Experimental quantum learning of a spectral decomposition

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Currently available quantum hardware allows for small-scale implementations of quantum machine learning algorithms. Such experiments aid the search for applications of quantum computers by benchmarking the near-term feasibility of candidate algorithms. Here we demonstrate the quantum learning of a two-qubit unitary by a sequence of three parameterized quantum circuits containing a total of 21 variational parameters. Moreover, we variationally diagonalize the unitary to learn its spectral decomposition, i.e., its eigenvalues and eigenvectors. We illustrate how this can be used as a subroutine to compress the depth of dynamical quantum simulations. One can view our implementation as a demonstration of entanglement-enhanced machine learning, as only a single (entangled) training data pair is required to learn a 4×4 unitary matrix.

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I. INTRODUCTION

Quantum simulation and machine learning are among the most promising applications of large-scale quantum computers. Of these, the discovery of algorithms with provable exponential speedup has been more challenging in the machine learning domain, in part because it is harder to port established machine learning techniques to the quantum setting [1]. Notable exceptions include linear system solvers [2–4], kernel methods [5,6], and Boltzmann machines [7,8]. But quantum simulation demonstrations [9–13] appear to be ahead of machine learning [14–20] in terms of the maximum problem sizes achieved, suggesting that quantum simulation might yield the earliest applications with quantum advantage.

Variational quantum algorithms [21–23] will likely facilitate near-term implementations for these applications. Such algorithms employ a problem-specific cost function that is evaluated on a quantum computer, while a classical optimizer trains a parameterized quantum circuit to minimize this cost.

Some variational quantum algorithms have interest beyond their ability to achieve quantum advantage on their own and can serve as subroutines for larger quantum algorithms. These include quantum autoencoders for data compression [24,25] and linear algebra methods [26–28]. A common subroutine is the training of a variational quantum state to approximate the ground state of a given n -qubit Hamiltonian, which can be the Hamiltonian of a simulated model [29] or some other opti-

mization objective [30–32]. Variational quantum algorithms to learn and diagonalize density matrices have also been developed [33–35], which is a fundamental subroutine that will have many uses including principal component analysis and estimation of quantum information quantities [36,37]. Another subroutine is the learning of one quantum state by a second state, where the output of a variational circuit is optimized to maximize the overlap with an input state that might itself be the output of another algorithm [38–41]. Although a minimum of $2(2^n - 1)$ real parameters are required to do this exactly in general, it is widely believed that for many cases of interest a polynomial number of parameters will suffice.

Beyond learning states, it is also useful to *variationally learn a unitary channel* $\rho \mapsto U\rho U^\dagger$. This is more challenging because now all of the $4^n - 1$ matrix elements must match for an exact replica V of an arbitrary U , up to a global phase. A hybrid protocol for learning a unitary is provided by the quantum-assisted quantum compiling algorithm [38]. This is a low-depth subroutine appropriate for both near-term and fault-tolerant quantum computing.

Given a target unitary U and parameterized unitary $V(\theta)$, both acting on n qubits, quantum-assisted quantum compiling uses a maximally entangled Bell state on $2n$ qubits to compute the Hilbert-Schmidt inner product, $|\text{Tr}(UV(\theta)^\dagger)|$. Since this inner product is directly related to the average fidelity between states acted on by U and $V(\theta)$ [42,43], this allows the action of U on all possible input states to be studied using a single entangled input state. Consequently, with this entanglement-enhanced learning strategy, only a single training state is needed to fully learn U , in contrast to the $\approx 2^n$ input-output pairs that are required in the absence of entanglement [44,45].

Although more challenging than state learning, learning a unitary can be used for a wide variety of quantum information applications, including circuit depth compression,

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noise-tailoring, benchmarking, and the “black box uploading” of an unknown experimental system unitary [38]. Quantum-assisted quantum compiling has been demonstrated on $1 + 1$ qubits, where a single-qubit variational circuit $V(\theta)$ learned the value of a single-qubit unitary U [38].

