\alpha} w_{\alpha}(\theta) \Phi_{\alpha}(\vec{x})$$

- Classification rule

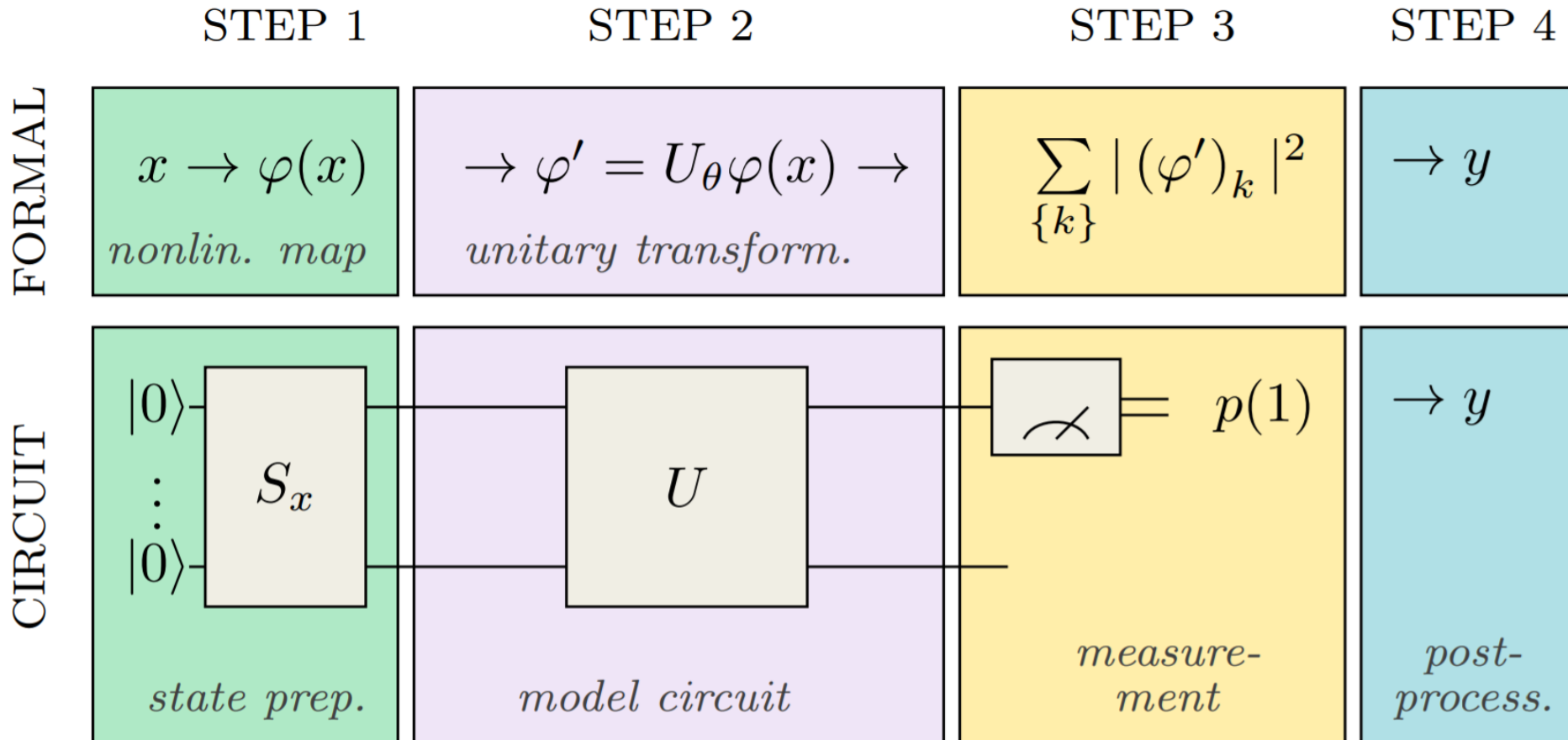
$$\tilde{m}(\vec{x}) = \text{sign} \left(\frac{1}{2^n} \sum_{\alpha} w_{\alpha}(\theta) \Phi_{\alpha}(\vec{x}) + b \right)$$



Quantum Neural Networks (QNN)

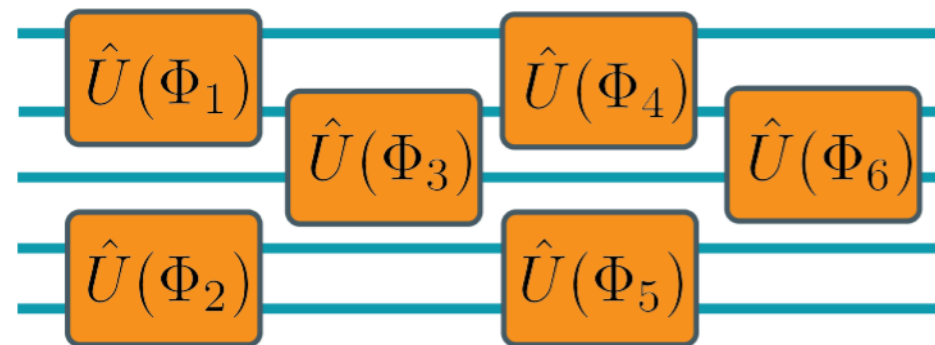
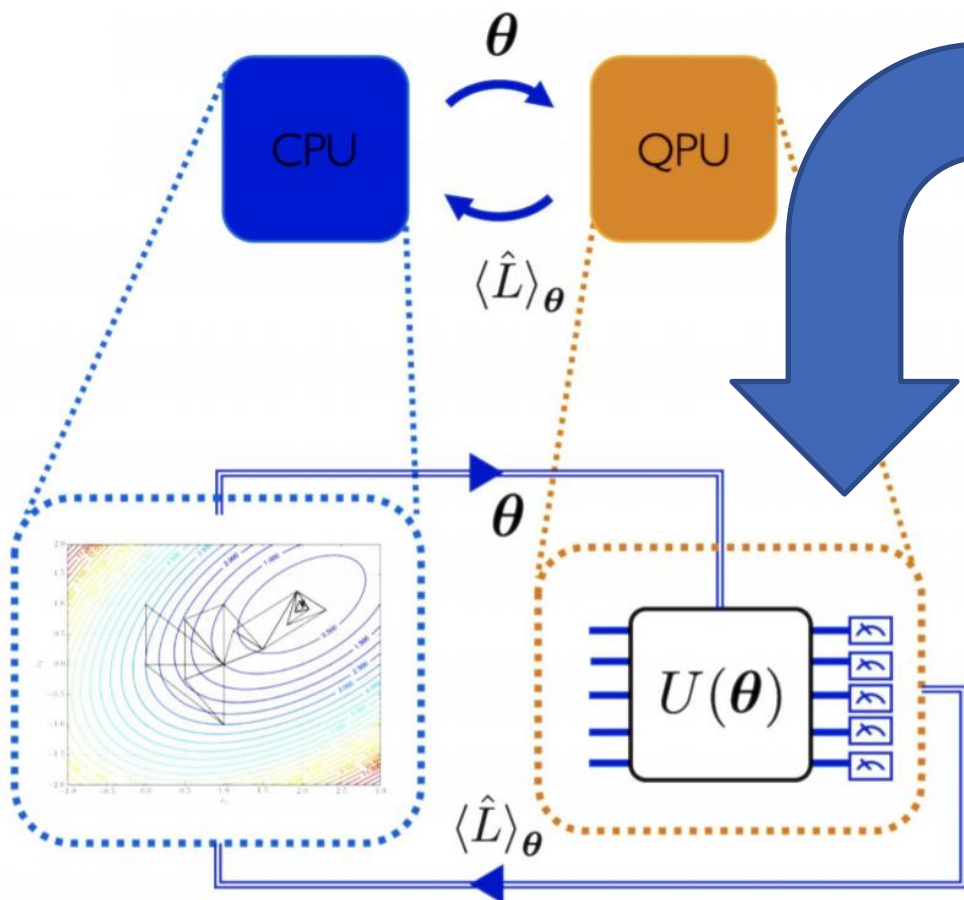
VARIATIONAL QUANTUM ALGORITHM

General idea



QUANTUM NEURAL NETWORK

Definition



- Sequence of continuously-parametrized rotations executed on QPU
- Measure observable expectation value (non-linearity)
- CPU optimization suggests new parameters to minimize the expectation value

