



Tutorial on QuantumFlow: A Co-Design Framework of Neural Network and Quantum Circuit towards Quantum Advantage

Session 5: Roadmap of Quantum Machine Learning

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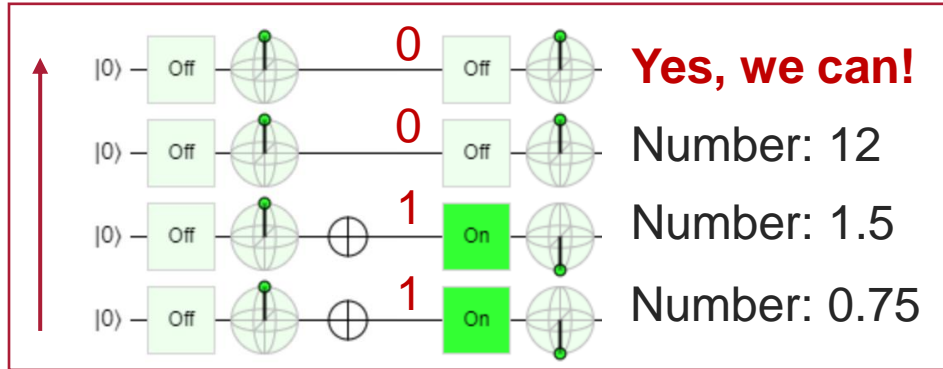
Agenda – Session 1: Introduction

- **Roadmap of Quantum Machine Learning**
 - Data Encoding
 - HHL Algorithm
 - Variational Quantum Circuit
 - Quantum-based Neural Network Accelerator
 - Applications
- **Call for paper at “Electronics”**
- **Conclusion**
- **Q&A**

What Data Can Be Encoded to Quantum Computers, and how?

- Can we encode an arbitrary number into quantum computer? Is it efficient?

▪ **Yes / No**



No, because it uses too many qubits!

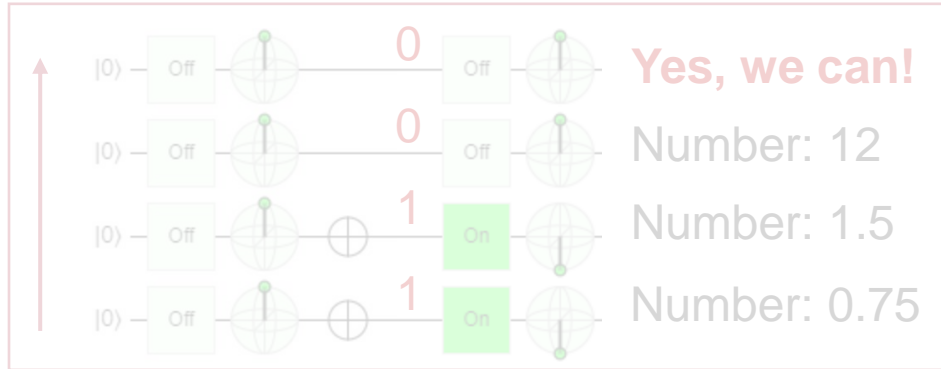
This encoding is similar to classical bits, where each qubit is regarded as a binary number!

1-to-N mapping! (Boolean Function)

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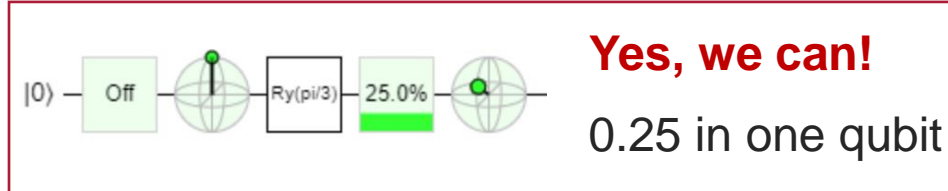
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1-to-N mapping! (Boolean Function)

- Can we take use of superposition of qubits to encode data? Is this solution perfect?

- **Yes / No**



No, (1) data needs in the range of $[0,1]$!

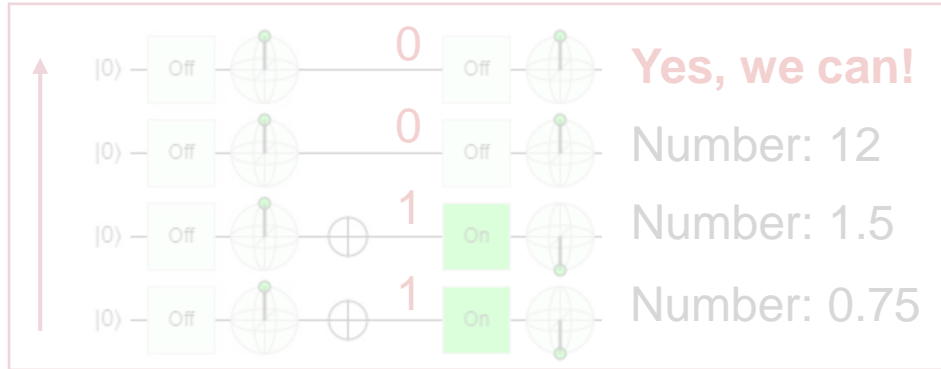
(2) same complexity $O(1)$ as classical

1-to-1 mapping! (Angle Encoding)

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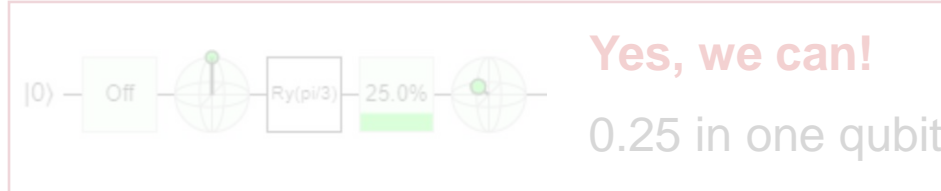
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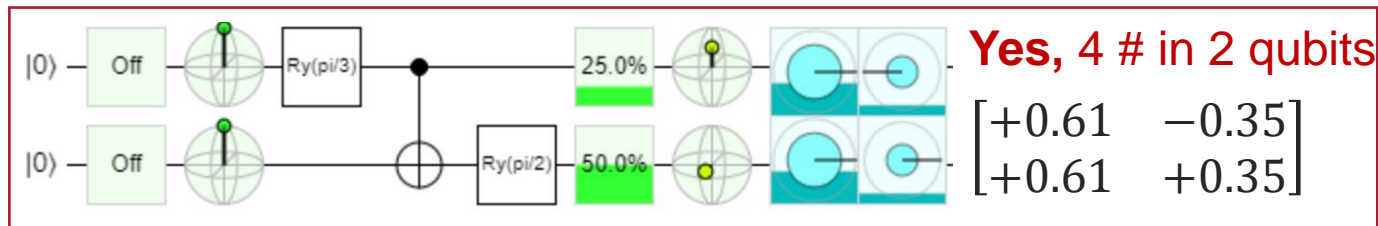
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1-to-1 mapping! (Angle Encoding)

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▪ Yes / No



No, (1) sum of the square of data need to be 1
 (2) may have high cost to encode data

N-to-logN mapping! (Amplitude Encoding)

Encoding: 1-to-N v.s. 1-to-1 v.s. N-to-logN

Data Encoding	# of Qubit (C v.s. Q)	Data Limitation	Encoding Complexity
1-to-N	$O(1)$ v.s. $O(N)$	Almost No!	Low
1-to-1	$O(1)$ v.s. $O(1)$	$[0,+1]$	Low
N-to-logN	$O(N)$ v.s. $O(\log N)$	$[-1,+1]$ and $\sum x^2 = 1$	High

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Quantum Fourier Transform (1-to-N)

Problem to be solved: Encoding the binary number represented by states to phase.

QFT, inspired by the discrete Fourier transform, is the **linear operator** defined over an orthonormal basis $|0\rangle, \dots, |N-1\rangle$ of a **N-dimensional complex vector space**, as

$$|a\rangle \xrightarrow{QFT} |a'\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{\frac{2\pi i}{N} ak} |k\rangle$$

Input:

$$|a\rangle = |01\rangle \rightarrow a=1$$

$$N = 2^2 = 4$$

$$QFT * |a\rangle = \frac{1}{\sqrt{N}} \times (x_0 \cdot |00\rangle + x_1 \cdot |01\rangle + x_2 \cdot |10\rangle + x_3 \cdot |11\rangle)$$

$$x_0 = e^{\frac{2\pi i}{N} ak} = e^{\frac{2\pi * a * k}{N} i} = e^{\frac{2\pi * 1 * 0}{4} i} = e^0$$

(note: k=0 since we consider $|k\rangle = |00\rangle$)

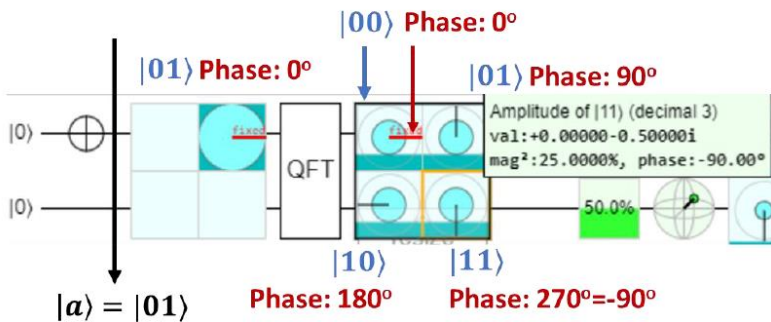
$$x_1 = e^{\frac{2\pi i}{N} ak} = e^{\frac{2\pi * a * k}{N} i} = e^{\frac{2\pi * 1 * 1}{4} i} = e^{\frac{1\pi}{2} i}$$

(note: k=1 since we consider $|k\rangle = |01\rangle$)

$$x_2 = e^{\frac{2\pi i}{N} ak} = e^{\frac{2\pi * a * k}{N} i} = e^{\frac{2\pi * 1 * 2}{4} i} = e^{\pi i}$$

$$x_3 = e^{\frac{2\pi i}{N} ak} = e^{\frac{2\pi * a * k}{N} i} = e^{\frac{2\pi * 1 * 3}{4} i} = e^{\frac{3\pi}{2} i}$$

$$\Rightarrow QFT * |a\rangle = \frac{1}{2} \times \left(e^0 \cdot |00\rangle + e^{\frac{\pi}{2} i} \cdot |01\rangle + e^{\pi i} \cdot |10\rangle + e^{\frac{3\pi}{2} i} \cdot |11\rangle \right)$$



Quantum Phase Estimation (1-to-N for Output)

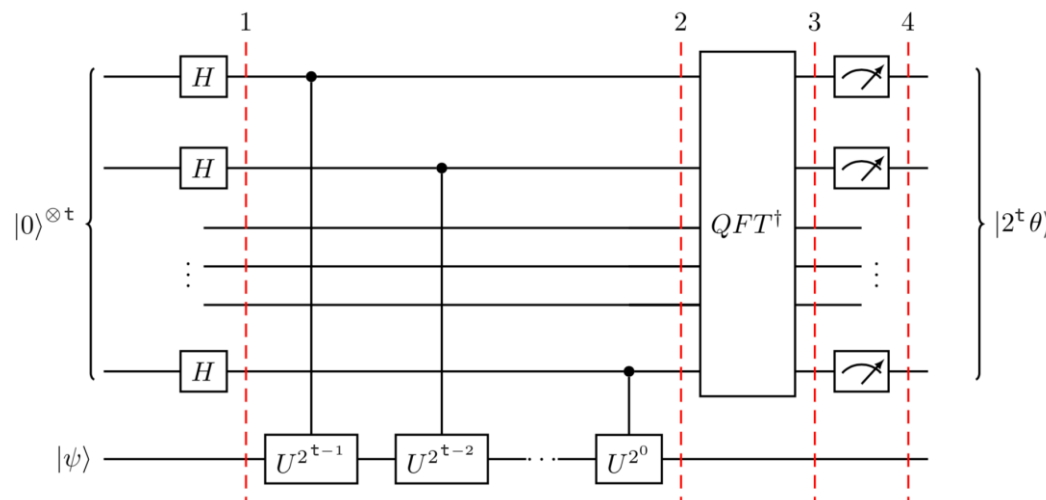
Problem to be solved: Extract the phase to binary number represented by states.

