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Two-Dimensional Convolutional Neural Networks for Predicting Non-Markovian Quantum Dissipative Dynamics

Zhiqian Huang[1], Cun Long[2], Qingdong Zhu[1], Jiaan Cao[2] and Xiao Zheng[1,3,*]

[1]*Department of Chemistry, Fudan University, Shanghai 200438, China;*

[2]*Hefei National Research Center for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China;*

[3]*Hefei National Laboratory, Hefei, Anhui 230088, China.*

[*] Corresponding author: xzheng@fudan.edu.cn

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Abstract: Simulating non-Markovian quantum dissipative dynamics remains a major challenge in theoretical and computational chemistry. While traditional numerical methods such as hierarchical equations of motion are numerically exact, they suffer from prohibitive computational costs when modeling systems with complex environmental couplings or strong non-Markovian effects. To address this limitation, we propose a deep learning framework based on two-dimensional convolutional neural networks (2D-CNN) for efficiently predicting long-time quantum dissipative dynamics using only short-time trajectory data. Our approach incorporates a 1D-to-2D feature reconstruction strategy, which transforms 1D time-series data into 2D images, and a multi-timescale fusion network to resolve complex dynamical features. We validate the framework on two paradigmatic cases -- dissipative relaxation in a two-level system and Rabi oscillations in a dissipative spin system -- achieving prediction mean absolute errors of 10^{-3} and 10^{-2}, respectively. The results highlight the effectiveness of our 2D-CNN approach in capturing long-time temporal correlations, providing a computationally efficient pathway for simulating quantum dynamics in realistic open systems.

Key words: deep learning, quantum dissipative dynamics, convolutional neural network.

1. Introduction

Non-Markovian quantum dissipative dynamics is widely observed in various fields ranging from photosynthesis to quantum computing [1-3]. Understanding these dynamics is essential to understand fundamental processes like quantum dissipation, decoherence and energy transfer [4-7]. Despite their universal significance, simulation of long-time open quantum dynamics remains an outstanding challenge, primarily due to the complex non-Markovian memory effects arising from strong system-environment correlations. This persistent theoretical bottleneck highlights the urgent need for developing accurate and computationally feasible methodologies that can simultaneously capture intricate memory effects while maintaining numerical tractability for practical applications.

Over decades, significant progress has been made in developing theoretical methods for modeling non-Markovian quantum dissipative dynamics. Established approaches include: numerical renormalization group (NRG) method [8-12] and its time-dependent extension [13-17], quantum Monte Carlo (QMC) method [18-30], real-time path integral (PI) method [31-37], hierarchical equations of motion (HEOM) [38-46], multi-configuration time-dependent Hartree (MCTDH) [47, 48] and its multilayer extension (ML-MCTDH) [49-53] and second-quantized version [54], density matrix renormalization group (DMRG) method [55-60] and its time-dependent extension [55, 61-65], stochastic quantum dissipation theory methods [66-71], and steady-state density functional theory (i-DFT) method [72]. While these methods have advanced our understanding of open quantum systems, their computational

demands typically scale exponentially with both system size and complexity of environment. This inherent complexity barrier fundamentally restricts applications to large-scale, long-time quantum dynamics. To overcome these limitations, recent efforts have turned to data-driven methods to enhance the efficiency for simulating long-time quantum dissipative dynamics. For instance, the transfer tensor method (TTM) [73-75], pioneered by Cerillo and Cao in 2014, offers a dimensionality-reduction framework to capture the critical dynamics feature by encoding short-time historical evolution into non-Markovian transfer tensors, which can be used to propagate long-time dynamics. Building on this paradigm, machine learning techniques have emerged as promising alternatives for tackling similar challenges.

Machine learning approaches for propagating long-time quantum dynamics can be conceptualized as time series prediction tasks [76], analogous to applications in weather forecasting or financial market modeling. However, quantum dissipative dynamics exhibits a critical distinction: its reduced system dynamics are governed by formally closed quantum dynamical equations rather than intricate real-world processes subjected to noise from countless external sources. The practical tractability stems from the fact that quantum memory effects arise from well-defined environmental interactions. For instance, within the HEOM framework, non-Markovian memory is fully encoded in the environmental hybridization correlation functions.

