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Neural Network in Schrodinger Equation with Deep Learning

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Abstract

The development of machine learning (ML) and artificial intelligence (AI) has elevated scientific research and studies, including physics, to new levels. the creation of animated visual simulations of the physical processes under study, powered by machine learning and neural network algorithms, which transform abstract theories and equations into clear and captivating visual representations of those phenomena. This paper aims to show how computational models can bridge the gap between the practical, educational uses of theoretical physics and its pure form. The simulation deals with solving and displaying the time-independent Schrödinger equation are presented in this study. This tool makes it easy to comprehend quantum behavior in constrained systems by showing potential wells, energy levels, and wave functions. Through the integration of mathematical datasets and physical limitations into a Python-based framework, this simulation employed machine learning and neural networks to handle massive amounts of data and solve intricate, mathematically stated equations that were previously believed to be beyond computing. By integrating physics-informed neural networks (PINNs), machine learning algorithms were utilized to solve the wave equation numerically for the Schrödinger equation simulation, providing a precise depiction of the quantum states.

Keywords: Neural Network in Physics, Machine Learning, Deep Learning, Quantum Mechanics, Artificial Intelligence.

Introduction

The most recent technologies for simulating and processing massive amounts of data and accurately solving intricate, mathematically specified equations are machine learning (ML) and neural networks (NN) [1, 2, 3]. Neural network feed forward and convolution architectures were employed to anticipate behavior based on input parameters and to approximate solutions [4,5]. Artificial intelligence (AI) and its models are becoming more and more prevalent in practically every aspect of life [6,7,8,9]. Through the integration of physical restrictions and mathematical datasets into a Python-based framework, these models made it possible to depict phenomena dynamically.

The basis for applying machine learning to physics is still supervised and unsupervised learning. CNN has been used, for example, to categorize phase transitions in physical systems [10]. In fact, it outperforms the conventional Monte Carlo approaches in terms of accuracy and performance [11, 12]. Similarly, it has been demonstrated that the use of deep reinforcement learning to improve quantum control protocols can solve optimization problems in quantum mechanics. Another review explores the evolution of machine learning in physics through dropout and regulation strategies that will help to enhance physics models. Effective methods that support the modeling of complex systems include random forests, neural networks, and cross validation. [13]. Computational techniques for comprehending and simulating complex systems have been transformed by the convergence of physics and machine learning. In any field, machine learning technologies have become strong substitutes for conventional numerical methods, providing both efficiency and novel insights [14].

Role of Physics Informed Machine Learning (PIML)

In the PIML framework, neural networks are trained and their architecture is influenced by physical rules to improve prediction in dynamic systems. In order to achieve strong generalization across datasets, sophisticated models take advantage of symmetry restrictions.

PDEs and BCs are incorporated into ML models via PIML. While PIML incorporates the knowledge of physical restrictions directly into the model design, standard techniques consider data as separate entities. As demonstrated by applications in fluid dynamics, structural mechanics, and plasma physics, this allows for reasonably accurate predictions with small amounts of data [13,15,16]. For instance, in the multi-physics problem, PIML may concurrently address stochastic processes and coupled systems [17]. In the meantime, it can effectively increase its generalization capability for different datasets by implementing symmetry restrictions such translation invariance [18].

The simulations' accuracy, scalability, and adaptability for educational purposes are guaranteed using machine learning and neural networks. Machine learning models are set to become increasingly significant in quantum physics and education as they get more sophisticated. It is anticipated that hybrid models that combine data-driven methodologies with limitations guided by physics would further enhance accuracy and interpretability. Furthermore, it is anticipated that developments in AI and quantum computing would enable simulations of hitherto unheard-of complexity, changing physics research and teaching [7,19].

Neural networks and machine learning have revolutionized physics by enabling the modeling of intricate systems and ideas that were previously thought to be incomprehensible. In order to simulate the Schrödinger equation, machine learning algorithms were utilized to numerically solve the wave equation while accurately visualizing the quantum states. Accuracy and interpretability were provided by the simulation's adherence to the fundamental laws regulating the system through the use of PINNs [11].

