Basics of Quantum Information Theory and Quantum Tangent Kernel

DA6300: Quantum Computing and Machine Learning

MD Karimulla Haque

Guided by,
Dr. Dhinakaran Vinayagamurthy and Dr. Chandrashekar Lakshminarayanan

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For more details on Cryptography and RSA:
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  - **Classical vs Quantum:** For classical computers, factoring a large number, such as those used in RSA keys (often hundreds of digits), is computationally infeasible and would take billions of years to break with current technology. In contrast, a quantum computer using Shor's Algorithm could factor these numbers in a matter of seconds or minutes.

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Cost of Building a Quantum Computer

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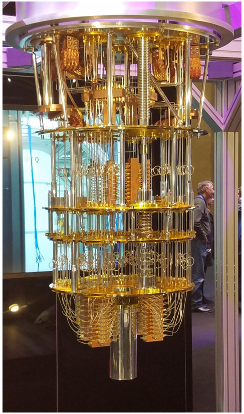

Figure: IBM Q quantum computer

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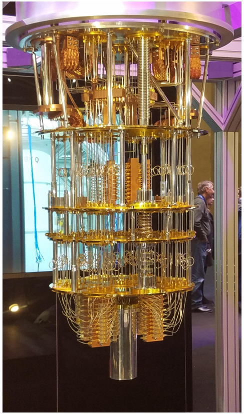

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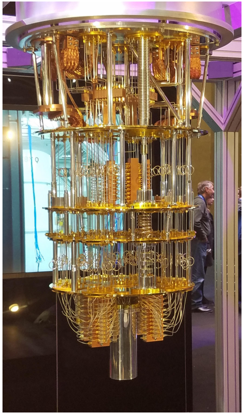
- **Development:** Quantum computing is still in the experimental phase, meaning significant resources are required to build and maintain these systems.
- Overall, the cost of building a quantum computer is in the range of **tens of millions of dollars**, and the technology is still in a nascent stage, meaning the cost could remain high for the next several years until it matures.



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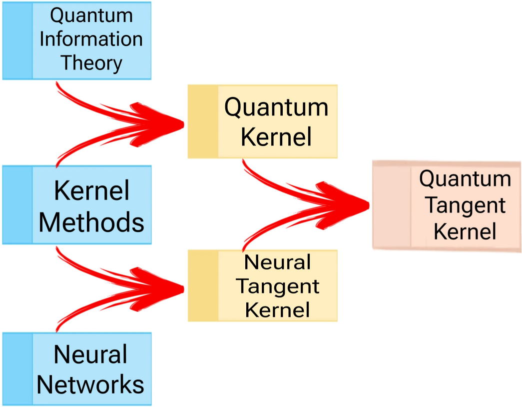
Roadmap


Quantum Information Theory
Quantum Kernel
Kernel Methods
Quantum Tangent Kernel
Neural Tangent Kernel
Neural Networks

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- **Vector Notations:** $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, standard Qubits.

  $\langle 0| = \begin{pmatrix} 1 & 0 \end{pmatrix}$ and $\langle 1| = \begin{pmatrix} 0 & 1 \end{pmatrix}$

Dirac notation

- $\langle a||b\rangle = \langle a|b\rangle = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases}$
- $|a\rangle\langle b|$ has a 1 in the (a,b)-entry and 0 for all other entries.

Pauli matrices

- $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

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- Example:
  - $$\sigma_x \otimes \sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

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- $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbb{C}$
- The fundamental requirement of quantum mechanics is that if we make measurement on $|\psi\rangle$ to see whether it is in $|0\rangle$ or $|1\rangle$, the outcome will be 0 (1) with the probability $|\alpha|^2(|\beta|^2)$,

- **Definition:** Quantum analog of classical bits; exists in superposition states $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbb{C}$ $= cos(\frac{\theta}{2})|0\rangle + e^{i\varphi} sin(\frac{\theta}{2})|1\rangle$, where $|\alpha|^2 + |\beta|^2 = 1$.

