Deep Learning for Ab Initio Nuclear Theory Extrapolations

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Abstract

We propose a feed-forward artificial neural network (ANN) as an extrapolation tool to obtain the ground-state (GS) energy and the GS point-proton root-mean-square (rms) radius along with their extrapolation uncertainties based on data calculated with the No Core Shell Model (NCSM). The designed ANNs produce results for these two very different observables in ^{6}Li that satisfy the theoretical physics condition: independence of basis space parameters in the limit of extremely large matrices.

Motivation

- Extrapolate results from NCSM calculations on High Performance Computing (HPC) machines to ultra-large basis spaces
- Quantify the extrapolation uncertainties
- Guide programs at DOE's major experimental facilities (FRIB, JLab, DUSL)

Introduction

The NCSM casts the nuclear quantum many-body problem as a Hamiltonian matrix eigenvalue problem expressed in a chosen, but truncated, basis space. Our three-dimensional harmonic-oscillator (HO) basis is characterized by the HO energy, $\hbar\Omega$, and the many-body basis space cutoff, $N_{\max}$ (defined as the maximum of the sum over all nucleons of their HO quanta above the minimum needed to satisfy the Pauli principle). Extrapolation tools are needed to estimate the converged results for eigenenergies and other observables as well as to quantify their uncertainties.

ANN design and filtering

1. Through experimentation, select a simple network design for initial applications (see Fig. 1)
2. Divide available NCSM results for ^{6}Li into training (90% of data) and testing (10% of data) sets
3. Train/test ensemble of ANNs and retain the 50 that best exceed minimum performance criteria
4. Develop histograms of results from best performers as function of increasing data set sizes (see Fig. 2)
5. Obtain extrapolation (mean) and uncertainty (standard deviation) from a Gaussian fit to each histogram

Current ANN design

Design features of our feed-forward ANN include Bayesian regularization, hyperbolic tangent sigmoid function for the activation function of the hidden layer, and randomly splitting the original data set for each ANN into 16/19 (for training/testing) and 3/19 for a post assessment of its performance.

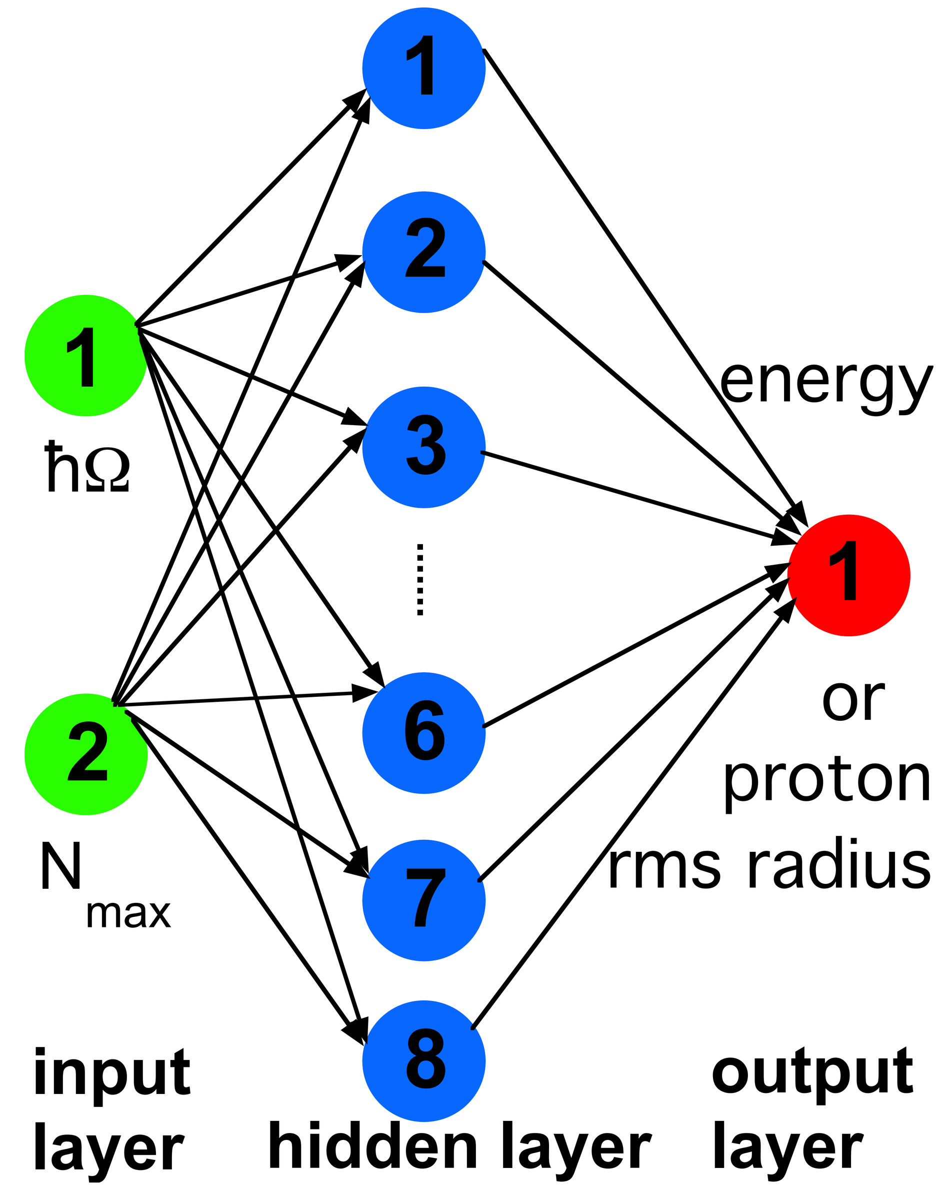

Figure 1: Neural network used to extrapolate the ^{6}Li GS energy and point-proton rms radius from currently achievable NCSM basis spaces ($N_{\max}$ datasets) to extreme basis spaces that attain basis parameter independence.

