# PROBLEM-DEPENDENT QUANTUM CIRCUIT DESIGN BASED ON ENTROPY MATCHING

Anonymous authors

Paper under double-blind review

#### ABSTRACT

Variational quantum machine learning (QML) have shown great promise for harnessing quantum advantage in machine learning tasks. However, architecture design of quantum circuits employed in these QML algorithms has been poorly explored for practical problems. Specifically, quantum circuits should have sufficient expressibility for modeling complex functions considering the inherent structures of real-world data. Naively increasing the circuit depth could enhance the expressibility of quantum circuits, which also induce the barren plateau problem as a by-product. In this work, we develop an architecture design framework to solve this problem. We use a simple yet effective metric of quantum entanglement, i.e. the linear entropy, to guide the circuit design from the perspective of the input data. First, we quantify the entanglement of input data by calculating the 1-qubit linear entropy of their amplitude encoding states. Then we implement an entropy matching approach to identify the optimal circuit depth that lead to the linear entropy being close the entropy of input data. The effectiveness of circuit designs based on entropy is verified by extensive experimental results. Specifically, we demonstrate that real-world datasets like MNIST images has limited quantum entanglement. Therefore, circuits designed with entropy matching exhibit relatively small depths being free from the barren plateau issue while maintaining benign performances in binary classification tasks. This work not only advances the efficiency of quantum circuit design but also sets the stage for further refinement of QML performance, with broad implications for practical quantum computing applications.

032 033 034

035

004

010 011

012

013

014

015

016

017

018

019

021

023

025

026

027

028

029

031

#### 1 INTRODUCTION

Quantum computing is a new paradigm for computing based on quantum mechanics(Nielsen & 037 Chuang, 2000), which has unimaginable advantages over its classical counterparts in many important applications(Shor, 1994; Grover, 1996). The physical implementation of quantum hardware has entered the Noisy Intermediate-Scale Quantum (NISQ) era, which is a significant milestone 040 towards realizing practical quantum computing(Preskill, 2018). The current quantum computing 041 devices, despite their noise and limited coherence times(), have demonstrated exponentially promo-042 tion in performing certain computing tasks over classical computers(Arute et al., 2019)(Zhong et al., 043 2020). Among the various approaches designed to exploit the power of NISQ devices, Variational 044 Quantum Algorithms (VQAs)(Cerezo et al., 2021a) stand out as a particularly effective algorithmic framework. VQAs have demonstrated potential in a wide range of applications, particularly in machine learning, where they have been used to solve complex tasks with notable success. 046

VQAs are fundamentally composed of two parts: the classical optimization process that updates parameters and the variational quantum circuit (VQC) Peruzzo et al. (2014). The depth of the VQC is a critical factor in determining the algorithm's expressibility, which is its ability to model complex functions. Shallow circuits, while easier to train, often suffer from limited expressibility, restricting their capacity to solve more complex problems. Conversely, deeper circuits, although more expressive, can encounter the barren plateau problem, where the optimization landscape becomes flat, making training difficult. This creates a fundamental dilemma in VQC design: balancing expressibility with trainability.

In this work, we propose a novel approach to quantum circuit design that is tailored to the specific problem at hand. Our method involves using linear entropy as a metric to evaluate the entanglement properties of both the problem dataset and the quantum states generated by the VQC. By adjusting the circuit depth to match the linear entropy of the dataset, our approach strikes a balance between the expressibility and trainability of the quantum circuit. We validate our method through experiments on quantum binary classification tasks using multiple datasets, demonstrating that our entropy-matching approach leads to improved performance, effectively navigating the trade-offs inherent in VQC design.

062 063

064

#### 2 PRELIMINARY

065 2.1 LITERATURE REVIEW

## 067 2.1.1 QUANTUM CIRCUIT ARCHITECTURE DESIGN

Quantum circuit architecture design is a foundational aspect of developing efficient quantum algorithms and optimizing their implementation on quantum hardware(Farhi & Neven, 2018). The architecture directly influences a circuit's computational power, efficiency, and ability to generalize across various tasks(Preskill, 2018). Various architectural strategies, including shallow circuits, deep circuits, hybrid designs, and hardware-efficient ansätze (HEAs), have been explored to enhance expressibility and performance(Mitarai et al., 2018)(Kjaergaard et al., 2020)(McClean et al., 2016).

Shallow circuits, characterized by fewer gates and layers, tend to be more robust against noise and easier to train, making them suitable for near-term quantum devices(Cerezo et al., 2021b)(Bravyi et al., 2018). Conversely, deep circuits provide greater expressibility, allowing them to capture complex relationships in data. However, deep architectures often encounter challenges such as overfitting and the barren plateau problem, where gradients vanish during optimization, complicating the training process.