Let, $\alpha = r_1 e^{i\theta_1}$ and $\beta = r_2 e^{i\theta_2}$

Then, $r_1^2 + r_2^2 = 1$ and $\theta_1 = \theta_2 + \varphi$

Take, $r_1 = cos(\frac{\theta}{2}), r_2 = sin(\frac{\theta}{2})$

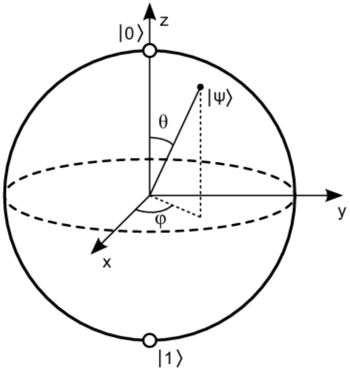

Figure: The Bloch sphere is a geometrical representation of a qubit. Qubits can take as value each point on the surface described by the two angles φ and θ. The pole points are $|0\rangle$ or $|1\rangle$.

Entangled States

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- However this decomposition is not possible since we must have $c_1 d_2 = c_2 d_1 = 0, c_1 d_1 = c_2 d_2 = \frac{1}{\sqrt{2}}$ simultaneously, and it is clear that the above equations have no common solution. Therefore the state $|\psi\rangle$ is not separable.

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- Such non-separable states are called **entangled** in quantum theory.

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- a quantum algorithm, is a part of a **quantum computation.**

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- Measurements to extract information we need.

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- The matrix expression of this gate as

$$I = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

NOT, shift gate

- Similarly we introduce
- $X : |0\rangle \rightarrow |1\rangle, |1\rangle \rightarrow |0\rangle$
- $Y : |0\rangle \rightarrow -|1\rangle, |1\rangle \rightarrow |0\rangle$
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- whose matrix representations are

$$X = |1\rangle\langle 0| + |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x$$

$$Y = |0\rangle\langle 1| - |1\rangle\langle 0| = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i\sigma_y$$

$$Z = |0\rangle\langle 0| - |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$$

$$\text{input} \; — \boxed{U} — \; \text{output}$$

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- $|00\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, |01\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, |10\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $|11\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

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- $U_{CNOT} : |00\rangle \rightarrow |00\rangle, |01\rangle \rightarrow |01\rangle, |10\rangle \rightarrow |11\rangle$ and $|11\rangle \rightarrow |10\rangle$ In the following, we use the standard basis vectors with components

Continue...

- whose matrix representation is

$$U_{CNOT} = |00\rangle\langle 00| + |01\rangle\langle 01| + |11\rangle\langle 10| + |10\rangle\langle 11|$$

$$= |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

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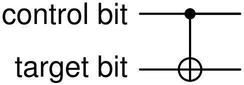
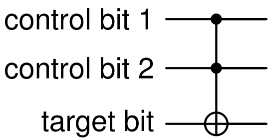
- The action of CNOT on the input state $|i\rangle|j\rangle$ is written as $|i\rangle|i \oplus j\rangle$,where $i \oplus j$ is an addition mod 2,
that is, $0 \oplus 0 = 0, 0 \oplus 1 = 1, 1 \oplus 0 = 1$ and $1 \oplus 1 = 0$.



Toffoli gate or, CCNOT(Controlled-Controlled-NOT) gate

- The explicit form of the CCNOT gate is

$$U_{CCNOT} = (|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10|) \otimes I + |11\rangle\langle 11| \otimes X$$



Hadamard gate

- $U_H : |0\rangle \to |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), |1\rangle \to |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

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$$\text{input} \;—\boxed{H}—\; \text{output}$$