Given a unitary operator U , the algorithm estimates θ in $U|\Psi\rangle = e^{2\pi i\theta} |\Psi\rangle$. Here, $|\Psi\rangle$ is an eigenvector and $e^{2\pi i\theta}$ is the corresponding eigenvalue. Since U is unitary, all of its eigenvalues have a norm of 1.

Why: Difficulty in Measuring the Phase.



How?



Given:

- We have the implementation of operator U .
- $U^t =$ Repeat the operator U for t times

HHL

Problem to solve:

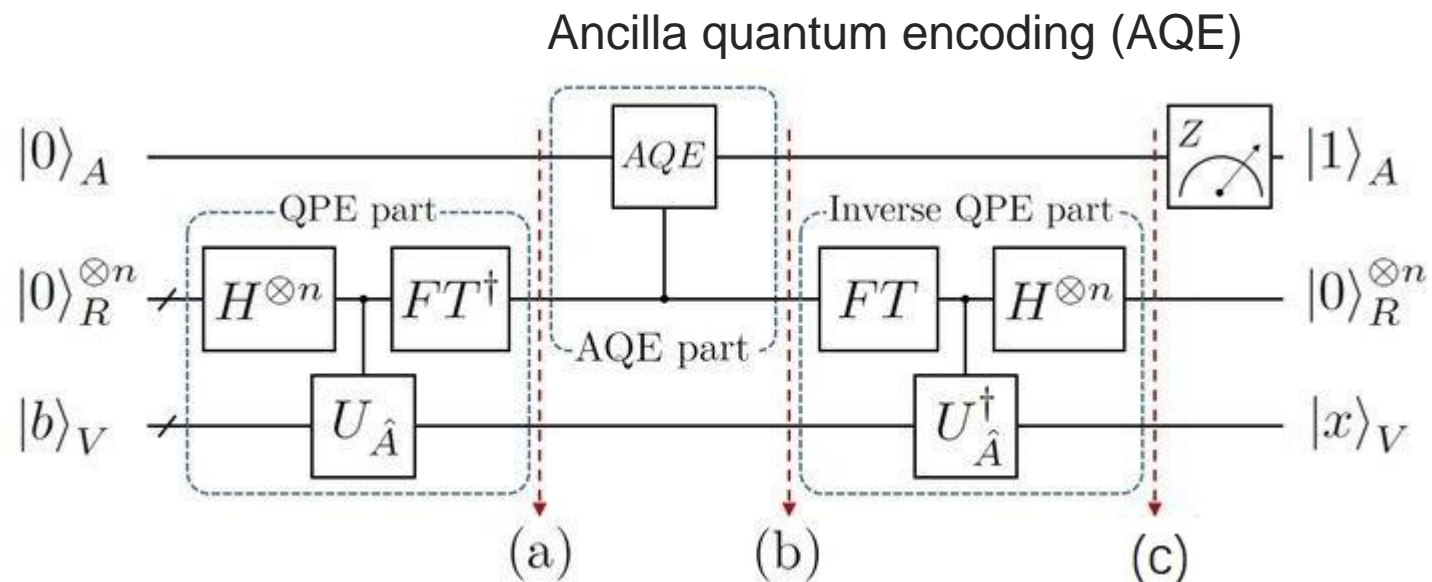
The problem can be defined as, given a matrix $\mathbf{A} \in \mathbb{C}^{N \times N}$ and a vector $\vec{b} \in \mathbb{C}^N$, find $\vec{x} \in \mathbb{C}^N$ satisfying $\mathbf{A} \vec{x} = \vec{b}$

Why: Classical has complexity of $O(N\kappa)$, can quantum reduce the complexity to $O(\log(N)\kappa^2)$. N is the number of variables in the linear system. κ is a low condition number.

How?

Given:

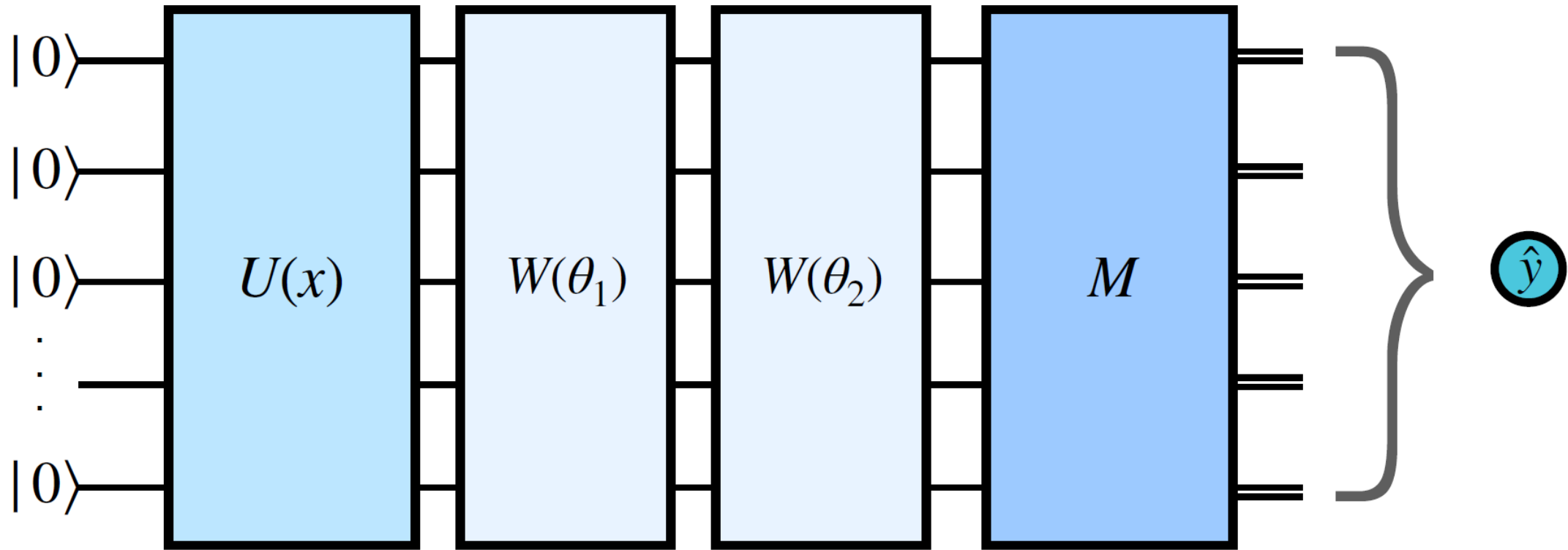
- Hermitian matrix A
- b



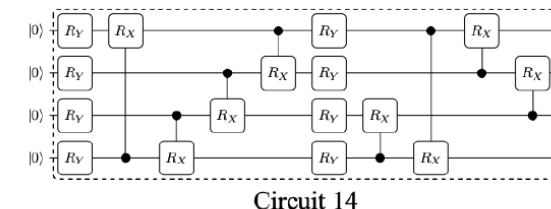
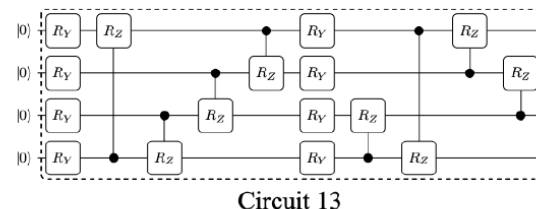
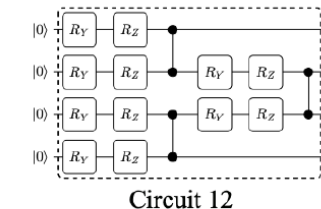
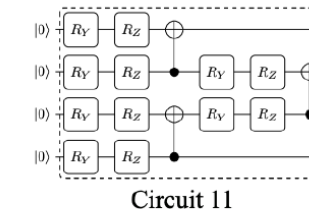
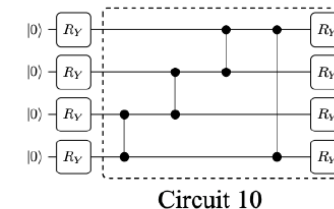
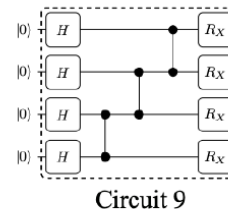
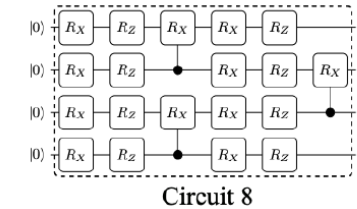
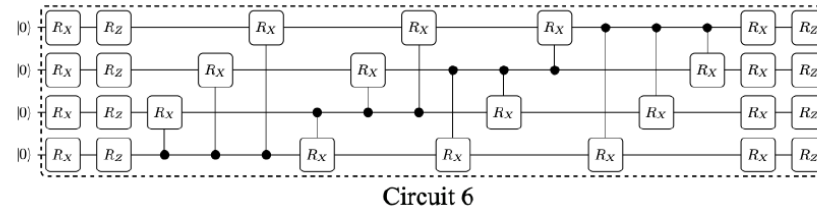
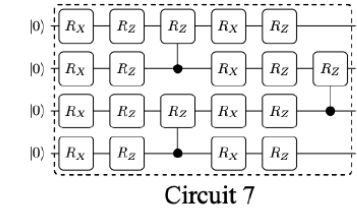
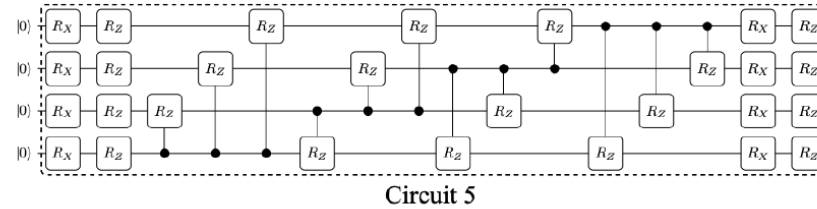
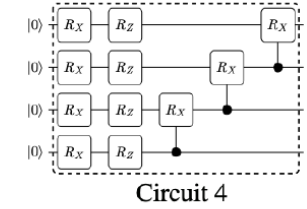
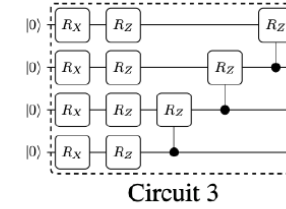
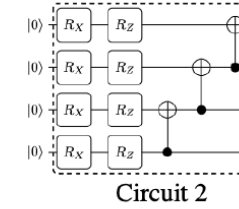
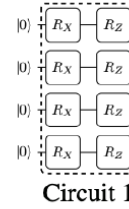
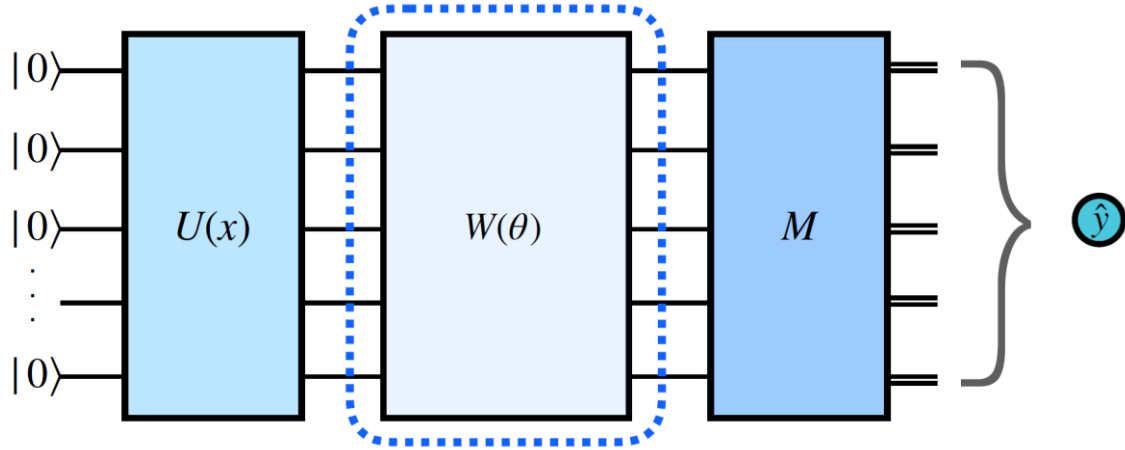
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Variational Classifier (1-to-N or 1-to-1 or N-to- $\log N$)

