Estimating the degree of non-Markovianity using quantum machine learning

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Several applications of machine learning in quantum physics encompass a measurement upon the quantum system followed by the training of the machine learning model with the measurement outcomes. However, recently developed quantum machine learning models, such as variational quantum circuits (VQCs), can be implemented directly on the state of the quantum system (quantum data). Here, we propose to use a qubit as a probe to estimate the degree of non-Markovianity of the environment. Using VQCs, we find an optimal sequence of interactions of the qubit with the environment to estimate, with high precision, the degree of non-Markovianity for the phase damping and amplitude damping channels. This work contributes to practical quantum applications of VQCs and delivers a feasible experimental procedure to estimate the degree of non-Markovianity.

I. INTRODUCTION

The last few years have seen a tremendous advance in using machine learning (ML) techniques for analyzing data in a wide variety of fields. Quantum physics has also benefited from ML in various aspects such as control of quantum systems, classification and estimation tasks [1-6]. In such cases, ML techniques have been used to analyze classical data, obtained from measuring quantum systems. On the other hand, considerable research has been done to take advantage of the quantum properties to improve machine learning techniques [7, 8]. Development of quantum artificial neural networks [9] and quantum kernel methods [10] are examples of which.

Towards quantum machine learning algorithms, learning circuits have proved to be a practical approach [11]. Considering the currently available noisy intermediate-scale quantum computers [12] with few qubits (50-100 qubits), hybrid quantum-classical algorithms have been designed to develop short-depth quantum circuits with free control parameters. These circuits have been termed as variational quantum circuits (VQCs) [13-16]. In VQCs, the optimization task is done over quantum (free parameters in the quantum circuit) and classical parameters (used in postprocessing) using classical optimization techniques [13].

One of the main obstacles in quantum technologies is the interaction of the quantum system with its surrounding environment which results in the loss of coherence of the quantum system [17]. Simplifications are generally imposed on the physical processes. For instance, the so-called Markovian approximation, in which it is assumed that the evolution of the system does not depend on the history of its dynamics, but only on its current state. Thus, memory aspects are ignored which, in many cases, works as a good approximation.

However, it is important to emphasize that non-Markovian signatures frequently appear in the dynamics of quantum systems [18, 19]. Furthermore, some physical processes are strongly subjected to non-Markovianity, such as reservoir engineering [20, 21], state teleportation [22], quantum metrology [23], and even current quantum computers [24, 25]. Moreover, non-Markovianity can be harnessed as a resource [26].

Accurate determination of the degree of non-Markovianity requires a large number of measurements. Moreover, for the measure of non-Markovianity based on entanglement dynamics, an ancillary qubit, protected from the interactions with the environment, needs to be considered. In order to surpass these challenges, ML techniques such as neural networks [27], support vector machines [28], random forest regressor [29], tensor network-based machine learning [30], and polynomial regression [31] have been used to determine the degree of non-Markovianity of a quantum process. In addition, it has been shown that quantum circuits can be used to simulate non-Markovian dynamics [32, 33] which is an important advance in the study of realistic sit-
oscillators, given by the Hamiltonian

\[ H = \omega_0 \sigma_+ \sigma_- + \sum_k \omega_k a_k^\dagger a_k + \sum_k (g_k \sigma_+ a_k + g_k \sigma_- a_k^\dagger). \]  

(1)

where \( \lambda \approx 1/\tau_r \) with \( \tau_r \) being the environment correlation time, \( \gamma_0 \approx 1/\tau_s \) where \( \tau_s \) is the typical time scale of the system.

The dynamics of the qubit that is coupled resonantly with the environment can be expressed as

\[ \rho(t) = \sum_{i=0}^{1} M_i(t)\rho(0)M_i^\dagger(t), \]  

(3)

where the Kraus operators are given by

\[ M_0(t) = |0\rangle\langle 0| + \sqrt{p(t)}|1\rangle\langle 1|, \]  

(4)

\[ M_1(t) = \sqrt{1 - p(t)}|0\rangle\langle 1|, \]  

(5)

in which

\[ p(t) = e^{-\lambda t} \left( \frac{\lambda}{d} \sinh(dt/2) + \cosh(dt/2) \right)^2, \]  

(6)

with \( d = \sqrt{\lambda^2 - 2\gamma_0 \lambda} \). The dynamics is known to be non-Markovian in the strong coupling regime \( \lambda < 2\gamma_0 \) (\( \tau_s < 2\tau_r \)).

