USING NEURAL NETWORKS TO PREDICT THE DENSITY PROFILES OF ISOTOPES.

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Isotope Program U.S. Department of Energy

US Department of Energy:
Isotope Program,
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^{155}Tb

- ^{155}Tb is a promising isotope for Theranostics; figure 1
  - Has computationally complex nucleus
  - Unknown reaction probabilities (cross sections)
  - Difficult to produce with high purity
- Auger electrons have low penetrative power, and travel between 0.7 and 33 μm, smaller than human cells[1]
  - High promise for highly precise cancer treatment
- Gamma rays are utilized in SPECT Imaging to diagnose tumors[1]

^{156}Gd

- Used in current, direct method of producing ^{155}Tb; eqn 1
- High overlap of cross sections with ^{154}Tb and ^{156}Tb[1]
  - Poor yield
- Novel method uses indirect production with the decay of ^{155}Dy via electron capture[1]; eqn 2

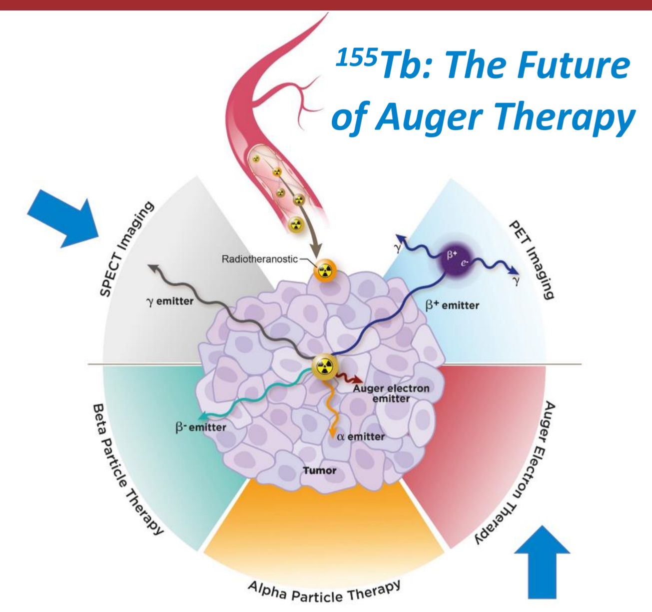

Figure 1: Uses of Auger electron emission[1]

Eqn 1: $$^{156}Gd(p,2n)^{155}Tb$$

Eqn 2: $$^{156}Gd(^{3}He,4n)\,^{155}Dy \qquad ^{155}Dy \xrightarrow{EC} {}^{155}Tb$$

JAX

- Accelerated learning algebra (XLA) application programming interface (API) that uses the Python language[4]
- Uses GPUs and TPUs which hold multiple discs
- Designed for construction and implementation of computationally large programs such as neural networks[4]
- Stax is a built-in library that efficiently constructs the architecture of neural networks.

Neural Networks

- A type of machine learning that are functionally digital brains; figure 2
- Each connection has a weight, a bias, and an activation function that compute the next neuron's value.
- Can be used to find patterns and be trained to predict with high accuracies
- Can save researchers both time and money.

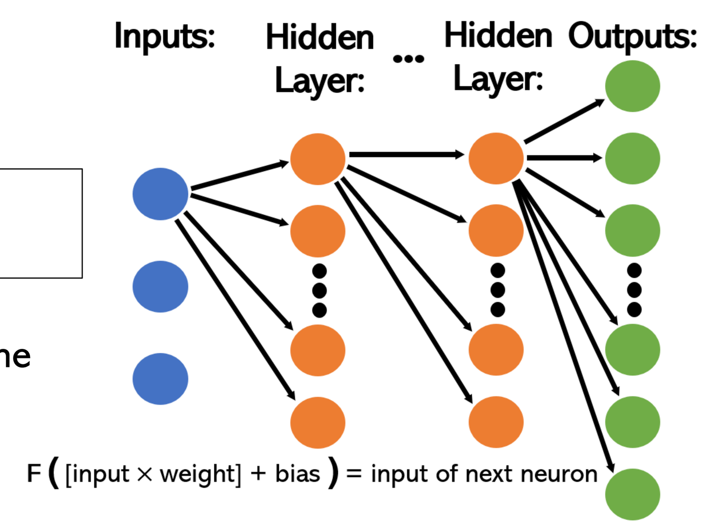

Figure 2: Diagram of a neural network

Objectives

- Create a neural networks capable of predicting the density profiles of isotopes
- Demonstrate the effects of different designs of neural networks on the predictions of density profiles
- Optimize the network's architecture for accuracy and run time.
- Predict the density profiles of ^{155}Tb and ^{156}Gd

