A physics-inspired neural network combined with a library-search algorithm in inverse problems of Schrödinger equation

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In this work, we solve inverse problems of a Schrödinger equation that can be formulated as a learning process of a convolutional neural network combined with a special projection technique which is called a library-search algorithm. The Schrödinger equation is $i\frac{\partial\psi}{\partial t} - \beta\frac{\partial^2\psi}{\partial x^2} + \gamma|\psi|^2\psi + V(x)\psi = 0$, where the wave function $\psi(x,t)$ is the solution to the forward problem and the potential $V(x)$ is the quantity of interest of the inverse problem. The main contributions of this work come from two aspects. First, we construct a special neural network directly from the Schrödinger equation, which is motivated by a splitting method. The physics behind the construction enhances the explainability of the neural network. In particular, each convolution layer and activation function correspond to different parts of the equation, which can be a useful guild when we train the network. Under this construction, it can be rigorously proved that the neural network has a convergence rate with respect to the length of input data and number of layers. The other part is using a library-search algorithm to project the solution space of the inverse problem to a lower-dimensional space. The motivation of this part is to alleviate the training burden in estimating functions. Instead, with a well-chosen library, we can greatly simplify the training process. More specifically, in one of the experiments, we analysis the landscape of the loss function with respect to the training parameters to easily obtain the optimal solution to the inverse problem. A brief version of analysis is given, which is focused on the well-possedness of some mentioned inverse problems and convergence of the neural network approximation. To show the effectiveness of the proposed method, we explore in some representative problems including simple equations and a couple equation. The results can well verify the theory part. In the future, we can further explore manifold learning to enhance the approximation effect of the library-search algorithm.