Machine Learning and the Schrödinger equation

Noah F. Berthusen,[1] Mathias S. Scheurer,[2] Peter P. Orth[3]

1 College of Engineering, Iowa State University, Ames, Iowa 50011
2 Department of Physics, Harvard University, Cambridge, Massachusetts 02138
3 Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011

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

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 + \lambda x^\alpha\right]|\psi\rangle = E|\psi\rangle$$

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

Discretization step of x

$$\Delta x = \frac{2}{(4b)^{1/4}\sqrt{L}}$$

$$x_m = \frac{\sqrt{L}}{(4b)^{\frac{1}{4}}}$$

Maximum absolute value of x

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

Hamiltonian in matrix form

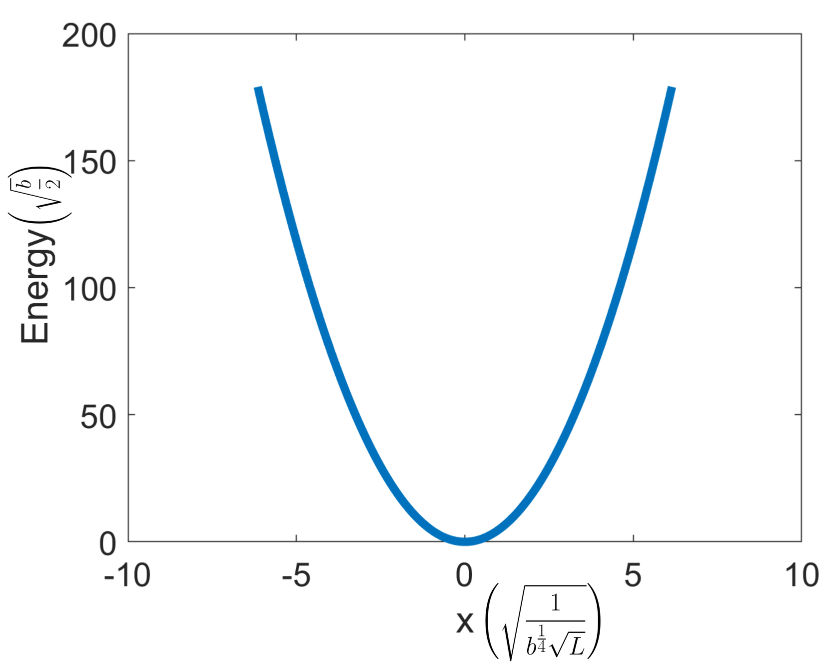
$$\begin{bmatrix} 2a + bx_1^2 + \lambda x_1^\alpha & -a & \dots & \dots & 0 \\ -a & 2a + bx_2^2 + \lambda x_2^\alpha & \dots & \dots & \vdots \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & -a \\ 0 & \dots & \dots & -a & 2a + bx_n^2 + \lambda x_n^\alpha \end{bmatrix}$$

