Nonadiabatic Dynamics and Machine Learning

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Nonadiabatic dynamics widely exist in photophysics, photochemistry and photobiology. We tried to develop theoretical approaches to study the photoinduced nonadiabatic dynamics. A few topics will be discussed.

We tried to combine deep leaning method and numerical accurate quantum dynamics approach to simulate the long-time quantum evolution of open quantum system. This approach allows us to obtain the evolution of reduced density matrix of open quantum system with a low computational cost. It demonstrates that the deep learning approach is the important tool to speed up the long-time quantum evolution. The similar time-series analysis tool can also be used to propagate all nuclear and electronic degrees of freedom in the trajectory evolution of the SQC-MM dynamics.

We showed the possibility to analyze the geometrical evolution of trajectory-based nonadiabatic molecular dynamics by the unsupervised machine learning and big data analysis, particularly the dimensionality reduction techniques. These approaches allow us to extract the major molecular motion from the very complicated time-dependent evolution from many trajectories without pre-knowledge of reaction pathway of excited state reactions. This opens a very interesting research topic in the future.