FINAL PROJECT REPORT

PREDICTING GROUND STATE ENERGY OF ELECTRON IN 2D POTENTIAL(S)

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INTRODUCTION

Solving the electronic structure problem for molecules, materials, & interfaces is of great importance in Scientific Fields, especially Physics. Paul Dirac was from start a proponent of an idea that approximate and practical methods of applying Quantum Mechanics should be developed, which can greatly reduce complex computation. With the advent of AI, it is now possible to peer into the weird domain of Quantum Mechanics and use tools of AI to approximate the problem and learn key principles by looking at the interaction between input and output layers. This may even help to us give certain insights of Quantum Worlds actually work, which is not possible by simply following the Math.

This Project pertains to ideas along the similar lines and one can demonstrate that even with very simple looking models, high degree of accuracy and further Insights could be gained.

In this project it has been implemented for the System of:

1)Simple Harmonic Potential

2)Infinite Potential Wells/Particle in a Box Potential

Both these potentials are analytically solvable and thus the results are used to establish Ground truth. A sufficiently large 'generated dataset' has been used to train and test a highly flexible model. This allows the Neural network to learn both the features (in weight space) and the mapping required to produce the desired output. The Schrödinger equation is used in its most basic form and Standard method of difference was used to solve the eigen value problem for the 2 cases. The potentials were generated with a dynamic range and length scale suitable to produce ground-state energies within a physically relevant range.

$$\hat{H}\psi \equiv (\hat{T} + \hat{V})\psi = \varepsilon\psi$$

Simple Harmonic Potential

It is one of the very basic examples of how classical systems can differ from Quantum Systems. Following form of S.H.O was implemented $(\varepsilon_0 = \frac{\hbar}{2}(\sqrt{k_x} + \sqrt{k_y})$

Infinite Well or Particle in a Box Potential

This System is also an Analytically Solved System. This represents the case when a particle is trapped in between a potential well and solving these problems is of great significance especially in Physics. The equations used were of the form given below. For the sake of clarity, all the constants are taken in natural units.

$\varepsilon_0 = \frac{1}{2}\pi^2\hbar^2(L_x^{-2} + L_y^{-2})$

METHODOLOGY

The methodology followed is Complex enough to require a great deal of computational resources, but the principle behind is relatively straightforward. Schrodinger Equation has been used to solve for the Ground Level Energies in a particular system and this data is used to Test and Train the Model.

This is implemented in 2 Different Notebooks, 'NB_1_SHO' has the code for Simple Harmonic Potential and 'NB_2_PIB' has the code for Particle in a Box System. The CNN model used for the both the datasets is almost identical which gives us more insight about the interconnected nature of both of these systems.

The Technique used for solving the Eigen Value Problem of Schrodinger Equation, to ultimately give the ground energy states is the 'method of finite difference'.

Data-Set Generation

Data Sets have been generated using a sophisticated yet affective manner. Functions like 'Solver_SHO' and 'Solver_PIB' are defined for specifically generating data for the Simple Harmonic Potential and Particle in a Box Potential respectively. These functions basically take in the input from the user in the form of Grid Size(L), Number of Data Set required(number) and limit and give 2 outputs namely 'Images' (multidimensional array of images generated) and Labels or Energy values.

The Potentials generated with a dynamic range and length scale suitable for producing Ground State Energies within a physically relevant range. Natural Units were used for all the constants (i.e., = 1). The Potentials generated thus were of the given form

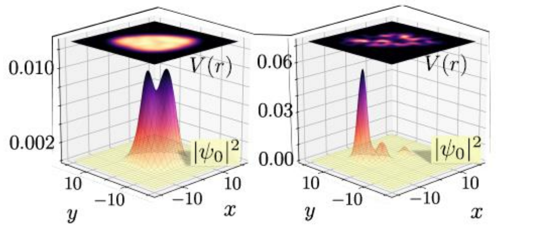

FIG. 2. Wavefunctions (probability density) $|\psi_0|^2$ and the corresponding potentials $V(r)$ for two random potentials.

1) **Simple Harmonic Potential**-These were generated using the basic function only while randomly varying the parameters within permissible limits set. A Data-Set of Size (8000,64,64) was generated which took a large amount of time.

2)**Infinite Well Potential**- Here much more elaborate work had to be done to keep the generated data consisted. The range of the 0 potential was determined each time through applicable randomization. To remove bias towards higher energies, the Lx & Ly values were interchanged sometimes, all of this resulted in a much more even distribution. A Data- Set of (12000,64,64) was generated, but not all were converted into an output.

Model/Deep Neural Network

The choice of model used is based on the Convolution Neural Network due to obvious reasons. There are certainly other models which also work well for the same type of problem but more often than not are lacking in some aspect. It was possible to achieve great deal of accuracy using relatively simple construct of the SAME model over two completely different datasets.

The ‘Sequential’ model used is described below:

- Convolution Layer with 128 Filters, Kernel(5x5), Stride(2x2)
- Max Pooling Layer(2x2)
- Batch Normalization
- Convolution Layer with 256 Filters, Kernel(3x3)
- Max Pooling Layer(2x2)
- Flattening
- Dense Layer of Size 256(ReLU), followed by a dropout layer
- Dense Layer of Size 128
- At last output Dense Layer of Size 3
- Various different parameters like the optimizers, loss functions, epochs etc were varied to get best possible results with least computational time.
- Total number of trainable parameters were between 4 and 4.5 million but many of the approaches like ***Drop Out***, ***Batch Normalization***, ***Early Stopping*** etc. helped in lowering the compute time to as low as possible.

RESULTS & OBSERVATIONS

The results were very reasonable given the Simplicity of model and the less amount of compute time. Compared to the original Paper, our model was much less complex and also had very less data to train upon. Despite these Limitations, the Result in the Case of ***Simple Harmonic Oscillator*** pointed to a mean squared error of about ***60mHa*** which is decent given the circumstances.

On the Other hand, in the Case of ***Particle in a Box Potential***, the model gave and error of just Single digit about ***6-8mHa*** on multiple iterations which is comparable to the results in the original research paper!

SOME OBSERVATIONS

- In the case of ***S.H.O potential***, the accuracy improved while using the data from 32x32 grid which to be expected as details get lost. Reducing the number of filters in the model negatively affected the accuracy of the predictions. Increasing the batch size resulted in a bit faster computation but poorer results
- In the case of ***P.I.B Potential***, the accuracy improved slightly. With some tweaks, the model was able to give single digit error score on a consistent basis.
- The loss function reached convergence in most of the iterations because the dataset was not the largest. Early Stopping approaches helped in getting best possible results.
- 'Mean_squared_error' loss function performed the best with 'adam' optimizer. Small learning rate gave better results in the case of S.H.O Potential (l.r= 0.0001 to 0.0002) with Beta1 (0.5 to 0.9). In the case of P.I.B Potential, default values were used which gave the best results.

CONCLUSION

While much of the projects focused on Solving the problems which are already pretty well understood by us and thus didn't add any new domain, the Main takeaway from here is that Problems like these can be solved much quickly and at a large scale with the help of the tools of AI. These concepts don't have any *'boundary condition'* where they can't be applied. Thus, this field is open for Exploration and we are getting new ways to look at the same results. To add to this, the AI performs much better in some situations like that of *'Random Potentials'*. These systems which are not analytically solvable can easily be approached using the tools of AI.

To conclude, this Project made me much more aware about how to apply AI to any problem and try to yield the maximum results from it in minimum time and in the process, maybe even discover something fundamental about Space-Time.

SOURCES

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