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

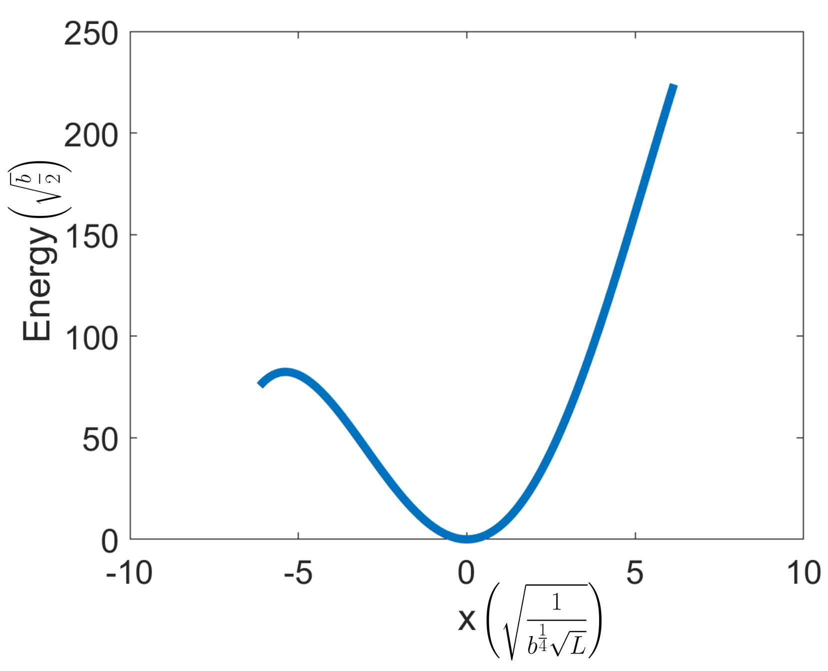
Machine Learning

- Generated 15,000 training examples with 150 features each

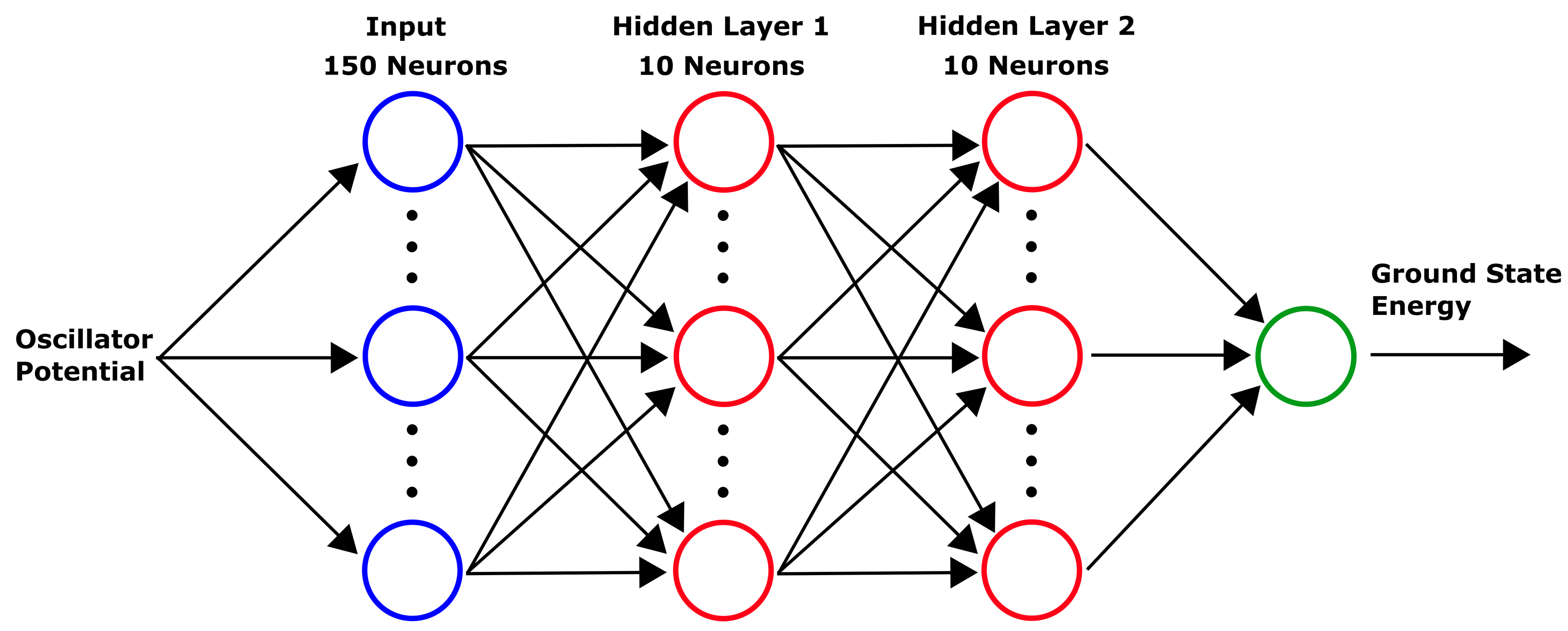
Harmonic Potential



Anharmonic Potential

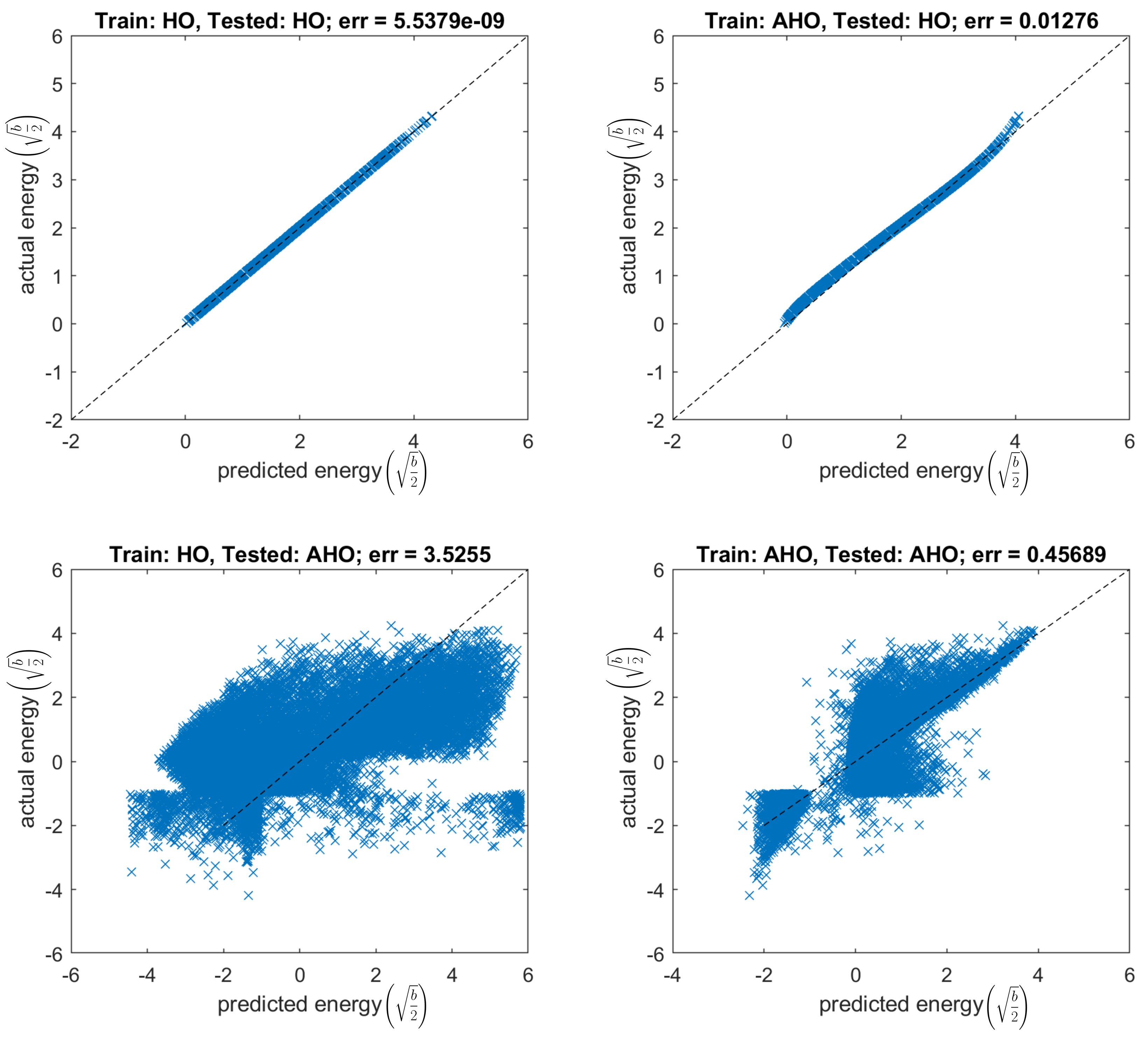


- Anharmonic ground state energies range from -3 to 4, Harmonic energies range from 0 to 4 (both in units of $\sqrt{b/2}$)
- A feedforward neural net was used for training both potentials. Harmonic architecture was two hidden layers with ten neurons each. Anharmonic architecture was three hidden layers with ten neurons each. Network was implemented using Matlab.

