Approximating Ground State Energies and Wave Functions of Physical Systems with Neural Networks

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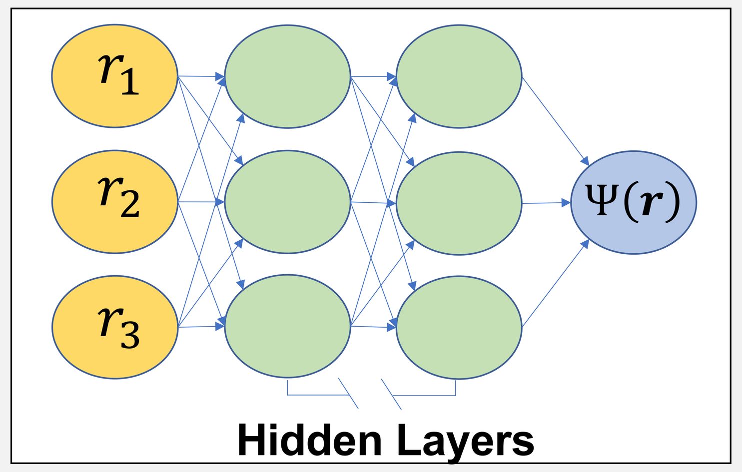
NEURAL INFORMATION PROCESSING SYSTEMS

Introduction

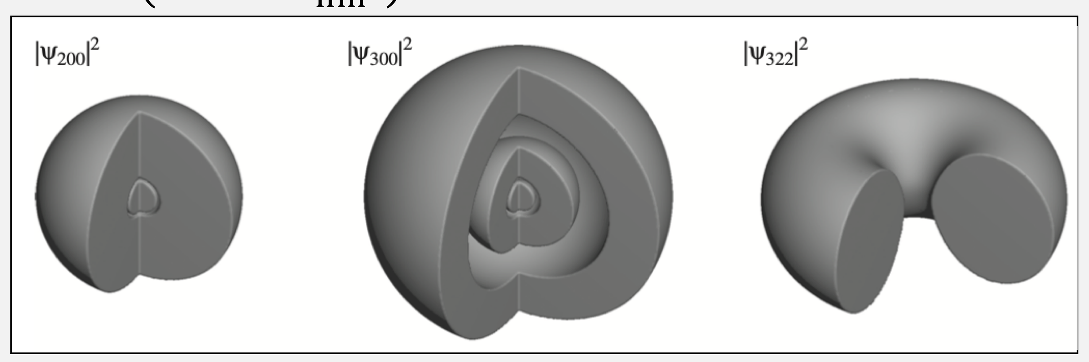
We propose using DNN, in an end-to-end deep learning approach, to directly model the wavefunction ansatz in a variational optimization scheme for approximating the ground state energies and wave functions of quantum mechanical systems.



Quantum Mechanical Systems

The state of a quantum mechanical system is given by a wave function. It obeys Schrödinger's equation and the modulus square gives the probability of the measurement of an observable at any given time.

Example: Electron density for hydrogen wave functions $\left(|\Psi|^2 > \frac{0.25}{nm^3}\right)$.

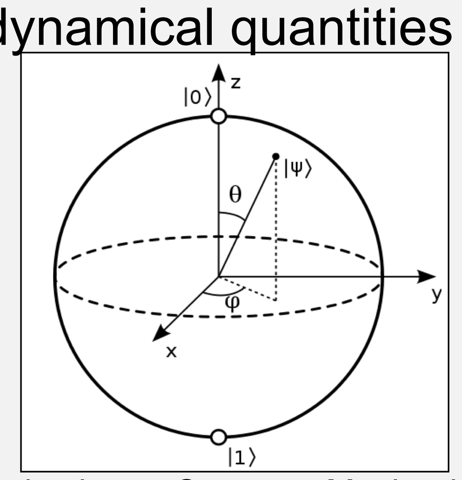


Observables

- Quantities of a physical systems that can be measured
- Mathematically represented by Hermitian operators
- Combination of position and momentum operators
- **Example**: Kinetic or angular momentum, energy, spin

Wave Functions $|\Psi\rangle$

- Abstract vector in a complex Hilbert space
- Access to the wave function of a physical system provides full knowledge of all dynamical quantities
- **Example**: Spin states in a complex 2 dimensional Hilbert space



1. David J. Griffiths and Darrell F. Schroeter. Introduction to Quantum Mechanics. Cambridge University Press, 3 edition, 2018.