HEAs are specifically designed to utilize the capabilities of current quantum hardware effectively(Chen et al., 2021). These architectures typically consist of layers of single-qubit gates with tunable parameters and two-qubit gates to enable entanglement. By structuring circuits in this way, researchers aim to optimize computational resources while minimizing noise susceptibility. The trade-offs between expressibility and trainability are critical in designing circuits that can learn effectively from data.

087 088

089

## 2.1.2 GENERALIZATION ERROR BOUND AND EXPRESSIBILITY ANALYSIS OF QUANTUM NEURAL NETWORKS

The performance of quantum neural networks (QNNs) depends significantly on their ability to generalize well to unseen data(Caro et al., 2022), a property that parallels the concept of generalization in classical machine learning. Generalization error bounds provide a theoretical framework for evaluating how well a QNN trained on a specific dataset will perform on new data. The generalization capability is influenced by several factors, including the architecture of the parameterized quantum circuit (PQC), the expressibility of the quantum circuit, and the complexity of the task(Cerezo et al., 2021a)(Abbas et al., 2021).

Expressibility can be quantified by comparing the distribution of states generated by a QNN with the uniform distribution of states, such as those from Haar random ensembles. A common method for quantifying expressibility involves calculating the Kullback-Leibler divergence between the fidelity probability distributions of the QNN and Haar random states(Sim et al., 2019). A lower divergence indicates higher expressibility, suggesting that the QNN can represent a wider range of functions effectively.

The interplay between expressibility and trainability is crucial in optimizing QNN architectures.
 Well-designed circuits should achieve high expressibility while maintaining effective training dy namics(Sim et al., 2019), allowing them to learn from the training dataset without succumbing to
 overfitting. Techniques derived from classical machine learning, such as regularization and model
 selection, have been adapted for quantum contexts to enhance the performance and generalization
 capabilities of QNNs(Cerezo et al., 2021a).(McClean et al., 2018)

## 108 2.2 QUANTUM COMPUTING KNOWLEDGE

110 Quantum computing(Nielsen & Chuang, 2000) is built upon fundamental concepts that bridge clas-111 sical computation and quantum mechanics. At its core lies the qubit, the basic unit of quantum 112 information. Unlike classical bits, which can exist in one of two states, 0 or 1, a qubit can exist in a 113 superposition of both. Mathematically, a qubit's state is described as  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ , where  $\alpha$ 114 and  $\beta$  are complex amplitudes such that  $|\alpha|^2 + |\beta|^2 = 1$ . This property allows quantum systems to 115 process information in fundamentally different ways, leading to potential computational advantages.

Building upon this, multi-qubit systems are described using tensor products of individual qubit states. For an N-qubit system, the quantum state exists in a  $2^N$ -dimensional Hilbert space, and the overall state is represented by the vector  $|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle$ . These quantum states are manipulated through quantum gates, the quantum analogue of classical logic gates. Quantum gates such as Pauli-X, Y, Z, and Hadamard, along with controlled gates like CNOT, enable the transformation of qubit states.

122 Quantum circuits provide the framework for organizing quantum gates to perform computations. A 123 quantum circuit can be viewed as a sequence of gate operations applied to a set of qubits, transform-124 ing an initial quantum state into a final state. This process is parameterized in variational quantum 125 circuits (VQCs), where the quantum gates depend on a set of classical parameters, denoted  $\theta$ . The 126 task in many quantum algorithms is to optimize these parameters to minimize a cost function, typi-127 cally defined as the expectation value of a quantum observable.

128 Measurement is a crucial aspect of quantum computation, where the outcome of a quantum process 129 is obtained by collapsing the quantum state into a classical result. Measurements are represented by 130 observables, which are Hermitian operators acting on the quantum state. For example, the Pauli-Z 131 observable measures the probability of a qubit being in the state  $|0\rangle$  or  $|1\rangle$ .

In quantum machine learning(Biamonte et al., 2017), loss functions quantify the difference between
 the predicted outcome and the actual target. These loss functions are typically defined in terms of
 the expectation value of an observable with respect to the quantum state produced by the quantum
 circuit. The general form of the loss function is given by:

- 136
- 137 138

 $\mathcal{L}(\theta) = \langle \psi_{\text{out}}(\theta) | \hat{O} | \psi_{\text{out}}(\theta) \rangle,$ 

where  $|\psi_{out}(\theta)\rangle$  is the output state of the quantum circuit with parameters  $\theta$ , and  $\hat{O}$  is the observable.

To optimize the parameters of the quantum circuit, gradient-based optimization methods are often employed. In quantum computing, gradients can be computed using the parameter-shift rule. This rule provides an efficient way to calculate the derivative of the loss function with respect to the circuit parameters, without requiring explicit knowledge of the circuit's internal workings. For a parameter  $\theta_j$  associated with a gate in the circuit, the gradient of the loss function with respect to  $\theta_j$ is given by:

$$\frac{\partial \mathcal{L}}{\partial \theta_i} = \frac{\mathcal{L}(\theta_j + \frac{\pi}{2}) - \mathcal{L}(\theta_j - \frac{\pi}{2})}{2}.$$

This rule leverages the structure of quantum operations to efficiently compute the gradients necessary for optimizing quantum neural networks, enabling quantum algorithms to learn from data and refine their parameters over time.