Arithmetic Circuit

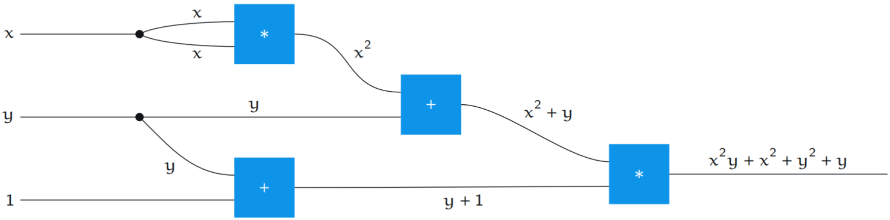

Figure: Wires store numbers and gates represent arithmetic operations, such as addition (+) and multiplication (*)

Example of Quantum Circuit

$$|0\rangle \;-\!\boxed{H}\!-\!\boxed{S}\!-\!\boxed{H}\!-\!\boxed{T}\!-\; \frac{1+i}{2}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

- where $H = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$, $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$ and $T = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix}$

We get $THSH = \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$

Why Kernel?

- Assume the feature map $\phi : \mathcal{X} \to \mathcal{F}$
- For example, $\phi\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) = \begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix} \in \mathcal{F}$, where $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \mathcal{X}$

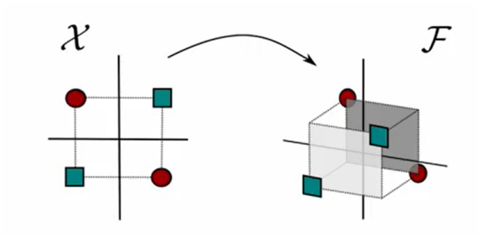

Figure: Separation may be easier in higher dimensions

Kernel Methods

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- Kernel method employs a non-linear map ϕ from the original space to the higher dimensional feature space: $\phi : \mathcal{X} \to \mathcal{F}$,
  i.e., $x_i \to \phi(x_i)$,
  where $\mathcal{X}$ is an original space of the data and $\mathcal{F}$ is a higher dimensional feature space.

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- Kernel method employs a non-linear map ϕ from the original space to the higher dimensional feature space: $\phi : \mathcal{X} \to \mathcal{F}$,
  i.e., $x_i \to \phi(x_i)$,
  where $\mathcal{X}$ is an original space of the data and $\mathcal{F}$ is a higher dimensional feature space.
- For two data x_i and x_j , we define $K(x_i, x_j) = \langle\phi(x_i), \phi(x_j)\rangle$, where $\langle\cdot, \cdot\rangle$ denotes the inner product on $\mathcal{F}$.

QML as a Kernel Method

- First, data are encoded into quantum states by $U_\phi(x)$ i.e.,

$$\begin{aligned} y(x,\theta) &= \langle 0^n | U^\dagger(x,\theta) O U(x,\theta) | 0^n \rangle \\ &= \langle 0^n | U_\phi^\dagger(x) V^\dagger(\theta) O V(\theta) U_\phi(x) | 0^n \rangle \qquad \{\because \mathrm{U(x,}\theta) = V(\theta) U_\phi(x)\} \\ &= Tr(O(\theta)\rho(x)), \end{aligned}$$

where weight vector $O(\theta) = V^\dagger(\theta) O V(\theta)$ and feature vector $\rho(x) = U_\phi(x)|0^n\rangle\langle 0^n|U_\phi^\dagger(x)$

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- Now the conventional quantum kernel is defined as
$K_q(x_i, x_j) = Tr(\rho(x_i)\rho(x_j)) = |\langle \phi(x_i) | \phi(x_j) \rangle|^2$, where $|\phi(x)\rangle = U_\phi(x)|0^n\rangle$

