Neural Nets and Quantum Physics

Schrödinger's wave equation

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Time independent Wave eqn

$$\frac{\partial^2\psi}{\partial t^2} = v^2\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) = v^2\nabla^2\Psi \tag{1}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Solution of the above equation is

$$\psi = \psi_0 \sin\omega t = \psi_0 \sin 2\pi v t$$

Where v is the frequency of the stationary wave associated with the particle

Time independent Wave eqn

By differentiating the above equation we get

$$\frac{\partial \Psi}{\partial t} = \psi_0(2\pi v)\cos 2\pi vt$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\psi_0(2\pi v)^2 \sin 2\pi vt$$

$$\frac{\partial^2 \psi}{\partial t^2} = -4\pi^2 v^2 \psi = -\frac{4\pi^2 v^2}{\lambda^2}\psi \quad \left(\because \quad v = \frac{\nu}{\lambda}\right)$$

Substituting the value of $\left(\frac{\partial^2 \psi}{\partial t^2}\right)$ from above equation in eq. (1), we get $v^2\nabla^2\psi = -\frac{4\pi^2 v^2}{\lambda^2}\psi$ $\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0$ Now from de-Broglie relation,

$$\lambda = \frac{h}{mv}$$

Time independent Wave eqn

$$\nabla^2\psi + \frac{4\pi^2}{h^2}m^2v^2\psi = 0$$

If E and V are total and potential energy of the particle then, kinetic energy $1/2\left(\mathrm{mv}^2\right)$ is given by

$$\frac{1}{2}mv^2 = E - V$$
$$m^2v^2 = 2m(E - V)$$

$$\nabla^2\Psi + \frac{4\pi^2}{h^2} \times 2m(E - V)\psi = 0$$

$$\nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

Time independent Wave eqn

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

$\left(\frac{\hbar^2}{2m}\right)\nabla^2\psi + (E - V)\Psi = 0$

$$\frac{\hbar^2}{2m}\nabla^2\psi - V\psi = -E\Psi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = E\Psi$$

$$\hat{H}\psi = E\Psi$$

where $\hat{H} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi,\quad$ where H is known as Hamiltonian operator For a free particle $V = 0$; Schrodinger wave equation for free particle is $\quad \nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0$

Wave equation

$$\frac{\partial^2 \psi}{\partial t^2} = \boldsymbol{v}^2 \boldsymbol{\nabla}^2 \Psi$$

By considering ψ to be complex function of space coordinates of particle and time, general solution for the above equation

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-i\omega t}$$
$$\psi = \psi_0 e^{-i\omega t}$$

Schrodinger equation

$$
\begin{aligned}
\frac{\partial \Psi}{\partial t} &= \psi_0(-i\omega)e^{-i\omega t} \\
&= \psi_0(-i2\pi v)e^{-i\omega t} = -2\pi i v\psi \\
&= -2\pi i(E/h)\psi \\
&= -\frac{iE}{\hbar}\Psi \\
E\psi &= i\hbar\frac{\partial \psi}{\partial t}
\end{aligned}
$$

Time Dependent Wave Equation

Substituting Eψ in Schrodinger time $-$ independent wave equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left[i\hbar\frac{\partial\psi}{\partial t} - V\psi\right] = 0$$

$$\nabla^2\psi = -\frac{2m}{\hbar^2}\left[i\hbar\frac{\partial\psi}{\partial t} - V\psi\right]$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

(Time dependent Schrodinger wave equation)

Time Dependent Wave Equation

$$
\begin{gathered}
\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = i\hbar\frac{\partial}{\partial t}\Psi \\
\hat{H}\psi = \hat{E}\Psi \\
\hat{H} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) = \text{ Hamiltonian operator} \\
\hat{E} = i\hbar\frac{\partial}{\partial t} = \text{ Energy operator}
\end{gathered} \tag{1}
$$