Role of Quantum Machine Learning (QML)

The intersection of quantum computing and traditional machine learning (CML) approaches is known as QML. Quantum neural networks and other hybrid quantum-classical models use quantum algorithms to handle issues that are beyond the scope of classical methods [10]. Applications of QML include error correction, quantum dynamics simulation, and quantum state tomography [20]. ML is useful in quantum physics for applications like quantum error correction and state tomography. In particular, QNNs show promise in bridging the gap between quantum hardware and classical algorithms.

Despite these advancements, there are still obstacles in applying machine learning to real-world situations, which calls for further study on adaptable algorithms and interdisciplinary approaches [11]. The creation of quantum-enhanced unsupervised learning for the identification of quantum states and the optimization of their representation in classical-quantum hybrid systems is one example. Certain computational barriers for quantum technology may be resolved by such advancements [20,21]. Quantum many body states with substantial entanglement are demonstrated to outperform conventional tensor-network techniques using restricted Boltzmann machines (RBMs). The paper demonstrates how an RBM may effectively bridge machine learning and quantum physics by simulating quantum systems through reinforcement learning [20]. This led to the conclusion that neural networks are a useful tool for solving challenging quantum problems that might not be solved conventionally.

Role of Neural Networks in Quantum Physics

In quantum many-body physics, machine learning, particularly with restricted Boltzmann machines (RBMs) [20], can represent quantum many-body states and their entanglement features. Additionally, the work demonstrates that random RBM states have distinct spectrum features that differ from normal random pure state entanglement. Because of the intricate correlations in the wave function, the many-body issue in quantum physics is difficult. Using a variant representation of quantum states with neural networks, machine learning can reduce this complexity [21].

Another strategy is the application of reinforcement techniques, which have been shown to be effective in resolving challenging quantum mechanical issues [22]. Deep reinforcement learning is used to improve quantum control protocols in order to achieve this.

In quantum physics, reinforcement learning (RL) has proven a game-changer, particularly for modeling time evolution in quantum systems and finding ground states. For the equilibrium and dynamic features of one- and two-dimensional spin models, RL models have advanced to the state-of-the-art level through the exploration of ideal configurations and tactics [23]. Understanding phenomena like phase transitions and quantum entanglement requires the use of such applications.

A class of machine learning methods known as PINNs naturally incorporates the underlying physical rules into the model's training process in order to solve PDEs. In contrast to conventional numerical solvers, PINNs employ neural networks to approximate differential equation solutions while simultaneously meeting the boundary and initial conditions, rather than discretizing the domain on grids [11]. Because of their adaptability, PINNs are particularly attractive for complicated or high-dimensional systems, such those seen in quantum mechanics [21,22].

Machine Learning in Physics: Challenges & Future

Even though machine learning (ML) has shown a lot of promise in physics, there are still many problems to be resolved. The majority of tests are conducted in idealized settings that are not representative of reality. Applications of ML models are hampered by noise, experimental heterogeneity, and a lack of labeled data [23, 24]. To improve the resilience and application of models, researchers are looking into transfer learning, generative models, and adaptive algorithms [12]. Furthermore, high-dimensional data representations are frequently necessary due to the complexity of physical systems, which may lead to overfitting and computational inefficiencies. To address these problems, automatic machine learning (AutoML), cross-validation, and regularization are being developed [13].

The way machine learning (ML) in physics will connect theoretical knowledge with real-world implementation is its future. For example, quantum computation would be considerably enhanced for PIML integration in multi-physics problem solving. Since explainable AI, or xAI, offers interpretability and transparency in model predictions, its significance in physics has been growing. Hybrid frameworks created by fusing data-driven methods with limitations guided by physics are promising areas for further research [13]. It is also anticipated that these methods will lead to advances in material science, cosmology, and other fields.

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Methodology
Integrated Schrödinger Equation
The loss function's definition included the Schrödinger equation:

$$\mathcal{L} = \left\| -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) - E\psi(x) \right\|^2$$

Where $\psi(x)$, $V(x)$ and E represent the wavefunction, potential and energy eigenvalues respectively. In order to guarantee that the generated neural network approximates wave functions that satisfy the equation and its given boundary conditions, this loss function was selected.

