
Density Functional Theory aided with Neural Networks

— By: Robert Branson —

Overview

Density Functional Theory helps predict charge radii

Finding the correct forms of the functionals can be difficult

Machine learning allows one to refine the process and increase accuracy

Relativistic Energy Density Functional

$$\begin{aligned}\mathcal{L}_{\text{int}} = & \bar{\psi} \left[g_s \phi - \left(g_v V_\mu + \frac{g_\rho}{2} \boldsymbol{\tau} \cdot \mathbf{b}_\mu + \frac{e}{2} (1 + \tau_3) A_\mu \right) \gamma^\mu \right] \psi \\ & - \frac{\kappa}{3!} (g_s \phi)^3 - \frac{\lambda}{4!} (g_s \phi)^4 + \frac{\zeta}{4!} g_v^4 (V_\mu V^\mu)^2 + \Lambda_v \left(g_\rho^2 \mathbf{b}_\mu \cdot \mathbf{b}^\mu \right) \left(g_v^2 V_\nu V^\nu \right)\end{aligned}$$

Machine Learning

Self Driving Cars

Image Recognition

Data Mining

Physics

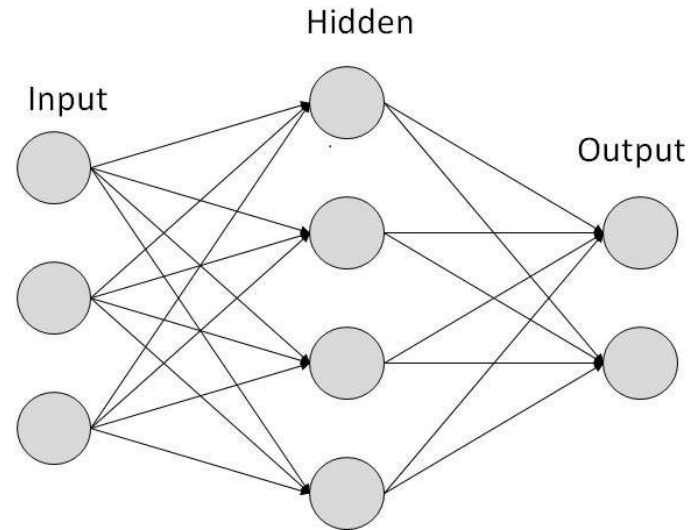
Neural Network

Consists of input layer, hidden layer, and output layer

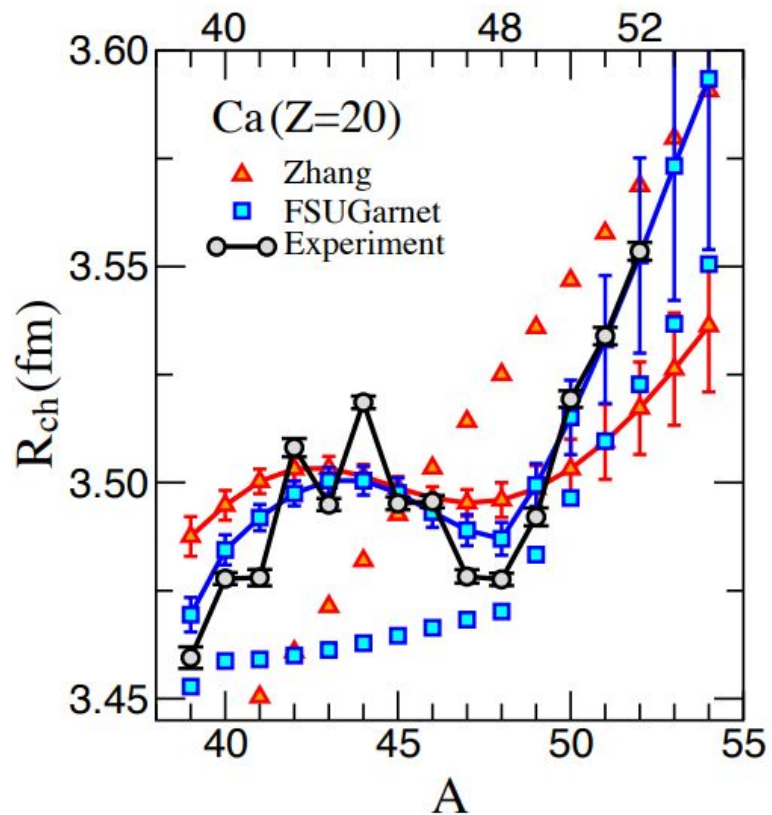
Each neural pathway has a certain weight

Weights are assigned randomly at first

Subsequent weights are trained from data set



Results



Results (cont.)

Increased accuracy of predictions by 40 percent

Still failed to predict strange behavior of calcium

Authors previously had success in increasing mass accuracy using neural networks

Source

R. Utama, W.-C. Chen, and J. Piekarewicz, J. Phys. G (2016).