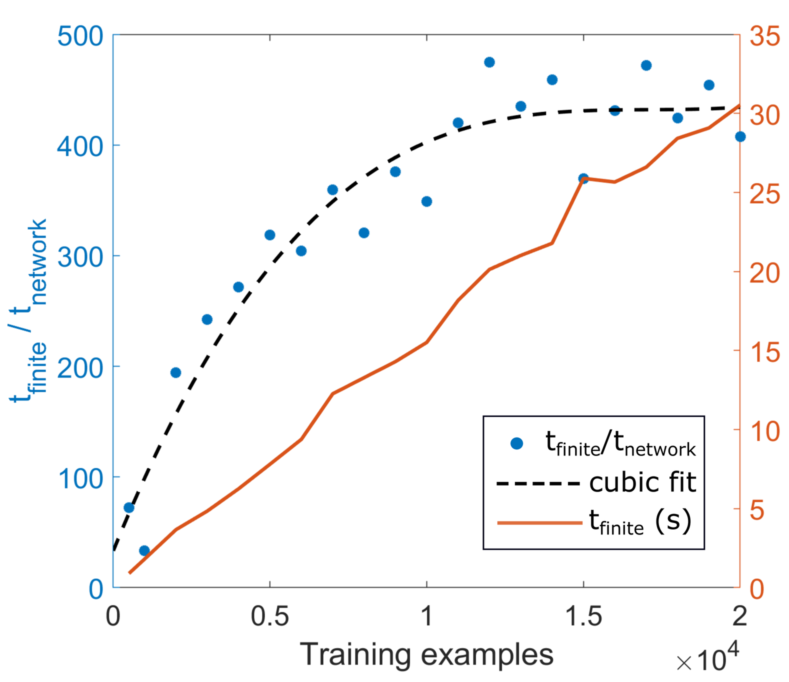


Results

Harmonic and anharmonic network evaluations



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_{finite} would be 27 minutes. $t_{network}$ 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 recieved 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:

[1] K. Mills, M. Spanner, I. Tamblyn, Physical Review A **96** 4104 042113 (2017)
[2] D. G. Truhlar, Journal of Computational Physics **10**, 123-132 (1972)

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