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A New Artificial Neural Network Method for Solving Schrödinger Equations on Unbounded Domains

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Abstract. The simulation for particle or soliton propagation based on linear or nonlinear Schrödinger equations on unbounded domains requires the computational domain to be bounded, and therefore, a special boundary treatment such as an absorbing boundary condition (ABC) or a perfectly matched layer (PML) is needed so that the reflections of outgoing waves at the boundary can be minimized in order to prevent the destruction of the simulation. This article presents a new artificial neural network (ANN) method for solving linear and nonlinear Schrödinger equations on unbounded domains. In particular, this method randomly selects training points only from the bounded computational space-time domain, and the loss function involves only the initial condition and the Schrödinger equation itself in the computational domain without any boundary conditions. Moreover, unlike standard ANN methods that calculate gradients using expensive automatic differentiation, this method uses accurate finite-difference approximations for the physical gradients in the Schrödinger equation. In addition, a Metropolis-Hastings algorithm is implemented for preferentially selecting regions of high loss in the computational domain allowing for the use of fewer training points in each batch. As such, the present training method uses fewer training points and less computation time for convergence of the loss function as compared with the standard ANN methods. This new ANN method is illustrated using three examples.

AMS subject classifications: 65N06, 65N12

Key words: Linear and nonlinear Schrödinger equations, artificial neural network method, convergence, soliton and particle propagations.

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1 Introduction

The linear and nonlinear Schrödinger equations (SE) in an unbounded domain can be expressed in a composite equation as follows:

$$i\frac{\partial u}{\partial t}(x,t)+\frac{1}{2}\frac{\partial^2 u}{\partial x^2}(x,t)-\left[V+\lambda|u(x,t)|^2\right]u(x,t)=0,\quad -\infty<x<\infty,\quad t>0, \tag{1.1a}$$

$$u(x,0)=u_0(x),\quad -\infty<x<\infty, \tag{1.1b}$$

$$\lim_{x\to\pm\infty}u(x,t)=0,\quad t>0, \tag{1.1c}$$

where $i=\sqrt{-1}$, $u=u(x,t)$ is a complex-valued scalar field, $V=V(x,t)$ is a linear potential, the nonlinear coupling constant λ is a real number, u_0 is the initial condition. The linear SE corresponds to the case where $\lambda=0$ while the nonlinear SE corresponds to the case where $V=0$.

It is well-known that for $V=0$ and $\lambda=0$, the SE exhibits dispersive wave packet solutions of the form

$$u(x,t)=\left(\frac{2}{\pi\sigma^2}\right)^{\frac{1}{4}}e^{-(x-k_0t)^2/\sigma^2}e^{i(kx-\omega t-\phi)}, \tag{1.2}$$

where the time-dependent width is determined by $\sigma=\sqrt{1+4t^2}$, k_0 is some initial wave number, $k=\frac{k_0+2tx}{1+4t^2}$ is the effective wave number, $\omega=\frac{1}{2}\frac{k_0^2}{1+4t^2}$ is the effective frequency, and $\phi=\frac{1}{2}\arctan(2t)$ is a time dependent phase shift. For $V=0$ and $\lambda<0$, the SE exhibits bright soliton behavior of the form

$$u(x,t)=A\text{sech}(a(x-vt))e^{i(kx-\omega t)}, \tag{1.3}$$

where $a=A\sqrt{|\lambda|}$, $v=k$, and $\omega=\frac{1}{2}(k^2+A^2\lambda)$. For $V=0$ and $\lambda>0$, the SE exhibits dark soliton behavior of the form

$$u(x,t)=A\tanh(a(x-vt)+i)e^{i(kx-\omega t)}, \tag{1.4}$$

where $a=A\sqrt{\lambda}$, $v=k+A\sqrt{\lambda}$, and $\omega=\frac{1}{2}k^2+2A^2\lambda$.

The simulation for particle/soliton propagations based on the above linear/nonlinear Schrödinger equations on unbounded domains requires the computational domain to be bounded. Within the bounded computational domain, there are many traditional computational methods for solving the above linear and nonlinear SEs, including finite difference methods [8, 28, 29, 31, 41, 44, 46, 47], finite element methods [16, 17], split-step methods [49], and pseudo-spectral methods [11], etc. However, if these numerical methods are used without imposing proper boundary conditions, outgoing waves would reflect back into the computational domain and destroy the simulation. To resolve this trouble,