<https://qml.entropicalabs.io/>

QUANTUM NEURAL NETWORK

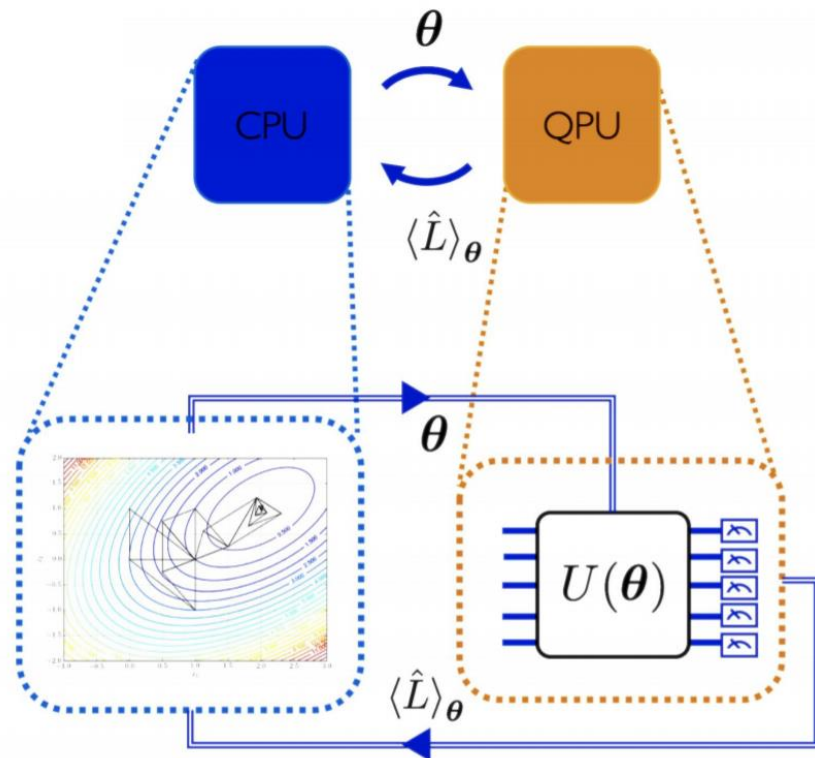
Problems

- Data must be prepared on the fly
- QPU needs full quantum program for each run (microseconds for each run)
- Relative high latency CPU-QPU (ms)