Methods

- Known data set of 80 nuclei, 60 for training, and 20 reserved for testing[2]
- Additional density profiles of nuclei calculated using 2pF, 3pF, and 3pG models[3]
- Created the architecture of a basic neural network for proof of concept (termed Original in figures)
  - Inputs: A and Z numbers
  - 1 hidden layer
  - 64 neurons per layer
  - Tanh used for the activation function
  - Cross Entropy function for calculating loss (error of the prediction from provided training data)
- Improved accuracy of network through the addition of a third input: Ground State Energy (GSE), and adding batches to the network's learning process; figure 3
  - The greater the GSE, the denser the nucleus
  - 10 batches of 6 nuclei from the training data set
  - Base network used to evaluate the effects of differing network architecture
- Evaluated different numbers of hidden layers, number of neurons, loss functions, steps, learning rates, activation functions, and initialization seeds; figures 4, 5

Results & Discussion

- Factors which affected the accuracy of the network the greatest; figure 3
  - Number of inputs
  - With/with out batches
  - Number of hidden layers
  - Number of neurons
- Most affective:
  - activation function: Gelu; figure 4
  - initialization seed: 119; figure 5
- ^{150}Sm produced a typical result; figure 6
- Lesser performance for nuclei with A & Z numbers approaching the end of the data set
- The final network performs the best overall
  - With ground state energy as an input
  - Batches used during network optimization
  - 64 neurons per hidden layer
  - 4 hidden layers
  - Cross Entropy loss function
  - 1000 steps with a learning rate of 0.0001
- Predictions of ^{155}Tb and ^{156}Gd are shown in figures 7 and 8

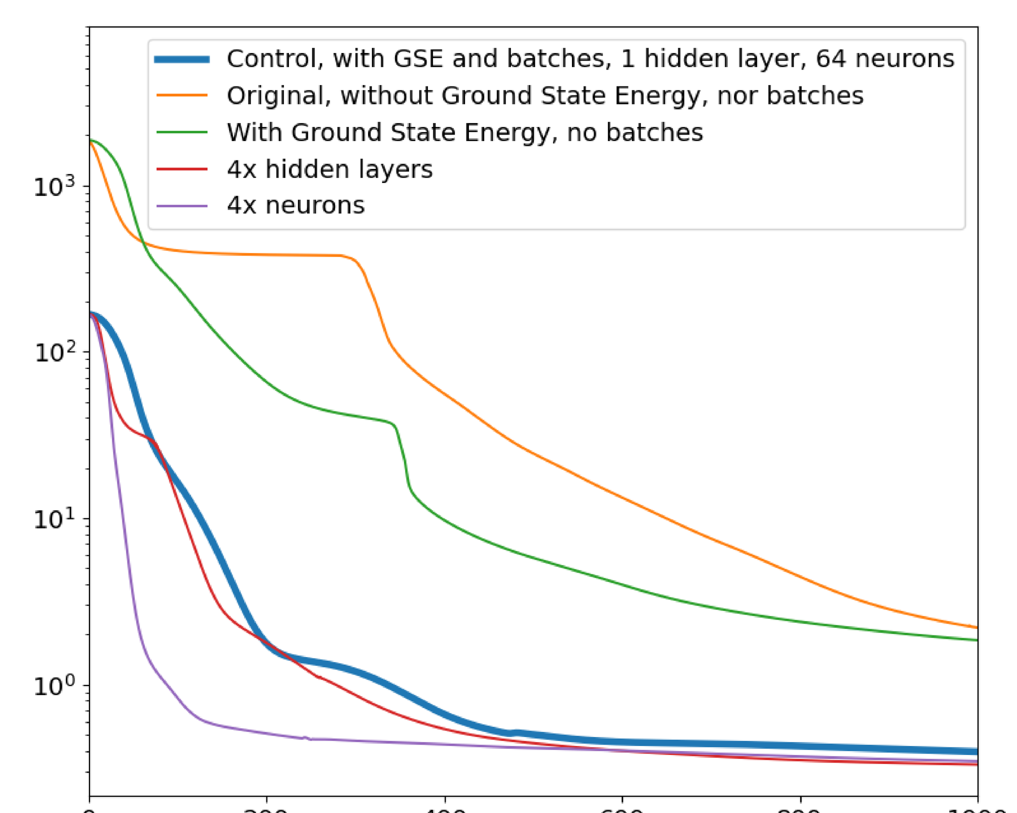

Figure 3: Path of gradient descent for the parameters of greatest affect.