Quantum-assisted quantum compiling can be generalized to learn not only a unitary, but also its Schur decomposition $W(\theta)D(\gamma)W(\theta)^\dagger$, where $W(\theta)$ is a parameterized unitary and $D(\gamma)$ is a parameterized diagonal unitary. That is, one can use quantum-assisted quantum compiling to *variationally diagonalize a unitary*. This is useful for a variety of quantum information science applications, since access to the spectral decomposition of a unitary U enables arbitrary powers of U to be implemented using a fixed depth circuit. Specifically, suppose we learn the optimal parameters θ_{opt} and γ_{opt} such that $U = W(\theta_{\text{opt}})D(\gamma_{\text{opt}})W(\theta_{\text{opt}})^\dagger$. We can then implement U^k using the fixed depth circuit $W(\theta_{\text{opt}})D(k\gamma_{\text{opt}})W(\theta_{\text{opt}})^\dagger$. We stress that the parameter k here can take any real value and hence this approach can be used to implement noninteger and negative powers of U .

One important application of variational unitary diagonalization is quantum simulation. Let U be a Trotterized (or other) approximation to a short-time evolution $e^{-iH\Delta t}$ by some time-independent Hamiltonian H . We assume that H is local [46–49], sparse [50–52], or given by a linear combination of unitaries [53–55], permitting efficient simulation with bounded error. Then $WD^{t/\Delta t}W^\dagger$ is an approximate *fast-forwarded* evolution operator with a circuit depth that is independent of t . By contrast, most of the best-known Hamiltonian simulation algorithms [49,52,55] have depths scaling at least linearly in t , inhibiting long time simulations on near-term hardware. Fast-forwarding can be applied to commuting time-dependent Hamiltonians of the form $f(t) \cdot H$ as well; in this case, after learning $e^{-iH\Delta\tau} = WDW^\dagger$ with a small $\Delta\tau$, we use $\exp(-iH\int_0^t f dt') = WD^{\tau(t)/\Delta\tau}W^\dagger$, where $\tau(t) = \int_0^t f dt'$ and $\Delta\tau = \tau(\Delta t)$.

This low-depth algorithm, called variational fast-forwarding [56], lies at an exciting intersection of machine learning and quantum simulation and is a promising approach in the burgeoning field of variational quantum simulation [57–68]. Variational fast-forwarding has been demonstrated on $1 + 1$ qubits [56]. Refinements of variational fast-forwarding for simulating a given fixed initial state [67] and for learning the spectral decomposition of a given Hamiltonian [68] have also been proposed. It is important to note that the unitary being diagonalized need not already be known. Therefore, variational unitary diagonalization could also be used to perform a “black box diagonalization” of the dynamics of an unknown experimental system. Thus, this approach provides an algorithmic tool for probing dynamics in an experimental setting.

In this work, we use `ibmq_bogota` to demonstrate the successful learning of a spectral decomposition on $2 + 2$ qubits. Specifically, we diagonalize the short time evolution unitary for an Ising spin chain. After only 16 steps of training by gradient descent, the spectral decomposition is used to fast forward the evolution of the Ising model, resulting in a dramatic reduction of simulation error compared with Trotterized Hamiltonian simulation and a significant ($\approx 10\times$) increase in the effective quantum volume of the simulation. Information

TABLE I. Ising model parameters.

	Parameter	Value
N	Number spins	2
Δt	Short evolution time	0.2
J	Exchange energy	1
B	Transverse field	1

about the qubits used in the experiment are provided in Appendix A.

II. METHODS

A. Learning task

We demonstrate the variational learning of the spectral decomposition of a unitary by learning a diagonalization of the short-time evolution operator of the two-spin Ising model

$$H = J \sum_{i=1} Z_i Z_{i+1} + B \sum_{i=1,2} X_i. \quad (1)$$

Here J quantifies the exchange energy, B is the transverse field strength, and Z_i and X_i are Pauli operators on the i th qubit. We approximate the short-time evolution $\exp(-iH\Delta t)$ of the spin chain using a two-step, second-order Trotter approximation; that is, we take

$$U = \left[\prod_i R_x(\theta_B)_i \times \prod_i R_{zz}(\theta_J)_{i,i+1} \times \prod_i R_x(\theta_B)_i \right]^2, \quad (2)$$

where $\theta_B = B\Delta t/2$ and $\theta_J = J\Delta t$. The simulated Ising model parameters are listed in Table I. The specific circuit we used for U is shown in Fig. 1.