QUANTUM NEURAL NETWORK

Hybrid approach

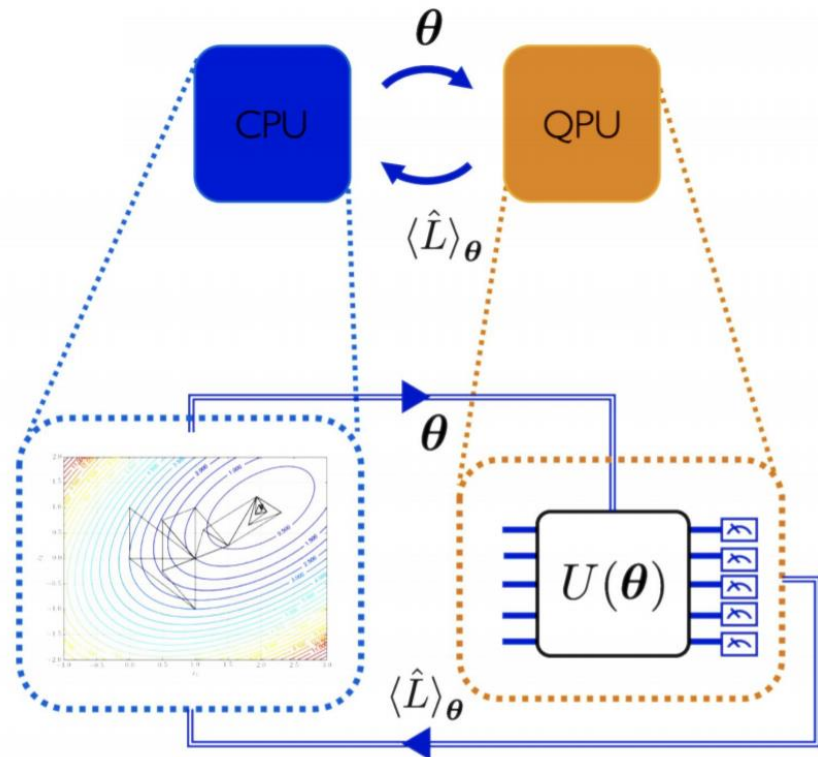
Classical optimization is used



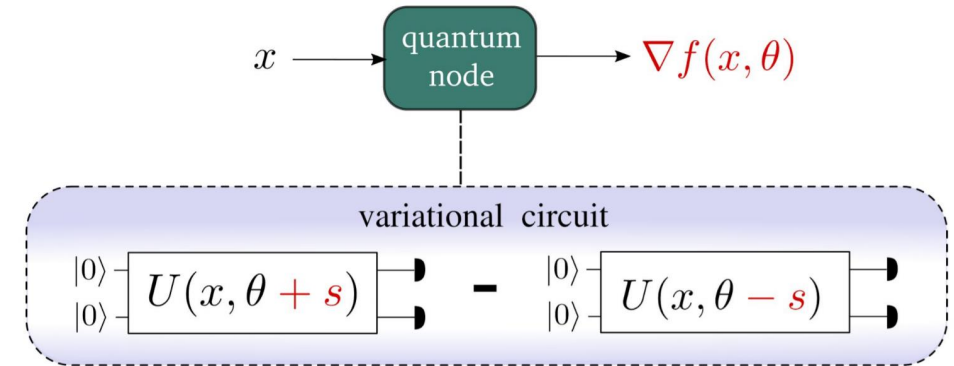
QUANTUM NEURAL NETWORK

Hybrid approach

Classical optimization is used



But the gradient is computed by QPU



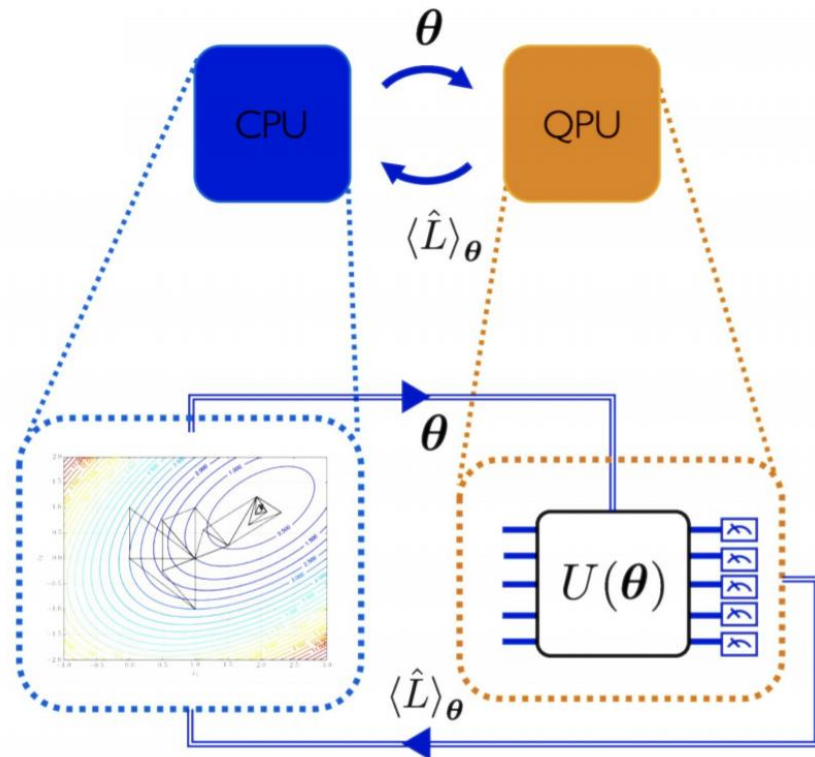
Parameter shift

$$\partial_{\theta} f(\theta) = c[f(\theta + s) - f(\theta - s)]$$

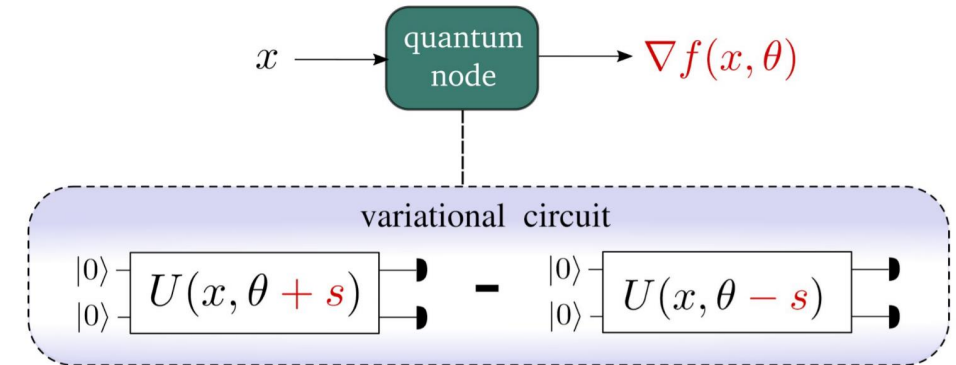
QUANTUM NEURAL NETWORK

Hybrid approach

Classical optimization is used



But the gradient is computed by QPU



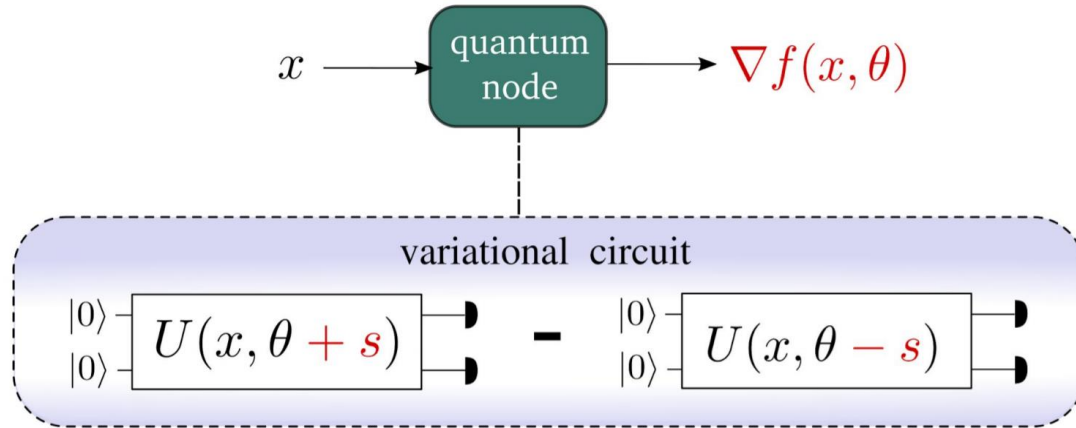
Parameter shift

$$\partial_\theta f(\theta) = c[f(\theta + s) - f(\theta - s)]$$

Exact

QUANTUM NEURAL NETWORK

Parameter shift



State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

Operator (Observable)

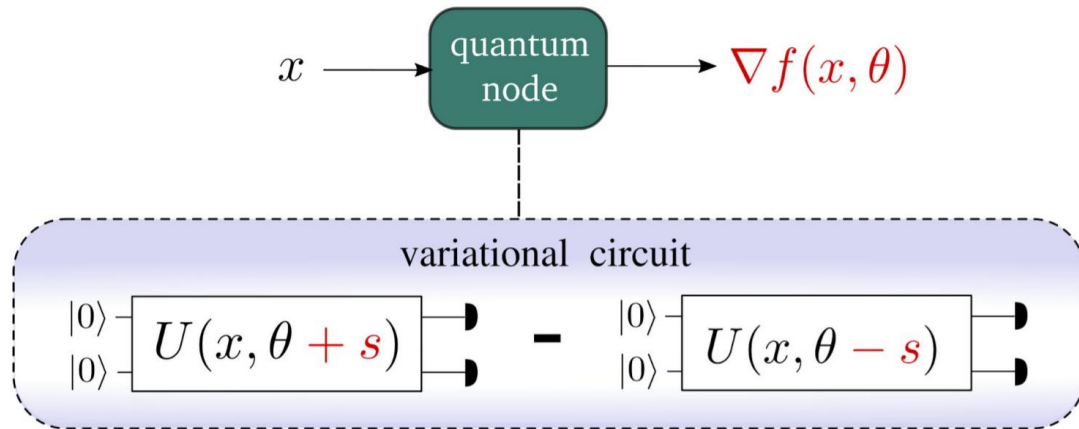
$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

QUANTUM NEURAL NETWORK

Parameter shift



State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

Operator (Observable)

$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

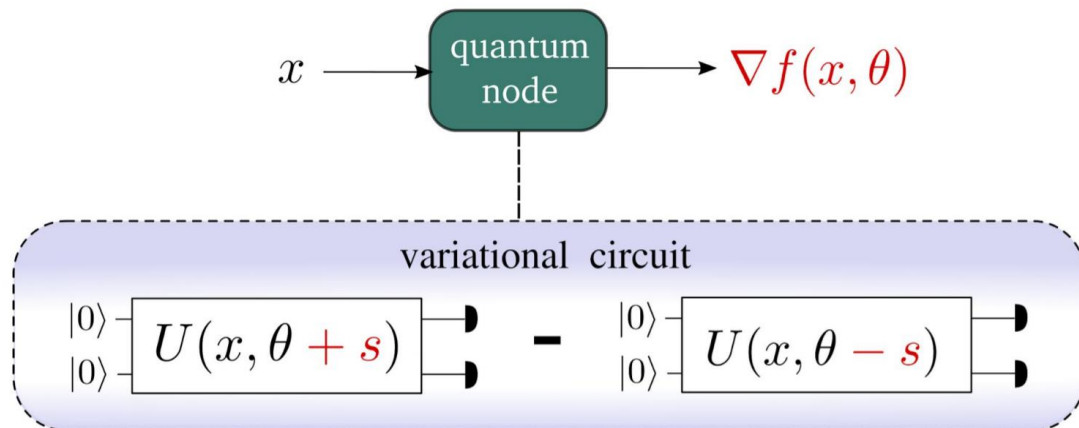
Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

$$\nabla_{\theta_i} f(x; \theta) = \langle \psi_{i-1} | \nabla_{\theta_i} \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle \quad ?$$

QUANTUM NEURAL NETWORK

Parameter shift



State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

Operator (Observable)

$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

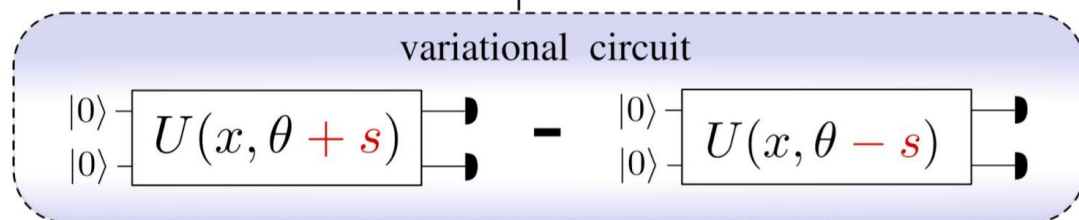
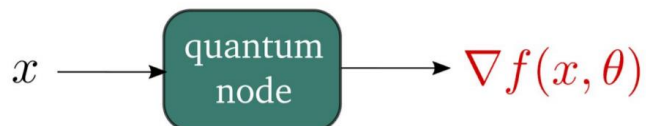
Pauli rotation

$$U_i(\theta_i) = \exp\left(-i \frac{\theta_i}{2} \hat{P}_i\right)$$

$$\nabla_{\theta_i} U_i(\theta_i) = -\frac{i}{2} \hat{P}_i U_i(\theta_i) = -\frac{i}{2} U_i(\theta_i) \hat{P}_i$$

QUANTUM NEURAL NETWORK

Parameter shift



$$\begin{aligned}\nabla_{\theta_i} f(x; \theta) &= \frac{i}{2} \langle \psi_{i-1} | U_i^\dagger(\theta_i) (P_i \hat{B}_{i+1} - \hat{B}_{i+1} P_i) U_i(\theta_i) | \psi_{i-1} \rangle \\ &= \frac{i}{2} \langle \psi_{i-1} | U_i^\dagger(\theta_i) [P_i, \hat{B}_{i+1}] U_i(\theta_i) | \psi_{i-1} \rangle,\end{aligned}$$

State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

Operator (Observable)

