Estimating the degree of non-Markovianity using variational quantum circuits

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Received: 18 January 2023 / Accepted: 21 June 2023 © The Author(s), under exclusive licence to Springer Nature Switzerland AG 2023

Abstract
Several applications of quantum machine learning (QML) rely on a quantum measurement followed by training algorithms using the measurement outcomes. However, recently developed QML 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 qubit-environment interactions that yield accurate estimations of the degree of non-Markovianity for the amplitude damping, phase damping, and the combination of both models. This work contributes to practical quantum applications of VQCs and delivers a feasible experimental procedure to estimate the degree of non-Markovianity.

Keywords Quantum machine learning · Variational quantum circuit · Decoherence · Non-Markovianity

1 Introduction
The last few years have seen a tremendous advance in 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 (Dunjko et al. 2018; Sarma et al. 2019; Fosel et al. 2018; Bukov et al. 2018), classification and estimation tasks (Palmieri et al. 2021; Papic et al. 2022), and quantum circuit compilation (Acampora et al. 2021; Zhang et al. 2020). 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 (Schuld et al. 2015; Biamonte et al. 2017). The development of quantum artificial neural networks (Beer et al. 2020) and quantum kernel methods (Schuld 2021) are examples of this.

Towards quantum machine learning algorithms, learning circuits have proved to be a practical approach (Mitarai et al. 2018). Considering the currently available noisy intermediate-scale quantum computers (Preskill 2018) 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) (McClean et al. 2016; Benedetti 2019; Cerezo et al. 2021; Bharti et al. 2022). 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 (McClean et al. 2016).

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 (Breuer and Petruccione 2007). 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 often works as a good approximation.
However, it is important to emphasize that non-Markovian signatures frequently appear in the dynamics of quantum systems (Breuer et al. 2016; De Vega et al. 2017). In recent years, non-Markovianity has been considered as a resource rather than noise (Berk et al. 2021; Li et al. 2020). Control of a non-Markovian dynamics can be harnessed for state teleportation (Laine et al. 2014), quantum key distribution (Vasile et al. 2011), quantum communication (Bylicka et al. 2014), quantum metrology (Chin et al. 2012), and quantum control (Reich et al. 2015). Even more, current quantum computers experience non-Markovianity (Morris et al. 2019; White et al. 2020).

In the present work, we show that the degree of quantum non-Markovianity can be estimated directly from measurements performed on the qubit. Using VQCs, through supervised learning, we find an optimal sequence of qubit-environment interactions to estimate the degree of non-Markovianity, reaching high precision. We apply this methodology to the paradigmatic amplitude and phase damping channels and the combination of both. For these damping channels, we will use exactly solvable models that provide a theoretical framework and parameter range to characterize non-Markovianity.

The remainder of this paper is organized as follows. In Sec. 2, we provide the theoretical framework for the open quantum dynamics and non-Markovianity. Section 3 contains a brief description of variational quantum circuits. In Sec. 4, we focus on the estimation of the degree of non-Markovianity of the quantum processes. We conclude the paper in Sec. 5.

## 2 Open quantum system dynamics

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

### 2.1 Amplitude damping

For the amplitude damping (AD) channel, we consider a qubit interacting with a bath of harmonic oscillators, given by the Hamiltonian ($\hbar = 1$) (Haikka et al. 2010; Whalen et al. 2016)

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

(1)

Where $\sigma_x = \sigma_x^\dagger = |1\rangle \langle 0| + |0\rangle \langle 1|$ 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

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

(2)

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

The evolved density matrix for the AD channel can be expressed as follows (super index $a$ refers to amplitude):

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

(3)

where the Kraus operators are given by (Nielsen et al. 2000; García-Perez et al. 2020)

\[
K_0^{(a)}(t) = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{p_a(t)} \end{pmatrix},
K_1^{(a)}(t) = \begin{pmatrix} 0 & \sqrt{1 - p_a(t)} \\ 0 & 0 \end{pmatrix}
\]

(4)

in which (Bellomo et al. 2007)

\[
p_a(t) = e^{-\lambda t} \left[ \frac{\lambda}{d} \sin \left( \frac{dt}{2} \right) + \cos \left( \frac{dt}{2} \right) \right]^2,
\]

(5)

with $d = \sqrt{2\gamma_0 \lambda - \lambda^2}$. The dynamics is known to be non-Markovian in the strong coupling regime $\lambda < 2\gamma_0 (\tau_s < 2\tau_r)$ (Bellomo et al. 2007). The non-Markovianity can be evidenced in Fig. 1a by the oscillations in the expectation value of the Pauli $z$ operator. Figure 1b shows the evolution of the Bloch vector initialized along the $x$ axis. This representation of the time evolution of the state provides insights for choosing the ansatz for the VQC. For the case of AD,
as time evolves, the length of the Bloch vector becomes smaller than 1, and after sufficiently long time, the vector decays to the ground state \(|0\rangle\) recovering its full length. This type of decoherence is also known as longitudinal relaxation which plays a fundamental role in color centers in diamond and superconducting qubits in circuit QED (Blais et al. 2020).

The AD process can be simulated for a general scenario with a quantum circuit via an ancilla qubit (Nielsen et al. 2000; Garcia-Perez et al. 2020). After tracing out the ancilla qubit, we obtain the desired mixed state. Figure 1c shows the quantum circuit. The Hadamard gate prepares the qubit in the superposition state \((|0\rangle + |1\rangle) / \sqrt{2}\), while the controlled \(y\) rotation and CNOT gates simulate the interaction of the qubit with the environment. In this circuit, the angle \(\theta_a\) is given by (Nielsen et al. 2000; Garcia-Perez et al. 2020)

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

where \(p_a(t)\) is given in Eq. (5)

### 2.2 Phase damping

For the phase damping (PD) channel, following Ref. (Daffer et al. 2004), we consider a qubit undergoing decoherence induced by a colored noise given by the stochastic Hamiltonian \((\hbar = 1)\)

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

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 Kraus operators (Daffer et al. 2004; Nielsen et al. 2000) (super index \(p\) refers to phase):

\[
K_0^{(p)}(t) = \sqrt{\frac{1 + \Lambda(t)}{2}} I, \quad K_1^{(p)}(t) = \sqrt{\frac{1 - \Lambda(t)}{2}} \sigma_z,
\]

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. 2a). We note that, in a PD channel, the off diagonal elements of the density matrix decay exponentially as depicted in Fig. 2a, where only in the cases \(\alpha \tau = \{0.4, 0.7\}\) we observe oscillations. We remind that \(|\sigma_z\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle) / \sqrt{2}\) for a two-level system where \(\rho\) is the density matrix and \(|0\rangle, |1\rangle\) are the qubit states. Figure 2b 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 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...
Phase damping (PD): The expectation value of the Pauli operator $\sigma_x$ versus $\alpha t$ for a range of values of $\alpha t$. Evolution of the Bloch vector. The qubit is initialized to $|0\rangle + |1\rangle$ / $\sqrt{2}$ and undergoes PD with $\alpha t = 0.2$. The Bloch vectors shown are at $\alpha t = 0$ (green), $\alpha t = 1$ (blue), and $\alpha t = 5$ (red). Quantum circuit for simulating PD of decoherence are nitrogen-vacancy center due to its interaction with lattice vibrations (Norambuena et al. 2020) and surrounding nuclear spins (de Lange et al. 2012), and superconducting qubits under low-frequency noise (Paladino et al. 2014).

The PD channel can also be simulated using a quantum circuit, as shown in Fig. 2c (Nielsen et al. 2000). 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. (9).

### 2.3 Combined amplitude and phase damping

There are several systems where phase and amplitude damping effects are present at the same time. This generates a more complex scenario from the point of view of non-Markovianity, as explained in Ref. (Norambuena et al. 2020). Thus, in order to extend the applicability of the proposed approach, we also consider a serial concatenation of AD and PD.

The Kraus operators of this combined channel are obtained by multiplication of the Kraus operators of AD and PD channels (Wilde 2013):

$$K_k^{(ap)}(t) = K_i^{(a)}(t)K_j^{(p)}(t),$$

where $i, j = 0, 1, k$ sweeps all possible combination of $i$ and $j$, and $K_i^{(a)}$ and $K_j^{(p)}$ are given in Eqs. 4 and 8, respectively. We note that the resultant density matrix of the evolved qubit is independent of the order of AD and PD channels, i.e., $\rho^{(ap)}(t) = \rho^{(pa)}(t)$.

This combined channel can be simulated with a quantum circuit that contains two ancillae, one for PD and one for AD, with the corresponding gates for each channel acting on the qubit and each ancilla.