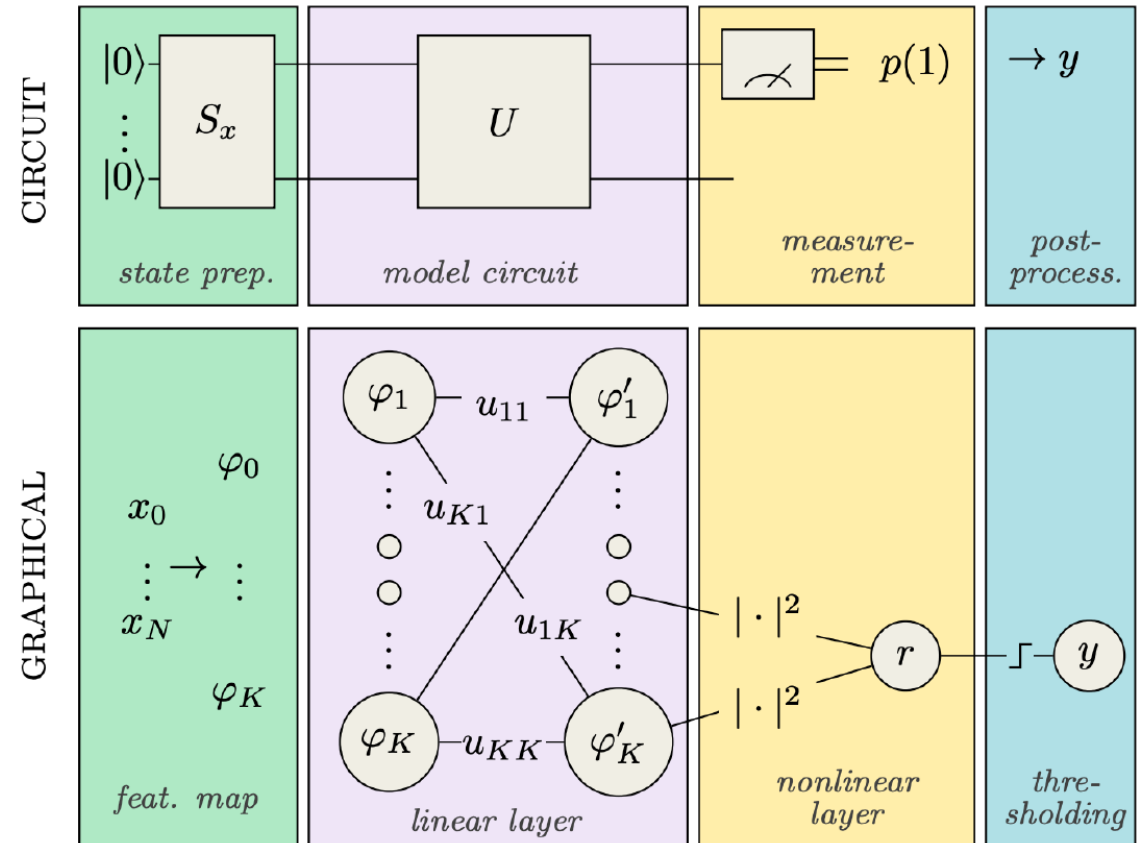
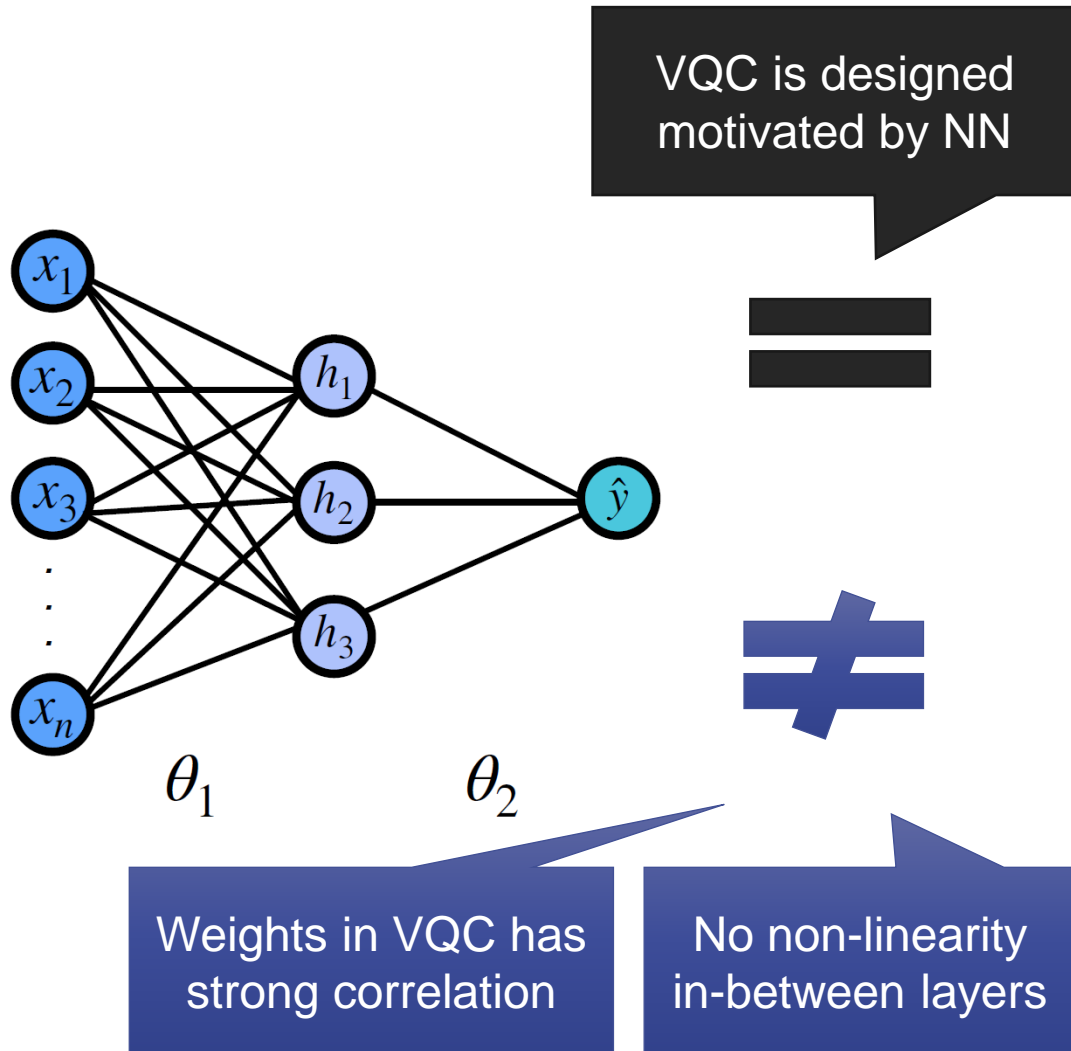


Variational Classifier



Sim et al. "Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms." Advanced Quantum Technologies 2.12 (2019): 1900070.

VQC-based Quantum Neural Network

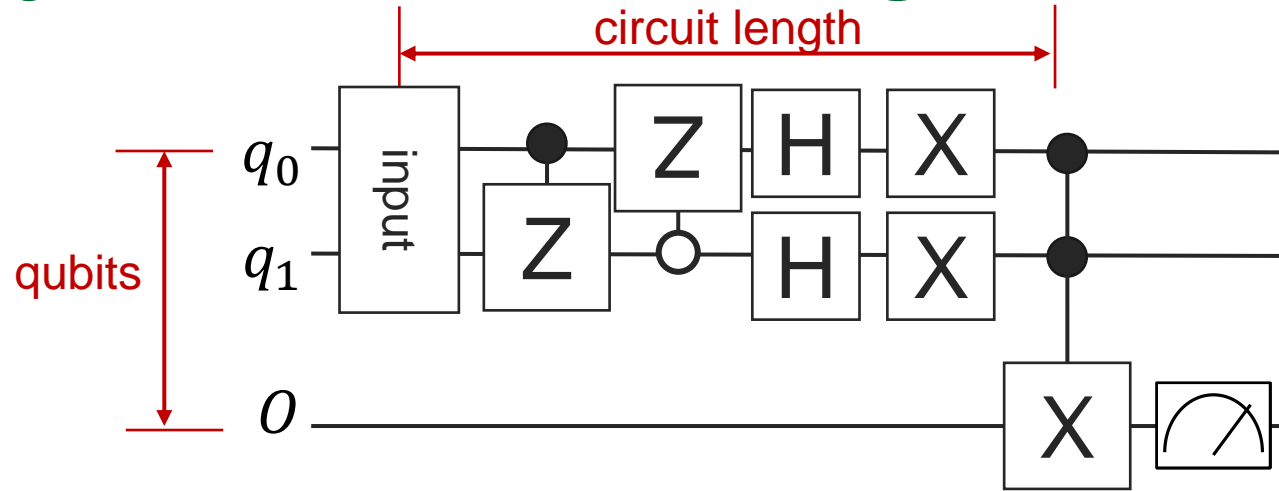
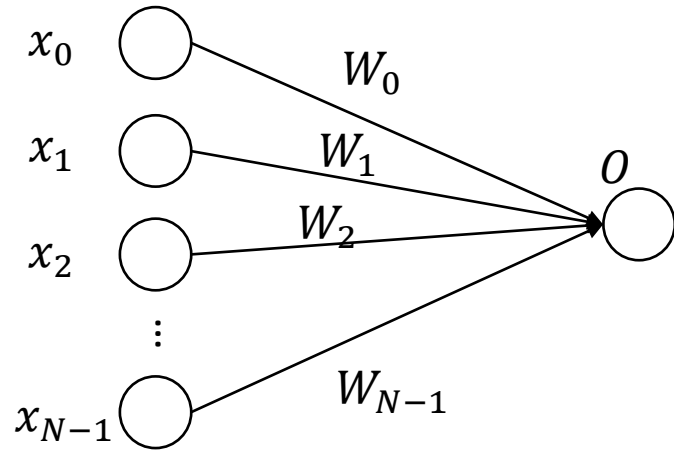


Schuld et al. "Circuit-centric quantum classifiers." *Physical Review A* 101.3 (2020): 032308.

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What's the complexity? Quantum Advantage?



