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Neural network approach for the calculation of potential coefficients in quantum mechanics

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ABSTRACT

A numerical method based on artificial neural networks is used to solve the inverse Schrödinger equation for a multi-parameter class of potentials. First, the finite element method was used to solve repeatedly the direct problem for different parametrizations of the chosen potential function. Then, using the attainable eigenvalues as a training set of the direct radial basis neural network a map of new eigenvalues was obtained. This relationship was later inverted and refined by training an inverse radial basis neural network, allowing the calculation of the unknown parameters and therefore estimating the potential function. Three numerical examples are presented in order to prove the effectiveness of the method. The results show that the method proposed has the advantage to use less computational resources without a significant accuracy loss.

1. Introduction

As known the Schrödinger equation is a partial differential equation developed during the first quarter of the 20th century and its a fundamental part of the quantum mechanics theory. Roughly speaking this equation describes the behavior of a system under the influence of different potentials, and one of the main goals is to find the dynamics of the system determined uniquely by the eigenvalues and eigenvectors. In the following we will review briefly the usage of numerical methods to solve the Schrödinger equation and in particular the use of neural networks.

In general, only in limited cases exact analytic solutions can be obtained, for example the free particle, linear harmonic oscillator or the hydrogen atom. On the other hand, there exist a number of useful approximation methods for more general hamiltonians, such as perturbation methods or the Wentzel–Kramers–Brillouin (WKB) method. Another well established methods for solving numerically the Schrödinger equation, are the ones based in variations of the Numerov's method, as shown in (Pillai et al. [1]) where the wave function is discretized over a lattice. However, to our best knowledge, when applied to practical physical problems, these methods have turn out to be less successful.

In (Braun et al.) [2], the Lanczos method is applied, on a grid, for obtaining eigensolutions of quantum systems. This methodology is used to solve one-, two-, and three-dimensional quantum problems. In (Ishikawa [3]) a numerical method is proposed in order to solve accurately the eigenvalue problem in quantum mechanics. In this case the efficiency is proved through the applications to the harmonic oscillator, in which they achieved 15-digit accuracy with double precision operations. In (Kannan and Masud [4]) two methods are presented in order to stabilize the Schrödinger wave equations, the first one consisting in a Garlekin/least-squares method, whose consistency and convergence was analyzed through potentials which have known analytic solutions. In (Watanabe and Tsukada [5]) the wave function evolution in a magnetic field is analyzed using a numerical method based on the finite elements, improving the accuracy without increasing the computational cost. Among other schemes proposed for solving numerically the Schrödinger equation it can be mentioned the study done by (Simos and Williams [6]) where they use a method based on phase-lag minimization in order to compute the eigenvalues, the method was tested in two types of potentials, an even function with respect of a one dimensional domain, and a general case of the Morse potential.

Other applications of ANN in partial differential equations can be found in (Ossandón and Reyes [7]) and (Ossandón et al. [8]), where the inverse eigenvalue problems for the linear elasticity operator and for the anisotropic Laplace operator are solved respectively. In (Poggio et al. [9]) it is shown that the ill-posed

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problem of function approximation through sparse data can be regularized using an appropriate class of approximation functions.

However, the ANNs have been less explored in quantum mechanics. Some works in this direction are given in (Lagaris et al. [10]), where a feedforward Artificial Neural Network (ANN) is used to find the eigenvalues of integro-differential operators, using the analytic solutions to test the accuracy of the solutions. In this case the neural network proved to be highly accurate, robust and efficient. Another use for the feedforward neural network can be seen in (Shirvany et al. [11]), where an energy term is derived from the boundary conditions which allows to use an unsupervised neural network to solve the equations, also the results given by the neural network were compared with the analytic solutions.

In the present work, our goal is to study the recovering of coefficients associated to the potential function through a finite set of eigenvalues in the quantum system. We assume that the function between the eigenvalues and the potential coefficients is smooth in the sense that two similar inputs correspond to two similar outputs. We emphasize that the error of any designed ANNs cannot have a better performance than the technique used to create the training data. As a consequence, the performance of any ANN is directly related to the training data. In general, all the computation process used by the neural networks, including the training, validation and simulation process, has lower computational time than the finite element method.