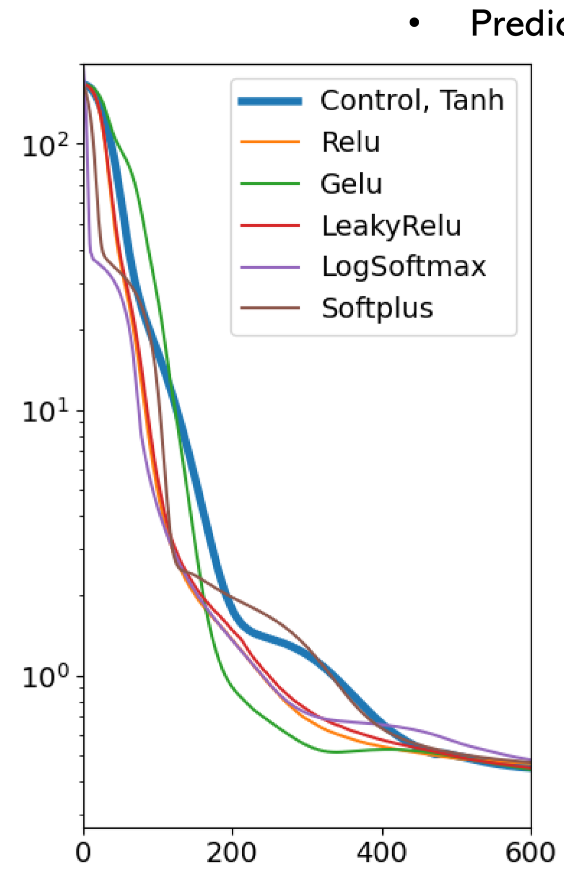

Figure 4: Path of gradient descent for different activation functions

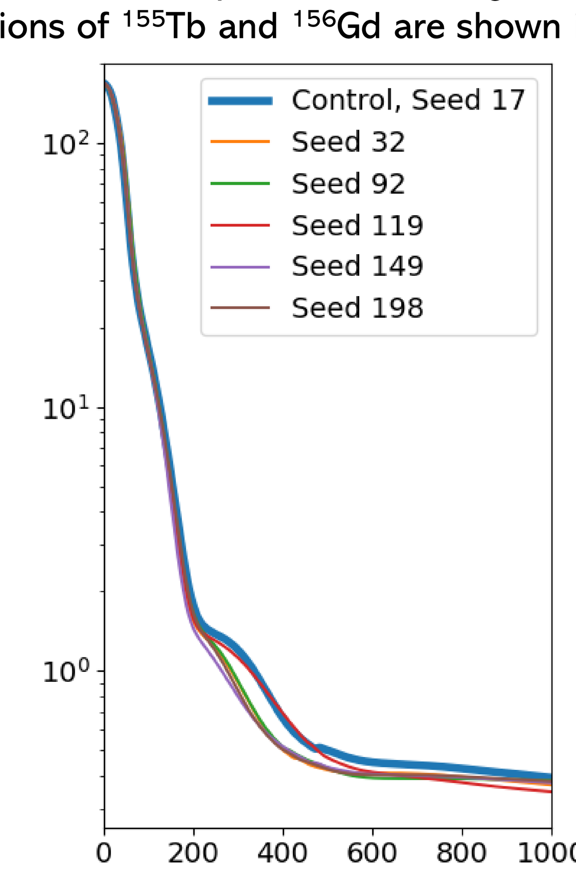

Figure 5: Path of gradient descent for different seeds to initialize weights and biases