$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

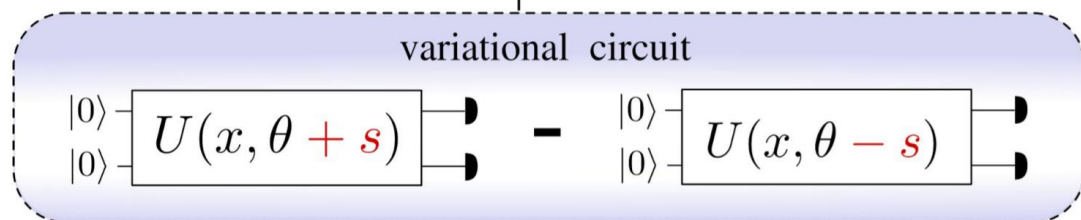
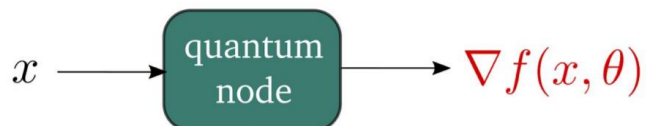
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$$\nabla_{\theta_i} U_i(\theta_i) = -\frac{i}{2} \hat{P}_i U_i(\theta_i) = -\frac{i}{2} U_i(\theta_i) \hat{P}_i$$

QUANTUM NEURAL NETWORK

Parameter shift



$$\begin{aligned}\nabla_{\theta_i} f(x; \theta) &= \frac{i}{2} \langle \psi_{i-1} | U_i^\dagger(\theta_i) (P_i \hat{B}_{i+1} - \hat{B}_{i+1} P_i) U_i(\theta_i) | \psi_{i-1} \rangle \\ &= \frac{i}{2} \langle \psi_{i-1} | U_i^\dagger(\theta_i) [P_i, \hat{B}_{i+1}] U_i(\theta_i) | \psi_{i-1} \rangle,\end{aligned}$$

Commutator $[X, Y] = XY - YX$

$$[\hat{P}_i, \hat{B}] = -i \left(U_i^\dagger \left(\frac{\pi}{2} \right) \hat{B} U_i \left(\frac{\pi}{2} \right) - U_i^\dagger \left(-\frac{\pi}{2} \right) \hat{B} U_i \left(-\frac{\pi}{2} \right) \right)$$

State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

Operator (Observable)

$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

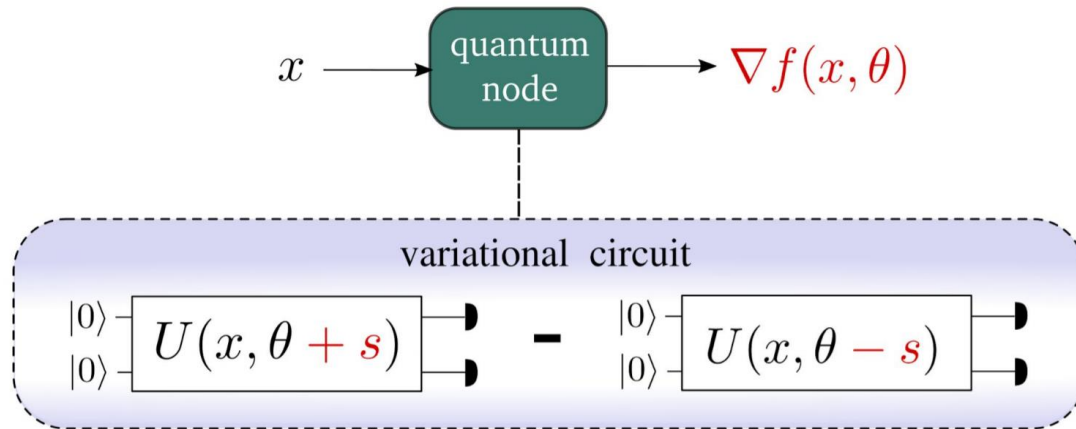
Pauli rotation

$$U_i(\theta_i) = \exp\left(-i \frac{\theta_i}{2} \hat{P}_i\right)$$

$$\nabla_{\theta_i} U_i(\theta_i) = -\frac{i}{2} \hat{P}_i U_i(\theta_i) = -\frac{i}{2} U_i(\theta_i) \hat{P}_i$$

QUANTUM NEURAL NETWORK

Parameter shift



State

$$|\psi_{i-1}\rangle = U_{i-1}(\theta_{i-1}) \cdots U_1(\theta_1) U_0(x) |0\rangle$$

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$$\hat{B}_{i+1} = U_N^\dagger(\theta_N) \cdots U_{i+1}^\dagger(\theta_{i+1}) \hat{B} U_{i+1}(\theta_{i+1}) \cdots U_N(\theta_N)$$

Expectation value

$$f(x; \theta) = \langle \psi_{i-1} | U_i^\dagger(\theta_i) \hat{B}_{i+1} U_i(\theta_i) | \psi_{i-1} \rangle = \langle \psi_{i-1} | \mathcal{M}_{\theta_i}(\hat{B}_{i+1}) | \psi_{i-1} \rangle$$

$$\nabla_{\theta} f(x; \theta) = \frac{1}{2} \left[f(x; \theta + \frac{\pi}{2}) - f(x; \theta - \frac{\pi}{2}) \right]$$

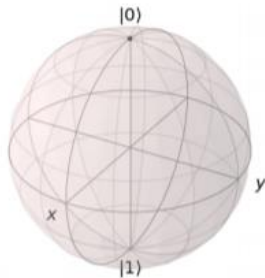
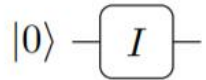
QUANTUM NEURAL NETWORK

Variational circuit ansatz

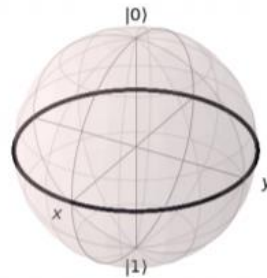
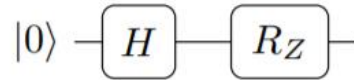
Choose a compromise between

- Computational cost (depth)
- Expressiveness of the unitary operator

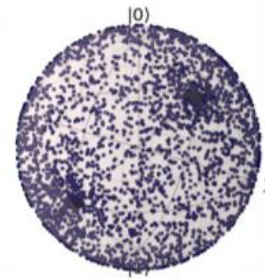
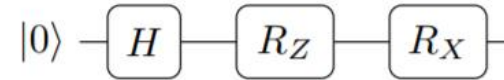
Idle circuit



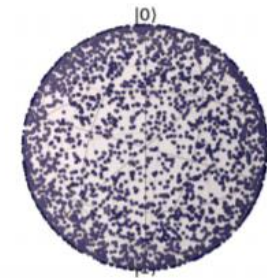
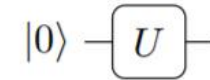
Circuit A



Circuit B



Arbitrary unitary



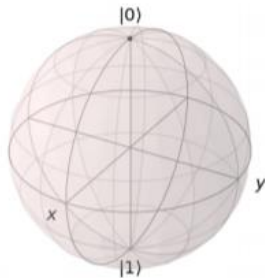
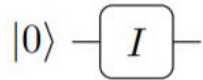
QUANTUM NEURAL NETWORK

Variational circuit ansatz

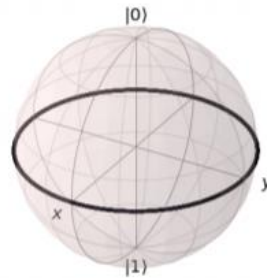
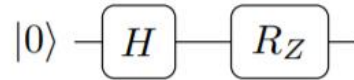
Choose a compromise between

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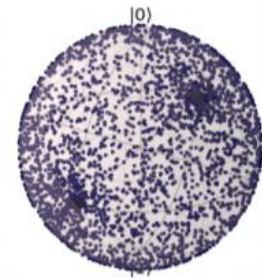
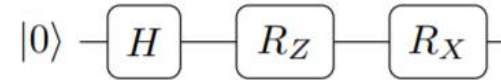
Idle circuit



Circuit A

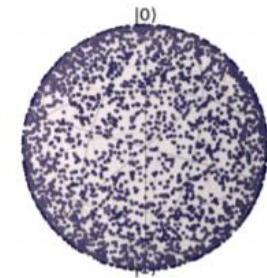
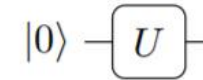


