
NORMALIZING FLOWS FOR CLASSICAL SIMULATION OF QUANTUM CIRCUITS IN PHASE SPACE

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ABSTRACT

We present a novel framework to learn a representation of quantum circuits based on the phase space formulation of many-qubit systems. Given that N -qubit states can be represented as quasi-probability distributions on a $2N$ -dimensional manifold, we show how unitary gates can be parameterized as normalizing flows between these distributions, opening a new avenue for AI-assisted quantum circuit simulation. We evaluate our method on two common families of quantum circuits, and show that it scales better than the current state-of-the-art to large numbers of qubits.

Keywords quantum computing, quantum circuits, phase space, generative models, normalizing flows

1 Introduction

The problem of classical simulation of quantum circuit is pertinent to both the existence of quantum advantage, and to inference and control of quantum hardware [1, 2]. Methods for classical simulation of quantum circuits range from exact state-vector methods to Feynman-style path integral schemes [3, 4, 5], to techniques that exploit a special circuit structure [6, 7] or low entanglement [8, 9, 10], to other approximation or Monte-Carlo sampling schemes [11, 12].

Machine-learning techniques have also been applied to this problem. Neural quantum states (NQS) and its variations [13, 14, 15, 16, 17] offer compact representations and were shown to be able to evolve nontrivial many-body states. More recently, generative models have been used to learn representations of quantum states in the probabilistic formulation of quantum dynamics [18, 19, 20].

In this paper, we present a novel method to learn the output state of a quantum circuit based on a different probabilistic formulation: the multi-qubit phase space formalism [21]. Each intermediate state is represented as a probability distribution, and unitary gates are represented as flow transformations that map from one distribution to the next. Unlike previous methods, ours is based on a continuous input space rather than a discrete domain such as $\{0, 1\}^N$ [18, 13, 14, 15]. Since deep neural networks naturally accept continuous-valued inputs, this lets us bypass many shortcomings of discrete input spaces, such as requiring continuous relaxations or one-hot encoding. In addition, our architecture is naturally composable due to the sequential nature of normalizing flows, in contrast with previous methods which employ a variational principle to a fixed architecture for each state [16, 17, 18]. We demonstrate our method on two common families of quantum state preparation circuit, the GHZ states and the 1D cluster states.

2 Methods

Our objective is to learn a representation of a quantum circuit from which measurement statistics and observable values can be extracted.

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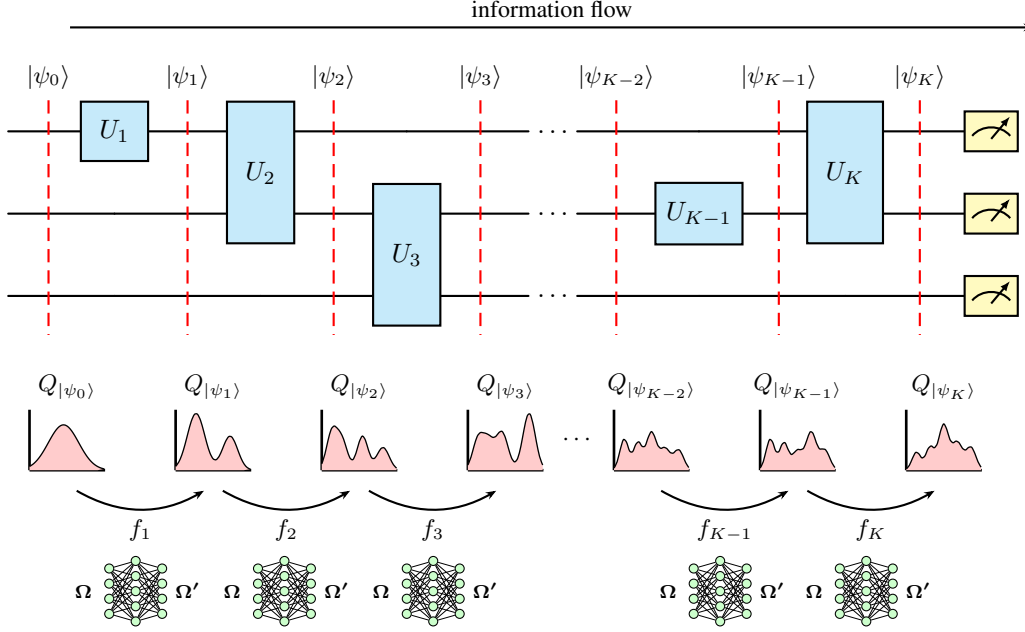