152 153 154

155

156

150

151

### 3 THEORETICAL

#### 3.1 HAAR MEASURE AND CIRCUIT EXPRESSIVITY

Haar measure is a type of invariant measure defined on a locally compact topological group G. The invariance property implies that for any element  $g \in G$  and any measurable subset  $A \subset G$ , the Haar measure  $\mu$  satisfies the following property:

161

$$\mu(gA) = \mu(A)$$

Here, gA represents the set obtained by left-multiplying each element of A by g. This means that the Haar measure is left-invariant on the group G, indicating that the measure of a set remains unchanged under translation by any group element. Similarly, Haar measure can also be rightinvariant, satisfying  $\mu(Ag) = \mu(A)$ .

On a compact topological group (such as the unitary group U(d)), the Haar measure is unique (up to a multiplicative constant) and can be normalized as a probability measure, meaning that the measure of the entire group is 1. This normalization is particularly important because it allows us to define a uniformly distributed quantum state by randomly selecting a unitary matrix in quantum computing.

In quantum computing, we often focus on the unitary group U(d), whose elements are unitary matrices in a *d*-dimensional Hilbert space. Unitary matrices are linear transformations that preserve inner products, satisfying  $U^{\dagger}U = UU^{\dagger} = I$ , where  $U^{\dagger}$  is the conjugate transpose of *U*, and *I* is the identity matrix.

The application of Haar measure on U(d) is evident in the uniform selection of a unitary matrix U, which generates a quantum state  $|\psi\rangle = U|\psi_0\rangle$  in the *d*-dimensional Hilbert space, where  $|\psi_0\rangle$  is a fixed initial state in the Hilbert space. Due to the uniformity of the Haar measure, the generated quantum state  $|\psi\rangle$  uniformly covers the entire Hilbert space, meaning that each possible quantum state is selected with equal probability, without any bias or inclination.

In practical computations, Haar measure is often expressed through integrals. For example, on the unitary group U(d), Haar measure can be used to calculate the expected value of certain statistical quantities. Suppose we have a function f(U) defined on the unitary group U(d), then its integral over the group (according to Haar measure) is given by:

$$\int_{U(d)} f(U) d\mu(U)$$

For the purity of a quantum state  $Tr(\rho^2)$ , Haar measure can be used to calculate its expected value, where  $\rho = |\psi\rangle\langle\psi|$  is the density matrix of the quantum state. In a *d*-dimensional Hilbert space, the expected purity of a pure state  $|\psi\rangle$  chosen according to the Haar measure is:

 $\mathbb{E}[\mathrm{Tr}(\rho^2)] = \frac{2}{d+1}$ 

191 192 193

194

195 196

This result indicates that a quantum state randomly chosen from the Haar measure distribution has lower purity, meaning the state exhibits high randomness and complexity. This uniform distribution ensures that each quantum state is equally likely to be selected, demonstrating that the quantum circuit can generate a wide variety of possible quantum states, comprehensively and randomly covering the Hilbert space.

In quantum computing, the significance of Haar measure lies in its use as a standard for evaluating the expressiveness of quantum circuits. The expressiveness of a quantum circuit refers to its ability to generate a wide range of quantum states, which is crucial for performing diverse quantum computational tasks.

A key mathematical criterion for evaluating the expressiveness of a quantum circuit is the extent to which the quantum states it generates approach the distribution defined by the Haar measure. If a quantum circuit can produce quantum states that closely approximate the Haar measure distribution, it indicates that the circuit has sufficient complexity and flexibility to execute a wide range of quantum computing tasks, rather than being limited to specific states or operations.

Approximating the Haar measure distribution implies that the quantum circuit can realize arbitrary
 quantum states, which is essential for universal quantum computing. The Haar measure corresponds
 to a maximum entropy distribution, where the generated quantum circuit has the greatest information
 processing capability. Furthermore, if the quantum states generated by the circuit are close to the
 Haar measure, it signifies that the circuit can achieve highly complex quantum state transformations,
 demonstrating high expressiveness.

## 216 3.2 LINEAR ENTROPY AS A MEASURE OF QUANTUM CIRCUIT EXPRESSIVENESS

To quantify circuit expressivity, we can use a mathematical measure known as linear entropy, defined as:

220

221 222 223

224

239

240 241

where  $\rho$  is the density matrix of the quantum state, and Tr( $\rho^2$ ) represents the trace of the square of the density matrix.