Circuit B

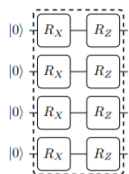


TARGET

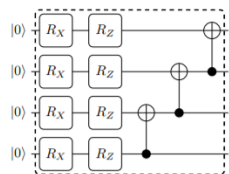
Arbitrary unitary



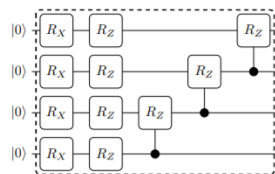
QUANTUM NEURAL NETWORK



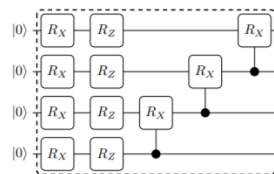
Circuit 1



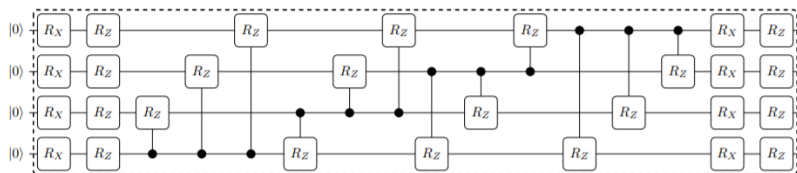
Circuit 2



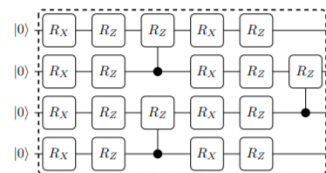
Circuit 3



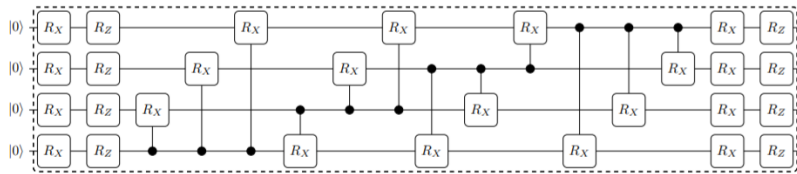
Circuit 4



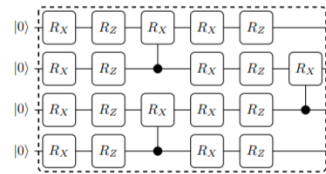
Circuit 5



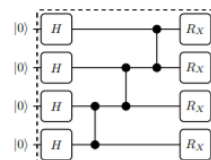
Circuit 7



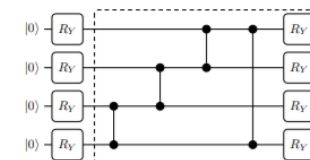
Circuit 6



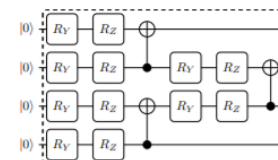
Circuit 8



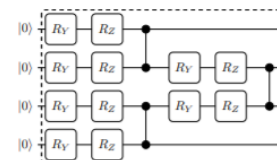
Circuit 9



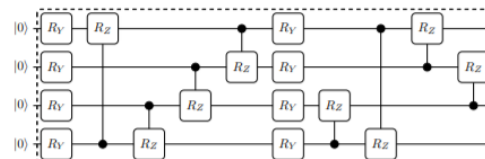