B. Ansatz

To learn the spectral decomposition of U , we variationally compile it to a unitary with a structure of the form

$$V(\theta, \gamma) = W(\theta)D(\gamma)W(\theta)^\dagger, \quad (3)$$

where W is an arbitrary unitary, D is a diagonal matrix, and θ and γ are vectors of parameters. After successful training, D will capture the eigenvalues of U , and W will capture the rotation matrix from the computational basis to the eigenbasis of U .

The parameterized circuits we used as ansatzes for the diagonal unitary D and basis transformation W are shown in Fig. 2. A general diagonal unitary $D \in \text{SU}(2^n)$ on n qubits contains $2^n - 1$ variational parameters. In our experiment, we implement a two-qubit version of this exact D containing three variables. In general, an arbitrary unitary W can be constructed from any general n -qubit parameterized quantum circuit with $\text{poly}(n)$ variables. The expressive power of different options has been investigated in Refs. [69,70]. The two-qubit circuit we use to implement the arbitrary unitary W consists of three layers of X , Y rotations and phase gates on each qubit, separated by two CNOT gates.

FIG. 1. Circuit for the short-time evolution of the Ising model. The boxes indicate individual Trotter steps. Here $R_x(\theta) = e^{-i\theta X/2}$ is a single-qubit Pauli X rotation, $P(\gamma) = \text{diag}(1, e^{i\gamma})$ is a single-qubit phase gate, and $R_{zz}(\theta) = e^{-i\theta Z \otimes Z/2}$ is a two-qubit diagonal unitary.

C. Cost function

To compile the target unitary into a diagonal form, we use the local Hilbert-Schmidt test cost function defined in Ref. [38], which can be written as

$$C = 1 - \frac{1}{n} \sum_{i=1}^n \text{Pr}(00)_{A_i, B_i}, \quad (4)$$

where $\text{Pr}(00)_{A_i, B_i}$ is the probability of observing outcome 00 on the pair of qubits (A_i, B_i) from registers A and B ; see Fig. 3.

The probabilities $\{\text{Pr}(00)_{A_i, B_i}\}_{i=1}^n$ are measures of the entanglement fidelity of the unitary channel $UV^\dagger$ with $V = WDW^\dagger$. As a result, this cost is faithful, vanishing if and only if the diagonalization $WDW^\dagger$ matches the target unitary U (up to a global phase). Furthermore, the cost is operationally meaningful for nonzero values in virtue of upper bounding the average gate fidelity between U and V . Hence, a small value of C guarantees that the diagonalization $WDW^\dagger$ is an accurate approximation of the target unitary U . We note that the cost (4) involves only local measures and hence mitigates trainability issues associated with barren plateaus [71–82]. For learning a 4×4 unitary matrix,

$$C = 1 - \frac{1}{2} [\text{Pr}(00)_{1,2} + \text{Pr}(00)_{3,4}], \quad (5)$$

where $\text{Pr}(00)_{1,2}$ and $\text{Pr}(00)_{3,4}$ are the 00-state probabilities measured after running the circuits shown in Figs. 4(a) and 4(b), respectively. For more details on the cost function, see Ref. [38].

D. Training

The parameters $(\theta_1, \dots, \theta_{18}, \gamma_1, \dots, \gamma_3)$ are initialized to minimize the cost (5) with the exchange energy J in (1) set

to zero, which can be simulated efficiently and solved exactly. This procedure reduces the chance of the optimization leading to a local but not global minimum of the cost, as C is not convex.