 $S_L(\rho) = 1 - \operatorname{Tr}(\rho^2)$ 

Linear entropy is a measure of the degree of mixture or randomness in a quantum state. It provides insight into how "mixed" a quantum state is, with higher values of linear entropy indicating greater randomness and complexity in the quantum state. In the context of quantum circuits, a higher linear entropy suggests that the quantum states generated by the circuit are spread across a larger portion of the Hilbert space, closely approximating a uniform distribution defined by the Haar measure.

The Haar measure, in quantum computing, is a uniform distribution over the unitary group U(d), where d is the dimension of the Hilbert space. If a quantum circuit can generate states that are distributed according to the Haar measure, it implies that the circuit has a high degree of expressiveness and can explore a wide range of possible quantum states.

Linear entropy provides a straightforward and effective way to quantify the randomness and complexity of quantum states produced by a circuit. Specifically, it directly measures the purity or mixedness of a quantum state. A pure quantum state, which is fully coherent and exhibits no randomness, will have a linear entropy of zero:

 $\operatorname{Tr}(\rho^2) = 1 \implies S_L = 0$ 

In contrast, a maximally mixed state, where the quantum state is evenly distributed across all possible
 states, will have a lower trace and hence a higher linear entropy:

$$\operatorname{Tr}(\rho^2) = \frac{1}{d} \implies S_L = 1 - \frac{1}{d}$$

Here, *d* represents the dimension of the Hilbert space. The linear entropy thus ranges from 0 for pure states to  $1 - \frac{1}{d}$  for maximally mixed states. This range provides a useful scale for assessing how well a quantum circuit can produce a distribution of quantum states that is close to the uniform distribution defined by the Haar measure.

When designing quantum circuits, especially for tasks in quantum machine learning, a key goal is to balance the circuit's expressiveness with its trainability. As the depth and complexity of a quantum circuit increase, so does its ability to generate complex quantum states. However, this increased complexity can also lead to what is known as the "barren plateau" problem, where the landscape of the optimization function becomes flat, making it difficult to find the optimal parameters using gradient-based methods.

The linear entropy serves as a diagnostic tool in this context. If a quantum circuit generates states with high linear entropy, it suggests that the circuit is highly expressive and can explore a large portion of the Hilbert space. This is beneficial for capturing complex data patterns but can also indicate a potential for optimization difficulties if the expressiveness is too high.

In practice, as the depth of a quantum circuit increases, the linear entropy of the states it generates
tends to stabilize at a certain value. This stabilization often indicates that the quantum states have
reached a level of distribution close to that defined by the Haar measure. From one perspective,
this stabilization is a positive indicator, showing that the circuit is capable of exploring the highdimensional quantum state space effectively.

However, from another perspective, it can be a warning sign. If the circuit's depth is too great, the
resulting quantum states may be so randomized that the optimization landscape becomes too flat,
leading to the barren plateau problem. In this scenario, while the circuit's expressiveness is high, its
ability to be trained effectively diminishes.

Therefore, when using linear entropy as a measure of quantum circuit expressiveness, it is crucial to find a balance. The goal is to design a circuit that is expressive enough to capture the necessary complexity of the problem at hand, without introducing excessive randomness that could hinder optimization.

274 One practical application of linear entropy in quantum circuit design is determining the optimal 275 circuit depth. By monitoring the linear entropy as the circuit depth increases, designers can identify 276 the point at which the entropy stabilizes. This stabilization point often corresponds to the optimal 277 depth, where the circuit is expressive enough to perform the task effectively without falling into 278 the barren plateau trap.In binary classification tasks using QNNs, the process involves encoding all 279 quantum states, calculating the linear entropy for single-qubit subsystems, and comparing the linear 280 entropy for different circuit depths. By analyzing these values, one can determine the optimal depth at which the quantum circuit has sufficient expressiveness to distinguish between different classes 281 of data while remaining trainable. 282

- 283
- 284 285

#### 3.3 DETERMINING THE OPTIMAL CIRCUIT DEPTH BASED ON ENTROPY MATCHING

In the broader context of quantum computation, the quantum circuit  $V(\theta)$  represents a dynamic and evolving framework where the interplay of parameters  $\theta$  governs the transformation of an initial quantum state  $|\psi_{in}\rangle$  into an output state  $|\psi_{out}\rangle = V(\theta) |\psi_{in}\rangle$ . This transformation encapsulates not just a technical procedure but the core essence of quantum machine learning, where the complexity of quantum operations mirrors the intricate nature of the information they process. The layers of parameterized gates, denoted as L, serve as fundamental building blocks, each subtly altering the trajectory of the quantum state through its vast state space.