Particle in a box

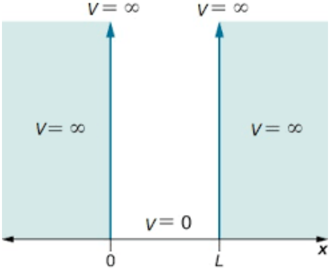


Figure: particle in a box

Consider that a particle of mass 'm'moving along $x-$ axis between two rigid walls A and B at $x = 0$ and $x = a$. Apart from that the particle is free to move between the walls. The potential energy of particle between two walls is constant as there is no force acting on particle For simplicity, the constant potential taken as zero When the particle strikes any of the walls, it is reflected back as the walls are perfectly rigid.

$$
\begin{aligned}
V(x) &= \infty \quad \text{for} \quad x < 0 \quad \text{and} \quad x > a \\
V(x) &= 0 \quad \text{for} \quad 0 \leq x \leq a
\end{aligned}
$$

Schrodinger wave equation for the particle is $\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$

Continued..

Between two walls, V = 0; Hence,

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\Psi = 0$$

$$\text{Let} \qquad \frac{8\pi^2 m}{h^2} E = k^2$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$\psi(x) = A\sin kx + B\cos kx \qquad A, B$ are constants;

Boundary Conditions

Here, the particle is enclosed between two rigid walls and ψ^2 represents the probability of finding particle at any instant The particle cannot penetrate the walls hence, $\psi = 0$ at $x = 0$

$$\psi = 0 \text{ at } x = a$$

Apply above boundary conditions Again

$$0 = A \sin 0 + B \cos 0, \text{ i.e., } B = 0$$

$$\psi(x) = A \sin kx$$

$$0 = A \sin ka \quad \therefore \psi(x) = 0 \quad \text{when } x = a$$

Here, either $A = 0$ or sin ka = 0; But A is not equal to zero. If A = 0, entire function would become zero

$$\sin ka = 0 \quad \text{or} \quad ka = n\pi (n = 0, 1, 2, 3, \ldots)$$

$$k = \frac{n\pi}{a}$$

Wave function would become as

$$\psi(x) = A \sin \frac{n\pi x}{a}$$

Eigen Values

$$k^2 = \frac{n^2\pi^2}{a^2}$$

$\frac{8\pi^2 mE_n}{h^2} = \frac{n^2\pi^2}{a^2}$ is evident that inside an infinitely deep potential well,
$E_n = \frac{n^2h^2}{8ma^2} = n^2\frac{\pi^2\hbar^2}{2ma^2}$,
the particle can have only
discrete set of values of energy. It means that (n=1,2,3, ...)
the energy is quantized.
and (n=h / 2 π)

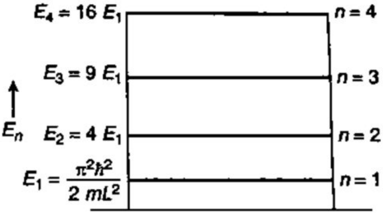
Energy levels

The discrete energy values are

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2} \text{ for } n = 1, E_2 = 4\frac{\pi^2 \hbar^2}{2ma^2} = 4E_1, \text{ for } n = 2$$

$$E_3 = 9\frac{\pi^2 \hbar^2}{2ma^2} = 9E_1 \text{ for } n = 3, E_4 = 16\frac{\pi^2 \hbar^2}{2ma^2} = 16E_1$$

The energy levels of a particle inside an infinite potential well



It is important to notice that classically particle can take continuous range of values between zero and infinite. But quantum mechanically energy is quantized and discrete values of energy are allowed

Harmonic Oscillator

For a simple harmonic oscillator, the restoring force F on a particle of mass m would linear. Essentially, the force i Proportional to displacement " x " from its equilibrium position and in the opposite direction

$$F = -kx$$

$$k - \text{ spring constant}$$
$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

Solutions would be $x = A\cos(2\pi\nu t + \phi)$

$$\nu = \frac{1}{2\pi} \cdot \sqrt{\frac{k}{m}}$$

v− frequency oscillations and A is amplitude $\phi-$ phase angle depends on what $'x'$ is at that time $t = 0$ Any system in which something executes small vibrations about an equilibrium position behaves like simple harmonic oscillator

