Objective
- The quantum mechanical Schrödinger equation for anharmonic oscillator potentials does not have an exact analytical solution. A trained neural network could predict the ground-state energy and significantly cut down on computation time [1]

The Schrödinger equation and the finite differences method
- The time-independent Schrödinger equation for a single particle in an anharmonic oscillator potential is given by

\[
\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 + \lambda x^n \psi(x) = E \psi(x)
\]

- Set \( \frac{1}{\sqrt{\hbar m \omega}} = b \), \( a = \frac{\omega^2}{2 \lambda b^2} \), and \( m = \hbar \) to derive the equations below, where \( L \) is number of discretizations, making the solution independent of discretization size

\[
\Delta x = \frac{2}{(ab)^{1/4} L} \quad x_a = \frac{L}{(ab)^{1/4}}
\]

- A solution to the Schrödinger equation can be approximated by utilizing the finite differences method [2]

Hamiltonian in matrix form
\[
\begin{pmatrix}
2a + bx^2 + \lambda x^n & -a & \cdots & 0 \\
-a & 2a + bx^2 + \lambda x^n & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & \cdots & -a & 2a + bx^2 + \lambda x^n
\end{pmatrix}
\]

- An eigenvalue solver can be used to solve the matrix and determine the ground-state energy of the potential

Results
Harmonic and anharmonic network evaluations
- Network accuracy could be greatly improved if a more complicated architecture (Convolutional Neural Network) was implemented

Finite Differences vs. Network Times
- At around 15,000 training examples, the network reaches max efficiency of about 400 times faster than the finite differences time
- Finite differences time increase linearly as number of training examples increases
- At 1,000,000 training examples, \( t_{\text{finite}} \) would be 27 minutes. \( t_{\text{network}} \) would be 4 seconds

- Net anharmonic oscillator (AHO) was able to accurately predict harmonic oscillator (HO) data. Prediction of AHO potentials could likely be improved by increasing the number of training examples.
- Since net HO had never seen negative energies, it had low accuracy at predicting negative values
- Similarly, net HO was not used to potentials that did not look like regular parabolas. When it received higher order potentials, it had no knowledge on the appropriate output
- Network accuracy could be greatly improved if a more complicated architecture (Convolutional Neural Network) was implemented

References: