Machine learning non-Markovian quantum dynamics

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Machine learning methods have proved to be useful for the recognition of patterns in statistical data. The measurement outcomes are intrinsically random in quantum physics, however they do have a pattern when the measurements are performed successively on an open quantum system. This pattern is due to the system-environment interaction and contains information about the relaxation rates as well as non-Markovian memory effects. Here we develop a method to extract the information about the unknown environment from a series of single-shot measurements on the system (without resorting to the process tomography). The method is based on embedding the non-Markovian system dynamics into a Markovian dynamics of the system and the effective reservoir of finite dimension. The generator of Markovian embedding is learned by the maximum likelihood estimation. We verify the method by comparing its prediction with an exactly solvable non-Markovian dynamics. The developed algorithm to learn unknown quantum environments enables one to efficiently control and manipulate quantum systems.

Introduction. Quantum systems are never perfectly isolated which makes the study of open quantum dynamics important for various disciplines including solid state physics [1], quantum chemistry [2], quantum sensing [3], quantum information transmission [4], and quantum computing [5]. Open quantum dynamics is a result of interaction between the system of interest and its environment. It is usually assumed that the environment is an infinitely large reservoir in statistical equilibrium, which has a well-defined interaction with the system [6]. However, the environments of many physical systems are rather complex and structured [7–18]. A model of the system-environment interaction is often heuristic and oversimplified (e.g., a harmonic environment), but even in this case the analysis is rather complicated and requires some elaborated analytical and numerical methods [19–21]. A theoretical model may also neglect some additional sources of decoherence and relaxation. The experimental analysis of the environmental degrees of freedom is difficult because of their inaccessibility in practice. In fact, one can only get some information about the actual environment by probing the system [22]. Therefore, one faces an important problem to learn the unknown environment and its interaction with the quantum system by probing and affecting the system only.

This problem can be partly solved within the assumption of fast bath relaxation, when the system density operator ρS experiences the semigroup dynamics ρS(t) = eCstSρS(0) with the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) generator LS [23, 24]. In this case, one can learn the generator by performing a process tomography of the quantum channel Φ(t1) = eCst1; for a fixed time t1 > 0 [25, 26]. Nevertheless, the actual dynamical map Φ(t) is usually much more involved and does not reduce to a semigroup [27, 28]. Thus, the problem of learning the environment is mostly attributed to memory effects accompanying the non-Markovian dynamics. In this case, one can still resort to the process tomography of channels Φ(t1), Φ(t2), ..., Φ(tn) by preparing various initial system states ρS(0) and performing different measurements on the system at time moments t1 < t2 < ... < tn. Such a procedure results in a discretized dynamical map {Φ(tn)}. The procedure is time consuming because one has to gather enough statistics for all times {tn}. A recently proposed transfer tensor method [29, 31] uses a finite set of reconstructed maps {Φ(tn)}Kn=1 to learn the Nakajima-Zwanzig equation [32–34] ρS(t) = t∫0K(t − t′)ρS(t′)dt′ with a memory kernel K that gives rise to non-Markovian effects [34]. Since the accuracy ε of statistical reconstruction of a general quantum process Φ on a dS-dimensional quantum system scales as ε ∼ dS√n with the number of measurements n [35, 36], the total number of required measurements N ∼ KdS/ε2 is rather large, with K being system specific [28]. Moreover, the tomographic reconstruction of the channel Φ(t) implies resetting the environment in the same initial state after each measurement, which is difficult to control in the experiment especially in the case of a strong coupling between the system and environment.

A recently suggested method of Ref. [37] uses recurrent neural networks for defining Lindblad operators and learning the convolutionless master equation with the convolutionless master equation ρS(t) = LS(t)ρS(t) + ρS(t). The idea is to perform the full quantum tomography of system states ρS(tn) for different times {tn} and the initializations ρS(0); then train the neural network by minimizing the cost function ∑n ∑i ∥ρS(tn) − ρS(tn)∥, where {ρS(tn)} are the states outputted by the neural network. An implementation of this method in practice encounters the same difficulties related with the necessity to perform tomography at different time steps.