Circuit 10



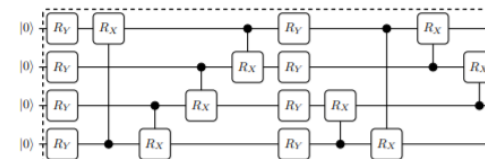
Circuit 11



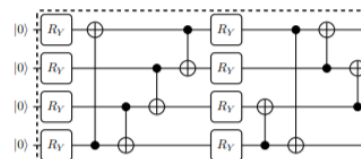
Circuit 12



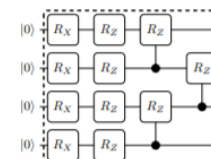
Circuit 13



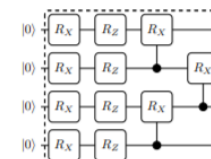
Circuit 14



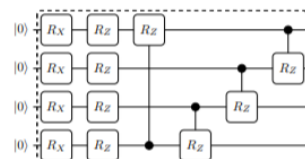
Circuit 15



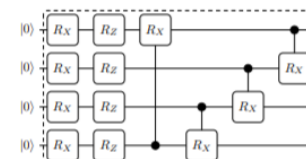
Circuit 16



Circuit 17

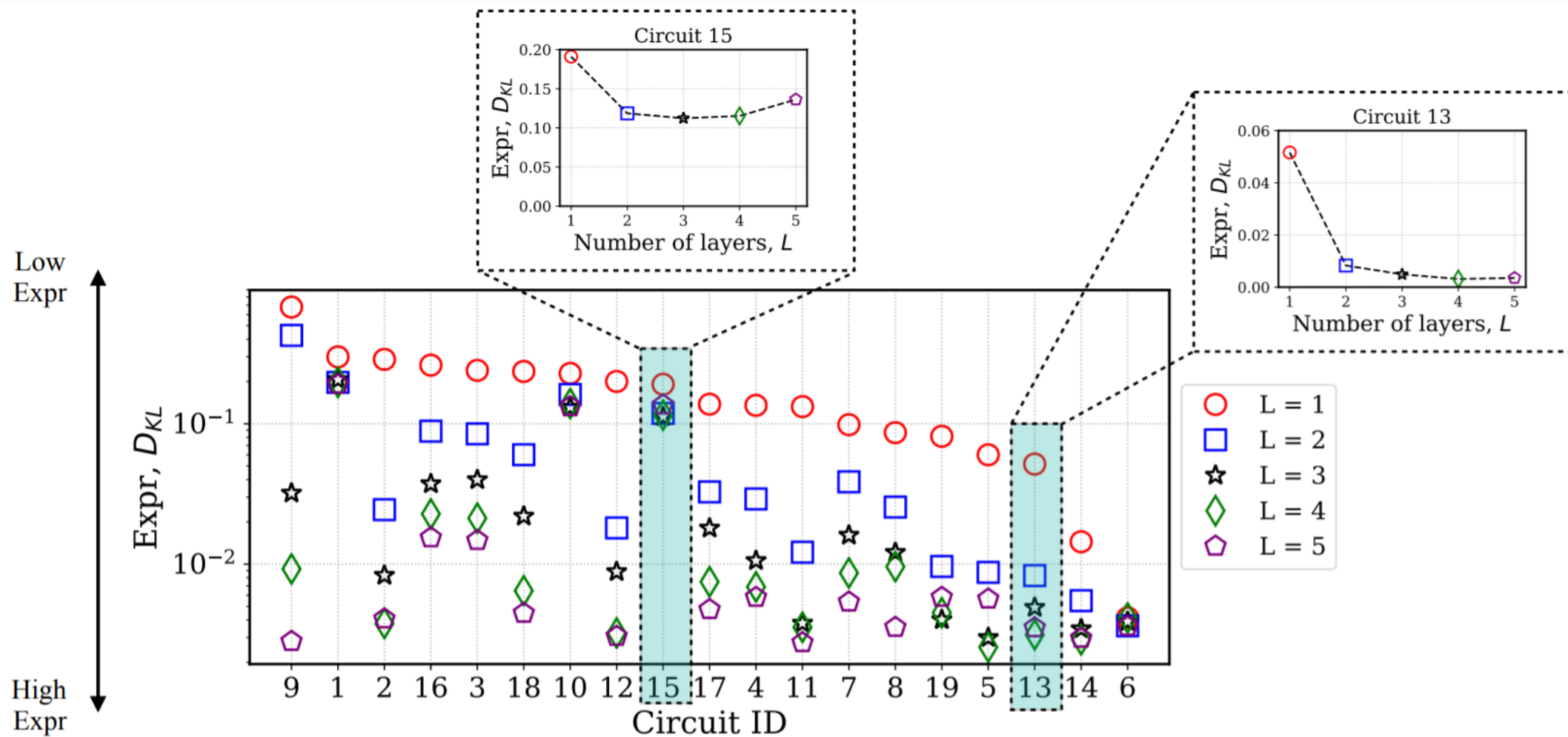


Circuit 18



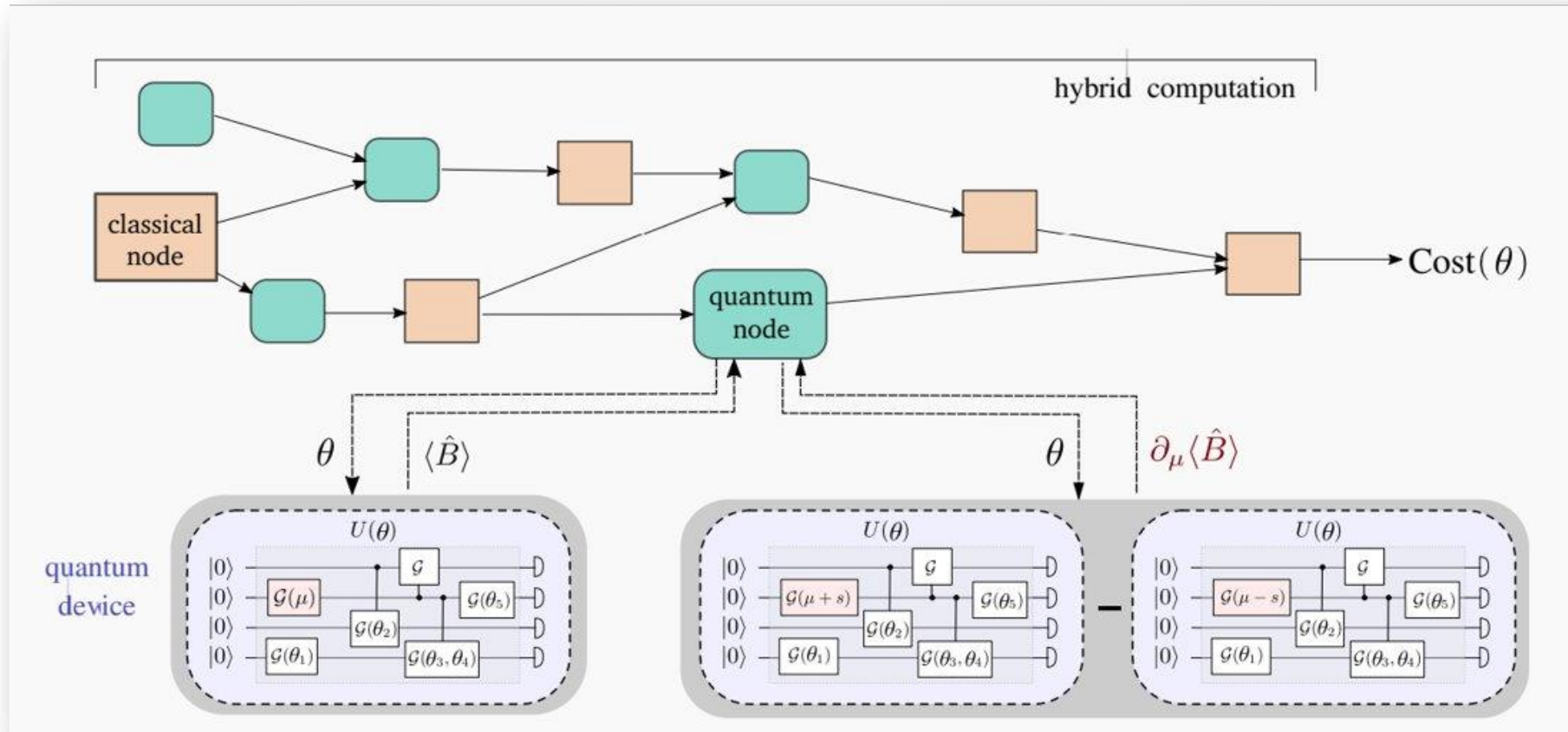
Circuit 19

QUANTUM NEURAL NETWORK



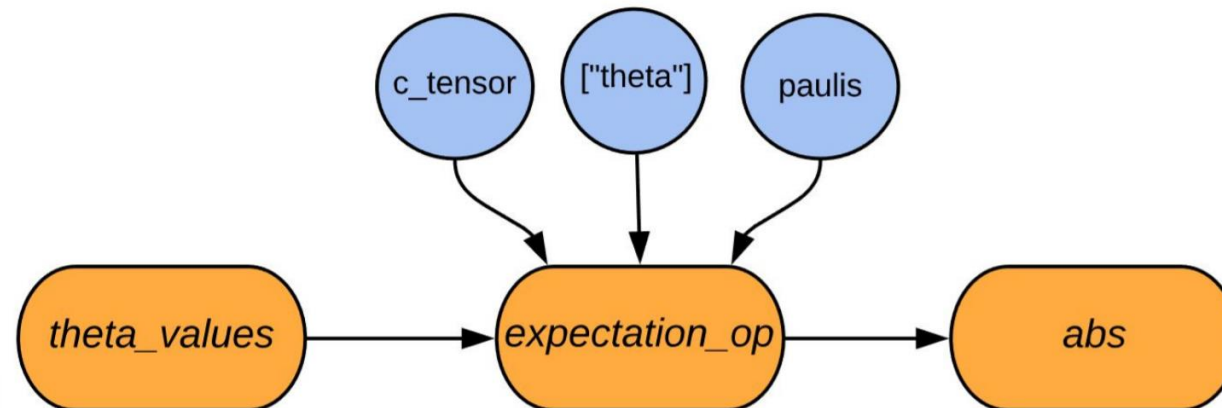
<https://arxiv.org/pdf/1905.10876>

HYBRID QUANTUM-CLASSICAL COMPUTING



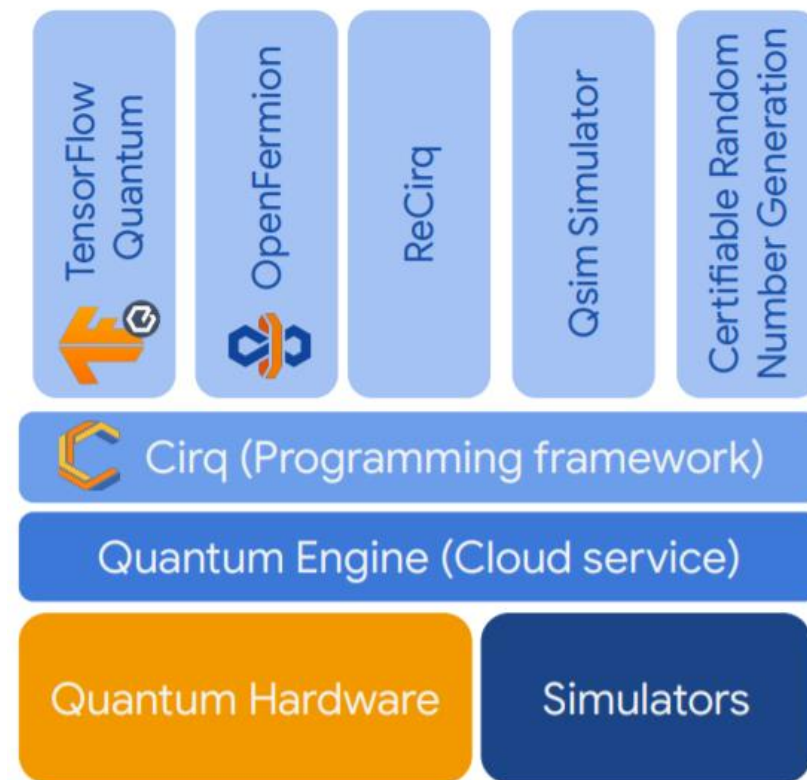
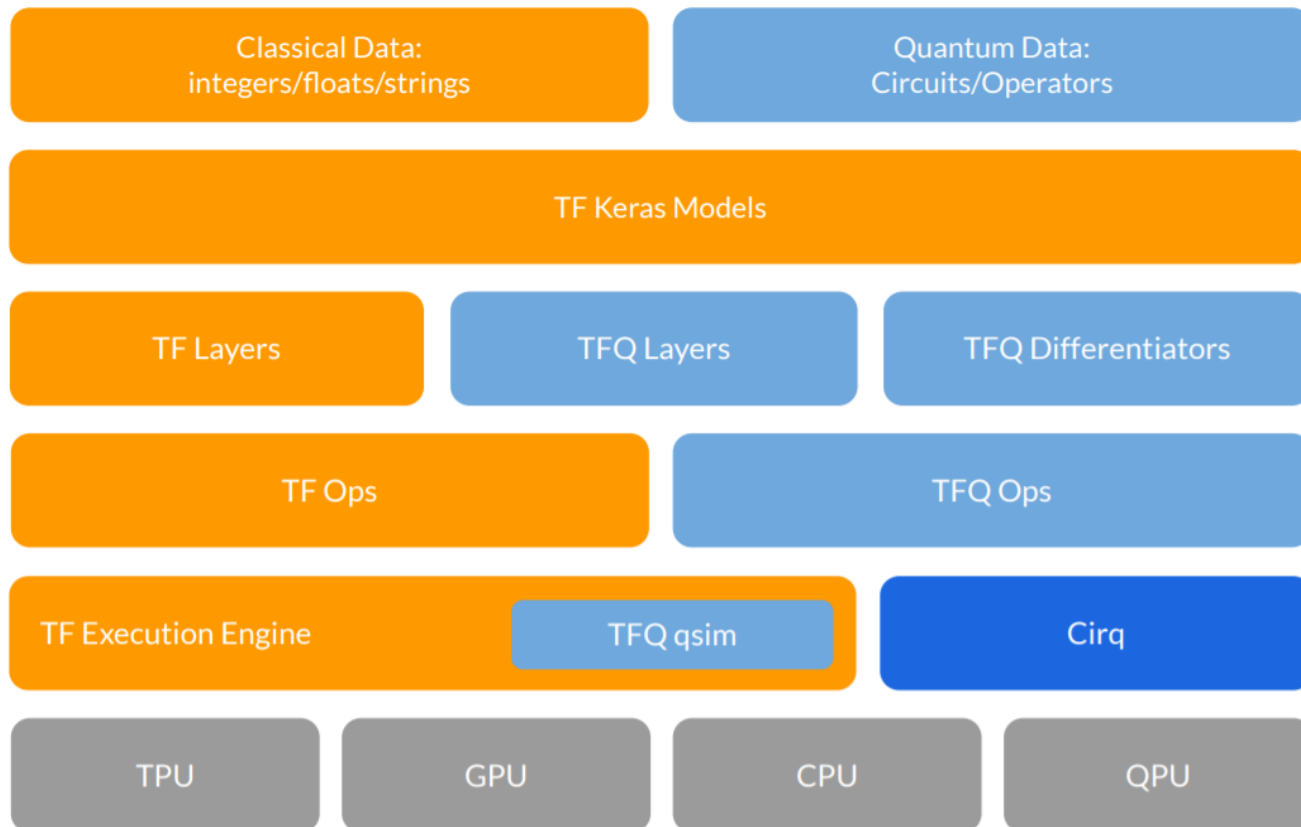
TensorFlow Quantum