- **Classical computer with 1 MAC**

Time: $O(N)$

Space (Comp. Res.): $O(1)$

Time \times Space: $O(N)$

- **Classical computer with N MAC**

Time: $O(1)$

Space (Comp. Res.): $O(N)$

Time \times Space: $O(N)$

- **Time-Space Complexity in Quantum computer**

Time: Circuit Length

Space (Comp. Res.): Qubits

Time \times Space ($T - S$): Qubits \times Circuit Length

- **Given that $T - S$ complexity on classical computer is $O(N)$, Quantum Advantage is achieved if $T - S$ complexity on Quantum can be $O(\text{polylog}N)$ or lower. ----- Exponential Speedup!**

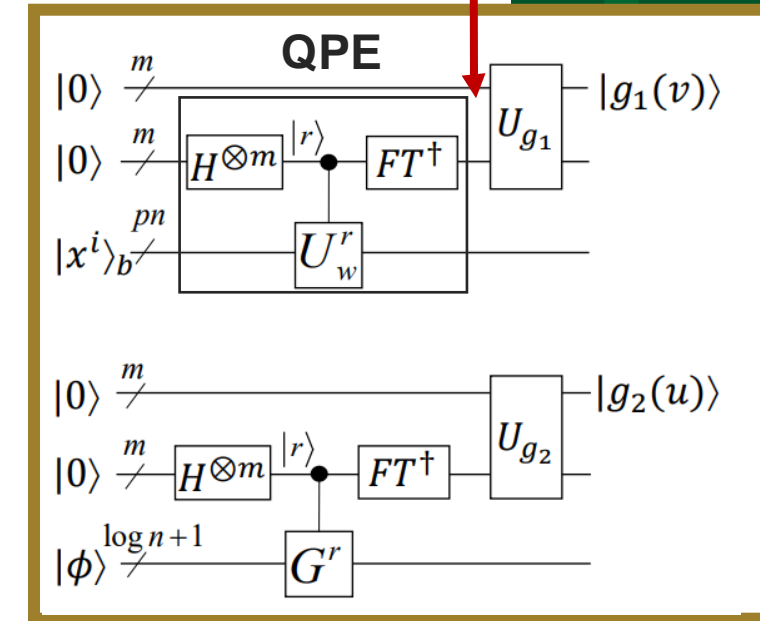
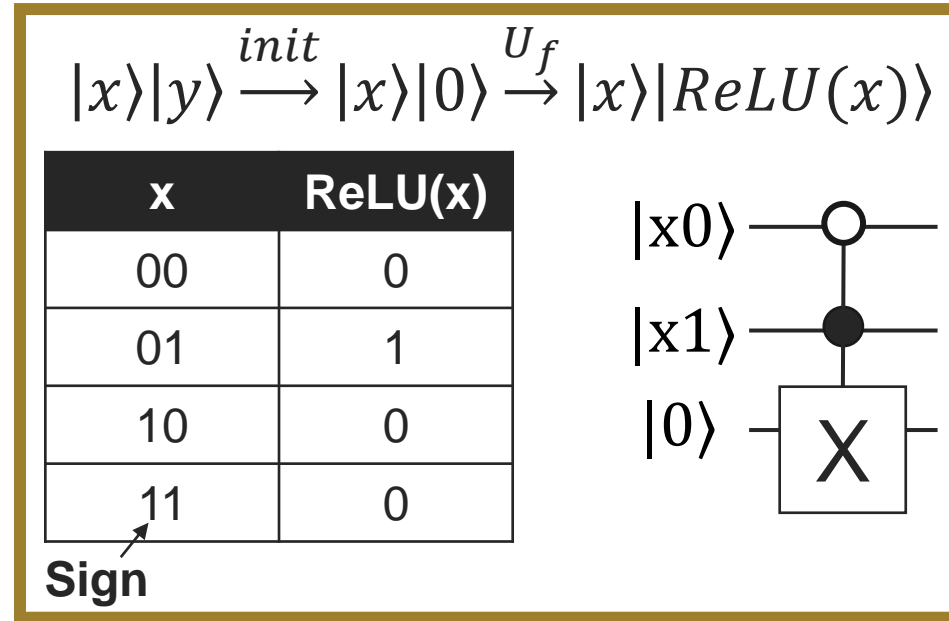
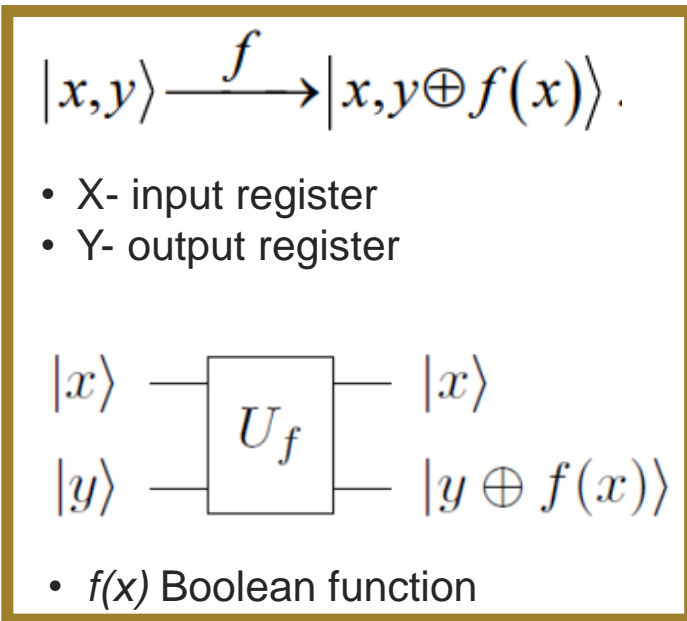
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Apply Boolean Function to Realize Any Non-Linear (1-to-N)

Problem to be solved: $U_f : |x\rangle |0\rangle^{\otimes m} \mapsto |x\rangle |f(x)\rangle$

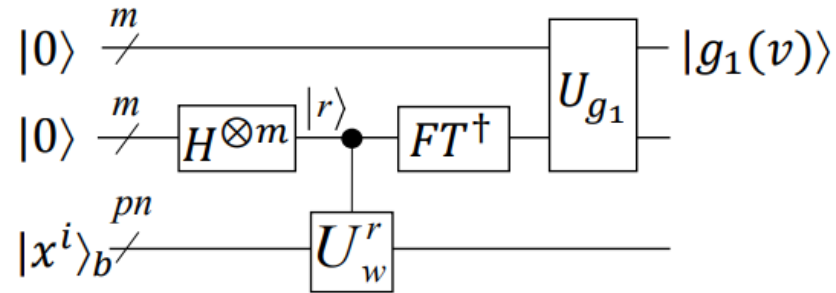
- f can be any non-linear function, say ReLU
- X is a $0.x_1x_2x_3\dots x_n$ binary format to hold the intermediate data



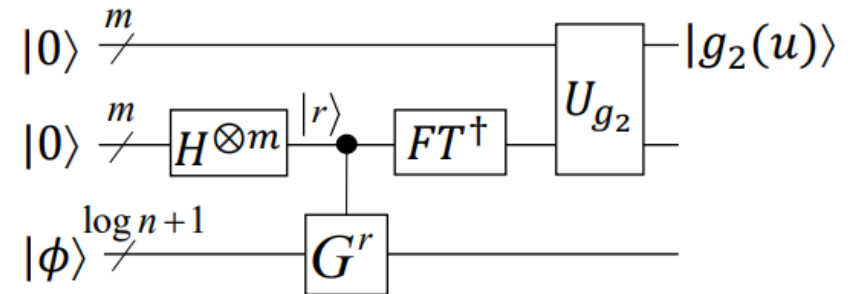
[ref 1] Shilu Yan, et al. , Nonlinear quantum neuron: A fundamental building block for quantum neural networks.
 [ref 2] F. M. de Paula Neto , et al. , Implementing Any Nonlinear Quantum Neuron, IEEE TNNLS

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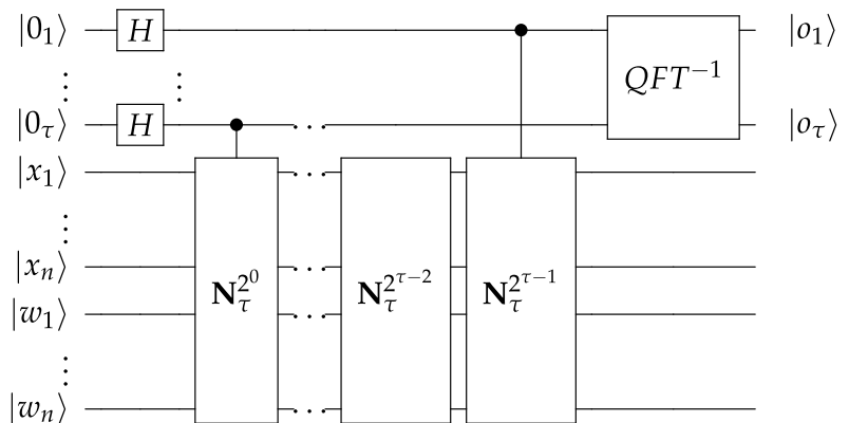
(a) angle encoding



(b) amplitude encoding



(c) [ref]



Comparison of different quantum neurons.

Quantum neurons	Input features	Number of qubits	Gate complexity
(a)	Binary	$pn + 2m$	$O(pn + m2^m)$
(b)	Continuous	$\log n + 2m + 1$	$O(mn^2 + m2^m)$
(c)	Binary	$2pn + m$	$O(m2^{2pn} + m^2)$

n: input data number
 p: precision for input
 m: precision for output
No Quantum Advantage

[ref] F. M. de Paula Neto, et al., Implementing Any Nonlinear Quantum Neuron, IEEE TNLS

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Quantum Neuron (1-to-1): Linear Part

Problem to be solved (Linear Function):

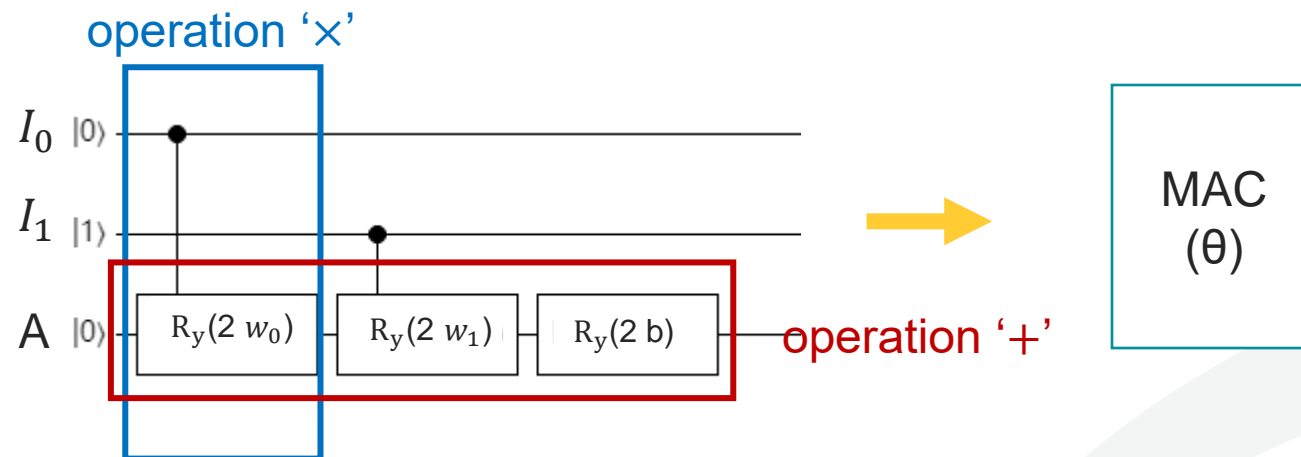
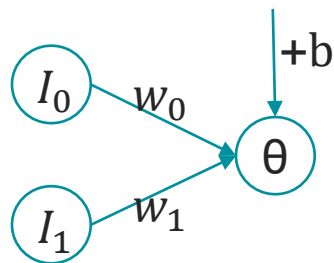
Classical: Given $I_0, I_1, \dots, I_n, b, w_0, w_1, \dots, w_n,$

$$\text{Output: } \theta = \sum_{i=0}^n I_i \times w_i + b$$

Quantum: Given $p_0, p_1, \dots, p_n, R_y(2b), R_y(2w_0), R_y(2w_1), \dots, R_y(2w_n)$

Output: $R_y(2\theta)$ ---- θ is computed on angle.