In this paper, we develop a method to learn the effective Markovian embedding [38–41] for non-Markovian...
processes instead of learning the master equation for the system $S$. Within such an approach, the environment is effectively divided into two parts: the first one carries memory of the system and is responsible for non-Markovian dynamics (effective reservoir, ER); the second one is memoryless and causes Markovian decoherence and dissipation of $S + ER$. Such a division of the environment is similar to the pseudomode method, where one derives a Markovian master equation in the GKSL form for the extended system comprising the system and the pseudomodes $\{42, 44\}$. The sufficient dimension $d_{ER}$ of the effective reservoir is found in Ref. $[45]$ and can also be estimated via an ensemble learning method $[46]$. Therefore, we reconstruct the system evolution

$$
\rho_S(t) = \text{tr}_{ER}[\rho_{S+ER}(t)]
$$

by learning the dynamics of the Markovian embedding:

$$
\frac{d\rho_{S+ER}(t)}{dt} = \mathcal{L}_{S+ER}[\rho_{S+ER}(t)].
$$

The data, which feed the learning algorithm, are the results of a series of single-shot projective measurements performed on the system at different times $t_1 < t_2 < \ldots < t_n$, see Fig. 1(a). A sharp distinction from many tomographic approaches is that the generator $\mathcal{L}_{S+ER}$ is reconstructed from a single series of such measurements. If the system evolution is Markovian ($d_{ER} = 1$), then the result of measurement at time $t_k$ depends on the measurement outcome at time $t_{k-1}$ only and does not depend on results of earlier measurements at times $t_{k-2}, t_{k-3}, \ldots \[47\]$. Instead, the non-Markovian dynamics is accompanied by correlations in the measurement outcomes $\[47, 50\]$, which can be analyzed via the process matrix $\Phi$ and the process tensor $\[52\]$. The process tensor is a particular form of a quantum network $[53]$, see Fig. 1(b), which is defined through the generator $\mathcal{L}_{S+ER}$ in our model. In subsequent sections, we implement machine learning for $\mathcal{L}_{S+ER}$ providing the observed series of measurement outcomes is given.

The problem that we address is similar to the tomographic reconstruction of the restricted process tensor via projective measurements $[54]$. The restricted process tensor infers the action of $n$ arbitrary intervening measurements at time moments $t_1 < t_2 < \ldots < t_n$ on an open quantum system of dimension $d_S$. To reconstruct the restricted process tensor one has to perform a series of $\frac{1}{2}[d_S^2(d_S+1)]^n$ tomographic measurements of the output state for linearly independent sequences of $n$ projections. As the process tensor has a peculiar form in our model [see Fig. 1(b)] and depends on the generator $\mathcal{L}_{S+ER}$ only, the latter can be reconstructed by maximizing the likelihood of getting the observed outcomes for a single series of measurements without resorting to the full quantum tomography.

Likelihood function and its gradient. Suppose the experimental setup allows for projective measurements of the system at times $t_i = i\tau$, $i = 1, \ldots, n$, with the measurement basis $\{\{\phi_k^{(m)}\}\}_{k=1}^{d_S}$ being randomly chosen at each time moment $t_i$. Observation of the particular measurement outcome $k_i$ transforms the system state into $|\phi_k^{(m)}\rangle/\langle\phi_k^{(m)}|$. Denote $E_i = |\phi_k^{(m)}\rangle/\langle\phi_k^{(m)}| \otimes I_{ER}$ the projector acting on the system and effective reservoir. The collection of projectors $\{E_i\}_{i=1}^{n}$ is the data set that feeds the learning algorithm.