- Circuits written with Cirq and converted into **tensors**
 - Expectation value of an operator (**OPs**)
 - Backpropagation for parameter optimization



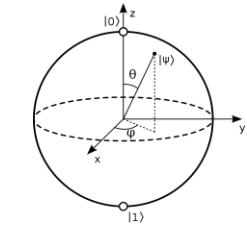
TENSORFLOW QUANTUM

TensorFlow Quantum

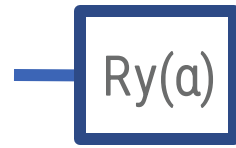


EXAMPLES

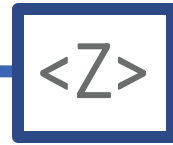
QNN example 1



Quantum data input

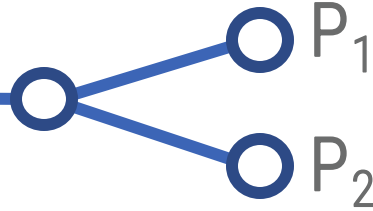


Quantum model



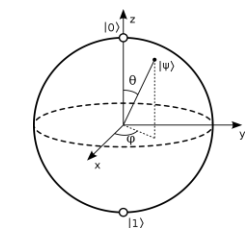
Expectation

Classifier

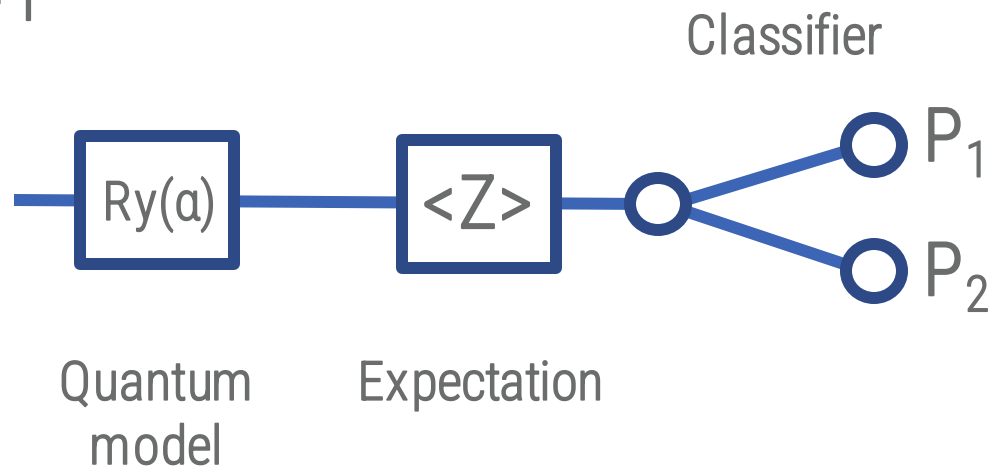


EXAMPLES

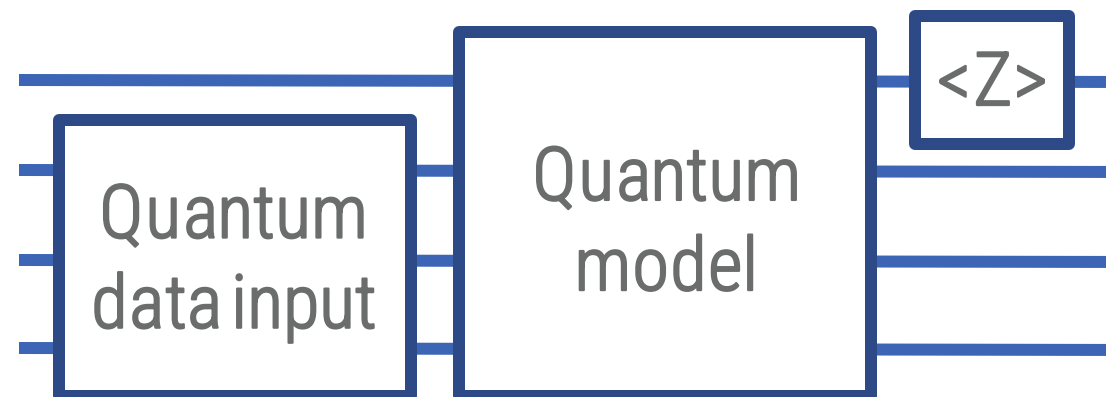
QNN example 1



Quantum data input



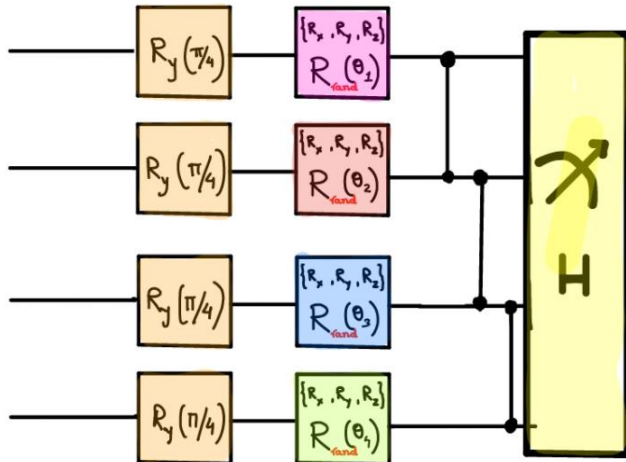
QNN example 2: mnist classification



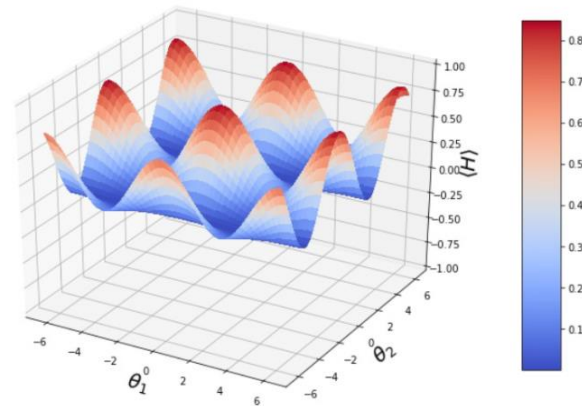
BARREN PLATEAUS

Pauli Rotation

$$\exp\left\{i\mathbf{P}\frac{\theta}{2}\right\} = \mathbf{I}\cos\frac{\theta}{2} + i\mathbf{P}\sin\frac{\theta}{2}$$