The AD process can be simulated for a general scenario with a quantum circuit via an ancilla qubit. After tracing out the ancilla qubit we obtain the desired mixed state. In this circuit, the angle \( \theta_a \) is given by

\[ \theta_a = 2 \arccos \left( \sqrt{p(t)} \right), \]  

(7)

where \( p(t) \) is given in Eq. (6).

B. Phase damping

For the phase damping (PD) channel, following Ref. [10], we consider a qubit undergoing decoherence induced by a colored noise given by the time

\[ J(\omega) = \frac{1}{2\pi} \frac{\gamma_0 \lambda^2}{(\omega_0 - \omega)^2 + \lambda^2}, \]  

(2)

Here, \( \sigma_+ = \sigma_+^\dagger = |1\rangle\langle 0| \) with \( |1\rangle \) \( (|0\rangle) \) corresponding to the excited (ground) state of the qubit with transition frequency \( \omega_0 \), \( a_k(a_k^\dagger) \) is the annihilation (creation) operator of the \( k \)-th mode of the bath with frequency \( \omega_k \), and \( g_k \) is the coupling between the qubit and the \( k \)-th mode. We assume that the bath has a Lorentzian spectral density

In the present work, we show that the degree of non-Markovianity of a quantum process can be estimated directly from the measurements performed on the qubit. Using VQCs, through supervised learning, we find an optimal sequence of interactions of the qubit with the environment to estimate the degree of non-Markovianity, with high precision, for amplitude damping and phase damping channels. We will assume that we know the type of the dominant decoherence process that the qubit undergoes, and the range of the parameters defining the Markovianity or non-Markovianity of the process.

The remainder of this paper is organized as follows. In Sec. II we provide the theoretical framework for the open quantum dynamics and non-Markovianity. Section III contains a brief description of variational quantum circuits. In Sec. IV we focus on the estimation of the degree of non-Markovianity of the process. We conclude the paper in Sec. V.

II. OPEN QUANTUM SYSTEM DYNAMICS

In what follows, we describe two paradigmatic mechanisms for simulating open quantum systems, namely amplitude damping and phase damping.

A. Amplitude damping

For the amplitude damping (AD) channel, we consider a qubit interacting with a bath of harmonic oscillators, given by the Hamiltonian \((\hbar = 1)\) \[34, 35\]

\[ H = \omega_0 \sigma_+ \sigma_- + \sum_k \omega_k a_k^\dagger a_k + \sum_k (g_k \sigma_+ a_k + g_k \sigma_- a_k^\dagger). \]  

Here, \( \sigma_+ = \sigma_+^\dagger = |1\rangle\langle 0| \) with \( |1\rangle \) \( (|0\rangle) \) corresponding to the excited (ground) state of the qubit with transition frequency \( \omega_0 \), \( a_k(a_k^\dagger) \) is the annihilation (creation) operator of the \( k \)-th mode of the bath with frequency \( \omega_k \), and \( g_k \) is the coupling between the qubit and the \( k \)-th mode. We assume that the bath has a Lorentzian spectral density

\[ J(\omega) = \frac{1}{2\pi} \frac{\gamma_0 \lambda^2}{(\omega_0 - \omega)^2 + \lambda^2}, \]  

where \( \lambda \approx 1/\tau_r \) with \( \tau_r \) being the environment correlation time, \( \gamma_0 \approx 1/\tau_s \) where \( \tau_s \) is the typical time scale of the system.

The dynamics of the qubit that is coupled resonantly with the environment can be expressed as

\[ \rho(t) = \sum_{i=0}^{1} M_i(t)\rho(0)M_i^\dagger(t), \]  

(3)

where the Kraus operators are given by \[32, 36\]

\[ M_0(t) = |0\rangle\langle 0| + \sqrt{p(t)}|1\rangle\langle 1|, \]  

(4)

\[ M_1(t) = \sqrt{1 - p(t)}|0\rangle\langle 1|, \]  

(5)

in which

\[ p(t) = e^{-\lambda t} \left( \frac{\lambda}{d} \sinh(dt/2) + \cosh(dt/2) \right)^2, \]  

(6)

with \( d = \sqrt{\lambda^2 - 2\gamma_0 \lambda} \). The dynamics is known to be non-Markovian in the strong coupling regime \( \lambda < 2\gamma_0 \) (\( \tau_s < 2\tau_r \)).