The circuits are trained to minimize the cost using gradient descent. At each step of the training, we measure the cost and gradients $\frac{\partial C}{\partial \theta_k}$ and $\frac{\partial C}{\partial \gamma_l}$ at a particular point (θ, γ) in the parameter space and use this to update (θ, γ) according to

$$\theta_k \leftarrow \theta_k - \eta \frac{\partial C}{\partial \theta_k}, \quad (6)$$

$$\gamma_l \leftarrow \gamma_l - \eta \frac{\partial C}{\partial \gamma_l}, \quad (7)$$

where η is the learning rate. The gradients $\frac{\partial C}{\partial \theta_k}$ and $\frac{\partial C}{\partial \gamma_l}$ are measured using the parameter shift rule derived in Ref. [56]. In each optimization step, the 21 components of the gradient are measured, requiring the measurement of 156 distinct circuits. For each cost evaluation, we took 8000 measurement shots, close to the maximum supported by the back end without incurring additional circuit overhead.

The learning rate was decreased as the optimization progressed according to the schedule

$$\eta(j) = \frac{\eta_0}{[1 + (j/\delta)]^\kappa}, \quad (8)$$

where $j \in \{0, 1, 2, \dots, 16\}$ is the optimization step number. The hyperparameters $\eta_0 = 1.1$, $\kappa = 0.5$, and $\delta = 12$ were optimized by classical simulation. Additional details about the training are provided in Appendix B.

FIG. 2. Ansatz circuits. Implemented circuits for the diagonal unitary D and basis transformation W . Here $R_{zz}(\gamma) = e^{-i\gamma Z \otimes Z/2}$ is a two-qubit diagonal unitary and $P(\gamma) = \text{diag}(1, e^{i\gamma})$ is a single-qubit phase gate. D contains three variational parameters. W has three layers and 18 variational parameters.

FIG. 3. Circuit for the learning of U by a variational circuit V . The input U can be known to the user and provided in the form of an efficient circuit construction, or unknown but provided by another algorithm. Measurements are performed on pairs of qubits (A_i, B_i) from registers A and B .

III. RESULTS

To assess the quality of the optimization, the parameters found at each step of the training were used to evaluate C both on the quantum computer and classically. The results are shown in Fig. 5. The classical cost, which we call the noise-free or *ideal* cost, reflects the true accuracy of the optimized circuits. We successfully reduced the raw cost to 0.110 corresponding to an ideal cost of 0.013. The raw cost from the quantum computer is higher than the ideal cost because of gate errors.

The inset of Fig. 5 confirms that the errors in D and $WDW^\dagger$ are both iteratively reduced as the cost is trained. Here the Frobenius distance between U and V is plotted, minimized over the arbitrary global phase $e^{i\varphi}$. The ideal and learned diagonals are also compared, accounting for the global phase $e^{i\varphi}$ and for a possible reordering, specified by a permutation matrix χ . Specifically, we plot the Frobenius distance $\min_{\varphi, \chi} \|D_{\text{exact}} - e^{i\varphi} \chi D \chi^\dagger\|$, where D_{exact} is a diagonal matrix with $\{\lambda_i^{\text{exact}}\}$, the ordered exact spectrum of U , along

FIG. 4. Cost function circuit. Circuits to learn the spectral decomposition $WDW^\dagger$ of a two-qubit unitary U on a four-qubit chain. Each cost function and gradient evaluation requires the estimation of $\text{Pr}(00)_{1,2}$ and $\text{Pr}(00)_{3,4}$, obtained by measuring the qubits in the dashed boxes of panels (a) and (b).