As illustrated in Figure 1, the circuit often initializes all qubits in the standard state  $|0\rangle$ , but this seem-293 ingly trivial starting point belies the immense potential of the quantum states that follow. By encoding classical input data x into quantum states through Y-rotation gates  $R_u(\hat{x}_i) = \exp(-i\hat{x}_i Y/2)$ , 295 we introduce classical features into the quantum domain. However, this process transcends mere 296 encoding—it is an act of transforming the very nature of data representation, where quantum states, 297 unlike classical bits, embody a superposition of possibilities. This endows the quantum circuit with 298 the power to represent and manipulate information in ways classical systems cannot. The structure 299 of the quantum circuit, characterized by alternating layers of parameterized single-qubit gates and 300 entangling operations (such as controlled-Z gates arranged in a circular topology), facilitates the 301 entanglement and interaction of qubits, forming a web of quantum correlations. These correlations, unlike classical dependencies, are non-local, entangling the qubits in a manner that makes them in-302 separable in a quantum mechanical sense. This entanglement is the source of the quantum circuit's 303 capacity for expressing complex transformations and interactions within the data. 304



315 316 317

305 306 307

308

310 311

312 313 314

Figure 1: A typical example of a quantum circuit with L layers of parameterized gates. All qubits are initialized in the state  $|0\rangle$ , followed by encoding the input x using Y-rotation gates. The circuit consists of parameterized single-qubit gates and controlled-Z entangling gates applied in a ring topology.

322

When evaluating the circuit in the context of a binary classification task, we move beyond classical notions of data processing. Each input quantum state, representing the encoded dataset, undergoes a

transformation through the circuit. The resulting quantum state  $|\psi_{out}\rangle$  is measured not only in terms of its final values but through the subtle lens of quantum entropy, specifically the linear entropy  $S_L(\rho)$ . This measurement provides a window into the degree of purity or randomness within the quantum system, with entropy reflecting the extent to which the quantum state remains coherent or has devolved into statistical noise.

In analyzing a dataset with different labels, we observe that the quantum circuit's ability to classify these states is tied to how the circuit balances complexity with stability. As the circuit depth *L* increases, it gains the capacity to explore a broader spectrum of quantum states. However, this comes at a cost—excessive complexity can push the quantum system toward randomness, diluting the very structure it is meant to capture. This phenomenon is akin to the system's entropy approaching the Haar measure, a point where the states resemble a random ensemble.

The key challenge lies in navigating the trade-off between expressiveness and optimization. A quantum circuit that is too shallow lacks the capacity to explore the rich space of quantum states necessary for distinguishing between classes. Yet, if the circuit becomes too deep, the system may encounter the barren plateau problem, where the landscape of the optimization becomes flat and gradients vanish, stalling the learning process. The optimal depth L is thus a delicate balance point, where the circuit is sufficiently complex to express the necessary transformations without succumbing to the randomness that hampers trainability.

By examining the entropy behavior of single-qubit subsystems across different circuit depths, we can identify this critical balance point. The entropy curves for states labeled +1 and -1 provide crucial insights into how the circuit processes and separates these states. When the difference in entropy between the two classes is minimized, the circuit is at its most effective, achieving maximum classification power without excessive entanglement or randomness.

Ultimately, this approach offers a pathway toward the optimization of quantum circuits, not just as a
 technical exercise but as a profound exploration of the boundaries between quantum randomness and
 structured information processing. It opens doors to more efficient quantum neural networks, where
 computational resources are judiciously conserved while achieving enhanced performance. The
 broader implications extend to the development of quantum technologies, where theoretical insights
 such as these pave the way for tangible advancements in quantum computing and its application to
 real-world problems.

354 355 356

357 358

359

#### 4 EXPERIMENTAL RESULTS

4.1 THEORETICAL DETERMINATION OF OPTIMAL LAYER DEPTH

360 To investigate this, we conducted experiments using the MNIST dataset (Modified National Institute 361 of Standards and Technology dataset). Each sample in the MNIST dataset is a grayscale image of 362 28x28 pixels. These images were first stored as 28x28 matrices and then flattened into vectors of length 784. Given that  $2^9 < 784 < 2^{10}$ , we designed a quantum circuit with 10 qubits, padding 363 these vectors to 1024 dimensions and normalizing them to ensure that each vector had a norm of 364 1. The data was then encoded into corresponding quantum states  $|\psi_{in}\rangle$  using amplitude encoding. 365 For the experiment, 40 samples labeled as +1 and 40 samples labeled as -1 were selected, and the 366 average linear entropy of the single-qubit subsystems was calculated for these samples. Preliminary 367 results showed that the average linear entropy for samples labeled as -1 was 0.45316231711829386, 368 while for samples labeled as +1, the average entropy was 0.4512322480823703. 369

The quantum circuit  $V(\theta)$  used in this study, designed based on the theoretical model, is shown in Figure 2. For samples labeled as +1, the output state  $|\psi \text{out}\rangle = V(\theta) |\psi \text{in}\rangle$  is expected to be close to the  $|0\rangle$  state, while for samples labeled as -1, the output state is expected to be close to  $|1\rangle$ .