Accuracy Compare

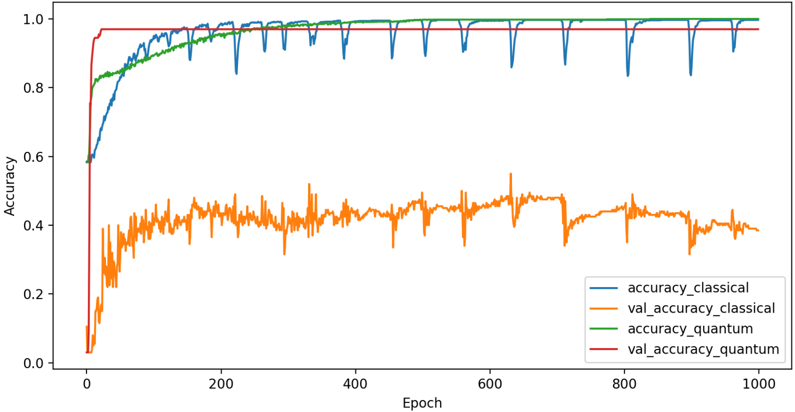

Figure: Comparison between Classical and Quantum Models

Neural Tangent Kernel (NTK)

- Suppose $f(x_i, \theta)$ is the output of a neural network where θ is parameters in the network, and x_i is the input data.

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- Now we approximated by the first-order expansion with respect to the parameters around the initial values:
  $f(x_i, \theta) \simeq f(x_i, \theta_0) + \nabla_\theta f(x_i, \theta_0)^T(\theta - \theta_0)$, where θ_0 is the initial values of parameters of a neural network.

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- This approximation allows us to interpret the neural network as a linear model with a feature map $\phi(x) = \nabla_\theta f(x, \theta_0)$
- Using this feature map, we define the following neural tangent kernel (NTK): $K_{ntk}(x_i, x_j) = \nabla_\theta f(x_i, \theta_0)^T \nabla_\theta f(x_j, \theta_0)$

- Now from K_q and K_{ntk}, we define the following quantum tangent kernel (QTK):
  $K_{qtk}(x_i, x_j) = \nabla_\theta y(x_i, \theta_0)^T \nabla_\theta y(x_j, \theta_0)$,
  where $y(x, \theta) = \langle 0^n | U^\dagger(x, \theta) O(\theta) U(x, \theta) | 0^n \rangle$

Numerical Experiment

- First one is a circuit where x is encoded only at the first layer as in the bellow Figure. $U_{shallow}(x,\theta) = V(\theta)U_{\phi}(x)$, where $V(\theta)$ is a parameterized unitary and $U_{\phi}(x)$ is a quantum feature map to encode data.

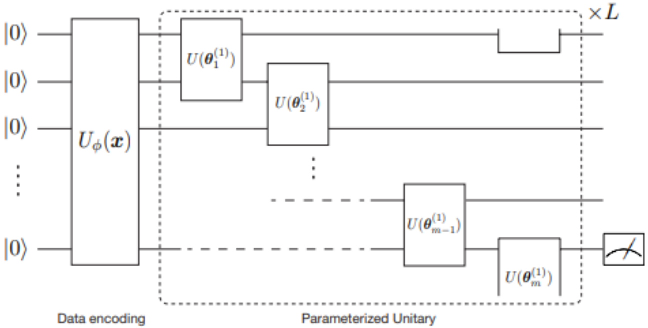

Figure: The m-qubit ansatz used for numerical simulations. $U_{\phi}(x)$ is the quantum feature map for encoding classical data. $U(\theta_j^{(i)}) \in SU(4)$ is the parameterized unitary of the i-th layer. At the output, we measure the Pauli Z expectation value of the final qubit.

- Next, in order to increase the non-linearity, we consider a multi-layered circuit that alternates between data encoding and a parameterized unitary as shown in the bellow Figure. $U_{deep}(x, \theta) = \Pi_{i=1}^{L} V(\theta_i) U_{\phi}(x)$,

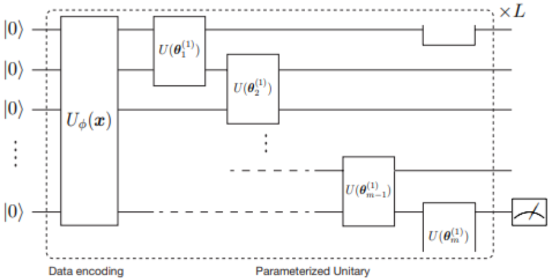

Figure: Quantum circuit that defines deep quantum tangent kernel. $U_{\phi}(x)$ is the feature map and $U(\theta_j^{(i)}) \in SU(4)$ is the parameterized unitary of the i-th layer. To increase the non-linearity of the kernel, the feature map $U_{\phi}(x)$ and the parameterized unitary are iteratively applied. At the output, we measure the Pauli Z expectation value of the final qubit.