Harmonic Oscillator (Classical)

A restoring force which is a function of $'x'$ can be expressed in a Maclaurin's series about the equilibrium position

$$F(x) = F_{x=0} + \left(\frac{dF}{dx}\right)_{x=0} x + \frac{1}{2}\left(\frac{d^2F}{dx^2}\right)_{x=0} x^2 + \frac{1}{6}\left(\frac{d^3F}{dx^3}\right)_{x=0} x^3 + \cdots$$

Higher terms can be neglected due to the fact that for small values of $x2$ and $x3$ are very small Significant term is

$$F(x) = \left(\frac{dF}{dx}\right)_{x=0} x$$

F(x) is hooks law when dF/dx at x = 0 is negative Conclusion: All oscillations are simple harmonic oscillations if their amplitudes are sufficiently small The potential energy function $U(x)$ that corresponds to a Hook's law force can be found by determining the Work needed to bring particle from $x = 0$ to $x = x$ against such force

$$U(x) = -\int_0^x F(x)dx = k\int_0^x x dx = \frac{1}{2}kx^2$$

Harmonic Oscillator (Quantum)

Energy levels: Schrodinger's equation for harmonic oscillator with $u(x) = 1/2kx^2$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0$$
$$\frac{2m}{\hbar^2}E = \alpha \quad \text{and} \quad \sqrt{\frac{mk}{A^2}} = \beta$$
$$\frac{d^2\psi}{dx^2} + \left(\alpha - \beta^2 x^2\right)\psi = 0$$

Introduce a dimensionless independent variable ξ such that $\xi = \sqrt{\beta}x$

$\frac{d^2}{dx^2} = \beta\frac{d^2}{d\xi^2}$

$\beta\frac{d^2\psi}{d\xi^2} + \left(\alpha - \beta^2\frac{\xi^2}{\beta}\right)\psi = 0$

$$\frac{d^2\psi}{d\xi^2} + \left(\frac{\alpha}{\beta} - \xi^2\right)\psi = 0.$$

Solutions would be in terms of Hermite polynomial $\mathrm{H}_n(\xi)$

$$\psi(\xi) = CH_n(\xi)e^{-\xi^2/2}$$

These solutions are acceptable only if $n = 0, 1, 2,$

Harmonic Oscillator

As there is a restriction on the values of 'n', there would also be restriction on E; The mathematical properties are such that this condition would be fulfilled only when

$$\frac{\alpha}{\beta} = (2n+1)$$

$$\frac{2mE/\hbar^2}{\sqrt{mk/\hbar^2}} = (2n+1) = 2\left(n+\frac{1}{2}\right)$$

$$E = \left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}$$

$$\frac{1}{2\pi}\sqrt{\frac{k}{m}} = v$$

$$E = \left(n+\frac{1}{2}\right)hv = \left(n+\frac{1}{2}\right)\hbar v$$

Neural Nets

Rather than seeking an appropriate input representation to capture the relevant physical attributes of a system, we train a highly flexible model on an enormous collection of ground-truth examples. In doing so, the deep neural network learns both the features (in weight space) and the mapping required to produce the desired output.
This approach does not depend on the appropriate selection of input representations and features; we provide the same data to both the deep neural network and the numerical method. As such, we call this **"featureless learning"**.

