XpookyNet: Advancement in Quantum System Analysis through Convolutional Neural Networks for Detection of Entanglement

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(Dated: January 30, 2024)

The applications of machine learning models in quantum information theory have witnessed a surge in recent years, driven by the sophistication of quantum computing (QC). However, relying on inappropriate models has often resulted in suboptimal accuracy. A custom deep convolutional neural network (CNN), XpookyNet, has been developed to address this. XpookyNet is explicitly tailored for quantum systems analysis and aims to detect fundamental quantum attributes, such as entanglement in two- and three-qubit systems and potentially more qubit systems. It harnesses the power of CNNs to provide instantaneous and meticulous results. With an accuracy of 98.53% achieved in merely a few epochs, XpookyNet effectively handles the inherent complexity of quantum information, providing deeper insights into QC. The study also investigates quantum features and their relation to the purity of a density matrix directly related to noise in NISQ-era quantum computation. Preparing the density matrix in a format compatible with customary CNNs is vital in dissecting quantum systems. Quantum-applied CNNs must also be refined utilizing recent methods and extensive metrics to enhance and ensure their performance.

I. INTRODUCTION

In quantum mechanics, an uncanny phenomenon known as quantum entanglement arises when two or more particles interact so that their quantum states become related in a way that the neither state $\psi_{AB} \neq \psi_A \otimes \psi_b$ nor $\langle A \otimes B \rangle \neq \langle A \rangle \otimes \langle B \rangle$ [1, 2]. Instantaneous changes in one particle are simultaneously mirrored in others, irrespective of their spatial separation, with the non-locality condition of $P(A = a, B = b) \neq P(A = a) \cdot P(B = b)$ holding [3]. Quantum Computing needs entanglement to form and rise, as it allows the system to perform multiple calculations simultaneously using many qubits, achieves secure and high key rates, and underpins quantum annealing and variational quantum algorithms to solve intractable problems and optimization problems [4–8].

The first step in manipulating systems is to detect the presence and amount of entanglement, so various entanglement detection criteria have been proposed [9–11]. However, the positive partial transpose (PPT) criterion can determine entanglement with certainty for systems $\mathcal{H}_A$ and $\mathcal{H}_B$ where the Hilbert space is $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ with the necessary size of $2 \otimes 2$ or $2 \otimes 3$ non-mixed states. In other words, Hilbert space includes entangled mixed states that still meet the PPT conditions called bound-entangled states [12].

Comprehensively assessing quantum entanglement requires choosing the right criterion. While criteria like concurrence, negativity, and relative entropy of entanglement have advantages, the entanglement of formation (EoF) stands out for its operational interpretation of the resources needed to create a specific state. Unlike its counterparts, it provides a deeper understanding of entanglement phenomenon [13–15].

Quantifying and classifying entanglement beyond three qubits is an NP-Hard problem. The generalized concurrence still measures entanglement, but its calculation is computationally intensive for mixed states and it cannot pinpoint individual qubits [16]. Entanglement witnesses are another practical tool to detect entanglement in many-body quantum systems. A witness W is a Hermitian operator that for all separable states, $\langle W \rangle_{\rho_{sep}} = \mathrm{Tr}(W\rho_{sep}) \geq 0$ but for some entangled states $\langle W \rangle_{\rho_{ent}} = \mathrm{Tr}(W\rho_{ent}) < 0$ [17]. It detects entanglement without fully characterizing the system or performing a tomography; however, due to the exponential growth of variables with higher qubit counts, it requires optimization in high-dimensional spaces. Quantum witnesses can be optimized using machine learning (ML) because they can quickly identify patterns in large datasets, making them ideal for solving complex problems [18, 19]. Illustrations in Fig. 1 give a grasp of compartmentalizing methods for classifying states.

Among ML techniques, CNNs are versatile and robust,