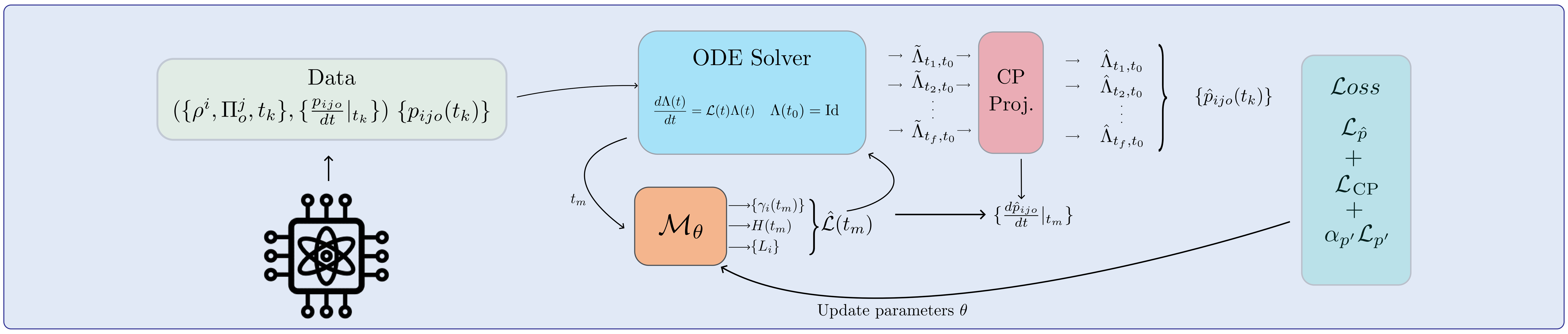
Neural assisted time-dependent Lindblad tomography

Antonio Ruiz-Molero[1,2], Daniel Manzano[3,4], Michalis Skotiniotis[3,4]

[1] INL – International Iberian Nanotechnology Laboratory, Braga, Portugal.
[2] Departamento de Informática, Universidade do Minho, Braga, Portugal .
[3] Electromagnetism and Condensed Matter Department, Universidad de Granada, 18071 Granada, Spain.
[4] Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, 18071 Granada, Spain.

QOpen Kick-off: MC Meeting & Scientific Workshop (Lisbon - 2026)



Motivation and results

The task of inferring the open dynamics of a system that interacts with a, possibly unknown, environment has gained attraction when building and mitigating errors in current quantum computers. In this work, we propose a method to estimate the time-dependent Lindbladian that evolves a system of interest combining different techniques from Machine Learning. As a feature, the technique can be used to estimate non-Markovian dynamics. We present a case study using synthetic data to learn non-trivial non-Markovian dynamics.

Time dependent Lindblad tomography

We consider the family of CPTP maps that evolves a system of dimension d, $\{\Lambda_{t_i,t_0}\}$ generated by the so-called canonical Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) time-local master equation[1]:

$$\frac{d\Lambda(t)}{dt} = \mathcal{L}(t) \circ \Lambda(t),$$

$$\mathcal{L}(t)[\bullet] \coloneqq -i[H(t), \bullet] + \sum_{i=0}^{d^2-1} \gamma_i(t) \left(L_i(t) \bullet L_i^\dagger(t) - \frac{1}{2}\{L_i^\dagger(t) L_i(t), \bullet\} \right).$$

The complete positivity of the maps $\Lambda_{t,t_0} = \mathcal{T} e^{\int_{t_0}^{t} ds \mathcal{L}(s)}$ is determined by the sign of the decay rates $\{\gamma_i(t)\}$. Positive decay rates are guaranteed to generate CPTP and CP-divisible maps (Markovian). Non-CP divisible maps (non-Markovian) are characterized by one or more decay rates becoming negative for some t.

We choose at least d^2 states $\{\rho^i\}$, and a set of measurement bases j defined by the POVM operators $\{\Pi_o^j\}$ such that the joint set is informationally complete in the Quantum Process Tomography (QPT) sense.

Given a set of evolution times $\{t_k\}$. For each combination of initial state i, measurement basis j and time k, one prepares the initial state, let the system be affected by the noise for the given time, and measure in the corresponding basis. The complete data is given by the observed frequencies $p_{ijo}(t_k)$.