Hence, the main issue of this proposed study is to solve the inverse problem associated to the Schrödinger equation, that is to say, calculate a set of coefficients associated to a potential function, through eigenvalues of the Schrödinger operator using ANNs. The ANN proposed is a multilayered Radial-Basis Function (RBF) network (see Ossandón and Reyes [7] and Ossandón et al. [8]). As discussed in (Schilling et al. [12]), a RBF ANN can approximate a function f using nonlinear functions which provides the best fit to the training data. An evaluation of the performance (computational time and accuracy) of the ANN methodology proposed will be done, comparing the results to a classical numerical method based on FEM.

The article is organized as follows. In Section 2, we give an introduction to the eigenvalue problem in quantum mechanics. In Section 3, we present the solution to the direct and inverse problem associated to the calculation of the eigenvalues of the time-independent Schrödinger equation. Numerical results and discussion are given in Section 4. Finally, in Section 5, the conclusions of this work are presented.

2. Eigenvalue problem in quantum mechanics

Let $\Omega \subset \mathbb{R}^k$ $(k \geqslant 1)$ be a nonempty, open, connected and bounded domain, with a Lipschitz-continuous boundary $\Gamma := \partial\Omega$. The unit normal vector pointing to the exterior of Ω is denoted by $\boldsymbol{n} = (n_1, n_2, \ldots, n_k)^T \in \mathbb{R}^k$ and $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)^T \in \mathbb{R}^k$.

Let $\widehat{\Lambda}$ be an observable associated to a physical quantity Λ. Let us say that ψ_γ is an eigenfunction of this operator, and λ_γ its associated eigenvalue, if $\psi_\gamma \neq 0$ and

$$\begin{cases} \widehat{\Lambda} \cdot \psi_\gamma = \lambda_\gamma \psi_\gamma & \text{in} \quad \Omega, \\ \psi_\gamma = 0 & \text{on} \quad \Gamma. \end{cases} \tag{1}$$

It is worth noting that the eigenvalues of a hermitian operator lie in the real line. Indeed, if we multiply Eq. (1) by ψ_γ^* and integrate in Ω, we obtain

$$\lambda_\gamma = \frac{\int \psi_\gamma^*(\boldsymbol{x})[\widehat{\Lambda}\psi_\gamma(\boldsymbol{x})]d\boldsymbol{x}}{\int |\psi_\gamma(\boldsymbol{x})|^2 d\boldsymbol{x}} \tag{2}$$

which is real.

In the case that the observable $\widehat{\Lambda}$ is the hamiltonian operator $\widehat{H} = -\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{x}) + V(\boldsymbol{x}, \boldsymbol{\theta})$, we have the well known time-independent Schrödinger equation $\widehat{H}\psi_\gamma(\boldsymbol{x}) = E_\gamma \psi_\gamma(\boldsymbol{x})$. In this equation $\hbar$ is the Planck's constant, m is the mass associated to the quantum system, and $V(\boldsymbol{x}, \boldsymbol{\theta})$ is the potential function, coming from the potential energy and, in our case, depending on a set of coefficients grouped in the vector $\boldsymbol{\theta} \in \mathbb{R}^l$, $l \geqslant 1$. Thus the energy E_γ is an eigenvalue, and $\psi_\gamma(\boldsymbol{x})$ its related eigenfunction, associated to the hamiltonian operator $\widehat{H}$.