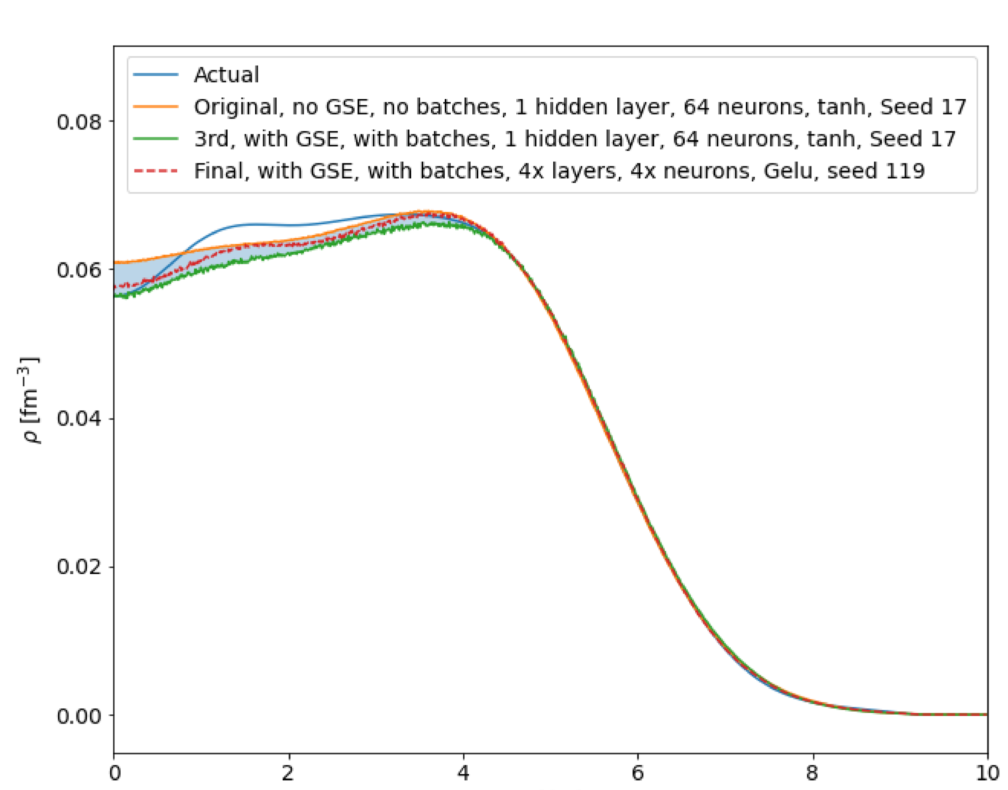

Figure 6: Density profile of ^{150}Sm, mapped from three progressive versions of the network

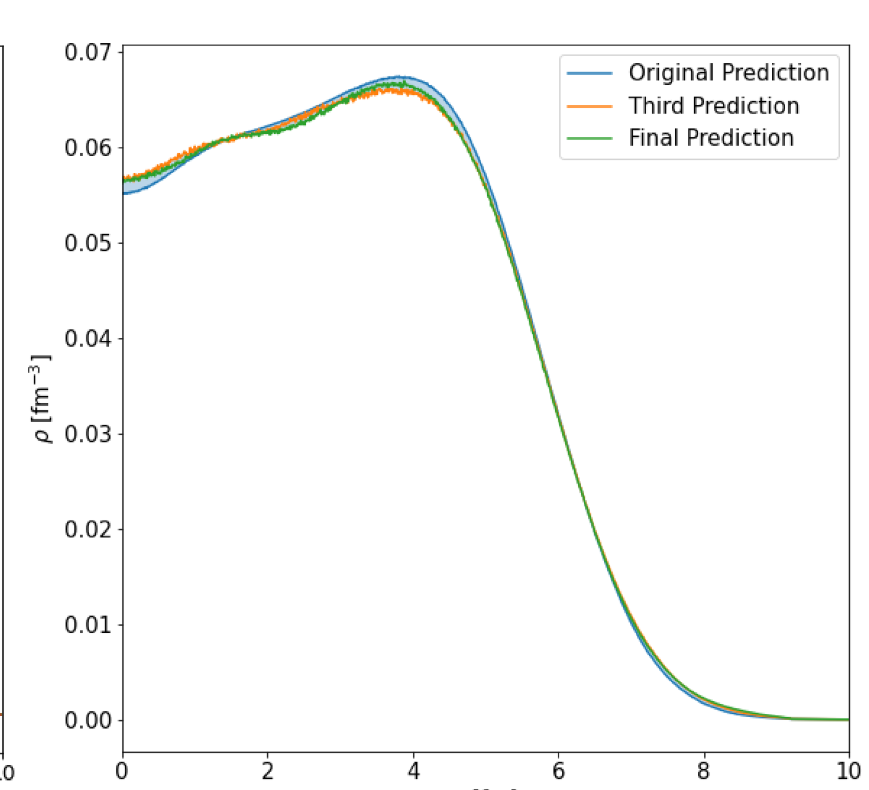

Figure 7: Density profile prediction of ^{155}Tb, mapped from three progressive versions of the network

