Training of Quantum Circuits on a Hybrid Quantum Computer

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(Dated: 24 December 2018)

Generative modeling is a flavor of machine learning with applications ranging from
computer vision to chemical design. It is expected to be one of the techniques most
suited to take advantage of the additional resources provided by near-term quan-
tum computers. We implement a data-driven quantum circuit training algorithm on
the canonical Bars-and-Stripes data set using a quantum-classical hybrid machine.
The training proceeds by running parameterized circuits on a trapped ion quantum
computer, and feeding the results to a classical optimizer. We apply two separate
strategies, Particle Swarm and Bayesian optimization to this task. We show that
the convergence of the quantum circuit to the target distribution depends critically
on both the quantum hardware and classical optimization strategy. Our study rep-
resents the first successful training of a high-dimensional universal quantum circuit,
and highlights the promise and challenges associated with hybrid learning schemes.
I. INTRODUCTION

Hybrid quantum algorithms use both classical and quantum resources to solve potentially difficult problems. This approach is particularly promising for current quantum computers of limited size and power. Several variants of hybrid quantum algorithms have recently been demonstrated, such as the Variational Quantum Eigensolver (VQE) for quantum chemistry and related applications and the Quantum Approximate Optimization Algorithm (QAOA) for graph or other optimization problems. Hybrid quantum algorithms can also be used for generative models, which aim to learn representations of data in order to make subsequent tasks easier. Applications of generative modeling include computer vision, speech synthesis, the inference of missing text, de-noising of images, and chemical design. Here, we apply a hybrid quantum learning scheme on a trapped ion quantum computer to accomplish a generative modeling task.

Data-driven quantum circuit learning (DDQCL) is a hybrid framework for generative modeling of classical data where the model consists of a parameterized quantum circuit. The model is trained by sampling the output of a quantum computer and updating the circuit parameters using a classical optimizer. After convergence, the optimal circuit produces a quantum state that captures the correlations in the training data sets. Hence the trained circuit serves as a generative model for the training data. Theoretical results suggest that such generative models have more expressive power than widely used classical neural networks. This is because instantaneous quantum polynomial circuits – special cases of the parameterized quantum circuits used for generative modeling – cannot be efficiently simulated by classical means.

The Bars-and-Stripes (BAS) data set is a canonical body of synthetic data for generative modeling. It can be easily visualized in terms of images containing horizontal bars or vertical stripes, where each pixel represents a qubit. Here, we use the 2-by-2 BAS shown in Fig. 1 in a proof-of-principle generative modeling task on a trapped-ion quantum computer. This is the first successful demonstration of generative quantum circuits trained on quantum hardware. We compare the performance of different classical optimization algorithms and conclude that Bayesian optimization shows significant advantages over Particle Swarm Optimization for this task.
II. DDQCL ON A TRAPPED ION QUANTUM COMPUTER

The experiment is performed on four qubits within a seven-qubit fully programmable trapped ion quantum computer \(^\text{[10]}\) (Appendix A). With individual addressing and readout of all qubits, the system can perform sequences of gates from a universal gates set, composed of Ising gates and arbitrary rotations \(^\text{[15]}\). In order to run the large number of variational circuit instances necessary for the data-driven learning, we calibrate single- and two-qubit gates and execute lists of circuits in an automated fashion. The system also features an application program interface (API) that can be incorporated with external optimization packages.

![Diagram of a quantum circuit](image)

**FIG. 1.** Data-driven quantum circuit learning (DDQCL) is a hybrid quantum algorithm scheme that can be used for generative modeling, illustrated here by the example of 2-by-2 Bars and Stripes (BAS) data. From top left, clockwise: A parametrized circuit is initialized at random. Then at each iteration, the circuit is executed on a trapped ion quantum computer. The probability distribution of measurement is compared on a classical computer against the BAS target data set. Next, the quantified difference is used to optimize the parametrized circuit. This learning process is iterated until convergence.

The training pipeline is illustrated in Fig. 1. The quantum circuits are structured as layers of parameterized gates. We use two types of layers, involving single-qubit rotations and two-qubit entangling gates. A single-qubit layer sandwiches an X-rotation between two Z-rotations on each qubit \(i\), or \(R_x^{(i)}(\alpha_i)R_z^{(i)}(\beta_i)R_x^{(i)}(\gamma_i)\), involving twelve rotation parameters.
for the four qubits (see Fig. 2). An entangling layer applies Ising or XX gates between all pairs of qubits according to any imposed connectivity graph. This is expressed as a sequence of $XX_{i,j}^{i,j}(\chi_{i,j})$ operations as shown in Fig. 2, with up to six entangling parameters for four qubits. Due to the universality of this gate set, a sufficiently long sequence of layers of these two types can produce arbitrary unitaries.

