Quantum machine learning simulations of photosynthetic light harvesting

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Abstract

Understanding the natural processes of excitation energy transfer (EET) in photosynthetic light-harvesting complexes (LHCs) is one of the essential keys to the design of efficient photovoltaic devices [1]. As LHCs are open quantum systems, the understanding of this energy transfer requires the simulation of its dynamics [2], taking into account the quantum effects and the protein environment in which these LHCs are embedded. According to spectroscopic studies, these effects would favor the EET [3–6]. However, dissipative quantum dynamics frameworks for simulating this transfer, taking into account these effects, encounter not only computational cost problems, in time and storage for the most accurate methods, but also an error accumulation problem for the less accurate ones [7–10]. Machine learning (ML), which is a tool that has already proven itself in several domains, makes it possible to predict this energy transfer with a lower computational cost in time and storage [11–14]. Moreover, thanks to convolutional neural networks (CNN), the problem of error accumulation is also circumvented, based on predictions made over an infinite time. In this last method, the prediction of the dynamics is made on a single Fenna-Matthews-Olson (FMO) complex, from data on the relaxation rate of the environment, the reorganization energy of the studied system, the temperature, the number of molecules necessary for the collection of light, as well as the information on the molecule receiving the excitation first [9, 12, 15]. Although the latter method has shown its feasibility on a single FMO complex, we wonder to what extent it can be extended to the study of several LHCs. With the evolution of the Noisy Intermediate Scale Quantum (NISQ) era, Quantum Convolutional Neural Networks (QCNNs) are receiving more and more attention, due to the fact that they are able to handle higher dimensional data, compared to simple quantum neural networks. Thus, in order to answer the question raised above, we propose a method using quantum convolutional neural networks to predict the EET dynamics of several LHCs in parallel, over infinite time. The LHCs we work with are the FMO complex and the FCP (Fucoxanthin-Chlorophyll) protein.

Keywords: Light harvesting, excitation energy transfer (EET), open quantum system, Lindblad master equation (LME), quantum machine learning, quantum convolutional neural networks

References

[1] P. Cheng, P. Cheng, and Y. Yang, "Narrowing the band gap: the key to high-performance organic photovoltaics", Account of Chemical Research **53**, 1218–1228 (2020), https://doi.org/10.1021/acs.accounts.0c00157.

[2] J. Brédas, E. Sargent, and G. Scholes, "Photovoltaic concepts inspired by coherence effects in photosynthetic systems.", Nature materials **16**, 35–44 (2017).

[3] B. González-Soria, F. Delgado, and A. Anaya-Morales, "Parametric mapping of quantum regime in fenna–matthews–olson light-harvesting complexes: a synthetic review of models, methods and approaches", Applied Sciences **10**, 10.3390/app10186474 (2020), https://www.mdpi.com/2076-3417/10/18/6474.

[4] R. Fenna and B. Matthews, "Chlorophyll arrangement in a bacteriochlorophyll protein from chlorobium limicola", Nature **258**, 573–577 (1975).

[5] B. Palmieri, D. Abramavicius, and S. Mukamel, "Lindblad equations for strongly coupled populations and coherences in photosynthetic complexes", The Journal of chemical physics **130**, 204512 (2009).

[6] M. Busch, F. Müh, M. Madjet, and T. Renger, "The eighth bacteriochlorophyll completes the excitation energy funnel in the fmo protein", The Journal of Physical Chemistry Letters **2**, 10.1021/jz101541b (2010).

[7] Y. Tanimura, "Reduced hierarchical equations of motion in real and imaginary time: correlated initial states and thermodynamic quantities", The Journal of Chemical Physics **141**, 044114 (2014), https://doi.org/10.1063/1.4890441.

[8] Y. Tanimura and R. Kubo, "Time evolution of a quantum system in contact with a nearly gaussian-markoffian noise bath", Journal of the Physical Society of Japan **58**, 101–114 (1989).

[9] A. Ullah, Pavlo, and Dral, "Predicting the future of excitation energy transfer in light-harvesting complex with artificial intelligence-based quantum dynamics", Nature Communications **13**, 10.1038/s41467-022-29621-w (2022).

[10] D. M. Wilkins and N. S. Dattani, "Why quantum coherence is not important in the fenna-matthews-olsen complex", Journal of Chemical Theory and Computation **11**, 3411–3419 (2015).

[11] K. Lin, J. Peng, F. L. Gu, and Z. Lan, "Simulation of open quantum dynamics with bootstrap-based long short-term memory recurrent neural network", The Journal of Physical Chemistry Letters **12**, 10225–10234 (2021).

[12] L. E. H. Rodríguez and A. A. Kananenka, "Convolutional neural networks for long time dissipative quantum dynamics", Journal of Physical Chemistry Letters **12**, 2476–2483 (2021).

[13] K. Naicker, I. Sinayskiy, and F. Petruccione, "Machine learning for excitation energy transfer dynamics", 10.48550/ARXIV.2112.11889 (2021), https://arxiv.org/abs/2112.11889.

[14] K. Lin, J. Peng, F. L. Gu, and Z. Lan, "Simulation of open quantum dynamics with bootstrap-based long short-term memory recurrent neural network", The Journal of Physical Chemistry Letters **12**, 10225–10234 (2021), https://doi.org/10.1021%2Facs.jpclett.1c02672.

[15] K. O'Shea and R. Nash, *An introduction to convolutional neural networks*, 2015, https://arxiv.org/abs/1511.08458.