The AD process can be simulated for a general scenario with a quantum circuit via an ancilla qubit \[32, 36\]. After tracing out the ancilla qubit we obtain the desired mixed state. In this circuit, the angle \( \theta_a \) is given by \[32, 36\]

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(7)

where \( p(t) \) is given in Eq. (6).

B. Phase damping

For the phase damping (PD) channel, following Ref. [10], we consider a qubit undergoing decoherence induced by a colored noise given by the time
FIG. 1. Amplitude damping (AD): (a) The expectation value of the Pauli operator $\sigma_z$ versus $\gamma_0 t$ for a range of values of $\lambda/\gamma_0$. (b) Evolution of the Bloch vector. The qubit is initialized to $|0\rangle + |1\rangle/\sqrt{2}$ and undergoes AD with $\lambda/\gamma_0 = 0.25$. The Bloch vectors shown are at $\gamma_0 t = 0$ (green), $\gamma_0 t = 2.5$ (blue), $\gamma_0 t = 5$ (red), $\gamma_0 t = 10$ (cyan). The Bloch sphere is plotted using qutip [41]. (c) Quantum circuit for simulating AD.

Kraus operators [40]

\[ M_0(t) = \sqrt{\frac{1 + \Lambda(t)}{2}} I, \]
\[ M_1(t) = \sqrt{\frac{1 - \Lambda(t)}{2}} \sigma_z, \]

where

\[ \Lambda(t) = e^{-t/(2\tau)} \left[ \cos\left(\frac{\mu t}{2\tau}\right) + \frac{1}{\mu} \sin\left(\frac{\mu t}{2\tau}\right) \right], \]

with $\mu = \sqrt{(4\alpha\tau)^2 - 1}$, and $I$ being the identity matrix.

For $\alpha\tau > 1/4$ the dynamics is non-Markovian, while for $\alpha\tau < 1/4$ it is Markovian (see Fig. 2(a)). We note that, in a PD channel, the off diagonal elements of the density matrix decay exponentially as depicted in Fig. 2(a). We remind that $\langle \sigma_x \rangle = \Sigma_{i\neq j} \rho_{ij}$. Figure 2(b) shows the evolution of the Bloch vector initialized along the $x$ axis. For such initialization, after sufficiently long time, the vector length decays to zero. In other words, the probability of qubit states ($|0\rangle$ and $|1\rangle$) is conserved but the phase information between them is lost. Phase damping is also known as transverse relaxation. Examples of systems that undergo this type of decoherence are nitrogen-vacancy center due to its interaction with lattice vibrations and surrounding nuclear spins [42, 43], and superconducting qubits under low-frequency noise [44].

The PD channel can be simulated using a quantum circuit, shown in Fig. 2(c) [36]. In this circuit, the Hadamard gate prepares the qubit into the superposition state and the controlled $y$ rotation simulates the interaction with the environment. The angle $\theta_p$ is given by

\[ \theta_p = 2 \arccos(\Lambda(t)), \]

where $\Lambda(t)$ is given in Eq. (11).

C. Non-markovianity measure

Several measures of non-Markovianity have been introduced [45, 49]. In this work, we consider the measure based on entanglement dynamics of a bipartite quantum state, the system and an ancilla that is isolated from the environment [45]. It is worth noticing that this ancilla only serves the purpose of quantifying non-Markovianity and it is not implemented in the quantum circuits, in contrast to

\[ H(t) = \Gamma(t) \sigma_z. \]

Here, $\Gamma(t)$ is a random variable which obeys the statistics of a random telegraph signal defined as $\Gamma(t) = \alpha(-1)^{n(t)}$, where $\alpha$ is the coupling between the qubit and the external influences, $n(t)$ is a random variable with Poisson distribution with mean $t/(2\tau)$, and $\sigma_z$ is the Pauli $z$ operator. In this case, the dynamics of the qubit is given by the following dependent Hamiltonian ($\hbar = 1$)
FIG. 2. Phase damping (PD): (a) The expectation value of the Pauli operator $\sigma_x$ versus $\alpha t$ for a range of values of $\alpha t$. (b) Evolution of the Bloch vector. The qubit is initialized to $(|0\rangle + |1\rangle)/\sqrt{2}$ and undergoes PD with $\alpha t = 0$ (green), $\alpha t = 1$ (blue), and $\alpha t = 5$ (red). (c) Quantum circuit for simulating PD.