A random variational circuit with gates chosen from the set $\{RX, RY, RZ\}$

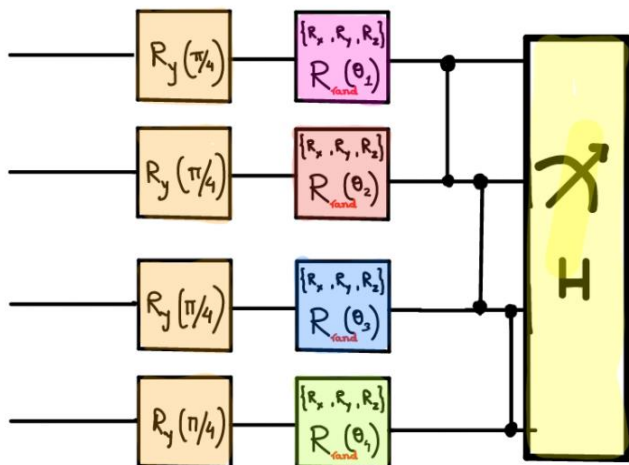


Expectation value of a Hermitian observable along a slice in the parameter space

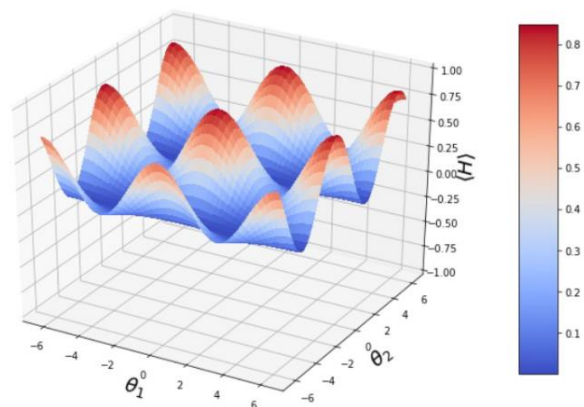
BARREN PLATEAUS

Pauli Rotation $\exp\left\{i\mathbf{P}\frac{\theta}{2}\right\} = \mathbf{I}\cos\frac{\theta}{2} + i\mathbf{P}\sin\frac{\theta}{2}$

Periodic function \longrightarrow Saddle points



A random variational circuit with gates chosen from the set $\{RX, RY, RZ\}$

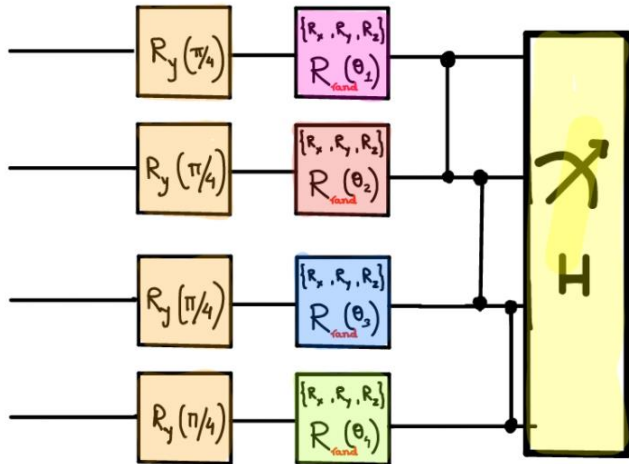


Expectation value of a Hermitian observable along a slice in the parameter space

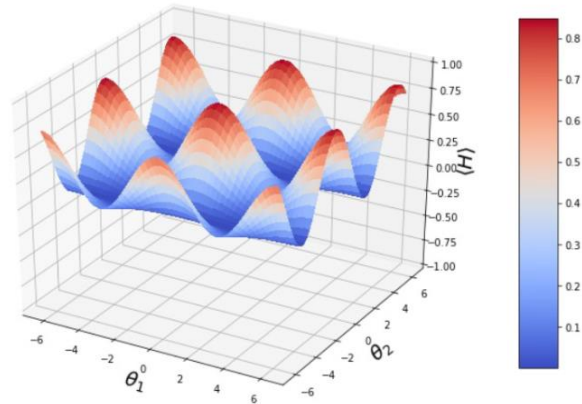
BARREN PLATEAUS

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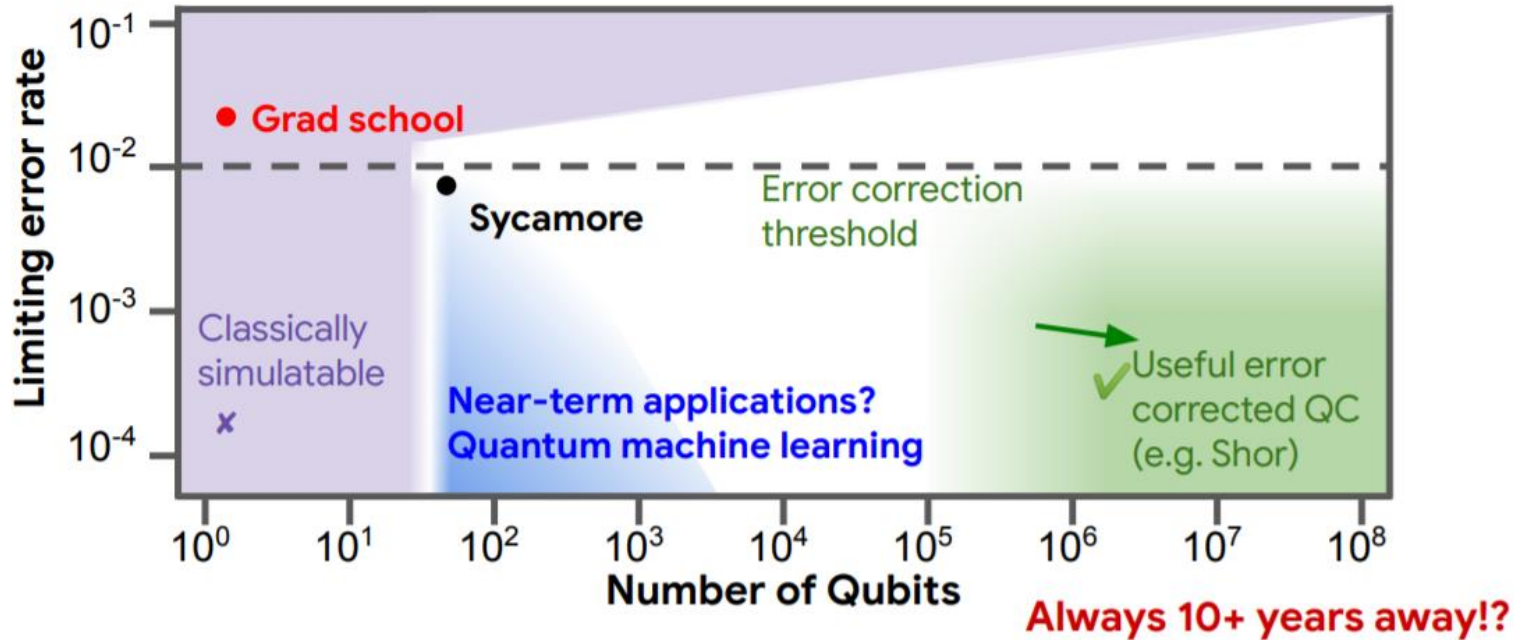
A random variational circuit with gates chosen from the set $\{RX, RY, RZ\}$



Expectation value of a Hermitian observable along a slice in the parameter space

- *In classical optimization, it is suggested that saddle points, not local minima, provide a fundamental impediment to rapid high-dimensional non-convex optimization. (Dauphin et al., 2014)*
- *For a wide class of reasonable parameterized quantum circuits, the probability that the gradient along any reasonable direction is non-zero to some fixed precision is exponentially small as a function of the number of qubits. (McClean et al., 2018)*

FUTURE PERSPECTIVES



- QRAM for data encoding
- Fault tolerant QC for better variational circuit ansatz
- More qubits

Third generation of QML

- No barren plateaus
- No heuristic model