Recent advances in deep learning have driven a paradigm shift in simulating quantum dissipative dynamics [77-82]. Neural network approaches for time series prediction, including feed-forward neural network (FFNN) [83, 84], recurrent neural networks (RNNs) such as gated recurrent units (GRUs) [85] and long short-term memory networks (LSTMs) [86-88], convolutional neural networks (CNNs) [89-91], and hybrid CNN-LSTM (CNN-LSTM) [92], have demonstrated success in systems like spin-boson models [4, 93] and Fenna-Matthews-Olson (FMO) complexes [94-97]. For example, Lin et al. have applied LSTM to simulate excited-state energy-transfer dynamics, successfully predicting long-time behavior under strong coupling and non-Markovian conditions. By integrating bootstrap sampling with LSTM, they developed a statistical framework to quantify prediction uncertainty and assess model reliability in long-time quantum dynamics simulations [86]. Ullah and Dral have proposed the artificial intelligence quantum dynamics method [90], which uses machine learning to directly predict quantum dynamics trajectories, avoiding the high computational costs and error accumulation inherent to traditional recursive methods. When validated on the FMO complex, the model captured long-time memory effects in quantum dynamics. They further developed a one-shot trajectory learning method [91] based on one-dimensional (1D) CNN, enabling single-step prediction of full trajectories while significantly reducing training time and memory usage. Wu et al. have proposed a 1D-CNN-LSTM based model with feature fusion network for predicting the long-time nonadiabatic quantum dynamics of spin-boson model, achieving high accuracy, robustness and transferability [92]. Furthermore, Zeng et al. have revealed the impact of memory time on the performance of TTM and deep learning approaches and proposed a practical method to estimate the effective memory time [98]. However, determining the appropriate length of short-time historical dynamics in machine learning remains an empirical process. The fundamental principle is to strike a balance between accuracy and efficiency: sufficiently long to encompass key characteristics while as short as possible to minimize resource consumption for training.

By circumventing explicit treatment of system-environment interactions, these methods substantially reduce computational cost while demonstrating unique advantages in long-time dynamics prediction. However, existing methods face certain limitations. For example, their effectiveness in complex systems remains unverified [89-92], such as the Rabi oscillation of a local spin subject to Kondo exchange couplings with environmental spins -- a scenario experimentally demonstrated by Yang et al. [99] and Willke et al. [100] using scanning tunneling microscope-radio frequency (STM-RF) protocols [100-102] to control coherent spin manipulation in hydrogenated Ti atoms and iron phthalocyanine molecules on surfaces. These Rabi oscillations exhibit multi-timescale characteristics, featuring low-frequency oscillations superimposed with high-frequency Larmor precession, and coherence times extending to several hundred nanoseconds (ns). For such complex, long-time quantum dissipative dynamics, RNN architectures risk substantial increases in training costs and complexity due to their inherently sequential nature, which precludes parallelization [103,104]. While 1D-CNNs avoid this issue [105], their long-time prediction accuracy diminishes significantly due to architectural constraints, as discussed in later sections.

To address this challenge, we propose a deep learning framework based on two-dimensional (2D) CNN for accurate long-time dynamics prediction in dissipative quantum systems, including the relaxation of a two-level system and the Rabi oscillations of a local spin. Our approach integrates a "1D-to-2D" temporal reconstruction strategy [106] coupled with multi-timescale feature fusion techniques [92], enhancing the model's ability to capture complex quantum dissipative dynamics.

The remainder of this paper is organized as follows: Section 2 outlines the framework of the 2D-CNN model. Section 3 presents the results and discussion. Section 4 provides the conclusion.

2. Theoretical method

Our deep learning model focuses on long-time quantum dissipative dynamics exhibiting multi-timescale characteristics. The architecture of the proposed model is illustrated in **Figure 1**. The inputs consist of a series of reduced density matrix (RDM) elements of the system at discrete times (e.g., $t_1, t_2, t_3, \ldots, t_n$). First, the input undergoes preprocessing to construct datasets compatible with a 2D-

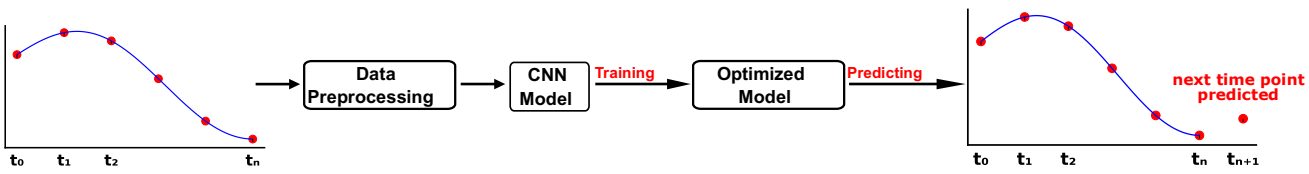

Figure 1. Schematic of the quantum dissipative dynamics prediction framework. Reduced density matrix elements at discrete times $(t_1, t_2, t_3, \ldots, t_n)$ are input, preprocessed, and used to train the 2D-CNN model. The optimized model predicts the next discrete time point t_{n+1}.