To precisely determine the optimal circuit depth, we computed the linear entropy of the single-qubit subsystems for the states  $V(\theta)^{\dagger}|0\rangle$  and  $V(\theta)^{\dagger}|1\rangle$  across different layers *L*. As the depth of the circuit increases, the distribution of quantum states tends to become more random, with the linear entropy approaching 0.5. This indicates that the quantum states have reached a distribution similar to that defined by the Haar measure. While this level of randomness suggests high expressiveness in the quantum circuit, it can also lead to the barren plateau problem, where optimization becomes difficult  $R_Y(\theta_1')$ 

 $R_Y(\theta_2)$ 

 $R_Y(\theta_3)$ 

 $R_Y(\theta_4')$ 

 $R_Y(\theta_m')$ 

U(Θ1)

 $R_X(\theta_1)$ 

 $R_X(\theta_2)$ 

 $R_X(\theta_3)$ 

 $R_X(\theta_4)$ 

 $R_X(\theta_m)$ 

 $U_{\phi}(\boldsymbol{x})$ 

Figure 2: The quantum circuit used in the study. The circuit consists of L layers, where each layer contains parameterized single-qubit gates and controlled-Z gates, arranged in a ring topology.

 $R_X(\theta_{1+(L-1)m})$ 

 $R_X(\theta_{2+(L-1)m})$ 

 $R_X(\theta_{3+(L-1)m})$ 

 $R_X(\theta_{4+(L-1)m})$ 

 $R_X(\theta_{Lm})$ 

V(θ)

 $R_Y(\theta_{1+(L-1)m'})$ 

 $\overline{R}_{Y}(\theta_{2+(L-1)m'})$ 

 $R_Y(\theta_{3+(L-1)m})$ 

 $R_Y(\theta_{4+(L-1)m})$ 

 $R_Y(\theta_{Lm'})$ 

U(Θ₂)

7

7

7

due to vanishing gradients. To refine the determination of the optimal layer count, we plotted the graph using  $\ln(0.5 - \text{entropy})$  as the vertical axis, as shown in Figure 3.



419 420

378 379

380

381 382

384

386 387

388

389

390 391

392

393 394 395

396

421 422

423

Figure 3: Linear entropy of the single-qubit subsystems across different layers L.

#### 4.2 EXPERIMENTAL VERIFICATION

The previous analysis identified that the theoretically optimal circuit depth is 9 or 10 layers based on entropy matching. We proceeded with experiments to validate the accuracy of this theoretical prediction.

As shown in Figure 4, the experimental results demonstrate that by statistically analyzing the linear entropy of single-qubit subsystems of encoded quantum states and matching it with the linear entropy of quantum states generated by circuits of varying depths, the optimal number of layers for a quantum circuit can be effectively determined. In this experiment, quantum neural networks with circuit depths of L=9 and L=10 exhibited the best error rate convergence on the test set, validating the effectiveness of this method in optimizing circuit design. In contrast, while circuits with L=8

and L=11 also significantly reduced error rates, they fell slightly behind in terms of stability and
 convergence speed. Additionally, circuits with too few layers (such as L=1) showed slow error rate
 reduction and large fluctuations, indicating insufficient expressivity. Conversely, circuits with ex cessive layers (such as L=20) experienced slightly higher error rates, likely due to the barren plateau
 problem, which suggests that deeper circuits can lead to optimization difficulties and reduced com putational efficiency.



Figure 4: Error rates on the test set for circuits with different layers.

456 This method of determining the optimal circuit depth by matching linear entropy not only enhances 457 the performance of quantum neural networks in classification tasks but also significantly conserves 458 computational resources. By optimizing quantum circuit design, we can achieve superior perfor-459 mance in practical applications. These findings provide strong theoretical and experimental support 460 for the future development of quantum computing technology, showing that designing and optimizing the structure of quantum neural networks by quantifying the complexity of quantum states is 461 an effective approach to improving performance. This lays the groundwork for applying quantum 462 machine learning to tasks such as classification and regression, further advancing the prospects of 463 quantum computing technology in real-world applications. 464