### 2.4 Non-Markovianity measure

Several measures of non-Markovianity have been introduced (Chruscinski 2011; Wilde 2009; Luo and Song 2012; Pollock et al. 2018; Rivas 2010). In this work, we consider the measure based on entanglement dynamics of a bipartite quantum state. This bipartite system is composed of the system and an auxiliary qubit that is isolated from the environment (Rivas 2010). It is worth noticing that this auxiliary qubit only serves the theoretical purpose of quantifying non-Markovianity and it is not implemented in the quantum circuit.

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. Using this criteria, the degree of non-Markovianity can be calculated as

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

where the maximization is done over all initial states $\rho(0)$ and $E(t)$ is the measure of entanglement where we use concurrence (Hill and Wootters 1997). It has been found that the maximization is achieved for Bell states (Neto et al. 2016). Therefore, we consider a bipartite system in a Bell state.
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, AD, and the combination of both dissipative channels.

3 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) (Benedetti 2019). We label the free quantum parameters of the circuit by $w$. In addition, we consider classical parameters, labeled by $\phi$, in post-processing the measurement outcomes of the quantum circuit.

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

$$C(x, \phi, w) = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{f}_{\phi,w}(x_i) - f_i(x_i) \right)^2,$$  \hspace{1cm} (13)

where $n$ is the number of input data. In this approach, $\hat{f}_{\phi,w}(x)$ is the estimate of $f_i(x)$ obtained from the output of the VQC.

The output $\hat{f}_{\phi,w}(x)$ is calculated as a linear combination of the measurement outcomes $\langle M_i \rangle_{x,\phi}$ (Benedetti 2019):

$$\hat{f}_{\phi,w}(x) = w_0 + \sum_{i=1}^{k} w_i \langle M_i \rangle_{x,\phi}. \hspace{1cm} (14)$$

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 (Robbins and Monro 1951) gradient-free techniques such as Nelder-Mead method (Nelder et al. 1965), or particle swarm optimization (Zhu 2019). The gradient can also be calculated using the quantum circuit (Schuld et al. 2019).

4 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 first consider each of these channels independently. We found that a precise estimate of $N$ can be obtained using a sequence of qubit-environment interactions. Our proposed scheme is the following: the qubit, initially in the state $|0\rangle$, is

rotated along the $y$ axis with angle $\phi_0$. 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 $\phi_i$ ($i = 1, 2$). Finally, the qubit is measured in the Pauli $z$ basis. The estimate of $N$ is obtained as

$$\hat{N} = w_0 + w_1 \langle \sigma_z \rangle. \hspace{1cm} (15)$$

We consider $\phi_i$ ($i = 0, 1, 2$), $t_j$ ($j = 1, 2$), $w_0$, and $w_1$ as the training parameters. The VQCs for AD and PD channels are shown in Fig. 3a and c, respectively. The optimal values of these parameters are found by minimizing the cost function, Eq. (13), 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 ancillae ($a_1$ 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 remark that the selection of this ansatz for the structure of the circuit relies on our observation of the Bloch vector as a function of the characteristic parameter of the environment, $\lambda/\gamma_0$ (for AD) and $\alpha \tau$ (for PD).

We performed our simulations using the quantum simulator of PennyLane (Bergholm et al. 2020). We used a combination of RMSprop (Hinton et al. 2012) and Adagrad optimizers (Duchi et al. 2011) (see Appendix A and Appendix B for some details about the optimizers). In order to find the optimal values of the parameters, we generated $100$ 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. The values of $N$ for each value of the characteristic parameter are calculated using Eq. (12) for a Bell state ($|0,0\rangle + |1,1\rangle$) $\sqrt{2}$ as the initial state and concurrence as the measure of the entanglement.

We used $70\%$ of the whole data points (which are chosen randomly) to train the VQC for each channel. For AD channel, we obtained $4.2 \times 10^{-6}$, and for the PD channel, we obtained $1.2 \times 10^{-5}$ for the MSE over the test data points. \footnote{For the PD channel, using $\hat{N} = \max (w_0 + w_1 \langle \sigma_z \rangle, 0)$ as the estimate of the degree of non-Markovianity, we obtained $1.7 \times 10^{-6}$ for the MSE over the test data.} Figures 3b and d show the target (dotted red line) and the predicted values (solid blue line) of $N$ versus $\lambda/\gamma_0$ (for AD) and 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 $N$ where $N = 0$.\footnote{For the PD channel, using $\hat{N} = \max (w_0 + w_1 \langle \sigma_z \rangle, 0)$ as the estimate of the degree of non-Markovianity, we obtained $1.7 \times 10^{-6}$ for the MSE over the test data.}
Fig. 3 VQCs for estimating the degree of non-Markovianity $N$ for AD channel (a) and PD channel (c). In each circuit, the system qubit ($s$) is first initialized by the rotation $R_y(\varphi_0)$. The qubit $s$ then interacts with the environment in a sequence of two interactions with time $t_i$. After each interaction, a rotation $R_y(\varphi_i)$ acts on the qubit $s$. The two ancilla qubits ($a_1$ and $a_2$) simulate the effect of the environment for each interaction, one ancilla for each interaction. In the output, the qubit $s$ is measured in $\sigma_z$ basis.