In between two sequential measurements, the system and the effective reservoir evolve as follows: $\rho_{S+ER}(t_{i+1} - 0) = \Phi[\rho_{S+ER}(t_i + 0)]$, where the quantum channel $\Phi = \exp\{\tau\mathcal{L}_{S+ER}\}$. The probability to get the particular sequence of measurement outcomes $\{k_i\}_{i=1}^{n}$ (the data $\{E_i\}_{i=1}^{n}$) equals $\[55\]

$$
p(\{E_i\}_{i=1}^{n}) = \text{tr}\left[ E_n \ldots \text{tr} \left[ E_2 \Phi[\rho_{S+ER}(0)] E_1 \right] \right].
$$

Eq. (3) is the likelihood function to be maximized over parameters of the generator $\mathcal{L}_{S+ER}$. Such a maximization is the most common approach in the supervised machine learning $[50]$. To simplify the implementation of the gradient decent method $[57]$ we use the Stinespring dilation for the channel $\Phi$ (see, e.g., $[55]$):

$$
\Phi[X_{S+ER}] = \text{tr}_A \left[ U(H) X_{S+ER} \otimes \varrho_A U^\dagger(H) \right],
$$

where $\varrho_A$ is a fixed pure state of the $(d_S d_{ER})$-dimensional ancilla $A$, $U(H) = \exp(-i\tau H)$ is a unitary evolution operator, and $H$ is the effective Hamiltonian of $S + ER + A$. Let $\tilde{\varrho}_{S+ER}(t_m)$ be the subnormalized state of $S + ER$ at time moment $t_m$ such that $\text{tr}[\tilde{\varrho}_{S+ER}(t_m)] = p(\{E_i\}_{i=1}^{n})$. Then we get the recurrence relation

$$
\tilde{\varrho}_{S+ER}(t_{m+1}) = \text{tr}_A \left[ E_m \otimes I_A U(H) \tilde{\varrho}_{S+ER}(t_m) \otimes \varrho_A \right. \\
\left. \times U^\dagger(H) E_m \otimes I_A \right]
$$

with $\tilde{\varrho}_{S+ER}(0) = \varrho_{S+ER}(0)$. The ancillary operator $\varrho_A$ plays the role of a renewable subenvironment in quantum
collision models \cite{59,61} and memoryless (Markovian) part of the environment \cite{40}. The recurrent calculation \cite{52} is associated with the forward propagation along the tensor network in Fig. 4. Similarly, we introduce the operator $\mathcal{E}_{S+ER}(t_m)$, which propagates backward (in the Heisenberg picture) by formula

$$\mathcal{E}_{S+ER}(t_m) = t_{A}[U^{\dagger}(H)(E_{m+1}\mathcal{E}_{S+ER}(t_{m+1})E_{m+1} \otimes I_A)$$

$$\times U(H)(I_{S+ER} \otimes \varrho_A)]$$ \hfill (6)

with $\mathcal{E}_{S+ER}(t_0) = I_{S+ER}$.

Merging the forward and backward propagations at a fixed time $t_m$, we express the likelihood function in the various forms:

$$p\{(E_i)_{i=1}^n|H\} = \text{tr}[\tilde{\varrho}_{S+ER}(t_m)\mathcal{E}_{S+ER}(t_m)] \quad \forall m = 0, \ldots, n, \ t_0 = 0$$

$$= \text{tr}[U(H)\tilde{\varrho}_{S+ER}(t_{m-1}) \otimes \varrho_A U^{\dagger}(H)$$

$$\times E_m \mathcal{E}_{S+ER}(t_m) E_m \otimes I_A] \quad \forall m = 1, \ldots, n.$$ \hfill (7)

The latter expression (7) is a “sandwich” composed of the forward propagation till time $t_{m-1}$ [the state $\tilde{\varrho}_{S+ER}(t_{m-1})$], the backward propagation till time $t_m$ [the operator $\mathcal{E}_{S+ER}(t_m)$], and the unitary transformation $U(H) \cdot U^{\dagger}(H)$ followed by the $m$-th measurement in between. Since the likelihood function is the $n$-degree monomial with respect to both operators $U(H)$ and $U^{\dagger}(H)$, we readily express its gradient operator as follows:

$$\frac{\partial p\{(E_i)_{i=1}^n|H\}}{\partial H} = \sum_{m=1}^n t_r \left\{ E_m \mathcal{E}_{S+ER}(t_m) E_m \otimes I_A$$

$$\times \left[ \frac{\partial U(H)}{\partial H} \tilde{\varrho}_{S+ER}(t_{m-1}) \otimes \varrho_A U^{\dagger}(H)$$

$$+ U(H)\tilde{\varrho}_{S+ER}(t_{m-1}) \otimes \varrho_A \frac{\partial U^{\dagger}(H)}{\partial H} \right]\right\}.$$ \hfill (8)

The operator (8) is Hermitian provided the Hamiltonian $H$ is Hermitian. The derivative $\frac{\partial U^{\dagger}(H)}{\partial H}$ is $\frac{\partial U^{\dagger}(H+t\nu V)}{\partial \nu}|_{\nu=0} = \sum_{k,l} \lambda_k \langle \psi_k | \psi_l \rangle e^{-i\lambda_k \tau}$$

$$\delta V = \exp[-i(H + V)\tau] = \exp[-iH\tau]T_\nu \exp[-i\int_0^\nu \exp(iH(t')dt')V\exp(-iH(t')dt')dt' + a(V)]$$

and the spectral decomposition $H = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k|$. To get

$$\frac{\partial U(H)}{\partial H} = \left(\frac{\partial U^{\dagger}(H)}{\partial H}\right)^\dagger = \sum_{k,l} e^{-i\lambda_k \tau} - e^{-i\lambda_l \tau} \langle \psi_k | \psi_l \rangle.$$ \hfill (9)

Finally, we find the gradient of the logarithmic likelihood $\log p\{(E_i)_{i=1}^n|H\}$ with respect to the unknown parameter $H$:

$$\frac{\partial \log p\{(E_i)_{i=1}^n|H\}}{\partial H} = \frac{1}{p\{(E_i)_{i=1}^n|H\}} \frac{\partial p\{(E_i)_{i=1}^n|H\}}{\partial H}.$$ \hfill (10)

Note that (10) is insensitive to the normalization of $p\{(E_i)_{i=1}^n|H\}$, which significantly simplifies the calculation. Eqs. (5)–(10) enable us to efficiently calculate the gradient of the logarithmic likelihood in $O(n)$ steps. The logarithmic likelihood $\log p\{(E_i)_{i=1}^n|H\}$ is a non-convex function with respect to $H$, so its optimization is accompanied with overcoming the convergence to local extremums and the slow convergence rate. In what follows, we use the techniques, which were shown to perform well in such non-convex optimization problems as neural network learning \cite{62}.

**Learning algorithm.** To learn the Markovian embedding is to estimate the channel $\Phi$ that governs dissipative and decoherence processes on the system and the effective reservoir. Since the system is being repeatedly measured, its initial state does not affect the learning algorithm. Neither does the initial state of the effective reservoir as long as the measurements last longer than the relaxation time of the environment ($\tau T$ is much greater than the environment relaxation time $T$). The latter condition implies that the system and the effective reservoir “forget” about their initial states after time $\tau T$.

The learning algorithm, which estimates $\Phi$ (and the corresponding generator $\mathcal{L}$) based on the data set $\{E_i\}_{i=1}^n$, is as follows \cite{63}:

1. Initialize the model by randomly choosing the factorized state $\tilde{\varrho}_{S+ER}(0) = \tilde{\varrho}(0) \otimes \varrho_{ER}(0)$ and the factorized Hamiltonian $H = H_{S+ER} \otimes I_A$. (Starting with a Hamiltonian, which is factorized with respect to $S+ER$ and $A$, fastens the learning process of memory effects. Otherwise, the correlations between $S+ER$ and $A$ induce irreducible decoherence and dissipation on $S+ER$ that smear out the memory effects.)