Proposed algorithm

The time-ordered integral requires a continuous modelling of $\mathcal{L}(t)$ to predict the observed probabilities, given by the Born rule,

$$\hat{p}_{ijo}(t_k) = \mathrm{Tr}\left[\Pi_o^j \mathcal{T} e^{\int_{t_0}^{t_k} ds \hat{\mathcal{L}}(s)} [\rho^i]\right].$$

We propose a model compound of three neural networks that map $t \to \{\hat{\gamma}_i(t)\}, \{\hat{L}_i\}, \{\hat{H}(t)\}$, allowing to reconstruct $\mathcal{L}(t)$ for $i: 1, \ldots, k \leq d^2 - 1$ where k is a maximum of active independent decay channels one expects to be active.

For the given configuration of the input data $\{\rho^i, \{\Pi_o^j\}, t_k\}$ of each iteration, the GKSL master equation is solved using a differentiable ode solver with $\Lambda(t_0) = \mathrm{Id}$ for the corresponding times t_k.

At each internal step of the ode solver t_m, the rhs of the master equation is constructed by interrogating the networks to produce $\mathcal{L}(t_m)$, obtaining a final set of $\{\tilde{\Lambda}_{t_k,t_0}\}$

CP projection There is no restriction on the positivity of the decay rates to allow learning non CP-divisible maps. Yet, negative decay rates can yield non CP maps. Training will make the network produce non-CP maps that best explain the data.

To encourage learning CP dynamics, we project the predicted maps to the closest CP ones, yielding $\{\hat{\Lambda}_{t_k,t_0}\}$. These CP maps are used to compute the predicted probabilities $\hat{p}_{ijo}(t_k)$. This translates in two loss terms, corresponding to the mean squared error between the predicted and observed probabilities; and the mean Hilbert-Schmidt distance between $\{\tilde{\Lambda}_{t_k,t_0}\}$, and $\{\hat{\Lambda}_{t_k,t_0}\}$.

Mitigating spectral bias Vanilla Multilayer Perceptrons (MLPs) struggle to learn functions with high frequency contents in a finite number of training epochs (Frequency bias). Low frequencies components are learned first, and only for very long training times higher frequencies are learned. To mitigate this phenomenon, and learn any type of decay rates evolution, we consider an architecture inspired in neural ordinary differential equations (NODES).

We define a latent vector $h(t)$ for each decay rate that evolves according to the ode: $h' = f_\theta(t, h(t))$, where f_θ is a MLP. Each latent vector is evolved alongside the maps inside the ode solver. We use a trainable linear layer that maps $h(t) \mapsto \gamma(t)$.

To allow learning high frequencies, we enocde the input time using Random Fourier Features. While this encoding tends to overfit and produce highly wiggling outputs, the integration of $h(t)$ acts as a natural low pass filter, producing smooth predictions.