Using only one interaction of the qubit with the environment, for the AD channel, we obtained $1.7 \times 10^{-4}$ for the MSE over the test data, while for the PD channel, we were not able to obtain a good estimate of $N$. 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 with a properly chosen initial state and interaction time, the degree of non-Markovianity can be estimated well as a linear function of $\langle \sigma_z \rangle$ after only one interaction. From Fig. 1a, we can see that at about $\gamma_0 t \approx 3$, the Markovian curves (the curves with $\lambda/\gamma_0 > 2$) have similar values of $\langle \sigma_z \rangle$, while the non-Markovian curves are well separated. Therefore, $\langle \sigma_z \rangle$ versus $\lambda/\gamma_0$ has the same functional form as $N$ versus $\lambda/\gamma_0$. On the other hand, for the case of PD, Fig. 2a shows that the Markovian curves ($\alpha\tau < 1/4$) are widely separated, i.e., a large range of $\langle \sigma_z \rangle$ corresponds to $N = 0$. Thus, only one interaction can not result in a linear relation between $N$ and the expectation value of the Pauli operator. 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 $N$ with high precision.

We also considered serial concatenation of AD and PD channels. In this case, we considered $17 \times 17 = 289$ data points in the range $[0.1,3]$ for $\lambda/\gamma_0$ and $[0.1,0.75]$ for $\alpha\tau$ (17 uniformly distributed data points for each range), and defined the estimate of $N$ as

$$\hat{N} = \max (w_0 + w_1 \langle \sigma_z \rangle, 0)$$

(16)

to avoid negative values. Training of the circuit is done using 70% of the data points. We obtained a precise estimate of $\hat{N}$ ($1.8 \times 10^{-5}$ for the MSE over the test data) using a sequence of four interactions of the qubit with the environment. As the dynamics (in this case) depends on two parameters, $\alpha\tau$ and $\lambda/\gamma_0$, a larger number of interactions of the qubit with the environment is required to achieve a precise estimate. After each combined AD and PD interaction, a $R_y(\varphi)$ gate is applied on the qubit (Fig. 4a). The optimization is done over the interaction times $t_i$, $i = 1, ..., 4$, the rotation angles $\varphi_j$, $j = 0, ..., 4$, and the parameters $w_0$ and $w_1$. Note that $R_y(\varphi_0)$ is the initialization gate, and we have taken the interaction time of AD and PD channels to be equal.

5 Conclusions

In summary, we proposed an experimentally feasible scheme to estimate the degree of non-Markovianity based on entanglement dynamics. We implemented this approach to the paradigmatic models of phase, amplitude damping, and com-
Fig. 4  a VQC for estimating the degree of non-Markovianity $\mathcal{N}$ for the case of combined amplitude and phase damping. The system qubit $s$ is first initialized by the rotation $R_y(\phi_0)$. The qubit $s$ then interacts with the environment in a sequence of four interactions with time $t_i$. After each interaction, a rotation $R_y(\phi_i)$ acts on the qubit $s$. For each interaction, two ancilla qubits are used to simulate the effect of the environment, one for AD and one for PD. In the output, the qubit $s$ is measured in $\sigma_z$ basis. b and c show the contour plots of the degree of non-Markovianity, $\mathcal{N}$, and $\hat{\mathcal{N}}$ (estimate of $\mathcal{N}$) versus $\lambda/\gamma_0$ and $\alpha\tau$, respectively.