2. Calculate $n$ operators $\{\tilde{\varrho}_{S+ER}(t_i)\}_{i=1}^n$ via the forward recurrent propagation formula (5) and $n$ operators $\{\mathcal{E}_{S+ER}(t_i)\}_{i=0}^{n-1}$ via the backward recurrent propagation formula (6). Keep these 2n operators in the computer memory.

3. Calculate the logarithmic likelihood $\log p\{(E_i)_{i=1}^n|H\}$ via formula (7).

4. Find the spectral decomposition of the $(dSd_{ER})^3$-dimensional operator $H = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k|$ and calculate $\frac{\partial U^{\dagger}(H)}{\partial H}$ and $\frac{\partial U^{\dagger}(H)}{\partial H}$ via formula (9).

5. Calculate the gradient (10) via formula (8) and results of items 2–3.

6. Feed the calculated gradient to an advanced optimization method \cite[e.g., the adaptive moment estimation (Adam)]{64} and get the increment $\Delta H$ of the effective Hamiltonian for $S+ER+A$.

7. Update the Hamiltonian $H \rightarrow H + \Delta H$ and repeat items 2–6 until the logarithmic likelihood $\log p\{(E_i)_{i=1}^n|H\}$ converges.

8. Make use of the final update of $H$ to find the channel $\Phi$ via formula (4) and the generator $\mathcal{L}_{S+ER} = \frac{1}{\tau} \ln \Phi$. 
Data generation. We apply the learning algorithm above to the in silico data set \( \{E_i\}_{i=1}^n \) generated in a non-Markovian composite bipartite collision model \[65\]. We consider a bipartite system that successively interacts with qubit subenvironments \( R \) during collision time \( \Delta t \), with the bipartite system being composed of the very open qubit system under study \( S \) and one auxiliary qubit system \( S_1 \), see Fig. 2b. Such a model is quite rich and describes, e.g., a qubit subject to random telegraph noise.

The composite bipartite collision model \[65\] allows to find the system evolution \( \rho_S(t) = \text{tr}_{S_1}[\rho_{S+S_1}(t)] \) invaded by measurements on the system. We fix the (dimensionless) interaction Hamiltonian between \( S, S_1 \), and \( R \) in the form

\[
H_{S+S_1+R} = 0.6 \rho_S \otimes I_{S_1} \otimes I_R + 0.6 \rho_S \otimes H_{S_1} \otimes I_R + 0.6 I_S \otimes I_{S_1} \otimes H_R + 0.3 h_{\text{int}} S_{S_1} \otimes I_R + 0.15 h_{\text{int}} S_{S_1} \otimes I_S + 0.1 h_{\text{int}} R \otimes I_{S_1},
\]

where each operator \( h \) is a random Hermitian matrix from the Gaussian unitary ensemble with unit scale parameter. The coefficients in the interaction Hamiltonian correspond to the case when strong memory effects are present in the evolution whereas the relaxation time is much longer than the recurrence time of memory effects — the hardest open dynamics to reconstruct. Each collision results in the transformation

\[
\rho_{S+S_1}(t+\Delta t) = \tau_{S_1} \exp(-iH_{S+S_1+R} \Delta t) \rho_{S+S_1}(t) \otimes \rho_R \exp(iH_{S+S_1+R} \Delta t).
\]

Suppose the qubit system is in the state \( \rho_S(t_i) \) at time \( t_i = i\tau \). We randomly choose a direction \( r^{(i)} \in \mathbb{R}^3 \), \( |r^{(i)}| = 1 \), on a Bloch ball and calculate eigenvectors \( |\varphi_+^{(i)}\rangle \) and \( |\varphi_-^{(i)}\rangle \) of the polarization operator \( I_S \sigma_x + r_y^i \sigma_y + r_z^i \sigma_z \), where \( \sigma_x, \sigma_y, \sigma_z \) is the conventional set of Pauli operators. The transformation \( \{\pm\} \rightarrow |\varphi_+^{(i)}\rangle |\varphi_-^{(i)}\rangle \) is an observable at time \( t_i = i\tau \). One of the two measurement outcomes \( \{\pm\} \) is accepted, with the probability to accept the result + being \( \langle \varphi_+^{(i)} | \rho_S(t_i) | \varphi_+^{(i)} \rangle \). As a result, one of the operators \( |\varphi_+^{(i)}\rangle \langle \varphi_-^{(i)}| \otimes I_{ER} \) is accepted as \( E_i \). Observation of the outcome \( \pm \) in the \( i \)-th measurement of the system results in the transformation