465 466 467

438 439

440 441

442

443 444

445

446 447

448

449 450

451

452 453 454

455

#### 5 CONCLUSION

468 In this work, we have explored the critical role of Haar measure and linear entropy in evaluating the 469 expressiveness of quantum circuits, particularly in the context of quantum machine learning. The 470 theoretical framework established in this study underscores the importance of ensuring that quan-471 tum circuits can generate quantum states that approximate the Haar measure distribution, which is indicative of a circuit's ability to explore the entire Hilbert space and perform complex quantum 472 computations. Our approach utilized linear entropy as a diagnostic tool to quantify the randomness 473 and complexity of quantum states produced by quantum circuits. By examining the linear entropy 474 across various circuit depths, we were able to identify the optimal number of layers that balance 475 expressiveness with trainability. This balance is crucial for avoiding the barren plateau problem, 476 where excessive circuit depth leads to a flat optimization landscape, making it difficult to effectively 477 train the quantum circuit. The experimental validation conducted on the MNIST dataset demon-478 strated that the theoretically determined optimal circuit depth, identified through entropy matching, 479 significantly enhances the performance of quantum neural networks in binary classification tasks. 480 The results showed that circuits with the optimal depth not only achieved lower error rates but also 481 maintained stability across different test scenarios. The findings of this study have several impor-482 tant implications for the future of quantum computing. The entropy-based approach presented here 483 offers a promising pathway for developing more efficient and effective quantum algorithms, with potential applications across a wide range of computational tasks. As quantum computing technol-484 ogy continues to evolve, the principles and methodologies discussed in this paper will play a pivotal 485 role in shaping the design and optimization of future quantum circuits.

#### 486 REFERENCES 487

491

518

527

- Amira Abbas, David Sutter, Christa Zoufal, Aurelien Lucchi, Alessio Figalli, and Stefan Woerner. 488 The power of quantum neural networks. *Nature Computational Science*, 1(6):403–409, June 489 2021. ISSN 2662-8457. doi: 10.1038/s43588-021-00084-1. URL http://dx.doi.org/ 490 10.1038/s43588-021-00084-1.
- 492 Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C. Bardin, Rami Barends, Rupak 493 Biswas, Sergio Boixo, Fernando G. S. L. Brandao, David A. Buell, Brian Burkett, Yu Chen, Zi-494 jun Chen, Ben Chiaro, Roberto Collins, William Courtney, Andrew Dunsworth, Edward Farhi, Brooks Foxen, Austin Fowler, Craig Gidney, Marissa Giustina, Rob Graff, Keith Guerin, Steve 495 Habegger, Matthew P. Harrigan, Michael J. Hartmann, Alan Ho, Markus Hoffmann, Trent Huang, 496 Travis S. Humble, Sergei V. Isakov, Evan Jeffrey, Zhang Jiang, Dvir Kafri, Kostyantyn Kechedzhi, 497 Julian Kelly, Paul V. Klimov, Sergey Knysh, Alexander Korotkov, Fedor Kostritsa, David Land-498 huis, Mike Lindmark, Erik Lucero, Dmitry Lyakh, Salvatore Mandrà, Jarrod R. McClean, 499 Matthew McEwen, Anthony Megrant, Xiao Mi, Kristel Michielsen, Masoud Mohseni, Josh Mu-500 tus, Ofer Naaman, Matthew Neeley, Charles Neill, Murphy Yuezhen Niu, Eric Ostby, Andre 501 Petukhov, John C. Platt, Chris Quintana, Eleanor G. Rieffel, Pedram Roushan, Nicholas C. Rubin, Daniel Sank, Kevin J. Satzinger, Vadim Smelyanskiy, Kevin J. Sung, Matthew D. Trevithick, Amit Vainsencher, Benjamin Villalonga, Theodore White, Z. Jamie Yao, Ping Yeh, Adam Zalcman, 504 Hartmut Neven, and John M. Martinis. Quantum supremacy using a programmable supercon-505 ducting processor. Nature, 574(7779):505-510, October 2019. ISSN 1476-4687. doi: 10.1038/ s41586-019-1666-5. URL http://dx.doi.org/10.1038/s41586-019-1666-5. 506
- 507 Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe, and Seth Lloyd. 508 Quantum machine learning. *Nature*, 549(7671):195–202, September 2017. ISSN 1476-4687. doi: 509 10.1038/nature23474. URL http://dx.doi.org/10.1038/nature23474. 510
- 511 Sergey Bravyi, David Gosset, and Robert König. Quantum advantage with shallow circuits. Science, 362(6412):308-311, October 2018. ISSN 1095-9203. doi: 10.1126/science.aar3106. URL 512 http://dx.doi.org/10.1126/science.aar3106. 513
- 514 Matthias C. Caro, Hsin-Yuan Huang, M. Cerezo, Kunal Sharma, Andrew Sornborger, Lukasz Cin-515 cio, and Patrick J. Coles. Generalization in quantum machine learning from few training data. Na-516 ture Communications, 13(1), August 2022. ISSN 2041-1723. doi: 10.1038/s41467-022-32550-3. 517 URL http://dx.doi.org/10.1038/s41467-022-32550-3.
- M. Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C. Benjamin, Suguru Endo, Keisuke Fujii, 519 Jarrod R. McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, and Patrick J. Coles. Vari-520 ational quantum algorithms. Nature Reviews Physics, 3(9):625–644, August 2021a. ISSN 521 2522-5820. doi: 10.1038/s42254-021-00348-9. URL http://dx.doi.org/10.1038/ 522 s42254-021-00348-9. 523
- 524 M. Cerezo, Akira Sone, Tyler Volkoff, Lukasz Cincio, and Patrick J. Coles. Cost function dependent 525 barren plateaus in shallow parametrized quantum circuits. *Nature Communications*, 12(1), March 2021b. ISSN 2041-1723. doi: 10.1038/s41467-021-21728-w. URL http://dx.doi.org/ 526 10.1038/s41467-021-21728-w.
- 528 Chih-Chieh Chen, Masaya Watabe, Kodai Shiba, Masaru Sogabe, Katsuyoshi Sakamoto, and Tomah 529 Sogabe. On the expressibility and overfitting of quantum circuit learning. ACM Transactions on 530 Quantum Computing, 2(2), July 2021. doi: 10.1145/3466797. URL https://doi.org/10. 531 1145/3466797. 532
- Edward Farhi and Hartmut Neven. Classification with quantum neural networks on near term pro-533 cessors, 2018. URL https://arxiv.org/abs/1802.06002. 534
- 535 Lov K. Grover. A fast quantum mechanical algorithm for database search. In Proceedings of the 536 twenty-eighth annual ACM symposium on Theory of computing, STOC '96, pp. 212–219, New York, NY, USA, 1996. ACM. doi: 10.1145/237814.237866. 538
- Morten Kjaergaard, Mollie E. Schwartz, Jochen Braumüller, Philip Krantz, Joel I.-J. Wang, Simon Gustavsson, and William D. Oliver. Superconducting qubits: Current state of play.