FIG. 5. Training curves. In the main plot, we show the cost as a function of the iteration step during training. The blue curve is the measured cost function C and the green curve is its noise-free “ideal” value. In the inset, the yellow curve indicates the total error in the learned unitary defined as Frobenius distances between U and V minimized over a global phase $e^{i\varphi}$, i.e., the quantity $\min_{\varphi, \chi} \|U - e^{i\varphi} V\|$. The red curve indicates the eigenvalue error, defined as the Frobenius distance between the learned and exact diagonal also minimized over a permutation χ , i.e., $\min_{\varphi, \chi} \|D_{\text{exact}} - e^{i\varphi} \chi D \chi^\dagger\|$.

the diagonal. This is equivalent to the sum of the eigenvalue errors $\sum_i |\lambda_i^{\text{exact}} - \lambda_i e^{i\varphi_{\text{opt}}}|^2$, where $\{\lambda_i\}$ is the ordered learned spectrum and φ_{opt} accounts for the global phase shift.

It is also interesting to monitor the training by using the measured gradient $\mathbf{g}_{\text{meas}}$ at each step to calculate the angle between $\mathbf{g}_{\text{meas}}$ and the exact gradient simulated classically. This is plotted in Appendix B. The data confirm that the optimization is correctly moving downhill in the cost function landscape.

Having learned the spectral decomposition, we use the result to fast forward the Hamiltonian simulation of the Ising model (1) for two spins on ibmq_bogota. In this experiment, we prepare an initial state $|+\rangle^{\otimes 2}$ and propagate it forward in time by both Trotterization and variational fast forwarding (with back-end circuit optimization disabled in both cases). The Trotterized evolution at times $t = K\Delta t$ is obtained by applying $K = 0, 8, 16, \dots, 96$ consecutive Trotter steps from Fig. 1. After each step, we experimentally measure the fidelity of the Trotterized evolution with the perfect evolution $e^{-iHt}|+\rangle^{\otimes 2}$, which contains no Trotter error. The variational fast-forwarding evolution at time t is obtained by applying the optimized variational circuits for $W^\dagger$, D , and W to $|+\rangle^{\otimes 2}$, but with D 's parameters $(\gamma_1, \gamma_2, \gamma_3)$ changed to

$$(\gamma_1, \gamma_2, \gamma_3) \frac{t}{\Delta t}. \quad (9)$$

The state fidelity with perfect evolution $e^{-iHt}|+\rangle^{\otimes 2}$ is also measured in this case. The results for this experimental fast forwarding and experimental Trotter simulation are indicated by the green and blue solid lines respectively in Fig. 6.

We compare the experimental fast forwarding to the ideal classical fast forwarding by also measuring the noise-free fidelities obtained by classical simulation. In this ideal

FIG. 6. Demonstration of variational fast forwarding. The plot shows the measured state fidelity vs evolution time. The data (circles) are obtained at multiples of $8 \Delta t$, out to $t = 19.2$.

simulation, the initial state $|+\rangle^{\otimes 2}$ is prepared perfectly and the Trotterized evolution includes Trotter errors but no gate errors. The measurement is also assumed to be ideal. The fidelities of these ideal simulations are indicated by the dashed lines in Fig. 6.

The ideal Trotterized evolution is nearly perfect in Fig. 6 due to the small value of Δt and use of a second-order Trotter step. The ideal variational fast-forwarding evolution is less accurate, due to the imperfect learning of U 's spectral decomposition (because noise during the learning prevents even the ideal cost, the green curve in Fig. 5, to reach zero). However, the real data taken on `ibmq_bogota` exhibit the opposite behavior: Whereas the variational fast-forwarding evolution is only slightly degraded by gate errors—because the circuit depth is independent of t —the Trotterized evolution quickly loses fidelity. Namely, while the fidelity of the variationally fast-forwarded simulation remains above 0.7 for all 20 times steps, the fidelity of the Trotterized simulation is less than 0.4 after only six times steps. Thus, Fig. 6 demonstrates a striking example of fast forwarding as well as provides further evidence that the spectral decomposition of U has been well learned.