3. The direct and inverse problems

3.1. The direct problem

From now on let us consider only two and three dimensional bounded domains, i.e. $k = 2$ or 3. In addition let us suppose that $V(\cdot, \boldsymbol{\theta}) \in L^\infty(\Omega)$, $V(\boldsymbol{x}, \boldsymbol{\theta}) \geqslant V_0 > 0$ for a.e. $x \in \Omega$ and $\forall \theta \in \mathbb{R}^l$. Our main goal is to solve the following eigenvalue problem:

Find $E \in \mathbb{R}$ and functions $\psi(\boldsymbol{x}) \not\equiv 0$ which are solution of

$$\begin{cases} -\dfrac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{x}, \boldsymbol{\theta})\psi = E\,\psi & \text{in} \quad \Omega, \\ \psi = 0 & \text{on} \quad \Gamma. \end{cases} \tag{3}$$

As known (see [13]) the only non-null solutions of Eqs. (3) are a pair sequence $\{(E_j, \psi_j)\}_{j\geqslant 1}$ of eigenvalues and eigenfunctions.

We define the following function $\mathcal{S}_{\overline{\Omega},N}$ associated to Eq. (3):

$$\mathcal{S}_{\overline{\Omega},N} : \mathbb{R}^l \to \mathbb{R}^N, \quad \overrightarrow{\boldsymbol{E}} := (E_1, E_2, \ldots, E_N)^{\mathbf{T}} = \mathcal{S}_{\overline{\Omega},N}(\boldsymbol{\theta}). \tag{4}$$

Given the values of the coefficients $\boldsymbol{\theta} \in \mathbb{R}^l$, the potential $V(\boldsymbol{x}, \boldsymbol{\theta})$ is completely well determined and consequently $\mathcal{S}_{\overline{\Omega},N}$ $(N \in \mathbb{N})$, for each domain Ω with regular boundary Γ, solves the direct problem associated to boundary-value problem (3), calculating the first N eigenvalues of the Schrödinger operator.

Let us define the functional space

$$\mathcal{V} = H_0^1(\Omega) = \left\{ v \in H^1(\Omega); \quad v = 0 \quad \text{on} \quad \Gamma \right\}, \tag{5}$$

equipped with the usual norm $\|v\|_{1,\Omega}^2 = \int_\Omega |\nabla v|^2 dx + \int_\Omega |v|^2 dx$.

Thus the eigenvalue problem for Schrödinger equation with homogeneous boundary conditions can be formulated as (weak formulation):

Find $(E, \psi) \in (\mathbb{R}, \mathcal{V})$ *such that*

$$a_{\boldsymbol{\theta}}(u, v) = E\,(u, v)_{0,\Omega} \qquad \forall v \in \mathcal{V} \tag{6}$$

where

$$a_{\boldsymbol{\theta}}(u, v) := \frac{\hbar^2}{2m}\int_\Omega \nabla u \cdot \nabla v dx + \int_\Omega V(\boldsymbol{x}, \boldsymbol{\theta}) uv dx \quad \text{and} \quad (u, v)_{0,\Omega} = \int_\Omega uv dx. \tag{7}$$

It is worth noting that the wellposedness of the discrete form of (6) can be guaranteed by the fact that the corresponding approximation space satisfies the Babuska–Brezzi condition (see [13–17] and [18]). Let $\{\mathcal{T}_h\}_{h>0}$ be a regular family of triangulations of Ω, made up of triangles T of diameter h_T, such that $h := \sup\{h_T | T \in \mathcal{T}_h\}$ and $\overline{\Omega} = \bigcup\{T : T \in \mathcal{T}_h\}$. In association with the mesh $\mathcal{T}_h$, let us select the finite element space $\mathcal{V}_h \subset \mathcal{V}$ of the continuous functions in Ω which are piecewise polynomials $\mathbb{P}_j$ of degree j, with $j \geq 1$, in each triangle $T \in \mathcal{T}_h$.

Let $(E_h, u_h) \in (\mathbb{R}, \mathcal{V}_h)$ be the eigenpair solution to the discrete form of (6). It is well known that the Rayleigh quotient for each eigenvalue E_h is given by:

$$E_h = \frac{a_{\boldsymbol{\theta}}(u_h, u_h)}{(u_h, u_h)_{0,\Omega}}. \tag{8}$$

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