Dataset Preparation, Architecture, Tools and Libraries
SchrodingerNet, a feed forward neural network, is used to represent the wave function ψ(x). This feed forward neural network that has input layer, hidden layers and output layer. The time-independent PyTorch and visualization tools are used to model Schrodinger's equation. For deep learning models, numerical data representation, visualizations, and animations, various libraries are utilized, including torch, numpy, matplotlib, and funcAnimation. Simulations utilizing deep learning, ML, neural networks like PINNs, and reinforcement approaches are configured with subsequent parameters.
The spatial domain for the quantum model has a defined range. With a set learning rate, training is carried out over a large number of epochs. The PyTorch framework for deep learning tasks is used to initialize the energy eigenvalues.
In machine learning, epochs represent the number of times the entire training dataset is passed through the model during training. For example, if you have 10 epochs, the model will see and learn from the entire dataset 10 times. In terms of the Schrodinger's equation, epochs represent how many times the neural network refines its prediction of the wave function to satisfy the Schrödinger equation for a given energy. Each epoch adjusts the model parameters to minimize errors, improving accuracy over time.

Simulating Time Independent Schrodinger's Equation using PINNs
One of the fundamentals of quantum physics is Schrodinger's equation. The equation's general principle controls how particles behave in quantum systems, and a quantum state of the system is currently evolving in both space and time. Analytical solutions are already available for straightforward issues like the harmonic oscillator, but there might not be many for more complicated potentials like the time-independent Schrodinger's equation. Numerical or approximative procedures are required in this situation. It is frequently necessary to quantize the domain and solve the extensive system of equations when using traditional numerical techniques like finite difference approaches. Neural networks, especially Physics informed neural networks (PINNs), provide an excellent substitute for this

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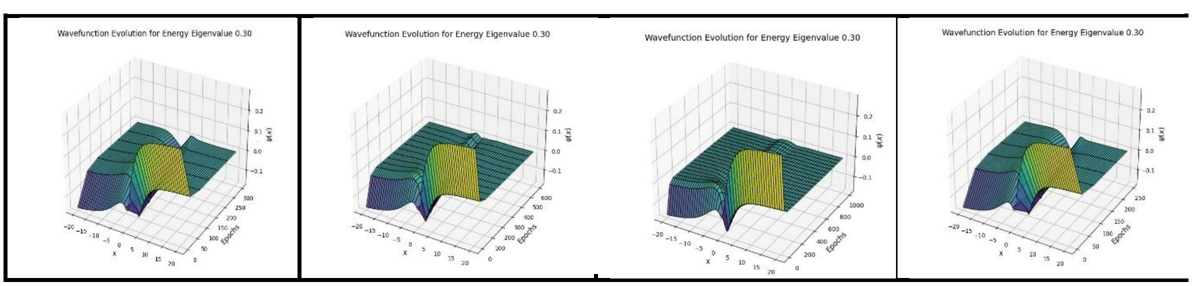
approach due to its potential computational complexity [4].
In order to enable the network to approximate solutions with exceptional efficiency and scalability, the governing equations are directly embedded into the loss function. In order to approximate the stationary solutions for a time-independent Schrodinger's equation for a harmonic oscillator potential $V(x) = 0.5x^2$, we have used a neural network in this study. This network is trained to guarantee adherence to the constraints of the equations and minimize a physics-informed loss. This network highlights the usefulness of neural networks in investigating the eigenstates and eigenvalues in quantum mechanics and shows how they may be used to solve differential equations. This method could be expanded to more complicated situations where it could be impossible to find analytical answers.

Discussion

Physics-Informed Neural Networks (PINNs) for the Simulation of Schrödinger's Equation: Coding

The fundamental concept of quantum mechanics that characterizes stationary states in quantum systems is the time-independent Schrödinger equation. However, it is difficult for academics and students to understand due to its mathematical complexity. In order to get around this, physics-informed neural networks (PINNs) were programmed to produce an animated visual representation that simplifies and makes sense of this equation. By turning abstract mathematics into a dynamic visual story, this method seeks to improve conceptual understanding in addition to computational correctness.
Using automatic differentiation for highly efficient computation of spatial and time derivatives, PINNs are coded in this study to simulate the wave-like model representing solutions to the Schrödinger equation. This ensures that the governing equation is satisfied at every point in the computational simulation domain. The simulation demonstrates the behavior of quantum particles by dynamically displaying wavefunctions fluctuating within potential wells.
Students can relate theoretical equations to real-world phenomena by using the animation's features, which include nodes, points of zero probability density, and the quantized energy levels connected to each wavefunction.