Example:



Idea: For I_j with $\text{Prob}\{I_j = |1\rangle\} = p_j$

If $p_j = 1$, then rotate the output qubit "A" by $2w_j$; otherwise, don't rotate A

Quantum Neuron (1-to-1): Non-Linear Part

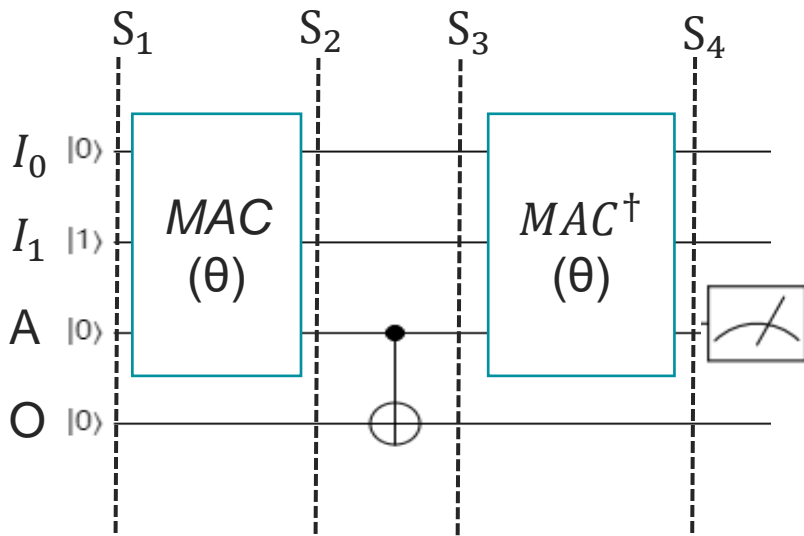
Problem to be solved (Non-Linear Function):

Classic: Given θ ,

Output: $\mathbf{q}(\theta) = \mathbf{arctan}(\mathbf{tan}^2\theta)$

Quantum: Given $R_y(2\theta)$

Output: $\mathbf{O} = R_y(2\mathbf{q}(\theta))$



$$S1: |0A\rangle = |00\rangle$$

$$S2: I \otimes R_y(2\theta) \times |00\rangle = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 & 0 \\ \sin(\theta) & \cos(\theta) & 0 & 0 \\ 0 & 0 & \cos(\theta) & -\sin(\theta) \\ 0 & 0 & \sin(\theta) & \cos(\theta) \end{bmatrix} \times \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \\ 0 \\ 0 \end{bmatrix}$$

$$S3: \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos(\theta) \\ 0 \\ 0 \\ \sin(\theta) \end{bmatrix}$$

$$S4: \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 & 0 \\ \sin(\theta) & \cos(\theta) & 0 & 0 \\ 0 & 0 & \cos(\theta) & -\sin(\theta) \\ 0 & 0 & \sin(\theta) & \cos(\theta) \end{bmatrix} \times \begin{bmatrix} \cos(\theta) \\ 0 \\ 0 \\ \sin(\theta) \end{bmatrix} = \begin{bmatrix} \cos^2(\theta) \\ -\sin(\theta)\cos(\theta) \\ \sin^2(\theta) \\ \sin(\theta)\cos(\theta) \end{bmatrix} \begin{matrix} |0A\rangle \\ |00\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$$

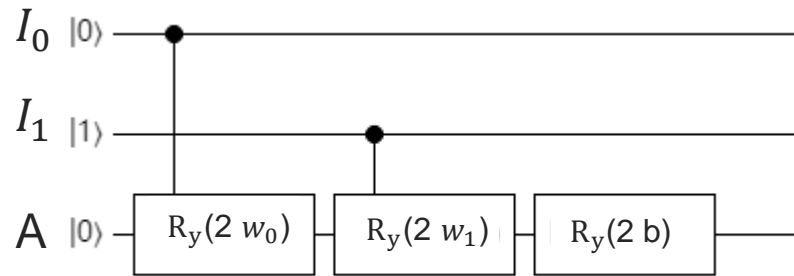
Measure A.

$|A\rangle = |0\rangle$: success

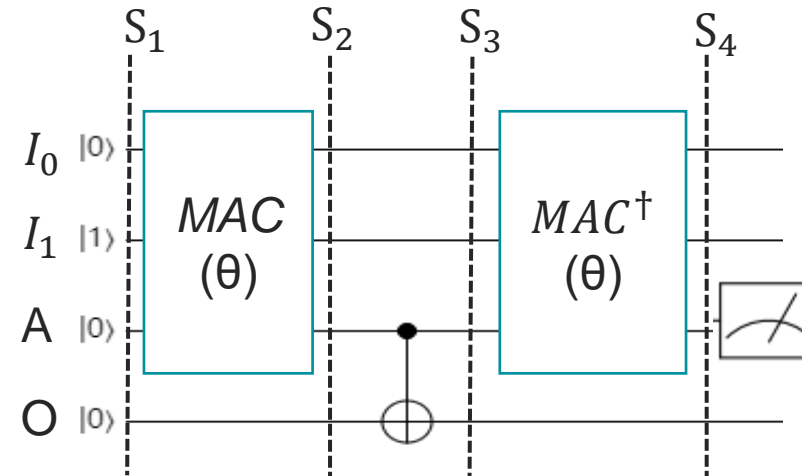
$|A\rangle = |1\rangle$: recover and repeat

$$\begin{bmatrix} \cos^2(\theta) \\ -\sin(\theta)\cos(\theta) \\ \sin^2(\theta) \\ \sin(\theta)\cos(\theta) \end{bmatrix} \rightarrow \begin{bmatrix} \cos^2(\theta) \\ 0 \\ \sin^2(\theta) \\ 0 \end{bmatrix} \rightarrow \tan^2 \theta$$

Quantum Neuron (1-to-1): Complexity



(a) Linear computation



(b) Non-linear computation

Input features	Number of Qubits	Number of Gates
Linear	$O(n)$	$O(n)$
Non-linear	$O(1)$	$O(m \cdot n)$

n: input data number
 m: repeat number
No Quantum Advantage

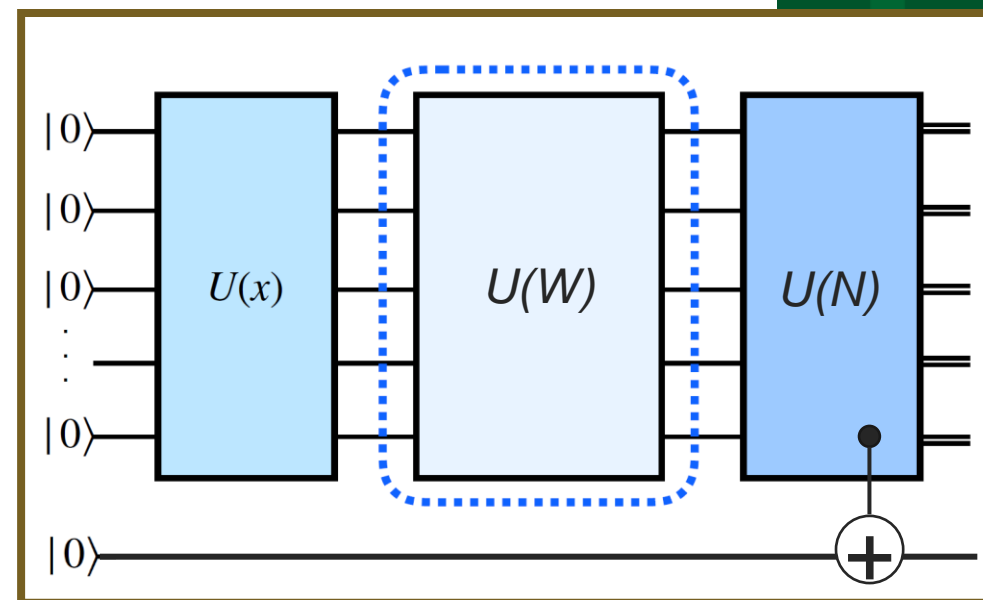
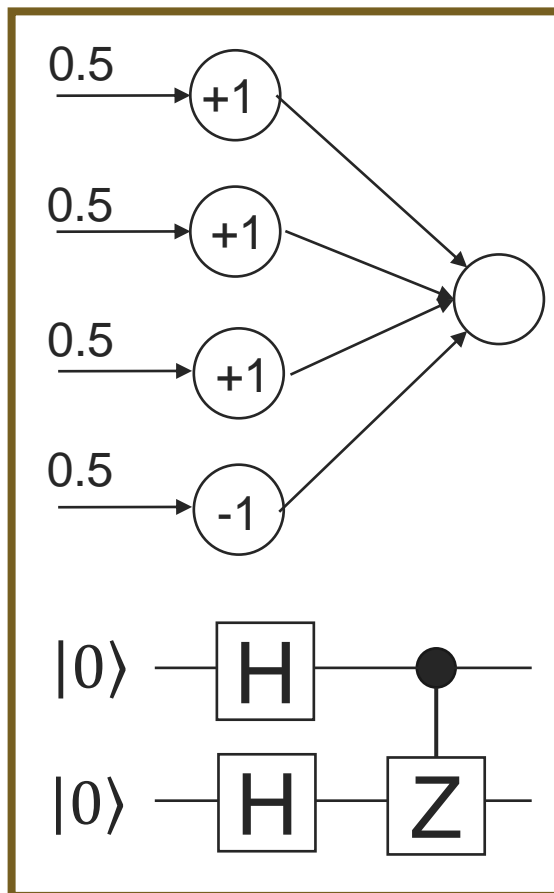
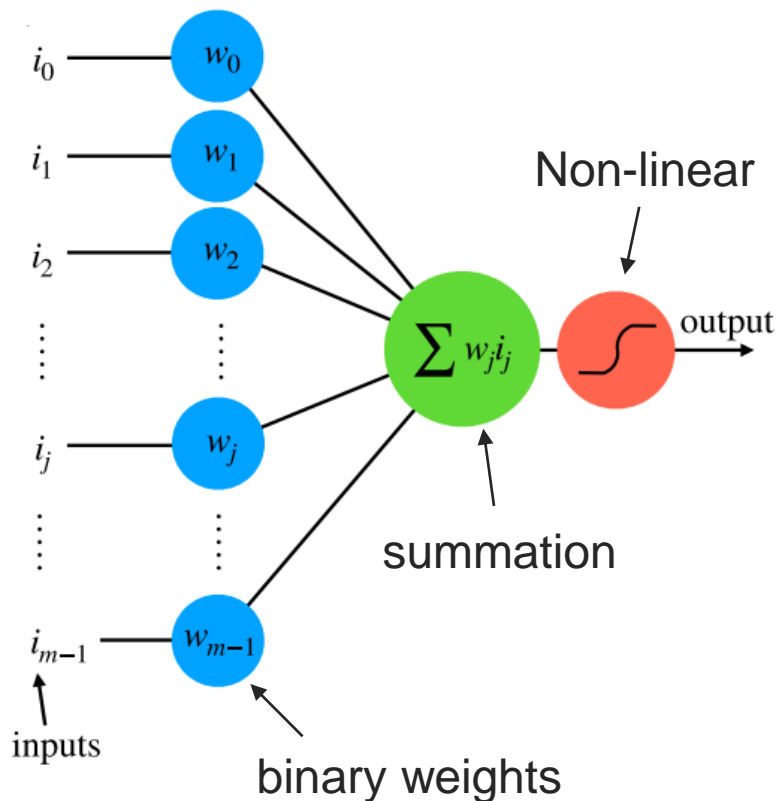
[ref] Cao, Yudong, et al. "Quantum neuron: an elementary building block for machine learning on quantum computers." *arXiv preprint arXiv:1711.11240* (2017).

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Sign Flip on Amplitude for Binary NN (N-to-logN)

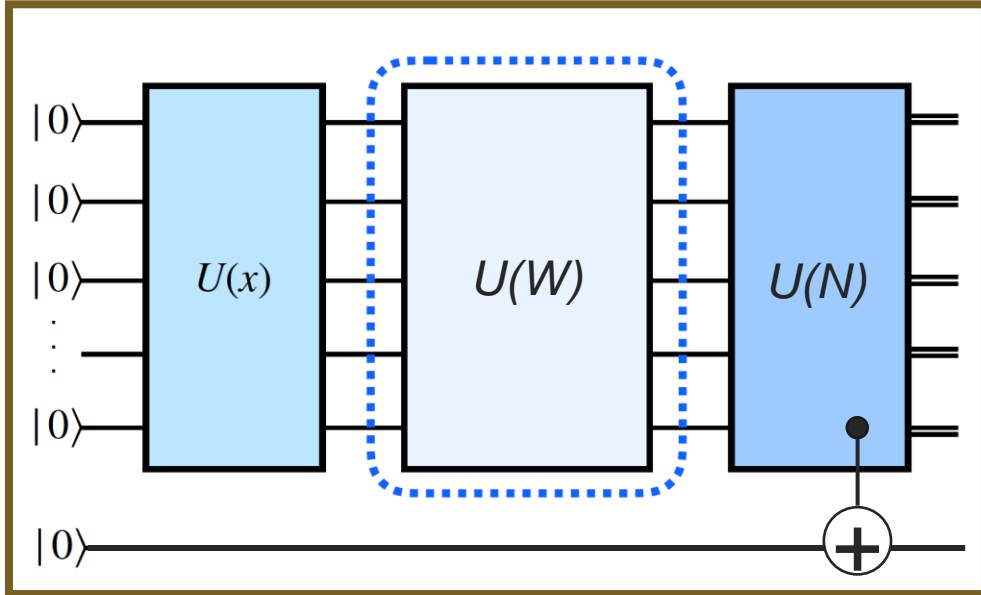
Problem to be solved (Binary Neural Network):



[Ref1] Tacchino, Francesco, et al. "An artificial neuron implemented on an actual quantum processor." *npj Quantum Information* 5.1 (2019): 1-8.