Figure 1: Our proposed framework for learning the output state of a quantum circuit. In the unitary picture (top half), the state of a quantum circuit is represented by the state vectors $|\psi_k\rangle$, and maps from one state to the next are given by unitary operators U_k . In the phase-space picture (bottom half), the state of a quantum circuit is represented by a probability distribution (i.e. the Q function), and maps from one state to the next are given by the normalizing flows f_k parameterized by neural networks. Here, the distributions are shown over R for illustrative purposes, but in reality are over $(S^2)^N$. Note that each f_k may in general contain many normalizing flow layers.

We choose to represent each state by a probability distribution over the phase space $(S^2)^N$, more specifically the Husimi Q representation [21]. We represent a unitary operator as the pushforward of the input distribution, under some diffeomorphism of the phase space. The diffeomorphism is parameterized as a normalizing flow layer and is trained to minimize the KL divergence.

The initial probability distribution is known, corresponding to some fiducial state, and the intermediate distributions are trained sequentially via the flow layers. The final state is a composition of each of the flow layers, allowing the model to represent increasingly complex distributions as the circuit gets deeper.

Our framework is illustrated in Fig. 1.

3 Results

We evaluate on two families of circuits, 1D cluster state preparation and GHZ state preparation, and compare with a similar method [18, 19] that uses IC-POVM probabilities and a transformer architecture. The results are shown in Fig. 2.

Overall, we see that our method performs better than the transformer architecture, achieving a fidelity of approximately 0.96 for the 1D cluster state preparation on 60 qubits, and approximately 0.965 for the GHZ state preparation on 60 qubits.

4 Conclusion and Outlook

In this paper, we introduced a novel framework to learn the output state of a quantum circuit based on normalizing flows in the phase space representation, and showed experimentally that the method is able to scale well to intermediate-size systems.

Further work can focus on applying the framework in this paper to other families of quantum circuits, for example those used in condensed matter simulation [22, 23, 24], or on improving the architecture of the flows to achieve higher per-gate fidelity, using e.g. [25, 26]. Overall, the results presented in

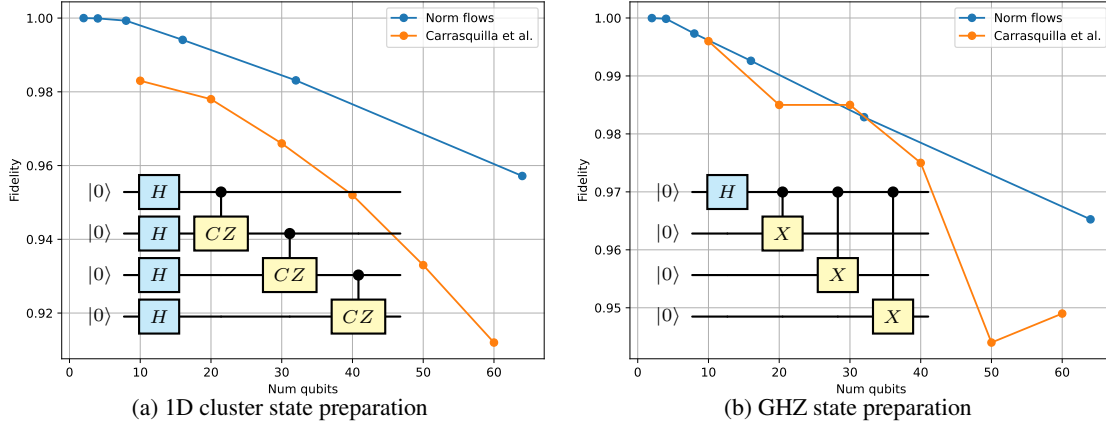


Figure 2: Classical fidelity between the exact Q representation of the final state and the output distribution of the normalizing flow model, as a function of the total number of qubits. Each flow transformation of the model has been trained for 20000 steps using the Adam optimizer with a learning rate of 10^{-3} and a batch size of 2^{10} .

this paper open up new avenues for the application of machine learning, and particularly generative models, to the problem of quantum simulation.

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