\[
\rho_{S+S_1} \rightarrow |\varphi_+^{(i)}\rangle \langle \varphi_+^{(i)}| \otimes \rho_{S_1}^{(i)} / \text{tr}[\rho_{S_1}^{(i)}], \quad \text{where} \quad \rho_{S_1}^{(i)} = \langle \varphi_+^{(i)} | \otimes I_{S_1} \rho_{S+S_1}(t) |\varphi_+^{(i)}\rangle \otimes I_{S_1} \rangle.
\]

The measurement is followed by another collision described above, which in turn is followed by a measurement, and so on until the set \( \{E_i\}_{i=1}^n \) is completed.

Verification and results. We run the learning algorithm for the data set \( \{E_i\}_{i=1}^n \), \( n \approx 10^5 \). Since the data set is generated in a collision model with qubits, we fix \( d_S = d_{ER} = 2 \). In the case of an actual experiment, \( d_{ER} \) should be estimated according to Refs. \[45, 46\]. The learning curve in Fig. 2(a) shows how the logarithmic likelihood increases during the learning process and approaches the theoretical prediction.

To verify the adequacy of the learned generator \( L_{S+ER} \) we compare the actual system dynamics in the non-Markovian composite bipartite collision model and the learned dynamics given by Eqs. (1)–(2), see Figs. 3(a-c) and 4(a-c) for short and long time scales, respectively. The initial state of the effective reservoir in both cases is the equilibrium state \( \text{tr}_S[\rho_S^{\infty} \rho_{ER}^{\infty}] = 0 \). At step \( n \) of the learning algorithm, we use the Adam optimizer \[64\] with the parameters \( \beta_1 = 0.9, \beta_2 = 0.95, \epsilon = 10^{-4} \), the learning rate equals \( 10^{-3} \).

Figs. 3(d) and 4(d) depict the dynamics of the trace distance \( \frac{1}{2}||\rho_S(t) - \rho_{ER}(t)|| \) for two different initial states of the system. Non-monotonicity of the trace distance is a clear indication of non-Markovianity \[60\], and the learned
Markovian embedding reproduces such a non-monotonic behavior quite well. The tests demonstrate that the presented learning algorithm actually extracts useful information from the correlation pattern in a sequence of measurements on the open quantum system.

Conclusions and outlook. We have proposed the method to learn the effective Markovian embedding for non-Markovian quantum evolution, which is based on successive single-shot measurements of the system without resorting to the full tomography. Correlations in the measurements at different times indicate non-Markovianity of the process and allow for the reconstruction of memory effects. The decay of correlations between apart measurements enables one to reconstruct the relaxation effects. Both memory and relaxation phenomena are taken into account by the generator $L_{S+ER}$ acting on the system and the effective reservoir of known dimension. We have tested learnability of the algorithm by analyzing the data set for the non-Markovian dynamics in the composite bipartite collision model.

The developed machine learning approach can be also adapted to the tasks of optimal control. Suppose the open system is coherently controlled via a time dependent Hamiltonian $H_S(t)$ and is subject to an uncontrollable quantum noise, which potentially induces non-Markovian effects. Once one can modify the algorithm and train it with a finite set of different control Hamiltonians $H_S^{(k)}(t)$ in such a way, that the algorithm will be able to predict the system dynamics under any time dependent Hamiltonian $H_S(t)$.

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