Extrapolations from best performing ANNs

As shown visually and in the labels (listing the means and standard deviations) of Fig. 2, we demonstrate reasonable consistency of ANN predictions with increasing $N_{\max}$. This quantifies the utility of ANNs for heavier nuclei where only lower $N_{\max}$ basis spaces are attainable.

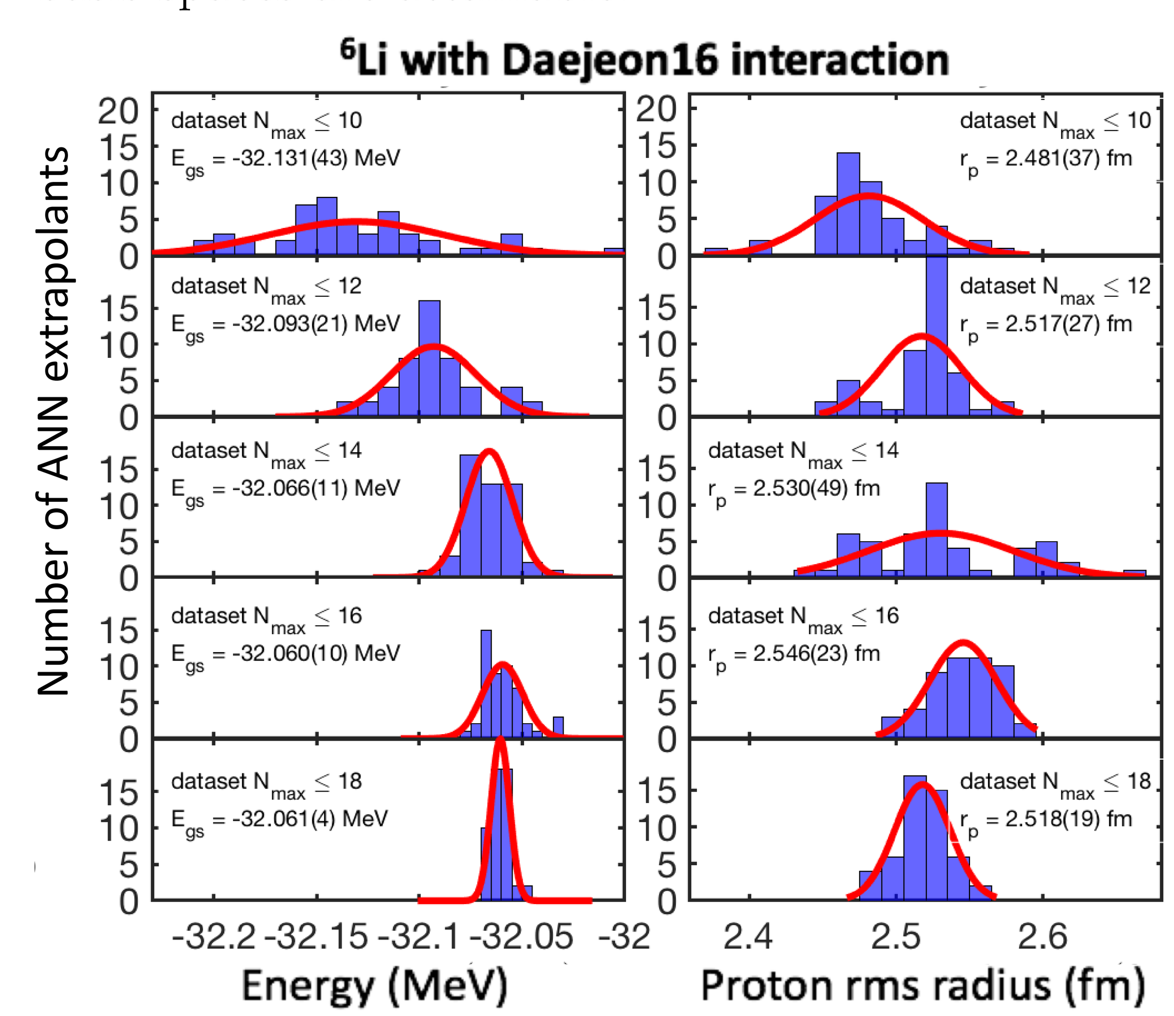

Figure 2: Distributions of the predicted GS energy (left) and GS point-proton rms radius (right) of ^{6}Li produced by 50 best-performing ANNs trained with ab initio NCSM data at increasing levels of truncation up to $N_{\max} = 18$. Each ANN predicted GS energy (GS point-proton rms radius) is obtained at $N_{\max} = 70$ (90).

Discussions and outlook

1. ANNs extend the predictive power of ab initio nuclear theory beyond the capabilities of current HPC machines
2. We will expand the range of applications to include electroweak moments and transition rates as well as scattering cross sections

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