[Ref2] Jiang, Weiwen, Jinjun Xiong, and Yiyu Shi. "When Machine Learning Meets Quantum Computers: A Case Study." *2021 26th Asia and South Pacific Design Automation Conference (ASP-DAC)*. IEEE, 2021.

Sign Flip on Amplitude (N-to- $\log N$): Complexity



Input features	Number of Qubits	Number of Gates
$U(x)$	$O(\log N)$	$O(?)$
$U(W)$	$O(\log N)$	$O(?)$
$U(N)$	$O(1)$	$O(\log N)$

n: input data number

Potential Quantum Advantage

Halfway Takeaway

- **3 typical data encoding without losing information**
 - 1-to-N encoding ([Boolean Function](#))
 - 1-to-1 encoding ([Angle Encoding](#))
 - N-to- $\log N$ encoding ([Amplitude Encoding](#))
- **Variational Quantum Circuit**
 - Designed **based on** neural network, but **no classical correspondence**
 - Can **integrate real-number weights** in the circuit
 - **Non-linearity** is difficult to be integrated, leading a 1-layer neural network

Halfway Takeaway

- Quantum-based Neural Network Accelerator

- Boolean function-based design

- High flexibility
 - High cost (**no quantum advantage**)

- Angle-based design

- Work for specific functions
 - Neutral cost (**still hard to have quantum advantage**)

- Amplitude-based design

- More limitations
 - Lower cost (**potential of quantum advantage**)

Comparison of different quantum neurons.

Quantum neurons	Input features	Number of qubits	Gate complexity
(a)	Binary	$pn + 2m$	$O(pn + m2^m)$
(b)	Continuous	$\log n + 2m + 1$	$O(mn^2 + m2^m)$
(c)	Binary	$2pn + m$	$O(m2^{2pn} + m^2)$

Input features	Number of Qubits	Number of Gates
Linear	$O(n)$	$O(n)$
Non-linear	$O(1)$	$O(m \cdot n)$

Input features	Number of Qubits	Number of Gates
U(x)	$O(\log N)$	$O(?)$
U(W)	$O(\log N)$	$O(?)$
U(N)	$O(1)$	$O(\log N)$

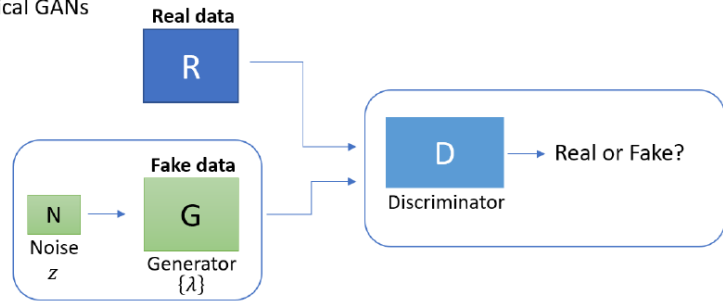
Data Encoding
Weight Embedding

Agenda – Session 1: Introduction

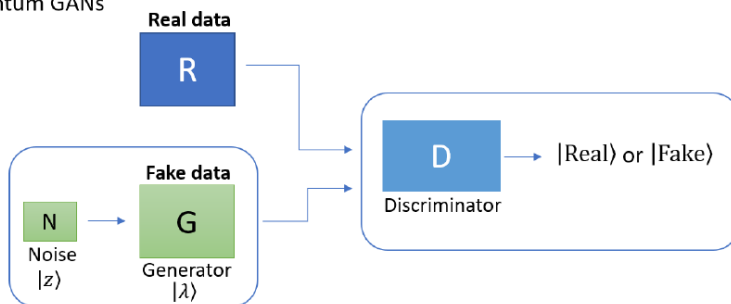
- **Roadmap of Quantum Machine Learning**
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QGAN'2018: Framework

(a) Classical GANs



(b) Quantum GANs



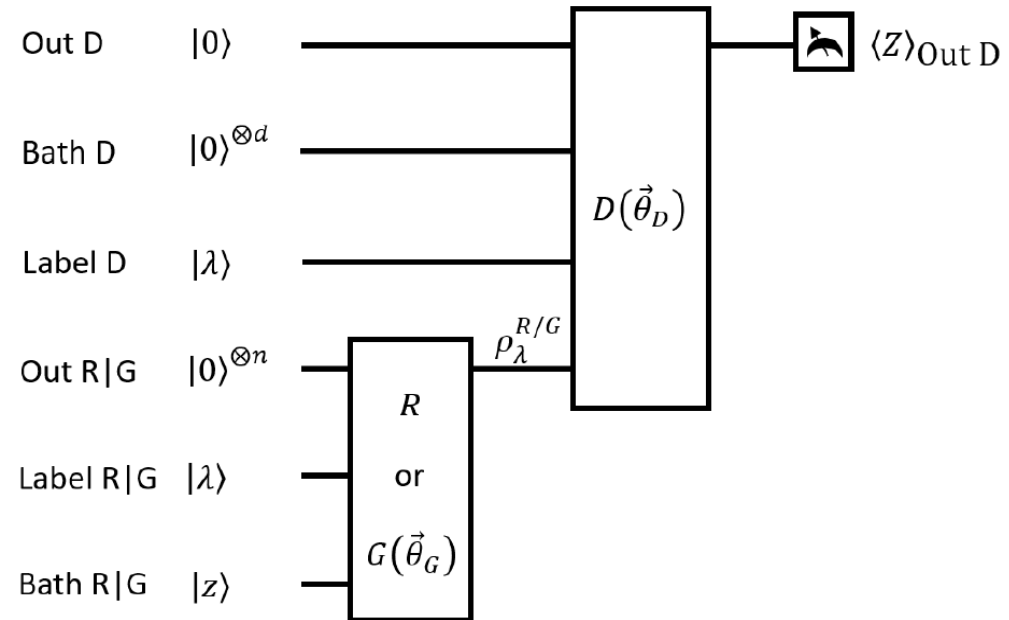
(a): A **discriminator** must determine **whether** the samples it is given are produced by a **real source R** or a generator **G(z)** equipped with a **source of noise z**.

(b): discriminator -> **quantum discriminator**

$G(z) \rightarrow G(|z\rangle)$

output(Real or Fake) -> output(|*real*> or |*fake*>)

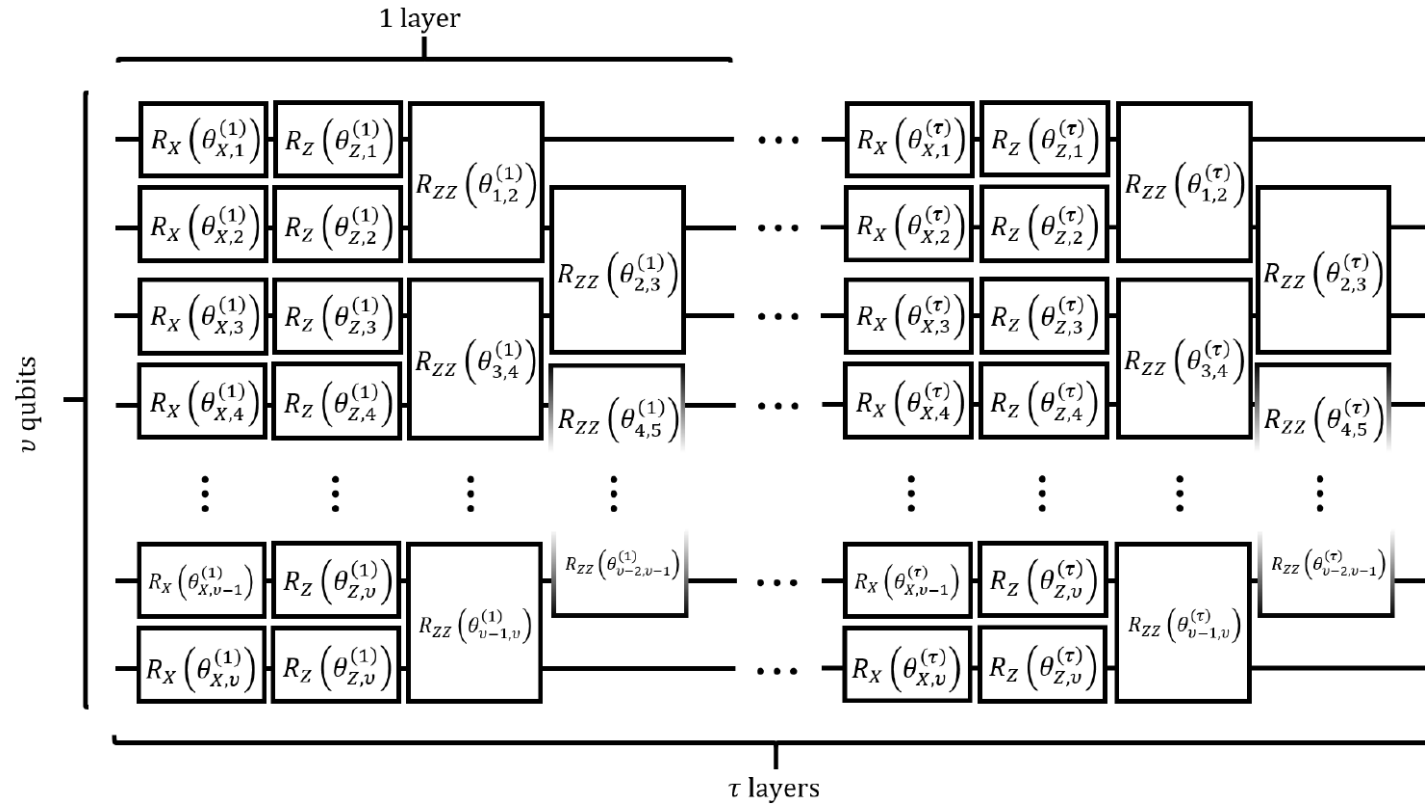
QuGANs:



- **R** or the parametrized generator $G(\vec{\theta}_G)$ is applied on an initial state $|0, \lambda, z\rangle$ defined on the **Label R|G**, **Out R|G** and **Bath R|G**.
- The discriminator $D(\vec{\theta}_D)$ uses the information $\rho_\lambda^{R/G}$ and an initial resource state $|0, 0, \lambda\rangle$ defined on the **Out D**, **Bath D** and **Label D** registers.
- D outputs its answer **|real>** or **|fake>** in the **Out D** register.
- The expectation value $\langle Z \rangle_{Out D}$ is proportional to the probability that D outputs **|real>**.