In conclusion, we have experimentally demonstrated the entanglement-enhanced quantum learning of a 4×4 unitary using a diagonal ansatz containing a total of six CNOTs and 21 variational parameters. A single input-output pair was used for training compared to the $2^2 = 4$ input-output pairs necessary for training without entangling ancillas. We both learn the unitary and its spectral decomposition, enabling the fast forwarding of an Ising model. This four-qubit experiment took 8000 shots for each of the 156 independent circuit evaluations, at each of the 16 steps of the optimization algorithm, for a total of ≈ 2500 distinct circuit implementations. It is among the most complex quantum machine learning demonstrations

FIG. 7. Layout of IBM Q device `ibmq_bogota`. In this work, we use qubits Q_0 , Q_1 , Q_2 , and Q_3 for the training and qubits Q_1 and Q_2 for the Trotter and VFF comparison.

TABLE II. Calibration data provided by IBM Q for the `ibmq_bogota` chip during the period of data acquisition.

Qubit	T_1 (μs)	T_2 (μs)	SPAM error ϵ	U_2 error
Q_0	136.6	178.0	0.056	3.70×10^{-4}
Q_1	132.3	117.4	0.045	2.01×10^{-4}
Q_2	65.4	132.4	0.024	2.48×10^{-4}
Q_3	103.6	158.3	0.020	4.74×10^{-4}
CNOT gates				CNOT error
CNOT _{0,1}		CNOT _{1,0}		1.04×10^{-3}
CNOT _{1,2}		CNOT _{2,1}		8.12×10^{-3}
CNOT _{2,3}		CNOT _{3,2}		3.81×10^{-2}

to date [14–20] and constitutes an important primitive in experimental quantum information science.

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FIG. 8. (a) Learning rate vs optimization step during training by gradient descent. This rate obeys $\eta(j) = \eta_0 / [1 + (j/\delta)]^\kappa$, where $j \in \{0, 1, 2, \dots, 16\}$ is the optimization step number and the hyperparameters $\eta_0 = 1.1$, $\kappa = 0.5$, and $\delta = 12$ were optimized by classical simulation. (b) Error in the measured gradient direction during training. Here we plot the angle between gradient measured on `ibmq_bogota` during training, and the true gradient calculated classically for the same set of parameters, for each optimization step.

APPENDIX A: QUBITS

Data were taken on the IBM Q processor `ibmq_bogota` using the BPQ software package developed by Geller and colleagues. BPQ is a PYTHON package developed to design, run, and analyze complex quantum computing and quantum information experiments using commercial back ends. We demonstrate the learning of a spectral decomposition using the qubits shown in Fig. 7. Calibration data supplied by the back end are summarized in Tables II(a) and II(b).

Here $T_{1,2}$ are the standard Markovian decoherence times, and

$$\epsilon = \frac{T(0|1) + T(1|0)}{2} \quad (\text{A1})$$

is the single-qubit state-preparation and measurement (SPAM) error, averaged over initial states. The U_2 error column gives the single-qubit gate error measured by randomized benchmarking. The CNOT errors are also measured by randomized benchmarking.

APPENDIX B: TRAINING

The variational circuits for W and D were trained by gradient descent

$$\begin{aligned} \theta_k &\leftarrow \theta_k - \eta \frac{\partial C_{\text{LHST}}}{\partial \theta_k} \\ \gamma_l &\leftarrow \gamma_l - \eta \frac{\partial C_{\text{LHST}}}{\partial \gamma_l}, \end{aligned} \quad (\text{B1})$$

where θ_k and γ_l are the variational parameters for the W and D circuits, respectively, and η is the learning rate. We used the variable learning rate plotted in Fig. 8(a), which was optimized by classical simulation. At each step of the training, we measure the cost C_{LHST} and gradients $\partial C_{\text{LHST}}/\partial \theta_k$ and $\partial C_{\text{LHST}}/\partial \gamma_l$ at a particular point $(\theta_1, \dots, \theta_{18}, \gamma_1, \dots, \gamma_3)$ in parameter space, and use this to update $(\theta_1, \dots, \theta_{18}, \gamma_1, \dots, \gamma_3)$ according to (B1). We also calculate the angle between the measured gradient and the exact gradient simulated classically, which is plotted in Fig. 8(b). These data show that the measured gradient is correctly pointing uphill until the end of the training when a local minimum is reached and the gradient becomes small and noisy.

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