A monotonic decrease in the entanglement of the bipartite system implies that the dynamics is Markovian. An increase in the entanglement during the evolution is a result of memory effects and thus non-Markovianity. The measure can be calculated as

$$N = \max \int_{dE/dt > 0} \frac{dE(t)}{dt} dt,$$

(13)

where the maximization is done over all initial states and $E$ is the measure of entanglement. It has been found that the maximization is achieved for Bell states [50]. Therefore, we consider a bipartite system in a Bell state and use concurrence as the measure of entanglement [51].

In the following sections, we first briefly review VQCs. We then use VQCs to find an optimal sequence to estimate the degree of non-Markovianity of a qubit under PD and AD channels.

III. VARIATIONAL QUANTUM CIRCUIT

VQCs also known as parametrized quantum circuits (sometimes also referred to as quantum neural networks) are a type of quantum circuit with some free parameters (normally for single qubit operations) [14]. We label the free parameters of the circuit by $\phi$. In addition, we consider classical parameters, labelled by $w$, in post-processing the measurement outcomes of the quantum circuit.

The optimization of the parameters $\phi$ and $w$ can be done in a supervised manner using a set of input data, $x$, and their corresponding labels, $f_t(x)$. We aim to minimize the cost function defined as the mean square error (MSE), i.e.,

$$C(x, \phi, w) = \frac{1}{n} \sum_{i=1}^{n} (\hat{f}_{\phi, w}(x_i) - f_t(x_i))^2,$$

(14)

where $n$ is the number of input data. $\hat{f}_{\phi, w}(x)$ is the estimate of $f_t(x)$ obtained from the output of the VQC which we take as a linear combination of the measurement outcomes, $\langle M_i \rangle_{x, \phi}$, performed on the qubits, i.e.,

$$\hat{f}_{\phi, w}(x) = w_0 + \sum_{i=1}^{k} w_i \langle M_i \rangle_{x, \phi}.$$

(15)

Here, $k$ is the number of measurement outcomes performed on the circuit. The whole optimization can be done through gradient-based techniques, such as stochastic gradient descent [52], or gradient-free techniques such as Nelder-Mead method [53], or particle swarm optimization [54]. The gradient can also be calculated using the quantum circuit [55].
IV. ESTIMATION OF THE DEGREE OF NON-MARKOVIANITY

We use VQCs to estimate the degree of non-Markovianity $N$ of the dynamics of a qubit, under AD and PD channels. We consider each of these channels independently. We found that a precise estimate of $N$ can be obtained using a sequence of interactions of the qubit with the environment. Our proposed scheme is as the following: the qubit, initially in the state $|0\rangle$, is rotated along the $y$ axis with angle $\varphi_0$. Next, it interacts with the environment in a sequence of two interactions, each with time $t_i$. Each interaction is followed by a rotation along the $y$ axis with angle $\varphi_i$ ($i = 1, 2$). Finally, the qubit is measured in the Pauli $z$ basis. The estimate of $N$ is obtained as

$$\hat{N} = w_0 + w_1 \langle \sigma_z \rangle.$$  \hspace{1cm} (16)

The VQCs that we used to find the optimal values of $\varphi_i$ ($i = 0, 1, 2$), $t_j$ ($j = 1, 2$), $w_0$, and $w_1$ for AD and PD channels, are shown in Fig. 3(a) and (c), respectively. The optimal values of these parameters are found by minimizing the MSE, Eq. (14), for a range of values of the parameters $\lambda/\gamma_0$ (for AD) and $\alpha\tau$ (for PD). Each VQC consists of a qubit ($s$) and two ancillas ($a_1$ and $a_2$). Each ancilla is used to simulate the dynamics of the qubit in each of its interactions with the environment. Note that, in the experiment, only one qubit (that interacts with the environment) is required to perform this estimation task, and no operation is required to be performed on the environment.