[ref] Pierre-Luc, et al.2018.Quantum generative adversarial networks . PHYSICAL REVIEW A 98,012324

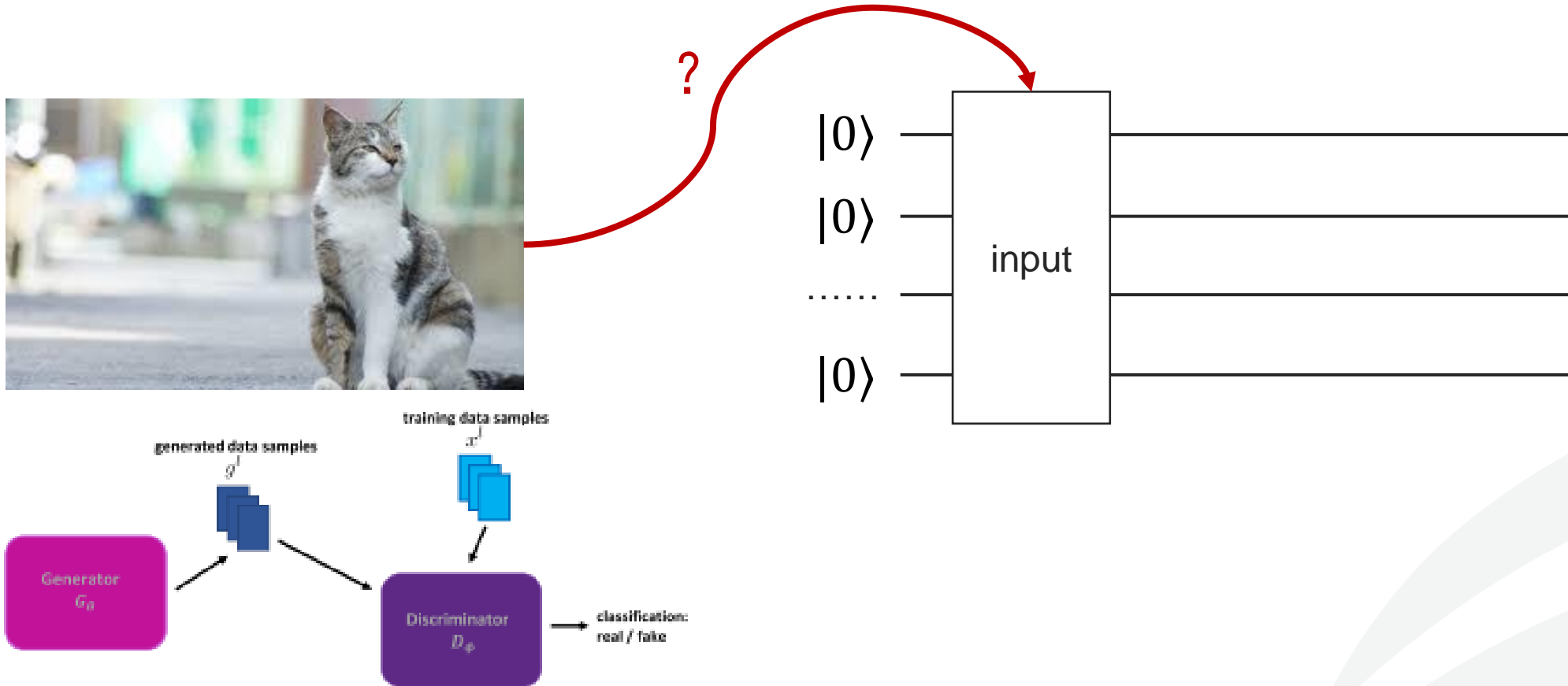
QGAN'2018: Applied VQC



[ref] Pierre-Luc, et al.2018.Quantum generative adversarial networks . PHYSICAL REVIEW A 98,012324

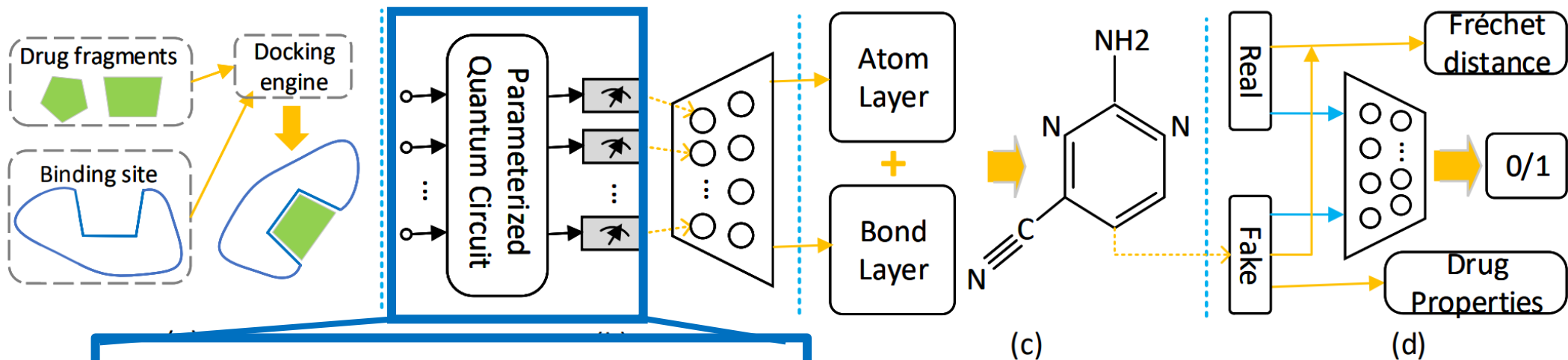
An Application of QGAN'2019

- Quantum State Preparation

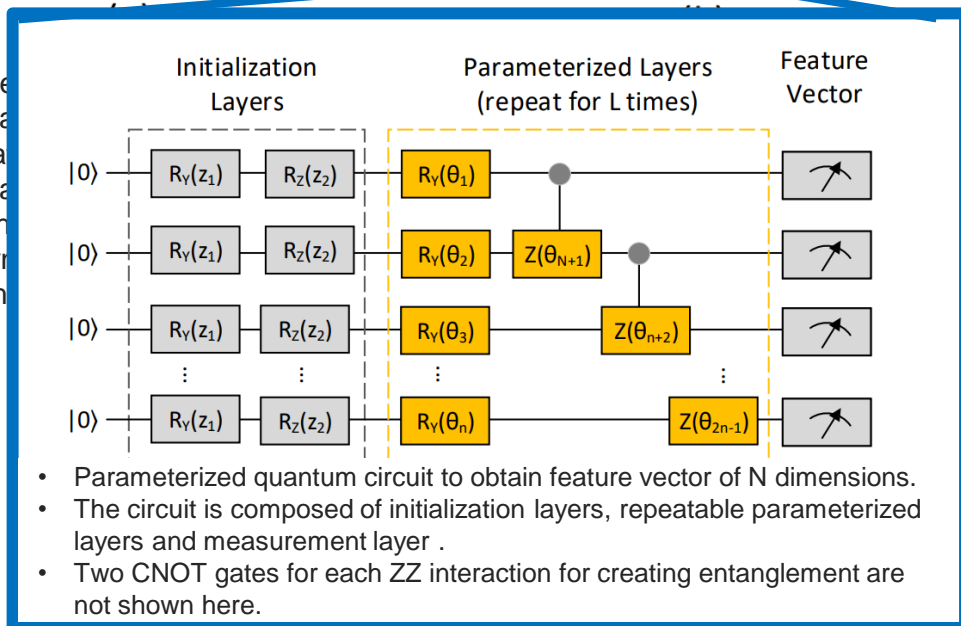


[ref] Christa Zoufal, et al., Quantum Generative Adversarial Networks for learning and loading random distributions. npj Quantum Information

Another Application of QGAN'2021



- (a) Only ge
- (b) (b) qua
- out-fea
- (c) applica
- (d) a batch
- real/syn
- discrim



s are considered as valid;
 measuring the expectation values) and classical stage (neural network with last-layer
 s (one example synthetic molecule is given);
 synthetic molecules generated from (c) are fed into classical discriminator for
 ic molecules are evaluated using RDKit package. The prediction losses from
 it for updating all parameters simultaneously in each training epoch.

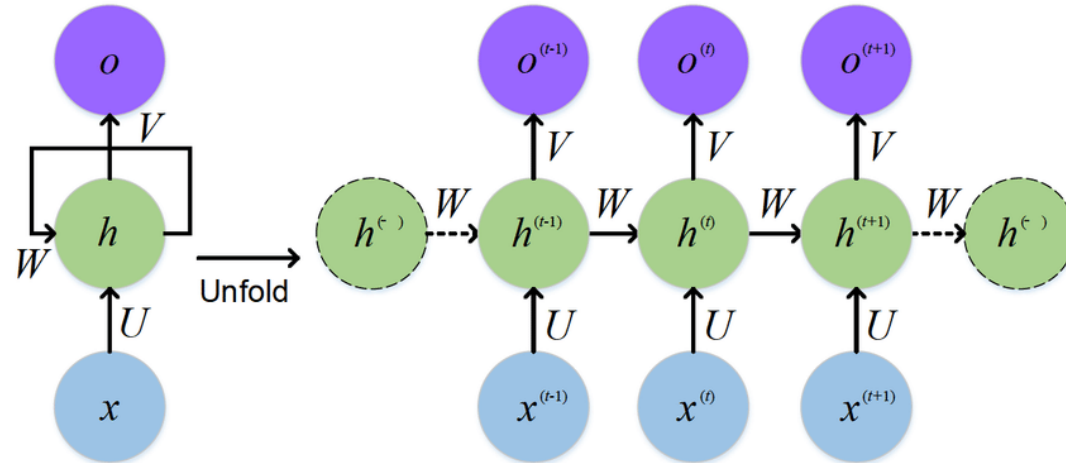
[ref] Junde Li, et al. , Quantum Generative Models for Small Molecule Drug Discovery. arXiv@2021

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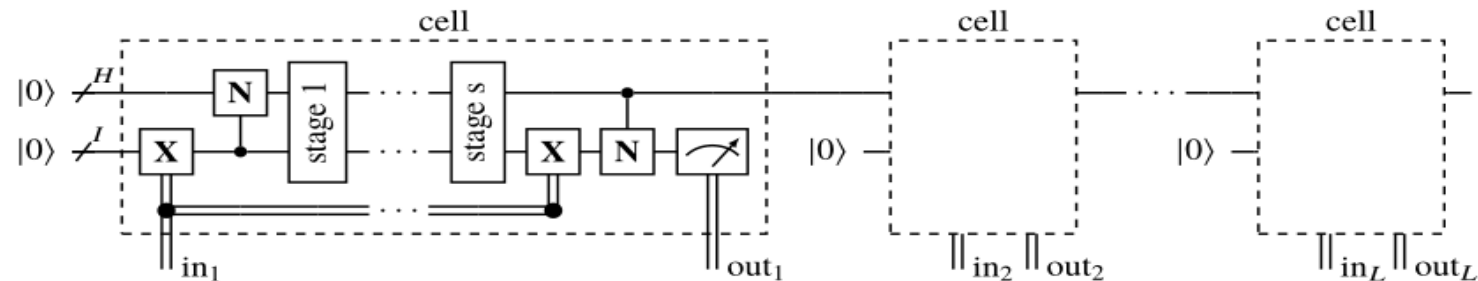
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QRNN --- Based on Quantum Neural (1-to-1)

Classical RNN



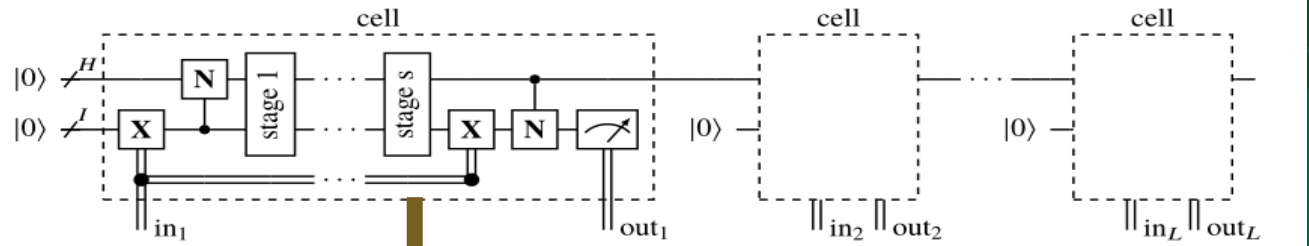
Quantum RNN



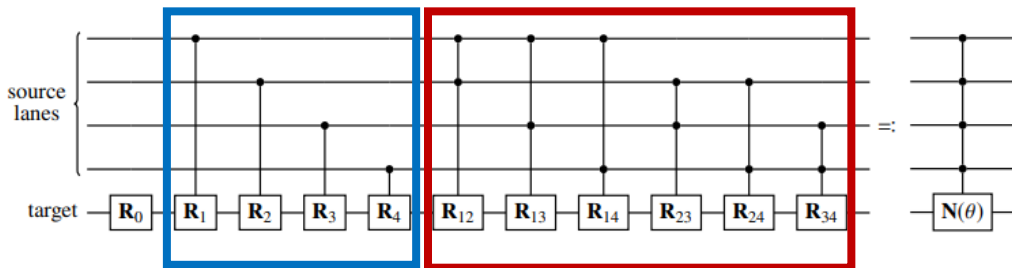
[ref] Johannes Bausch, et al. , Recurrent Quantum Neural Networks Johannes . arXiv @ Jun. 2020