At the start of DDQCL, all the rotation and entangling parameters are initialized with random values. Next the circuit is repeatedly executed on the trapped ion quantum computer in order to reconstruct the state distribution. A classical computer then compares the measured distribution with the target distribution and quantifies the difference using a cost function (see Appendix B for details). A classical optimization algorithm then varies the parameters. We iterate the entire process until convergence.

We impose two distinct connectivity graphs in a four-qubit circuit: all-to-all and star, as shown in Fig. 2. With star connectivity, entanglement between certain qubit-pairs cannot occur within a single gate layer, which means more layers are necessary for certain target distributions. Comparing the training process between circuits of different connectivity provides insight into the performance of DDQCL algorithms on platforms with more limited interaction graphs.

For each connectivity graph, we add layers until the goal of reproducing the BAS data with the trained model is achieved. The match between training data and model is limited by noise, experimental throughput rate, and sampling errors. The cost function used in optimization grades the result, but a successful training process must be able to generate data that can be qualitatively recognized as a BAS pattern to ensure that the system provides usable results in the spirit of generative modeling in machine learning.

We now describe the classical optimization strategies for the training algorithm. Although gradient-based approaches were recently proposed for DDQCL, we employ gradient-free optimization schemes that appear less sensitive to noise and experimental throughput. We explore two such schemes: Particle Swarm Optimization (PSO) and Bayesian Optimization (BO). PSO is a stochastic optimization scheme commonly used in machine learning that works by creating many “particles” randomly distributed across parameter space that explore the landscape collaboratively. We limit the number of particles to twice the number of parameters. BO is a global optimization paradigm that can handle the expensive sampling of many-parameter functions. It works by maintaining a surrogate model of the underlying
FIG. 2. Top: Fully-connected training circuit, with layers of rotations and entangling gates between any pair of the four qubits. Bottom: Star-connectivity training circuit layers, with restricted entangling gates. In either case, each rotation (denoted by X or Z) and each entanglement gate (denoted by XX) includes a distinct control parameter, for a total of 18 parameters for the fully-connected circuit and 15 parameters for the star-connected circuit. We remove the first Z rotation acting on the initial state $|0\rangle$. The connectivity figures on the left define the mapping between the four qubits and the pixels of the BAS images (see Fig. 1).

 cost function and, at each iteration, updates the model to guide the search for the global minimum. Essentially, the problem of optimizing the real cost is replaced with that of optimizing the surrogate model, which is designed to be a much easier optimization problem. We use OPTaaS, a BO software package developed by Mind Foundry\cite{OPTaaS} and adapted for this work.

III. RESULTS

Results from PSO optimization are shown in Fig. 3. We first simulate the training procedure using a classical simulator in place of the quantum processor (orange plots in Fig. 3). Since the PSO method is sensitive to the initial "seed" values of the particles, we simulate the convergence for many different random seeds (see Fig. 3). We choose a seed that converges quickly and reliably under simulated sampling error to start the training procedure on the trapped ion quantum computer illustrated in Fig. 1. We iterate the training until it
converges (blue plots in Fig. 3). In practice, which seeds are successful is unknown, and different seeds need to be tried experimentally until a good model is obtained. This incurs an additional cost in the form of multiple independent DDQCL training rounds.

For all-to-all connectivity, we find that a circuit with one rotation gate layer and one entangling gate layer is able to produce the desired BAS distribution (Fig. 3a). This is not the case for the star-connected circuit, with the closest state having two additional components in the superposition (states 6 and 9 in Fig. 3b). With two additional layers, the star-connected circuit is able to model the BAS distribution (orange plots of Fig. 3c). In the experiment however (blue plots in Fig. 3c), the PSO is unable to converge to an acceptable solution even using the best pre-screened seed value and sufficient sample statistics. We conclude that PSO fails because the throughput rate is too low for effectively training the circuit in the face of gate imperfections.

For these reasons, we instead employ a Bayesian optimization scheme for the circuit training procedure. We find that all circuits experimentally converge in agreement with the simulations, as shown in Fig. 4. Moreover, even the star-connected circuit with four layers now produces a recognizable BAS distribution (Fig. 4c). In contrast to PSO, BO dramatically reduces the number of samples needed for training and does not require any pre-selection of random seeds or other prior knowledge of the cost-function landscape.