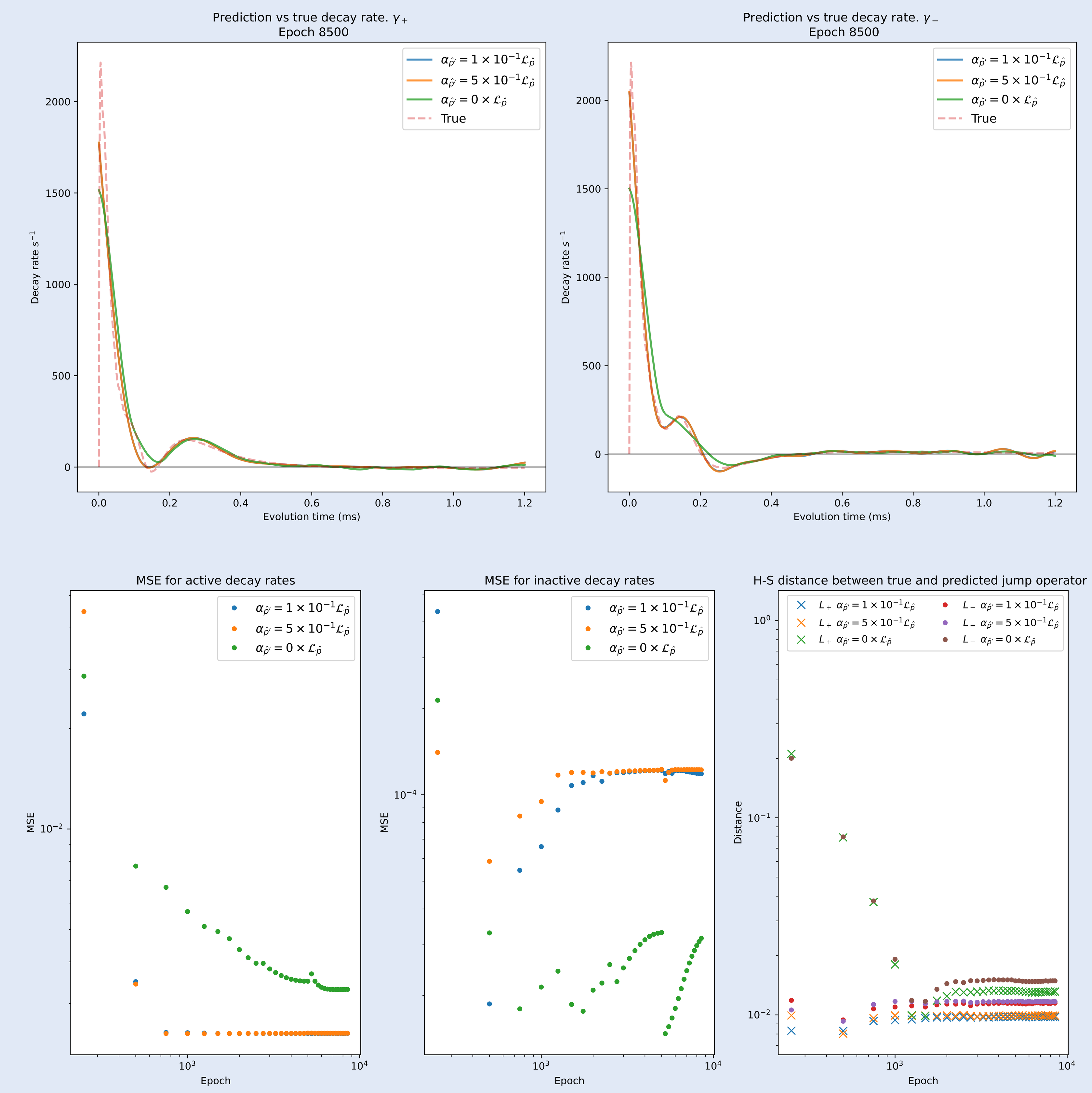
Sobolev training Backpropagation through the ode solver results in the network struggling to learn the initial dynamics. Sobolev training helps mitigating this problem, where the network has information about the evolution of the predicted probabilities. The prediction of the derivatives are $\hat{p}'_{ijo} = \mathrm{Tr}\left[\Pi_o^j \hat{\mathcal{L}}(t) \hat{\Lambda}_{t,t_0}[\rho^i]\right]$. We estimate the derivatives of the observed data using Gaussian Processes. We consider another loss term with the mean squared error between the "observed" and predicted time derivatives of the probabilities.

Loss function The parameters of the network are updated via backpropagation with the following loss function $\mathcal{L} = \mathcal{L}_{\hat{p}} + \mathcal{L}_{\mathrm{CP}} + \alpha_{p'}\mathcal{L}_{p'}$

Case study of Non-Markovian dynamics

We consider the two-qubits system studied in Ref. [2], where two impurity atoms each occupying a double-well potential with an optical supperlatice are infleuced by a common environment. The decay channels are given by $\gamma_+(t)$ with $L_+ = Z \otimes I + I \otimes Z$, and $\gamma_-(t)$, with $L_- = Z \otimes I - I \otimes Z$

The two decay rates depict a quick decay and become negative, yielding non-Markovian dynamics. We plot the results using synthetic data where we let the algorithm learn a maximum number of 5 decay channels. We consider three scenarios to compare the influence of including the time derivatives of the probabilities in the loss function, controlled by the scalar $\alpha_{p'}$.



Acknowledgements

ARM acknowledges support from FCT – Fundação para a Ciência e a Tecnologia (Portugal) through PhD Grant SFRH/BD/151453/2021. This work was supported by the ERC Advanced Grant QU-BOSS, GA no. 884676

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[3] Antonio Ruiz-Molero, Daniel Manzano, and Michalis Skotiniotis. Neural assisted time-dependent lindblad tomography. Manuscript in development, 2026.