QRNN

QRNN

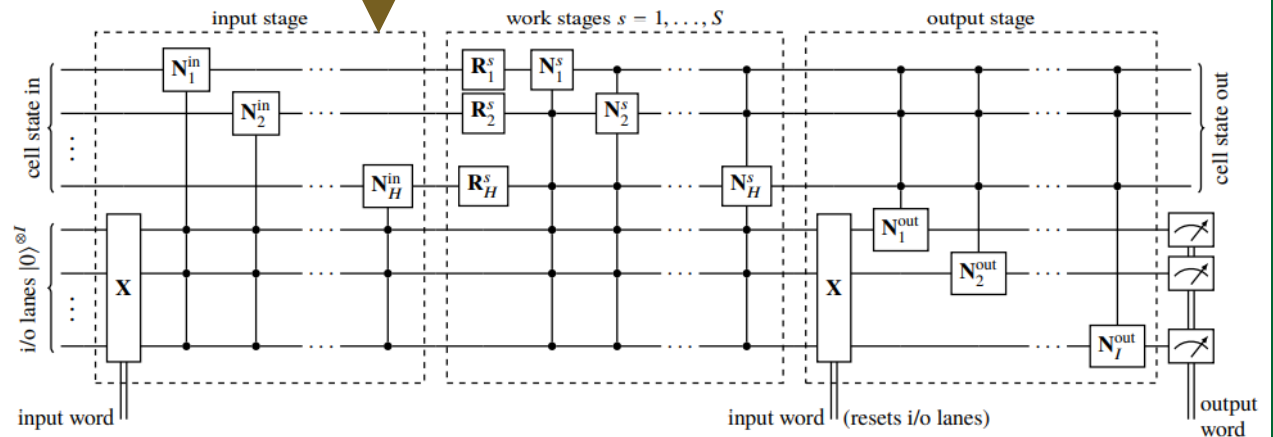


Quantum Neuron (1-to-1)



$$\eta' = \theta_0 + \sum_{i=1}^n \theta_i x_i + \sum_{i=1}^n \sum_{j=1}^n \theta_{ij} x_i x_j + \dots = \sum_{\substack{I \subseteq [n] \\ |I| \leq d}} \theta_I \prod_{i \in I} x_i,$$

QRNN Cell

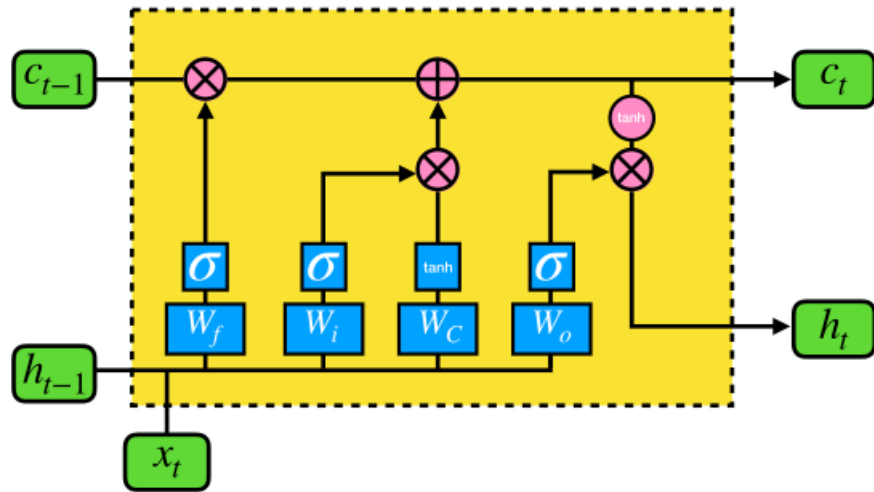


[ref] Johannes Bausch, et al. , Recurrent Quantum Neural Networks Johannes . arXiv @ Jun. 2020

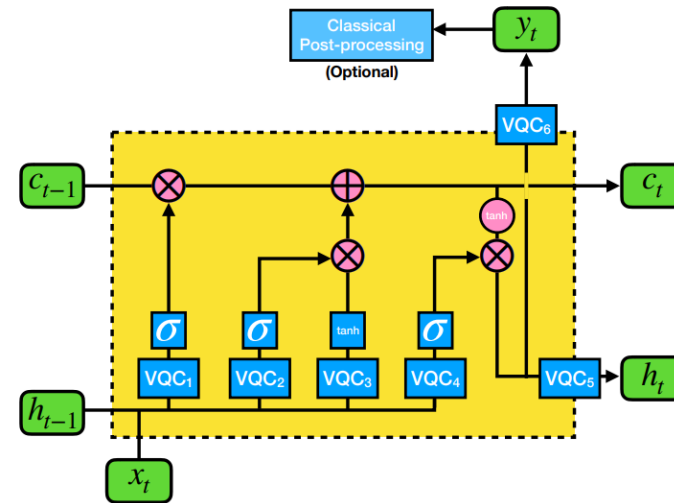
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LSTM v.s. QLSTM -- Based on VQC



$$\begin{aligned}
 f_t &= \sigma(W_f \cdot v_t + b_f) \\
 i_t &= \sigma(W_i \cdot v_t + b_i) \\
 \tilde{C}_t &= \tanh(W_C \cdot v_t + b_C) \\
 c_t &= f_t * c_{t-1} + i_t * \tilde{C}_t \\
 o_t &= \sigma(W_o \cdot v_t + b_o) \\
 h_t &= o_t * \tanh(c_t)
 \end{aligned}$$

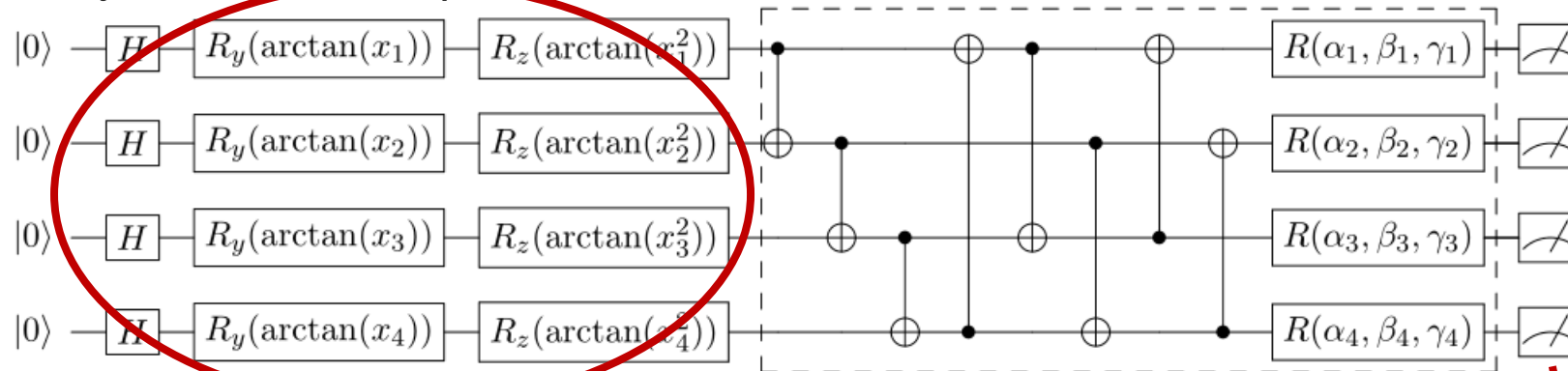


$$\begin{aligned}
 f_t &= \sigma(VQC_1(v_t)) \\
 i_t &= \sigma(VQC_2(v_t)) \\
 \tilde{C}_t &= \tanh(VQC_3(v_t)) \\
 c_t &= f_t * c_{t-1} + i_t * \tilde{C}_t \\
 o_t &= \sigma(VQC_4(v_t)) \\
 h_t &= VQC_5(o_t * \tanh(c_t)) \\
 y_t &= VQC_6(o_t * \tanh(c_t))
 \end{aligned}$$

[ref] Samuel Yen-Chi, et al. , Quantum Long Short-Term Memory.

VQC Used in Q-LSTM

VQCs are a kind of quantum circuits that have tunable parameters subject to iterative optimizations



Data Encoding Layer: classical input vector encoded into quantum state.

Variational Layer: Generate multi quantum entanglement.

Quantum Measurement Layer: Consider the expectation values of every qubit by measuring in the computational basis

[ref] Samuel Yen-Chi, et al. , Quantum Long Short-Term Memory.

Agenda – Session 1: Introduction

- Roadmap of Quantum Machine Learning

Special Issue "Quantum Machine Learning: Theory, Methods and Applications"

- [Special Issue Editors](#)
- [Special Issue Information](#)
- [Keywords](#)
- [Published Papers](#)

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A special issue of *Electronics* (ISSN 2079-9292). This special issue belongs to the section "Quantum Electronics".

Deadline for manuscript submissions: 20 April 2022.

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Guest Editor

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Guest Editor

Computational Science Initiative, Brookhaven National Laboratory, New York, NY 11973-5000, USA

Interests: Quantum computing; Quantum machine learning; Quantum optimal control; Quantum error correction



- **Call for paper at "Electronics"**
- **Conclusion**
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Special Issue:

Quantum Machine Learning Theory, Methods and Applications

Guest Editor:

Dr. Weiwen Jiang

Department of Electrical and Computer Engineering, George Mason University, USA

Dr. Ying Mao

Department of Computer and Information Science, Fordham University, New York, USA

Dr. Samuel Yen-Chi Chen

Computational Science Initiative, Brookhaven National Laboratory, New York, USA

Deadline for manuscript submissions:

20 April 2022

Topics are welcome to contribute:

- Quantum machine learning
- Quantum neural network
- Quantum supervised learning
- Quantum unsupervised learning
- Quantum reinforcement learning
- Quantum learning theory
- Variational quantum circuits
- Noisy intermediate-scale quantum devices (NISQ)



https://www.mdpi.com/journal/electronics/special_issues/quantum_machine_learning

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Takeaway

- Quantum Computing
 - # of qubits grows rapidly
 - Q-Circuit design is similar to classical ones, using quantum gates
- Machine Learning meets Quantum Computing
 - Potential to solve computation-bound / memory-wall in classical
 - What is quantum neural network? VQC v.s. Q-Based Accelerator
- What is the fair metric for comparison?
 - Time-space complexity
- What we want to achieve?
 - Quantum advantage for real-world applications in near-term Q!

Q&A



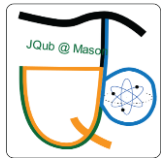
https://github.com/JQub/QuantumFlow_Tutorial (Source Code of All Hands-On in Tutorial)

<https://github.com/JQub/qfnn> (Source Code of QFNN API & Place to post Issues)



<https://pypi.org/project/qfnn/> (Package of QFNN on PYPI)

<https://libraries.io/pypi/qfnn/> (QFNN on Libraries.io)



<https://jqub.ece.gmu.edu> (JQub Website)

<https://jqub.ece.gmu.edu/categories/QF> (QuantumFlow Website for news and slides)

<https://jqub.ece.gmu.edu/categories/QF/qfnn/> (QFNN Documents)



<https://www.nature.com/articles/s41467-020-20729-5> (QuantumFlow Paper)



<https://arxiv.org/pdf/2012.10360.pdf> (Paper on How to Correct Map NN to Q)

<https://arxiv.org/pdf/2109.03806.pdf> (QF-Mixer)

<https://arxiv.org/pdf/2109.03430.pdf> (QF-RobustNN)



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