Appendix A. Adagrad

Here, following Ref. (Ruder 2016), we give some details about the Adagrad optimizer that we used in our simulations. Adaptive gradient (Adagrad) is a variation of the gradient descent (GD) optimizer. In the GD algorithm, the parameters, labeled by $\phi$ here, are updated in the opposite direction of the gradient of the cost function $C(\phi)$. In other words, for every parameter $\phi_i$ at each time step $t$, the update rule can be written as

$$\phi_{t+1,i} = \phi_{t,i} - \eta \nabla_{\phi_i} C(\phi),$$  \hspace{1cm} (A1)$$

where $\eta$ is the learning rate, which is assumed to be constant and independent of $\phi_i$ throughout the learning process.

In Adagrad, a different learning rate is used for every parameter $\phi_i$ at every time step. In the update rule for Adagrad, the learning rate at each time step $t$ for every parameter $\phi_i$ is based on the past gradients that have been calculated for $\phi_i$ (Ruder 2016)

$$\phi_{t+1,i} = \phi_{t,i} - \frac{\eta}{\sqrt{R_{t+1,i}} + \varepsilon} \nabla_{\phi_i} C(\phi).$$  \hspace{1cm} (A2)$$

This methodology can be used to estimate the degree of non-Markovianity for other decoherence channels that can be simulated with a quantum circuit such as Pauli channel and depolarizing channel. Moreover, sequences of the interaction of the qubit with its environment may find applications in other tasks such as estimating parameters related to the environment that could be either a bath of harmonic oscillators or surrounding qubits. In a multi-qubit system, a sequence of interactions between qubits inter-spaced with single qubit rotation gates, followed by measurements on each qubit can be used to estimate the desired parameter such as the degree of non-Markovianity or the coupling strength between the qubits.
Here, $g_{t+1,i}$ is the sum of the squares of the gradients with respect to $\phi_i$ up to time step $t + 1$,

$$g_{t+1,i} = g_{t,i} + \left( \nabla_{\phi_i} C(\phi) \right)^2,$$  

(A3)

where $g_0 = 0$, and $\epsilon$ (usually chosen on the order of $10^{-8}$) is for avoiding division by zero.

The weakness of Adagrad is the accumulation of the squared gradients in the denominator. The accumulated sum keeps growing during the training process as the added terms are all positive. As a result, the learning rate could approach zero, and therefore, the algorithm stops learning. To avoid this issue in our simulations, when the rate of learning became very small, we reinitialized the optimization process with the newly found hyperparameters as the initial values.

**Appendix B. RMSprop**

Root mean square propagation (RMSprop) is a variation of Adagrad algorithm which uses a decaying average of squared gradients in the adaptation of the step size for each parameter (Ruder 2016). The use of a decaying average allows the algorithm to forget early gradients and only focus on the most recent gradients during the optimization process. As a result, RMSprop overcomes the AdaGrad’s diminishing learning rates. In RMSprop, the parameter update rule is

$$\phi_{t+1} = \phi_t - \frac{\eta}{\sqrt{g_{t+1}} + \epsilon} \nabla_{\phi_i} C(\phi).$$  

(B1)

In this case, we have

$$g_{t+1,i} = \gamma g_{t,i} + (1-\gamma) \left( \nabla_{\phi_i} C(\phi) \right)^2,$$  

(B2)

where $g_0 = 0$, and for $\gamma$ it is suggested to use $\gamma = 0.9$ (Hinton et al. 2012).

In our simulations, using RMSprop algorithm, a local minima of the cost function reached quickly (in less number of steps than Adagrad). However, the algorithm then started to diverge, resulting in large values for the cost function. Therefore, once RMSprop reached the local minima, we followed the optimization process with Adagrad to reach the desired accuracy.

**Acknowledgements** The authors thank Mauro Cirio for helpful comments on the manuscript. H.T.D. acknowledges support from Universidade Mayor through a postdoctoral fellowship. D.T acknowledges financial support from Universidad Mayor through the Doctoral fellowship. F.F.F. acknowledges support from Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP), Project No. 2019/05445-7. A. N. acknowledges financial support from Fondecyt Iniciación No 11220266. R.C. acknowledges financial support from FONDECYT Iniciación No. 11180143.

**Author Contributions** H.T.D., R.C., and D.T. conceptualized the idea. F.F.F. provided the dataset for PD and AD channels. A.N. advised on the experimental implementations of the proposed scheme. H.T.D. performed the numerical simulations. All authors discussed the results and contributed to writing and review of the paper.

**Availability of data and materials** The data that supports the findings of this study are available from the corresponding author upon reasonable request.

**Declarations**

**Conflict of interest** The authors declare no competing interests.

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