BO updates the surrogate model using the experimental result of every iteration. Therefore, the classical part of each BO iteration consumes more time than with PSO, where the time cost on the classical optimizer is negligible. However, the BO procedure converges faster to the desired BAS distribution. More generally, these examples highlight the need to balance quantum and classical resources in order to produce acceptable performance and run time in a hybrid quantum algorithm.

As a measure of the performance of the various training procedures, we compute the Kullback-Leibler (KL) divergence and the qBAS score of the experimental results at the end of each DDQCL training run, shown in Table I. We also compute the entanglement entropy (S) averaged over all two plus two qubit partitions assuming a pure state, estimated via simulation of the quantum state from the trained circuits. This metric shows that the successfully trained circuits generate states that are consistent with a high level of entanglement. As a reference, the entanglement entropy of a GHZ state over any partition is $S = 1$. 
FIG. 3. Quantum circuit training results with Particle Swarm optimization (PSO), with simulations (orange) and trapped ion quantum computer results (blue). Column (a) corresponds to a circuit with two layers of gates and all-to-all connectivity. The circuit converges well to produce the bars-and-stripes (BAS) distribution. Columns (b) and (c) correspond to a circuit with two and four layers and star-connectivity, respectively. In (b), the simulation shows imperfect convergence with two extra state components (6 and 9), due to the limited connectivity, and the experimental results follow the simulation. In (c), the simulation shows convergence to the BAS distribution, but the experiment fails to converge despite performing 1,400 quantum circuits. The optimization is sensitive to the choice of initialization seeds. To illustrate the convergence behavior, the shaded regions span the 5th-95th percentile range of random seeds (500 for (a) and (b), 1000 for (c), and the orange curve shows the median. The two-layer circuits have 14 and 11 parameters for (a) all-to-all- and (b) star-connectivity, while the (c) star-connectivity circuit with four layers has 26 parameters. Number of PSO particles used per iteration is twice that of parameters, and each training sample is repeated 5000 times. Including circuit compilation, controller-upload time, and classical PSO optimization, each circuit instance takes about 1 min to be processed, in addition to periodic interruptions for the recalibration of gates.
FIG. 4. Quantum circuit training results with Bayesian optimization (BO), with simulations (orange) and trapped ion quantum computer results (blue). Column (a) corresponds to a circuit with two layers of gates and all-to-all connectivity. Columns (b) and (c) correspond to a circuit with two and four layers and star-connectivity, respectively. Convergence is much faster than with PSO (Fig. 3). Unlike the PSO results, the four-layer star-connected circuit in (c) is trained successfully. As before, the two-layer circuits have 14 and 11 parameters for (a) all-to-all- and (b) star-connectivity, while the (c) star-connectivity circuit with four layers has 26 parameters. We use a batch of 5 circuits per iteration, and each training sample is repeated 5000 times. Including circuit compilation, controller-upload time, and BO classical optimization, each circuit instance takes 2-5 minutes, depending on the amount of accumulated data.
| circuits | optimizer | $D_{KL}$ | qBAS score | $S$  |
|---------|-----------|---------|------------|------|
| ![Circuit 1] | PSO       | 0.116   | 0.91       | 1.628|
|         | BO        | 0.094   | 0.91       | 1.659|
| ![Circuit 2] | PSO       | 0.357   | 0.74       | 0.9950|
|         | BO        | 0.328   | 0.77       | 0.9999|
| ![Circuit 3] | PSO       | 0.646   | 0.59       | 0.8867|
|         | BO        | 0.100   | 0.91       | 1.709|

TABLE I. KL divergence ($D_{KL}$, see Appendix B), qBAS score, and entanglement entropy ($S$) for the state obtained at the end of each of the DDQCL trainings on hardware, for various circuits and classical optimizers used.

IV. OUTLOOK

This demonstration of generative modeling using reconfigurable quantum circuits of up to 26 parameters represents the most powerful hybrid quantum application to date. This approach can be scaled up to handle larger data sets with increased qubit number by adapting the cost function for sparser sampling\textsuperscript{16}. Moreover, this procedure can be adapted for other types of hybrid quantum algorithms.

Classical optimization techniques for hybrid quantum algorithms on intermediate-scale quantum computer do not always succeed\textsuperscript{27}. Recent work suggests that typical cost functions for medium to large scale variational quantum circuits landscape resemble “barren plateaus”\textsuperscript{28}, making optimization hard. As quantum computers scale up for larger problems, the cost of classical optimization such as BO must be weighed against the quantum algorithmic advantage.