Numerical Experiment

- The "ansatz-generated" dataset is generated in the following manner. Four dimensional random value data x_i are inputted into $U_{deep}(x, \theta)$ consisting of n = 4 qubits and L = 10 layers.

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- Then, evaluate the expectation value $I(x_i, \theta) = \langle 0^n | U^\dagger_{deep}(x_i, \theta) Z_4 U_{deep}(x_i, \theta) | 0^n \rangle$ with a randomly chosen θ. We label each x_i as 1 and -1 if $I(x, \theta) \geq 0$ and $I(x, \theta) < 0$, respectively.

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- Here, generate the 15,000 samples of the four dimensional input data x_i and its label y_i. They are splitted into 10,000 training and 5000 test data.

- Behavior of training losses and training accuracies for different number of layers during training.

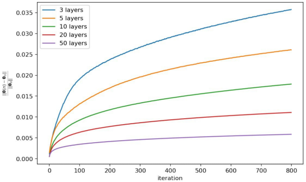

Figure: Relative norm change in the parameters of the quantum circuit from initial values during training by gradient descent. $\theta(n)$ is the parameter at the n-th iteration. θ_0 is initial value of the parameter.

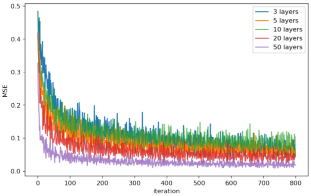

Figure: Mean Square Error

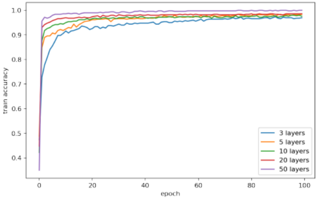

Figure: Train Accuracy

Classification accuracy for three types of kernels

- Classification accuracy for SVM with three types of kernels. Three SVMs classify the ansatz-generated dataset generated by a quantum circuit for deep QTK

Kernel	Accuracy
Quantum kernel	0.7842
Shallow quantum tangent kernel	0.7484
Deep quantum tangent kernel	0.812

The distribution of outputs

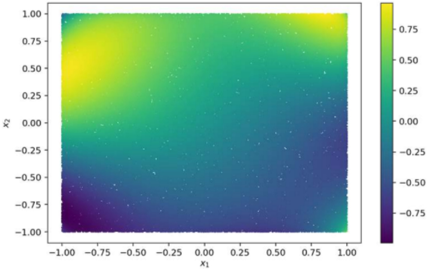

Figure: The distribution of outputs of the quantum circuit with L = 10 layers which can be interpreted as the conventional quantum kernel method.

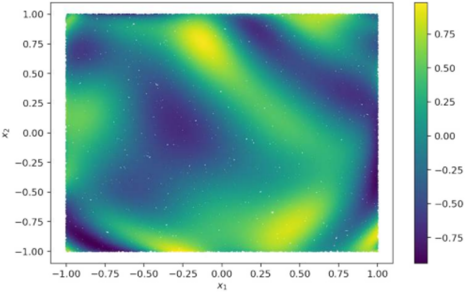

Figure: The distribution of outputs of the quantum circuit with L = 10 layers beyond the conventional quantum kernel

Conclusion

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- Here quantum tangent kernel (QTK) and deep quantum tangent kernel which cannot be interpreted as conventional quantum kernel methods
- QTK is defined by applying the formulation of NTK to parametrized quantum circuits.
- It imply that deep parameterized quantum circuits with repetitive data encoding unitary have a higher representation power and better performance for quantum machine learning than the conventional quantum kernel method.
- Hence, better ansatz constructions and parameter optimization methods are crucially important.

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- Pictures were taken from Google Images.

Thank You