TISE

Time Independent Schrödinger Equation (TISE)

$$\mathbf{H}|\Psi\rangle = \mathrm{E}|\Psi\rangle$$

- Hamiltonian operator, H
- Energy (real valued), E
- Eigenvalue problem

Hamiltonian

$$\mathbf{H} = \mathbf{T} + \mathbf{V} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2}{\partial x^2} + \mathrm{V(x)}$$

- Energy operator
- Equal to the sum of the kinetic energy $\mathbf{T}$ and potential energy $\mathbf{V}$ operators
- Describes a physical system in quantum theory

Objective Function

The Variational Principle

The expectation value of the Hamiltonian for an arbitrary state $|\Psi_{\mathrm{trial}}\rangle$ is greater than or equal to the ground state energy of the system.

$$\frac{\langle \Psi_{\mathrm{trial}}|\mathbf{H}|\Psi_{\mathrm{trial}}\rangle}{\langle \Psi_{\mathrm{trial}}|\Psi_{\mathrm{trial}}\rangle} \geq \mathrm{E}_{\mathrm{Ground\ state}}$$

Expectation value of Hamiltonian

$$\langle \mathrm{E}\rangle = \frac{\langle \Psi|\mathbf{H}|\Psi\rangle}{\langle \Psi|\Psi\rangle} = \frac{\sum_{i,j}\langle \Psi|\mathrm{b_i}\rangle\langle \mathrm{b_i}|\mathbf{H}|\mathrm{b_j}\rangle\langle \mathrm{b_j}|\Psi\rangle}{\sum_i|\langle \mathrm{b_i}|\Psi\rangle|^2}$$

- **Objective Function**
- Approximate $\mathrm{E}_{\mathrm{Ground\ state}}$ and $|\Psi_{\mathrm{Ground\ state}}\rangle$ by optimizing DNN wavefunction to minimize $\langle \mathrm{E}\rangle$
- Works for finite and Infinite dimensional Hilbert Spaces

Challenges

- Applying Hamiltonian to DNN wave function ansatz
- Infinite dimensional Hilbert space
- Multidimensional Integrals in function decomposition

Our Approach

- Use DNN to model a wave function and output its value
- Use basis of a finite subspace as the computational basis.
- Decompose DNN wave function onto computational basis using Riemann approximations and compute a matrix of $\langle \mathrm{H}\rangle$ using the basis

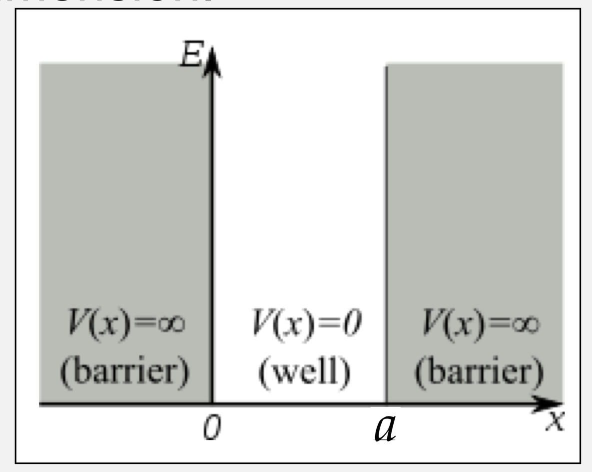
Experiments

Single particle quantum systems in 1 dimension.

Particle In a Box

Potential: $\mathrm{V}(x) = \begin{cases} 0, & 0 < x < \mathrm{a} \\ \infty, & \text{otherwise} \end{cases}$ well width, a

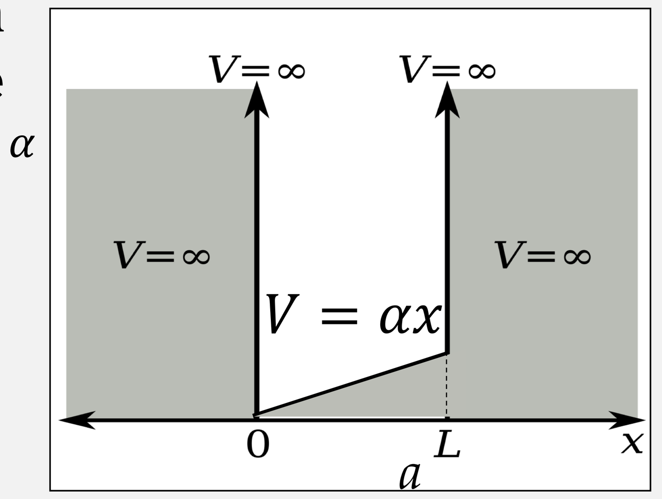
Hamiltonian: $\mathbf{H} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2}{\partial x^2}$