V. ACKNOWLEDGEMENTS

This work was supported by the ARO with funds from the IARPA LogiQ program, the ARO MURI program on Modular Quantum Circuits, the AFOSR MURI program on Optimal Quantum Measurements, the NSF STAQ Practical Fully-Connected Quantum Computer Project, and the NSF Physics Frontier Center at JQI.
VI. APPENDIX

A. Trapped Ion Quantum Computer

The trapped ion quantum computer used for this study consists of a chain of seven single $^{171}$Yb$^+$ ions confined in a Paul trap and laser cooled close to their motional ground state. Each ion provides one physical qubit in the form of a pair of states in the hyperfine-split $^2S_{1/2}$ ground level with an energy difference of 12.642821 GHz, which is insensitive to magnetic fields to first order. The qubits are collectively initialized through optical pumping, and state readout is accomplished by state-dependent fluorescence detection. Qubit operations are realized via pairs of Raman beams, derived from a single 355-nm mode-locked laser. These optical controllers consist of an array of individual addressing beams and a counter-propagating global beam that illuminates the entire chain. Single qubit gates are realized by driving resonant Rabi rotations of defined phase, amplitude, and duration. Single-qubit rotations about the z-axis, are performed classically with negligible error. Two-qubit gates are achieved by illuminating two selected ions with beat-note frequencies near motional sidebands and creating an effective Ising spin-spin interaction via transient entanglement between the two ion qubits and all modes of motion. To ensure that the motion is disentangled from the qubit states at the end of the interaction, we used a pulse shaping scheme by modulating the amplitude of the global beam.

B. Cost functions

We use a cost function to quantify the difference between the target BAS distribution and the experimental measurements of the circuit. The cost functions used to implement the training are variants of the original Kullback-Leibler Divergence ($D_{KL}$):

$$D_{KL}(p, q) = -\sum_i p(i) \log \frac{q(i)}{p(i)}$$  \hspace{1cm} (1)

For PSO, we use the clipped negative log-likelihood cost function:

$$C_{nll} = -\sum_i p(i) \log \{\max[\epsilon, q(i)]\}. \hspace{1cm} (2)$$

Taking $p(i)$ as the target distribution, Eq.2 is identical to Eq.1 up to a constant offset, so the optimization of these two functions is equivalent.
For BO, we use the clipped symmetrized Kullback-Leibler (KL) divergence as the cost function
\[
\tilde{D}_{KL}(p,q) = D_{KL}[^{\max}(\epsilon,p),^{\max}(\epsilon,q)] + D_{KL}[^{\max}(\epsilon,q),^{\max}(\epsilon,p)].
\] (3)
This is found to be the most reliable variant of \(D_{KL}\) for BO.

REFERENCES

1. J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, “The theory of variational hybrid quantum-classical algorithms,” New Journal of Physics 18, 023023 (2016).
2. J. Preskill, “Quantum Computing in the NISQ era and beyond,” Quantum 2, 79 (2018).
3. A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, “Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets,” Nature 549, 242 (2017).
4. A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O’Brien, “A variational eigenvalue solver on a photonic quantum processor,” Nature communications 5, 4213 (2014).
5. C. Hempel, C. Maier, J. Romero, J. McClean, T. Monz, H. Shen, P. Jurcevic, B. P. Lanyon, P. Love, R. Babbush, A. Aspuru-Guzik, R. Blatt, and C. F. Roos, “Quantum chemistry calculations on a trapped-ion quantum simulator,” Phys. Rev. X 8, 031022 (2018).
6. P. O’Malley, R. Babbush, I. Kivlichan, J. Romero, J. McClean, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, et al., “Scalable quantum simulation of molecular energies,” Physical Review X 6, 031007 (2016).
7. C. Kokail, C. Maier, R. van Bijnen, T. Brydges, M. K. Joshi, P. Jurcevic, C. A. Muschik, P. Silvi, R. Blatt, C. F. Roos, et al., “Self-verifying variational quantum simulation of the lattice schwinger model,” arXiv preprint arXiv:1810.03421 (2018).
8. E. Farhi, J. Goldstone, and S. Gutmann, “A quantum approximate optimization algorithm,” MIT-CTP/4610 (2014).
9. J. Otterbach, R. Manenti, N. Alidoust, A. Bestwick, M. Block, B. Bloom, S. Caldwell, N. Didier, E. S. Fried, S. Hong, et al., “Unsupervised machine learning on a hybrid quantum computer,” arXiv preprint arXiv:1712.05771 (2017).
10. J.-Y. Zhu, T. Park, P. Isola, and A. A. Efros, “Unpaired image-to-image translation using cycle-consistent adversarial networks,” arXiv preprint (2017).
A. Van Den Oord, S. Dieleman, H. Zen, K. Simonyan, O. Vinyals, A. Graves, N. Kalchbrenner, A. Senior, and K. Kavukcuoglu, “Wavenet: A generative model for raw audio,” CoRR abs/1609.03499 (2016).

