Parametric Quantum Circuit (PQC)

1 Introduction

A parametric quantum circuit is a type of quantum circuit that includes one or more parameters that can be adjusted or "tuned" during the execution of the circuit. These parameters can be used to control the behavior of the quantum circuit and can be set to different values to perform different computations.

Parametric quantum circuits are used in a variety of applications, including quantum machine learning, quantum chemistry, and optimization. They can be particularly useful for tasks that require the optimization of a function or the search for an optimal solution, as the parameters can be adjusted to explore different regions of the search space.

Consider a quantum circuit with two qubits and one parameter, denoted by the symbol $'\theta'$. The quantum circuit consists of a series of quantum gates, which are operations that perform quantum-mechanical transformations on the qubits. The sequence of gates in the quantum circuit defines the computation that is performed.

One possible quantum circuit with a parametric quantum gate might be as follows:

1. Initialize the two qubits in the state $|00\rangle$
2. Apply a Hadamard gate to the first qubit, which puts the qubits in the state $\frac{(|00\rangle+|01\rangle+|10\rangle+|11\rangle)}{2}$
3. Apply a parametric quantum gate, denoted by $'U(\theta)'$, to the two qubits. This quantum gate depends on the parameter $'\theta'$, which can be adjusted to control the behavior of the quantum circuit.
4. Measure the two qubits to obtain the output of the quantum circuit.

In this example, the parametric quantum gate $'U(\theta)'$ is a unitary gate that depends on the parameter $'\theta'$. Unitary gates preserve the inner product between the input and output states of the gate, which means that they preserve the norm (length) of the state vector. This is a useful property for many quantum algorithms, as it ensures that the probability of measuring a particular outcome is always between 0 and 1.

The value of $'\theta'$ can be adjusted to perform different computations with the quantum circuit. For example, if $'U(\theta)'$ is a rotation gate, then $'\theta'$ can be used to control the angle of the rotation. Alternatively, if $'U(\theta)'$ is a controlled gate, then $'\theta'$ might be used to control the operation that is performed on the second qubit based on the state of the first qubit.

To execute the quantum circuit, it is necessary to use a quantum computer or quantum simulator. The quantum computer or simulator will apply the quantum gates to the qubits according to the specified sequence and will return the measured output of the quantum circuit. By adjusting the value of $'\theta'$, it is possible to explore different regions of the search space and perform different computations with the quantum circuit.

2 Importance in QML

Parametric quantum circuits (PQCs) are important in quantum machine learning (QML) because they can be used to represent and optimize parametric quantum functions.

In QML, the goal is often to learn a function that maps inputs to outputs, where the function is represented by a quantum circuit. The quantum circuit can be optimized to fit the data by adjusting the parameters of the circuit, which can be done using a variety of techniques such as gradient-based optimization or quantum-assisted optimization. PQCs are a natural choice for representing parametric quantum functions in QML because they allow the parameters of the quantum circuit to be adjusted to fit the data.

PQCs are also useful in QML because they can exploit the unique capabilities of quantum computers, such as superposition and entanglement, to perform tasks that are difficult or impossible for classical computers. For example, PQCs can be used to implement quantum neural networks, which can perform tasks such as classification and regression using quantum algorithms.

Overall, PQCs are an important tool in QML because they allow quantum functions to be represented and optimized using quantum algorithms and quantum computers, which can lead to improved performance and new insights in a variety of machine learning tasks.

3 Parametrized Single-Qubit Gates

Pauli rotation matrices: A Pauli P-rotation matrix $R_P(\theta)$, with $P \in \{X < Y < Z\}$, is a unitary matrix whose generator is given by $\frac{\theta}{2} \cdot P$, i.e.,

$$R_P(\theta) = exp(-\iota \frac{\theta}{2} P) = \cos(\frac{\theta}{2})I - \iota \sin(\frac{\theta}{2})P$$

where θ is a real parameter.

general parametrized single-qubitcan be expressed, apart from a global phase, as the following cascade of two types of Pauli rotations

$$R(\theta^1, \theta^2, \theta^3) = R_P(\theta^1) R_{P'}(\theta^2) R_P(\theta^3)$$

where $P \neq P'$ with $P, P' \in \{X, Y, Z\}$. A typical choice is $P = Z$ and $P' = Y$. The general single qubit gate is specified by the three parameters, or rotation angles, θ^1, θ^2, and θ^3

4 Mean-field Ansatz

An ansatz $U(\theta)$ that uses only single-qubit gates is known as a mean-field ansatz as it is based on the idea of replacing the many-body wave function with a product of single-particle wave functions, which are themselves parameterized by some set of mean field variables.