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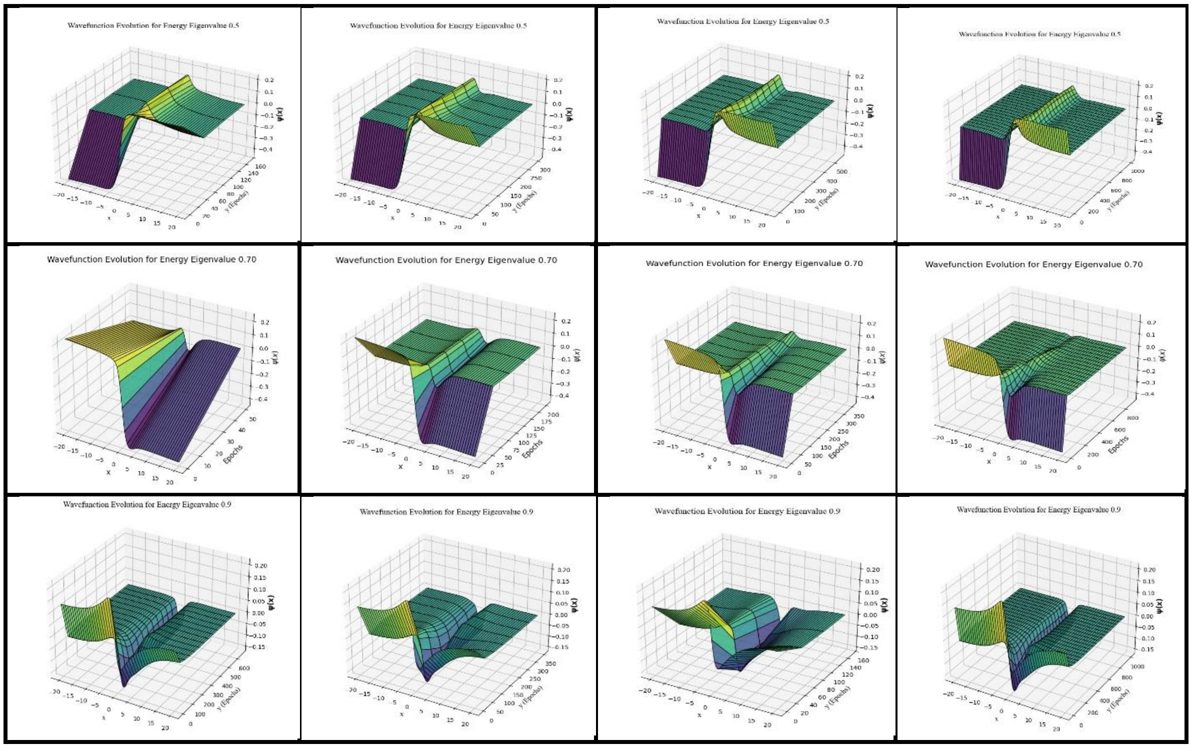

Fig. 1

Neural network is used in the simulation of these models for the evolution of wave functions of a particle for the same quantum harmonic oscillator potential $V(x) = 0.5x^2$, for different energy eigenvalues such as 0.30, 0.50, 0.70, and 0.90. Fig.1, represents four cases of each of these models (total 16 cases) for the evolution of wave functions of a particle for the same quantum harmonic oscillator potential $V(x) = 0.5x^2$, for different energy eigenvalues such as 0.30, 0.50, 0.70, and 0.90.These three-dimensional models are used to represent time-independent Schrodinger equation. They are discussed one by one.

$E = 0.30$, represents a low energy state with fewer nodes, e.g. 1 or 0, and decays slowly. This has a low probability density.

$E = 0.50$, represents a slightly higher energy level in which particle behavior significantly changes. This particle is easily found in the central region.

$E = 0.70$, represents higher energy state with more nodes, e.g. 2. The greater frequency, and higher probability density is needed to found the particle.

$E = 0.90$, represents higher energy than all previous cases and more nodes. This has higher frequency and more oscillations. The kinetic energy is high and the particle moves easily or freely and very high probability density is needed to found the particle.