We performed our simulations using the quantum simulator of Pennylane [56] with Adagrad optimizer [57] (see Appendix A for some details about the optimizer). In order to find the optimal values of the parameters, we generated 1000 data points (feature vectors) for each channel. The data is uniformly distributed for the parameter $\lambda/\gamma_0$ in the range [0.1,3] (for AD) and for the parameter $\alpha\tau$ in the range [0.1,0.75] (for PD). The feature vectors contain the values of the parameters $\lambda/\gamma_0$ (AD) and $\alpha\tau$ (PD) and the labels are the corresponding values of $N$ for each channel.

We used 50% of the whole data points (which are...
chosen randomly) to train the VQC for each channel. For AD channel, we obtained $7.2 \times 10^{-6}$ and for the PD channel we obtained $4.3 \times 10^{-5}$ for the MSE, testing on the whole data points. Figures 3(b) and (d) show the target (dotted red line) and the predicted values (solid blue line) of $\lambda/\gamma_0$ versus $\alpha \tau$ (for PD) respectively. For the AD channel, the predicted values are very close to the target values for the full range of $\lambda/\gamma_0$. For the PD channel, there is a small difference between the target and predicted values of $\lambda/\gamma_0$ where $\lambda/\gamma_0 = 0$.

Using only one interaction of the qubit with the environment, for the AD channel, we obtained $1 \times 10^{-4}$ for the MSE, while for the PD channel, we were not able to obtain a good estimate of $\lambda/\gamma_0$. A single interaction of the qubit with the environment is a nonlinear mapping from the characteristic parameter of the environment ($\lambda/\gamma_0$ for AD and $\alpha \tau$ for PD) to the state of the qubit, which is measured by $\langle \sigma_z \rangle$. For the case of AD, one interaction (with a properly chosen interaction time) is sufficient to obtain a good estimate of $\lambda/\gamma_0$, while for the case of PD, only one interaction is not sufficient. After the first interaction with the environment, each value of the characteristic parameter is mapped to a different Bloch vector, from which the nonlinear mapping of the second interaction gives $\lambda/\gamma_0$ with high precision. It is worth mentioning that, for the case of PD, we did not obtain a significant decrease in MSE by increasing the number of interactions of the qubit with the environment (up to 5 interactions).

V. CONCLUSIONS

In summary, we proposed an experimentally feasible scheme to estimate the degree of non-Markovianity based on entanglement dynamics for phase damping and amplitude damping channels. We assumed that we know the type of decoherence channel and the range of characteristic parameters of the channel that determine the non-Markovianity of the process. In contrast to previous works, here we took advantage of the quantum nature of the problem, and used a variational quantum circuit, through supervised learning, for this estimation task. We found an optimal sequence of interactions of the qubit with the environment to obtain an accurate estimate of the degree of non-Markovianity of its dynamics from measurement outcomes with minimal classical post-processing.

It is important to emphasize that this work presents a new strategy on how to estimate non-Markovianity using quantum machine learning. Naturally, it can be used for other quantum channels, considering different spectral densities, or phase covariant noise, which contains both amplitude damping and phase damping simultaneously [58, 59]. Our focus here is to present the procedure, and other studies considering different dissipative processes will be left for future work.

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Appendix A: Adagrad optimizer

In this appendix we give some details about the optimizer that we have used in our simulations. Adagrad is a variation of the gradient descent (GD) optimizer. In the GD algorithm the parameters, labelled by $\varphi$ here, are updated in the opposite direction of the gradient of the cost function $C(\varphi)$ [60]. In other words, for every parameter $\varphi_i$ at each time step $t$ the update rule can be written as

$$\varphi_{t+1,i} = \varphi_{t,i} - \eta \nabla \varphi_i C(\varphi_{t,i}), \quad (A1)$$

where $\eta$ is the learning rate. Note that, $\eta$ is the same for every parameter $\varphi_i$.

In Adagrad a different learning rate is used for every parameter $\varphi_i$ at every time step [60]. In the update rule for Adagrad, the learning rate at each time step $t$ for every parameter $\varphi_i$ is based on the past gradients that have been calculated for $\varphi_i$ [60]

$$\varphi_{t+1,i} = \varphi_{t,i} - \frac{\eta}{\sqrt{G_{t,ii}} + \varepsilon} \nabla \varphi_i C(\varphi_{t,i}). \quad (A2)$$

Here, $G_t$ is a diagonal matrix where each diagonal element of which, $G_{t,ii}$, is the sum of the squares of the gradients with respect to $\varphi_i$ up to time step $t$, and $\varepsilon$ is for avoiding division by zero.
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