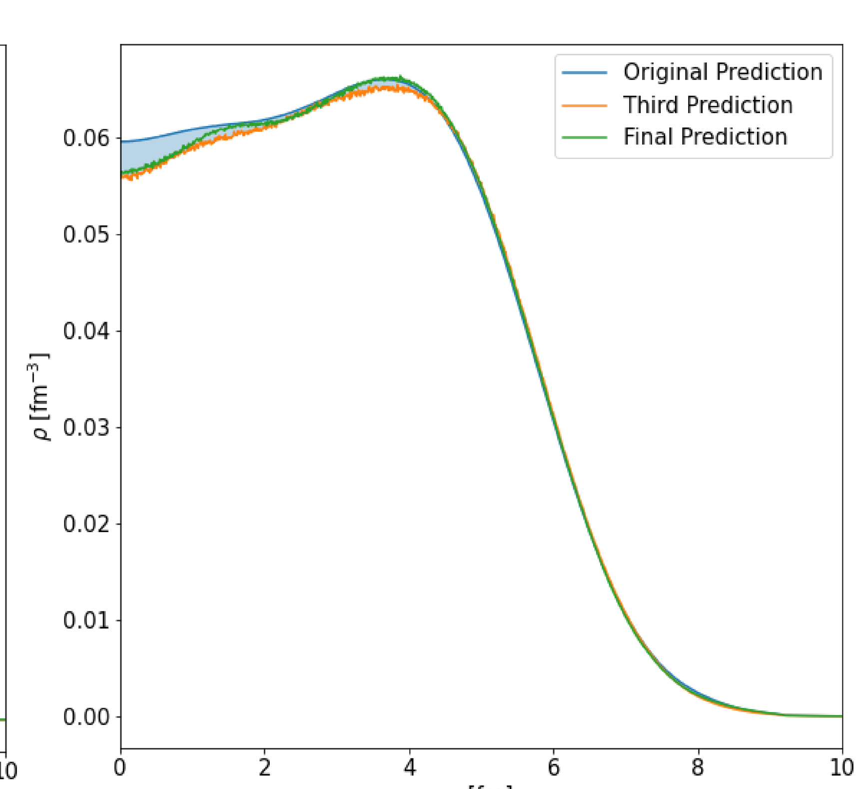

Figure 8: Density profile prediction of 156Gd, mapped from three progressive versions of the network

Conclusion and Further Research

By testing different architectures of the neural network, the optimal configuration was found, producing the lowest loss value, and providing sufficient predictions. With the optimal network created (dubbed "final") predictions for ^{155}Tb and ^{156}Gd were made; figures 7 and 8.

- High accuracy can be achieved with
  - Large enough data set
  - Greater number of hidden layers,
  - Greater number of neurons per layer
- Run time can be decreased with access to more or larger GPUs

Neural networks show high promise for the future of predicting properties of isotopes, but further research must be done to determine at what point they overtrain and begin to provide inaccurate predictions when faced with novel data for tests.

The next step in this line of research is to build a neural network that will understand the spectrum of energy levels of nuclei. From this, cross sections can be predicted, such as the cross sections of the reaction pathways for producing ^{155}Tb.

References

[1] H. Álvarez, Natalia, et al. *"Recent Advances in Radiometals for Combined Imaging and Therapy in Cancer."* ChemMedChem **16**, 2909 (2021). https://doi.org/10.1002/cmdc.202100135.

[2] University of Virginia: *Nuclear Charge Density Archive Downloads*, http://discovery.phys.virginia.edu/research/groups/ncd/download.html (Accessed 2 July 2022).

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[4] DeepMind: *Jax Reference Documentation*, https://jax.readthedocs.io/en/latest/index.html (Accessed 1 June 2022).

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