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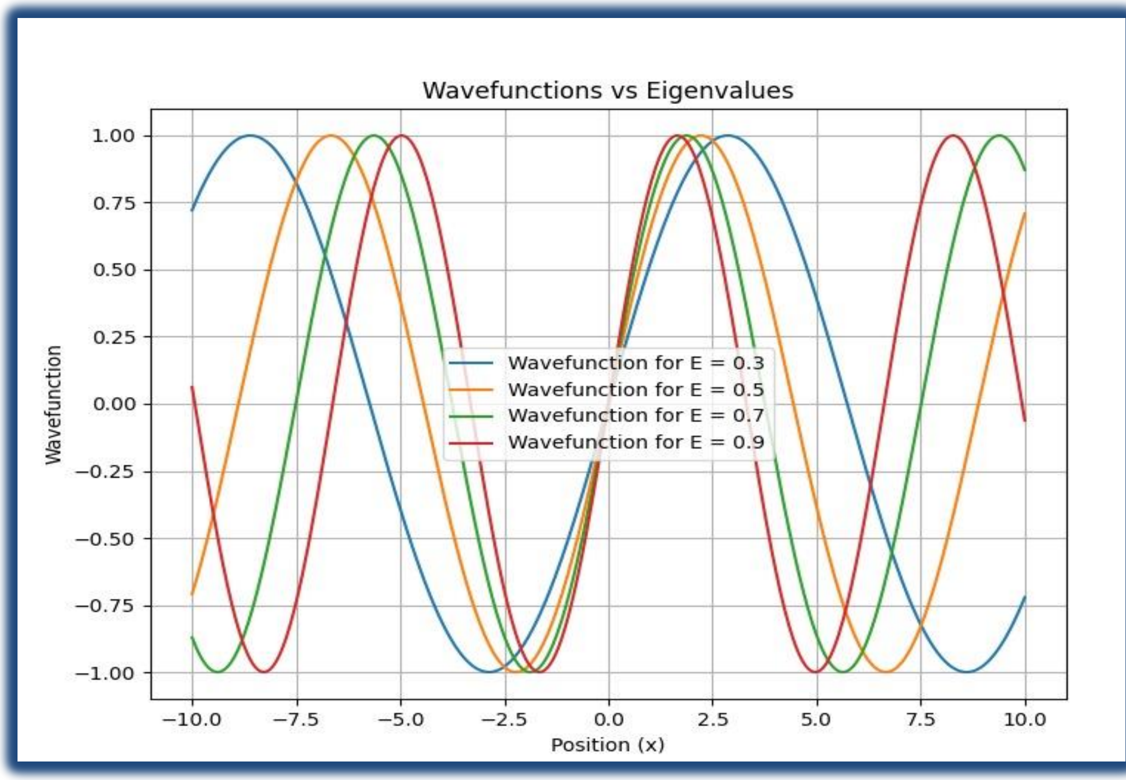

Fig. 2

To analyze the behavior of wavefunction a graph is plotted for different eigenvalues such as 0.30, 0.50, 0.70, and 0.90 between wavefunction and position of the particle, it is shown in fig. 2. This graph shows different eigenvalues in quantum states. The ascending order is used in coding. The sinusoidal wave function using the code gives eigenvalues.

The energy eigenvalues (0.3, 0.5, 0.7, 0.9) of this wave are different in frequency, energy, and amplitude. It is evident from fig. 2, that $E = 0.30$, represents a low energy state with fewer nodes, it decays slowly and has a low probability density. The $E = 0.50$, represents a slightly higher energy level in which particle is easily found in the central region. The $E = 0.70$, represents higher energy state with more nodes, greater frequency, and higher probability density, The $E = 0.90$, represents higher energy than all previous cases and more nodes, with higher frequency, greater kinetic energy is high and very high probability density is needed to found the particle. In all four cases the nodes form at different points shows the variation of different parameters.

Advantages of Visual Simulations

Complex algebraic operations and numerical approximations are used in the majority of approaches to solving and understanding the Schrödinger equation. Despite their accuracy, these techniques can occasionally mask the physical understanding that underlies quantum behavior. The advantage of PINNs is that they enable users to get closer to conceptual issues by avoiding some of the technical obstacles. Accessibility, adaptability, and interactivity are a few advantages of the visualization that PINNs generate [1, 3, 4, 6].