Architecture

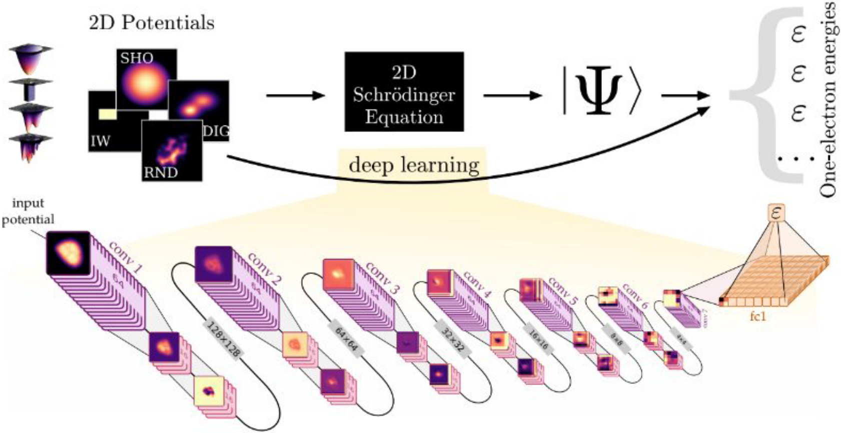


Figure: Architecture

Methods

Training set: choice of potentials

Developing a deep learning model involves both the design of the network architecture and the acquisition of training data. The latter is the most important aspect of a machine learning model, as it defines the transferability of the resulting model. We investigated four classes of potentials: simple harmonic oscillators (SHO), "infinite" wells (IW, i.e. "particle in a box"), double-well inverted Gaussians (DIG), and random potentials (RND). Each potential can be thought of as a grayscale image: a grid of floating-point numbers.

There is no closed-form equation to represent the potentials, and certainly not the eigenenergies. A convolutional neural network tasked with learning the solution to the Schr odinger equation through these examples would have to base its predictions on many individual features, truly "learning" the mapping of potential to energy.

DNN

We use two different types of convolutional layers, which we call "reducing" and "non-reducing". The 7 reducing layers operate with filter (kernel) sizes of 3×3 pixels. Each reducing layer operates with 64 filters and a stride of 2×2, effectively reducing the image resolution by a factor of two at each step. In between each pair of these reducing convolutional layers, we have inserted two convolutional layers (for a total of 12) which operate with 16 filters of size 4×4. These filters have unit stride, and therefore preserve the resolution of the image. The purpose of these layers is to add additional trainable parameters to the network. All convolutional layers have ReLU activation.

Continued..

The final convolutional layer is fed into a fully-connected layer of width 1024, also with ReLU activa- tion. This layer feeds into a final fully-connected layer with a single output. This output is the output value of the DNN. It is used to compute the mean-squared error between the true label and the predicted label, also known as the loss. We used the AdaDelta optimization scheme with a global learning rate of 0.001 to minimize this loss function (Shown in Figure), monitoring its value as training proceeded.
We found that after 1000 epochs (1000 times through all the training examples), the loss no longer decreased significantly.

Training Stats

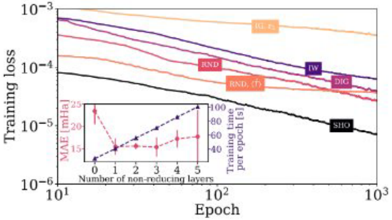


FIG. 3. The training loss curve for each model we trained. Since the training loss is based upon the training datasets, it does not necessarily indicate how well the model generalizes to new examples. The convergence seen here indicates that 1000 epochs is an adequate stopping point; further training would produce further reduction in loss, however 1000 epochs provides sufficient evidence that the method performs well on the most interesting (i.e. random) potentials. In the inset, we see that two non-reducing convolution layers is a consistent balance of training time and low error.

Results

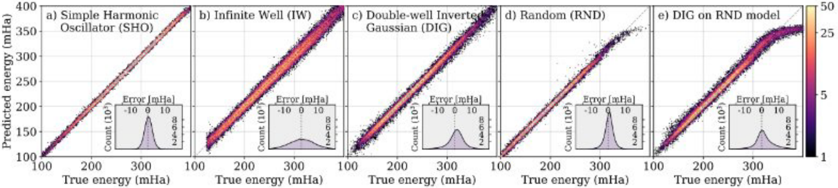


FIG. 4. Histograms of the true vs. predicted energies for each example in the test set indicate the performance of the various models. The insets show the distribution of error away from the diagonal line representing perfect predictions. A 1 mHa^2 square bin is used for the main histograms, and a 1 mHa bin size for the inset histogram. During training, the neural network was not exposed to the examples on which theses plots are based. The higher error at high energies in (d) is due to fewer training examples being present the dataset at these energies. The histogram shown in (d) is for the further-trained model, described in the text.