Given the input state $|0\rangle$, a Parametrized quantum circuit following the mean-field ansatz outputs the separable state where we have written as $|0\rangle$ both the multi-qubit ground state and the corresponding single-qubit states with some abuse of notation.
It sounds like you are describing a parametrized quantum circuit (PQC) that is designed to output a separable state (a product state) when given the input state $|0\rangle$. The PQC follows the mean field ansatz, which means that it is based on the idea of replacing the many-body wave function with a product of single-particle wave functions. In this context, it seems that you are using the notation $|0\rangle$ to represent both the multi-qubit ground state and the corresponding single-qubit states. This is a common abuse of notation, as it allows you to represent the state of a many-qubit system using a single ket vector.

In the context of a parametrized quantum circuit (PQC), the mean field ansatz may be used to design and analyze the behavior of the circuit. For example, the PQC may be designed to output the approximate ground state of a many-body quantum system, using the mean field ansatz to represent the state of the system. The PQC may also be used to study the phase transitions and critical behavior of many-body quantum systems, using the mean field ansatz to approximate the ground state of the system.

5 Hardware-Efficient Ansatz

includes parametrized single-qubit gates and a fixed entangling unitary
The hardware-efficient ansatz prescribes PQCs that implement a cascade of L layers of unitaries. These unitaries are parametrized by a set of angle variables $\theta = \theta_1, \theta_2, ..., \theta_L$. The PQC is designed such that each unitary layer $U(\theta)$ is a sequence of single- and two-qubit gates that can be implemented with a small number of qubits and gates.

The overall circuit is defined as: $U(\theta) = U_L(\theta) \cdot U_{L-1}(\theta) \cdots U_1(\theta)$, where each unitary matrix $U_l(\theta)$ at the $l-$th layer can be expressed as

$$U_l(\theta) = U_{ent}\left(R(\theta^1_{l,0}, \theta^2_{l,0}, \theta^3_{l,0}) \otimes \cdots \otimes R(\theta^1_{l,n-1}, \theta^2_{l,n-1}, \theta^3_{l,n-1})\right)$$

with $(\theta^1_{l,k}, \theta^2_{l,k}, \theta^3_{l,k})$ for $k \in 0, 1, ..., n-1$. In this way, the PQC can be controlled by adjusting the values of the angle variables θ, which in turn controls the operation of the single-qubit gates. And the fixed entangling unitary U_{ent}(linear, circular, or full entangling circuits) add the entanglement to the circuit..

This approach allows for a great flexibility in the design of the circuit, and it allows for the use of less complex and less resource-intensive circuits, while still being able to perform complex computations.

6 Parametrized Two-Qubit Gates

Two common types:

- Parametrized two-qubit controlled gates: A two-qubit controlled gate is a quantum gate that acts on two qubits, with one qubit (the control qubit) determining the operation that is applied to the other qubit (the target qubit). These gates are typically implemented using a combination of single-qubit gates and a two-qubit entangling gate. Parametrized two-qubit controlled gates, also known as parametrized two-qubit gates, are a variation of two-qubit controlled gates that have additional parameters that can be adjusted to control the operation of the gate. These parameters are typically represented by angle variables, and the gate operation is determined by the values of these parameters.
  Are of the form $C^{U(\theta)}_{jk}$, where j is the index of controlling qubit, k is the index of the controlled qubit, and $U(\theta)$ is a parametrized single-qubit gate. Example: Controlled-Rotation gate, defined as
  $$C^{U(\theta)}_{01} = |0\rangle \langle 0| \otimes I + |1\rangle \langle 1| \otimes U(\theta)$$
  where $U(\theta)$ is a single-qubit rotation gate and θ is a parameter that controls the rotation angle; applies a rotation to the target qubit only if the control qubit is in the state $|1\rangle$.

- Two-qubit Pauli rotations: : For a system with two qubits, a two-qubit Pauli PQ-rotation is defined as the unitary matrix
  $$R_{PQ}(\theta) = exp\left(-\iota\frac{\theta}{2}(P \otimes Q)\right)$$
  where $P, Q \in I, X, Y, Z$
  Two-qubit Pauli rotations are generally not local operators. A local operator is an operator that acts on a single quantum system and does not entangle the system with other quantum systems. In contrast, two-qubit Pauli rotations are non-local operators that act on two quantum systems and can entangle the systems. For example, the two-qubit Pauli X rotation (also known as the CNOT gate) flips the state of the second qubit if and only if the state of the first qubit is $|1\rangle$. This entangles the two qubits, as the state of the second qubit depends on the state of the first qubit.