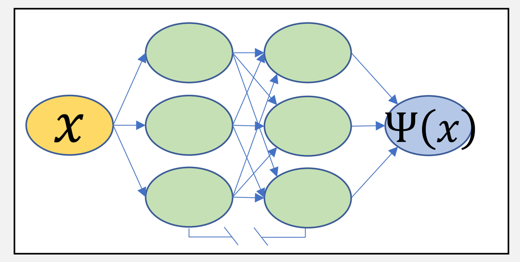
Perturbed Particle In a Box

Potential: $\mathrm{V}(x) = \begin{cases} \alpha x, & 0 < x < \mathrm{a} \\ \infty, & \text{otherwise} \end{cases}$ Perturbation constant, α

Hamiltonian: $\mathbf{H} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2}{\partial x^2} + \alpha x$

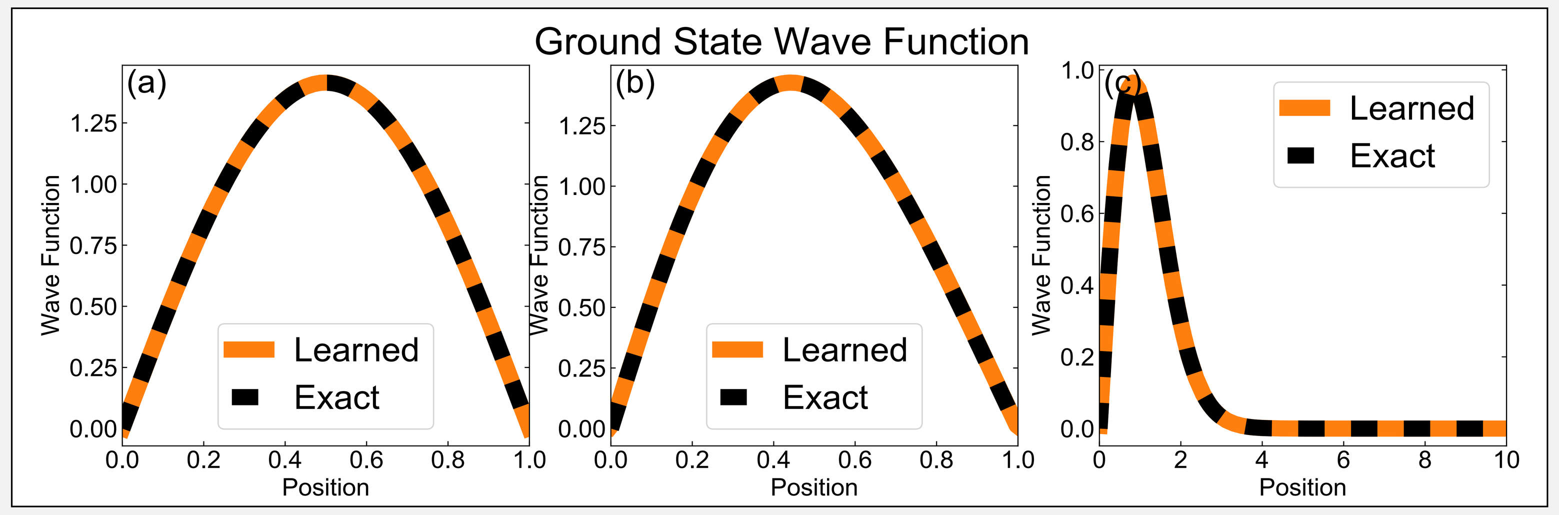


DNN Wave Function



Results

Wave Functions



Ground State Energies

Table 1: Ground state energies

System	$E_{\mathrm{ground\ state}}$ Computed	VMC[2]	Exact
Unperturbed	4.93484	4.9348	4.93480
Perturbed A	8.79510	8.7960	8.79507
Perturbed B	2.94583	NA	2.94583

- a) Unperturbed system
- b) Perturbed system A: $\mathrm{a} = 1$, $\alpha = 8$
- c) Perturbed system B: $\mathrm{a} = 10$, $\alpha = 2$

Challenges and Future Work

- Incorporating physical constraints to DNN wave function
- Extending to high dimensional systems
- Exploring other orthonormal computational basis

2. Teng Peiyuan. Machine learning quantum mechanics: solving quantum mechanics problems using radial basis function network. Phys. Rev. E, 98(033305), 2018.