

Deep Neural Network Approaches for Computing the Defocusing Action Ground State of Nonlinear Schrödinger Equation

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Abstract. The defocusing action ground state of the nonlinear Schrödinger equation can be characterized via three different but equivalent minimization formulations. In this work, we propose some deep neural network (DNN) approaches to compute the action ground state through the three formulations. We first consider the unconstrained formulation, where we propose the DNN with a shift layer and demonstrate its necessity towards finding the correct ground state. The other two formulations involve the L^{p+1} -normalization or the Nehari manifold constraint. We enforce them as hard constraints into the networks by further proposing a normalization layer or a projection layer to the DNN. Our DNNs can then be trained in an unconstrained and unsupervised manner. Systematical numerical experiments are conducted to demonstrate the effectiveness and superiority of the approaches.

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1 Introduction

The nonlinear Schrödinger equation (NLS) is widely applied in fields such as quantum physics, nonlinear optics, fluid dynamics, and plasma physics [3, 7, 11, 15, 16, 19, 40, 43, 44, 49, 51, 54]. Under the influence of an external potential field, the NLS equation reads as:

$$i\partial_t\psi(\mathbf{x},t)=-\frac{1}{2}\Delta\psi(\mathbf{x},t)+V(\mathbf{x})\psi(\mathbf{x},t)+\beta|\psi(\mathbf{x},t)|^{p-1}\psi(\mathbf{x},t), \quad t>0, \quad (1.1a)$$

$$\mathbf{x}=(x_1,\cdots,x_d)^\top\in\mathbb{R}^d, \quad (1.1b)$$

where $\beta\in\mathbb{R}$ and $p>1$ are given parameters, $\psi(\mathbf{x},t):\mathbb{R}^d\times\mathbb{R}\rightarrow\mathbb{C}$ is the unknown complex-valued wave function. Here, $V(\mathbf{x})$ is a real-valued potential function. A commonly employed example of such a potential is the harmonic oscillator potential, defined as

$$V(\mathbf{x})=\frac{1}{2}\sum_{j=1}^d\gamma_j^2x_j^2 \quad \text{with} \quad \gamma_j\geq 0.$$

The parameter β characterizes the strength of the nonlinear self-interaction, with $\beta>0$ corresponding to a defocusing interaction and $\beta<0$ corresponding to a focusing interaction. The standing wave/stationary solution of the NLS equation (1.1) is considered key quantities for understanding the evolution of wave systems. By setting $\psi(\mathbf{x},t)=e^{i\omega t}\phi(\mathbf{x})$ in (1.1), the stationary solution $\phi(x)$ satisfies the following elliptic equation:

$$-\frac{1}{2}\Delta\phi(\mathbf{x})+V(\mathbf{x})\phi(\mathbf{x})+\beta|\phi(\mathbf{x})|^{p-1}\phi(\mathbf{x})+\omega\phi(\mathbf{x})=0, \quad \mathbf{x}\in\mathbb{R}^d, \quad (1.2)$$

where $\omega\in\mathbb{R}$ represents the given chemical potential. In fact, there can be infinitely many nontrivial solutions ($\phi(\mathbf{x})\not\equiv 0$) that satisfy (1.2) [12, 50]. Among these non-trivial solutions, the one that minimizes the *action functional*

$$S_\omega(\phi):=\frac{1}{2}\|\nabla\phi\|_{L^2}^2+\int_{\mathbb{R}^d}V|\phi|^2d\mathbf{x}+\frac{2\beta}{p+1}\|\phi\|_{L^{p+1}}^{p+1}+\omega\|\phi\|_{L^2}^2 \quad (1.3)$$

is referred to as the *action ground state*, denoted by ϕ_g [11, 12].

The action ground state is of great importance in mathematical and physical studies [4, 11, 15, 19, 24, 25, 37, 38, 53]. Particularly, it is needed in the computations of the multichannel dynamics in NLS [47–49]. Also, the recent works [22, 30, 37] reveal its non-equivalence with the energy ground state, making its computation to own more independent interests. It can be rigorously defined as follows. Note that