Spatial and Computational Setup

Since the energy eigenvalues are crucial Schrödinger equation parameters, they were initialized using an array with a single eigenstate. This simplifies the initial testing and enables the treatment of many eigenstates in the experiments to follow. Deep learning potential was demonstrated by this implementation, which also demonstrated that non-traditional data-driven solutions can be applied to quantum-mechanical problems.

Applications of the Model

This model is useful in various research fields of interest in many ways, like, for the simulation of energy eigenvalues and eigenfunctions for quantum systems, for the approximation of wavefunctions for systems that are not amenable to analytical solutions, such as multi-dimensional issues or harmonic potentials, creation of comprehensible wavefunctions and quantum behavior simulation for research and teaching purposes. For the solution of other types of partial differential equations, generally the time evolution of quantum systems.

In conventional computation as a general tool for evaluating and testing quantum algorithms designed to solve the time-dependent Schrödinger equation. It provides the foundation for modeling semiconductors, superconductors, and a wide range of other materials by illuminating the behavior of electrons in potential wells.

To forecast molecular orbitals and characteristics, the Schrödinger equation for complicated molecular systems must be solved. modeling wavefunctions and potential energy surfaces for chemical reaction routes.

The knowledge gathered from training this model could be used to improve PINNs even more for use in scientific computing and engineering. Employing neural network wavefunctions to determine a physical system's ideal configuration, such as a quantum system's minimal energy state. Visualization of quantum theory ideas such as tunneling, quantized energy, and wave-particle duality enhancing the learning experience of quantum physics through the use of interactive animations and real-time simulations.

Results

Given the energy eigenvalues, this model trains a physics-informed neural network (PINN) to simulate the wavefunctions of the quantum harmonic oscillator. The loss function fulfills the governing differential equation of the quantum system that the neural network is to learn by using the physical limitations in the Schrödinger equation.

An approximation of the wavefunction $\psi(x)$ for various energy eigenvalues was successfully found using the model. As anticipated for the theoretical solutions of the quantum harmonic oscillator, the wavefunctions exhibit oscillation and symmetry.

For the selected energy eigenvalues, loss convergence was observed, demonstrating efficient learning of the wavefunction structure. During training, it was noticed that the wavefunction was periodically captured and refined in the direction of the real solution.

The wavefunction approximation changed dynamically with epochs, as the animated animation demonstrates. The capacity of PINNs to capture quantum mechanical features was demonstrated by the evolution of the wavefunction from an initial random state to a very accurate representation of the eigenstate.

The findings demonstrated that dynamic systems might be efficiently analyzed by combining machine learning methods with conventional physics models. In addition to increasing computation performance, the hybrid approach enables a more thorough examination of system characteristics.

The outcomes also confirm that physics-based neural networks provide a flexible method for resolving quantum problems. This method provides a prospective method of further inquiry for more complex potentials and high-dimensional quantum systems since it accurately approximates Eigen functions of the Schrödinger equation.

Conclusion

This work showed how to solve the quantum mechanical issue known as the "Time independent Schrodinger equation" using machine learning and PINNs. The training approach involved incorporating physical rules without the direct assistance of conventional numerical approximation techniques. At specific energy eigenvalue values, the PINN was able to approximate the wavefunctions of a quantum harmonic oscillator. The network's convergence to solutions that complied with the physical limitations was depicted by the wavefunction's time-evolution throughout training.

These concepts demonstrate how neural networks are highly flexible in simulating extremely large physical systems, bridging the gap between machine learning and physics.

PINNs' ability to generalize across domains and energy levels makes them a prime contender for additional research in physics, including quantum mechanics and vibrations.

The findings here suggest that machine learning holds promise as an additional instrument to improve our comprehension of physical phenomena, laying the groundwork for increasingly complex scientific and engineering applications.

Future Work

The focus of this paper is stationary systems. We are focusing on extending the methods to time-dependent Schrödinger equations or systems whose parameters change over time, which is a much broader topic for future research. By addressing these shortcomings, it will be possible to advance the use of PINNs and machine learning in tackling challenging physics problems and make them more useful, dependable, and adaptable in real-world applications.

Higher-dimensional quantum systems, time-dependent Schrödinger equations, high order potentials, and nonlinear dynamical systems are a few more examples of these multimodal strategies that combine models informed by physics with experimental evidence. To solve a multi-dimensional quantum system of atoms trapped in 2D or 3D potentials, train the model. a potential that has unpredictability, discontinuities, or practical limitations.

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