540 Annual Review of Condensed Matter Physics, 11(1):369-395, March 2020. ISSN 1947-541 5462. doi: 10.1146/annurev-conmatphys-031119-050605. URL http://dx.doi.org/10. 542 1146/annurev-conmatphys-031119-050605. 543

- Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik. The theory of vari-544 ational hybrid quantum-classical algorithms. New Journal of Physics, 18(2):023023, February 2016. ISSN 1367-2630. doi: 10.1088/1367-2630/18/2/023023. URL http://dx.doi.org/ 546 10.1088/1367-2630/18/2/023023. 547
- 548 Jarrod R. McClean, Sergio Boixo, Vadim N. Smelyanskiy, Ryan Babbush, and Hartmut Neven. 549 Barren plateaus in quantum neural network training landscapes. Nature Communications, 9(1), November 2018. ISSN 2041-1723. doi: 10.1038/s41467-018-07090-4. URL http://dx. 550 doi.org/10.1038/s41467-018-07090-4. 551
  - K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii. Quantum circuit learning. Phys. Rev. A, 98: 032309, Sep 2018. doi: 10.1103/PhysRevA.98.032309. URL https://link.aps.org/ doi/10.1103/PhysRevA.98.032309.
- Michael A. Nielsen and Isaac L. Chuang. Quantum computation and quantum information. Cam-556 bridge University Press, 2000.
- 558 Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, 559 Alá Aspuru-Guzik, and Jeremy L. O'Brien. A variational eigenvalue solver on a photonic quantum processor. Nature Communications, 5(1):4213, July 2014. doi: 10.1038/ncomms5213. URL 561 https://www.nature.com/articles/ncomms5213.
- John Preskill. Quantum computing in the nisq era and beyond. Quantum, 2:79, August 2018. ISSN 563 2521-327X. doi: 10.22331/q-2018-08-06-79. URL http://dx.doi.org/10.22331/ 564 q-2018-08-06-79. 565
- 566 Peter Williston Shor. Algorithms for quantum computation: discrete logarithms and factoring. In 567 Proceedings 35th Annual Symposium on Foundations of Computer Science, pp. 124–134, Santa Fe, New Mexico, November 1994. IEEE Computer Society Press. 568
- 569 Sukin Sim, Peter D. Johnson, and Alán Aspuru-Guzik. Expressibility and entangling capability 570 of parameterized quantum circuits for hybrid quantum-classical algorithms. Advanced Quantum Technologies, 2(12), October 2019. ISSN 2511-9044. doi: 10.1002/qute.201900070. URL 572 http://dx.doi.org/10.1002/qute.201900070.
- Han-Sen Zhong, Hui Wang, Yu-Hao Deng, Ming-Cheng Chen, Li-Chao Peng, Yi-Han Luo, Jian 574 Qin, Dian Wu, Xing Ding, Yi Hu, Peng Hu, Xiao-Yan Yang, Wei-Jun Zhang, Hao Li, Yuxuan 575 Li, Xiao Jiang, Lin Gan, Guangwen Yang, Lixing You, Zhen Wang, Li Li, Nai-Le Liu, Chao-576 Yang Lu, and Jian-Wei Pan. Quantum computational advantage using photons. Science, 370 577 (6523):1460-1463, December 2020. ISSN 1095-9203. doi: 10.1126/science.abe8770. URL 578 http://dx.doi.org/10.1126/science.abe8770. 579
- 580

552

553

554

555

562

571

573

- 581 582
- 583
- 584 585
- 586 587

588

- 589

- 592 593