Adapting reservoir computing to solve the Schrödinger equation

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Reservoir computing is a machine learning algorithm that excels at predicting the evolution of time series, in particular, dynamical systems. Moreover, it has also shown superb performance at solving partial differential equations such as chaotic time series prediction [1]. In the field of quantum chemistry, machine learning methods are proving to have advantages over the standard computational chemistry approaches [2, 3] , especially in the case of high-dimensional systems.

In this work, we aim to use RC to propagate wave packets with time, that is, to solve the time-dependent Schrödinger equation in continuous quantum systems. To do so, the RC model needs to be adapted to work with wavefunctions, which are complex-valued high-dimensional matrices. We adapted the regularized linear model to complex data by extending the ridge regression to the complex domain. We also propose here a new learning strategy that allows propagating wavefunctions while reducing the overfitting of the training data. Such learning strategy consists of a two-step training of the readout layer, where the reservoir is shown how predicting unseen data affects the evolution of the internal states. The learning algorithm is adapted to prevent fast error propagation during the test phase. The algorithm to train the Multi-setp RC model is schematically depicted in Fig. 1.

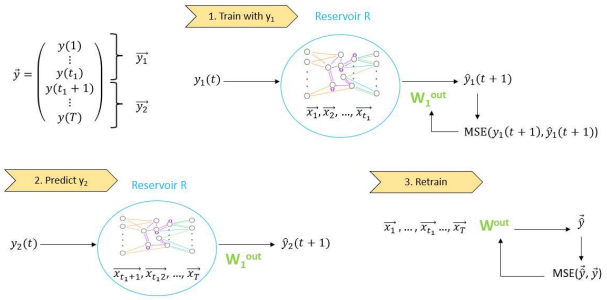

Fig. 1. Architecture of multi-step training of the reservoir computing model.

As an illustration, we have applied our method to four quantum systems: three 1D systems and one 2D system. The 1D systems include the harmonic oscillator, the Morse potential and a polynomial potential. The 2D system is a 2D harmonic oscillator. It is observed that the mean squared error of the propagated wavefunctions increases slower with time when using multi-step learning. This fact is critical in the 2D system, (see Fig. 2) which has higher-dimensional data, this leading to more overfitting. In this case, the standard RC model was not able to correctly reproduce the eigenenergies of the system, while the multi-step learning could. Moreover, the multi-step learning RC also allowed to recover the eigenfunctions of all the quantum systems, proving that the method can correctly predict the time evolution of the wavepackets and the corresponding eigenstates.

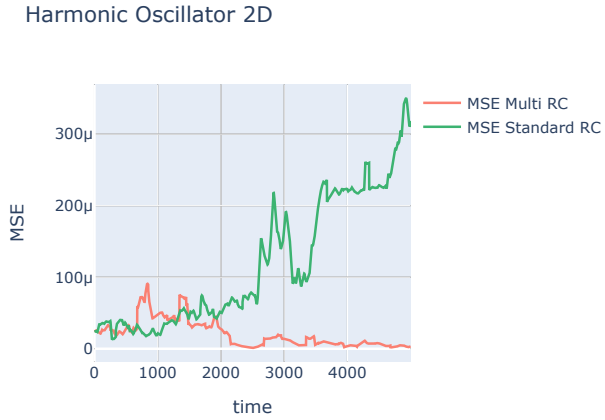

Fig. 2. Time evolution of the mean square error (MSE) of the 2D harmonic oscillator wavefunctions for the standard RC and the multi-step RC.

Once the efficiency of our multi-step RC has been proved, the present work can be extended by application to other interesting problems. This future work could include, among others, the application to more complex and realistic quantum systems, the computation of eigenstates in a high lying energy window [5], or the calculation of the so-called scarred functions [4] that play a very important role in the field of quantum chaos.

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