S. R. Bowman, L. Vilnis, O. Vinyals, A. M. Dai, R. Jozefowicz, and S. Bengio, “Generating sentences from a continuous space,” SIGNLL Conference on Computational Natural Language Learning (CONLL), 2016 (2016).

Y. Bengio, L. Yao, G. Alain, and P. Vincent, “Generalized denoising auto-encoders as generative models,” in Advances in Neural Information Processing Systems (2013) pp. 899–907.

R. Gómez-Bombarelli, J. N. Wei, D. Duvenaud, J. M. Hernández-Lobato, B. Sánchez-Lengeling, D. Sheberla, J. Aguilera-Iparraguirre, T. D. Hirzel, R. P. Adams, and A. Aspuru-Guzik, “Automatic chemical design using a data-driven continuous representation of molecules,” ACS central science 4, 268–276 (2018).

S. Debnath, N. M. Linke, C. Figgatt, K. A. Landsman, K. Wright, and C. Monroe, “Demonstration of a small programmable quantum computer with atomic qubits,” Nature 536, 63 (2016).

M. Benedetti, D. Garcia-Pintos, O. Perdomo, V. Leyton-Ortega, Y. Nam, and A. Perdomo-Ortiz, “A generative modeling approach for benchmarking and training shallow quantum circuits,” arXiv preprint arXiv:1801.07686 (2018).

Y. Du, M.-H. Hsieh, T. Liu, and D. Tao, “The expressive power of parameterized quantum circuits,” arXiv preprint arXiv:1810.11922 (2018).

D. J. MacKay and D. J. Mac Kay, Information theory, inference and learning algorithms (Cambridge university press, 2003).

K. A. Landsman, C. Figgatt, T. Schuster, N. M. Linke, B. Yoshida, N. Y. Yao, and C. Monroe, “Verified quantum information scrambling,” arXiv preprint arXiv:1806.02807 (2018).

L. Theis, A. v. d. Oord, and M. Bethge, “A note on the evaluation of generative models,” arXiv preprint arXiv:1511.01844 (2015).

J.-G. Liu and L. Wang, “Differentiable learning of quantum circuit born machine,” arXiv preprint arXiv:1804.04168 (2018).

R. C. Eberhart and X. Hu, “Human tremor analysis using particle swarm optimization,” in Proceedings of the congress on evolutionary computation (IEEE Press Piscataway, NJ,
1999) pp. 1927–1930.

23 P. I. Frazier, “A tutorial on bayesian optimization,” arXiv preprint arXiv:1807.02811 (2018).

24 Mind Foundry Limited, “OPTaaS: An API for general purpose bayesian optimization,” http://edu.optaas.mindfoundry.ai (since 2018).

25 S. Kullback and R. A. Leibler, “On information and sufficiency,” The annals of mathematical statistics 22, 79–86 (1951).

26 A. Higuchi and A. Sudbery, “How entangled can two couples get?” Physics Letters A 273, 213–217 (2000).

27 K. E. Hamilton, E. F. Dumitrescu, and R. C. Pooser, “Generative model benchmarks for superconducting qubits,” arXiv preprint arXiv:1811.09905 (2018).

28 J. R. McClean, S. Boixo, V. N. Smelyanskiy, R. Babbush, and H. Neven, “Barren plateaus in quantum neural network training landscapes,” arXiv preprint arXiv:1803.11173 (2018).

29 S. Olmschenk, K. C. Younge, D. L. Moehring, D. N. Matsukevich, P. Maunz, and C. Monroe, “Manipulation and detection of a trapped $yb^+$ hyperfine qubit,” Phys. Rev. A 76, 052314 (2007).

30 K. Mølmer and A. Sørensen, “Multiparticle entanglement of hot trapped ions,” Phys. Rev. Lett. 82, 1835–1838 (1999).

31 E. Solano, R. L. de Matos Filho, and N. Zagury, “Deterministic bell states and measurement of the motional state of two trapped ions,” Phys. Rev. A 59, R2539–R2543 (1999).

32 G. Milburn, S. Schneider, and D. James, “Ion trap quantum computing with warm ions,” Fortschritte der Physik 48, 801–810 (2000).

33 T. Choi, S. Debnath, T. A. Manning, C. Figgatt, Z.-X. Gong, L.-M. Duan, and C. Monroe, “Optimal quantum control of multimode couplings between trapped ion qubits for scalable entanglement,” Phys. Rev. Lett. 112, 190502 (2014).