Ensemble Neural Networks

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1 Research Task

The first step in our research is to create a neural network relating pictures of metal oxides to their spectra graphs. Once this is achieved, we will work to put predictive errors bars around the results produced by the neural network. Since neural networks work somewhat like a ”black box”, giving an input and seemingly magically getting a result, this has proven difficult in the past.

2 Neural Networks

A neural network is an algorithm modeled after the network of neurons in the human brain, which, when trained, is able to identify underlying relationships in a set of data. Similarly to how we learn, it takes in training data to understand what it is looking for and then uses that to predict future data. The neural network attempts to learn, from the input data, how to label new inputs.

3 NNSS

The Nevada National Security Site (NNSS) is part of the U.S. Department of Energy research and development complex, located in the Nevada desert. The NNSS's two primary missions are defense nuclear nonproliferation and the pursuit of science. Following an agreement to ban nuclear weapons testing, NNSS uses controlled underground experiments and simulations to verify the usability of the arms. They are currently interested in to the impact of neural networks on their work

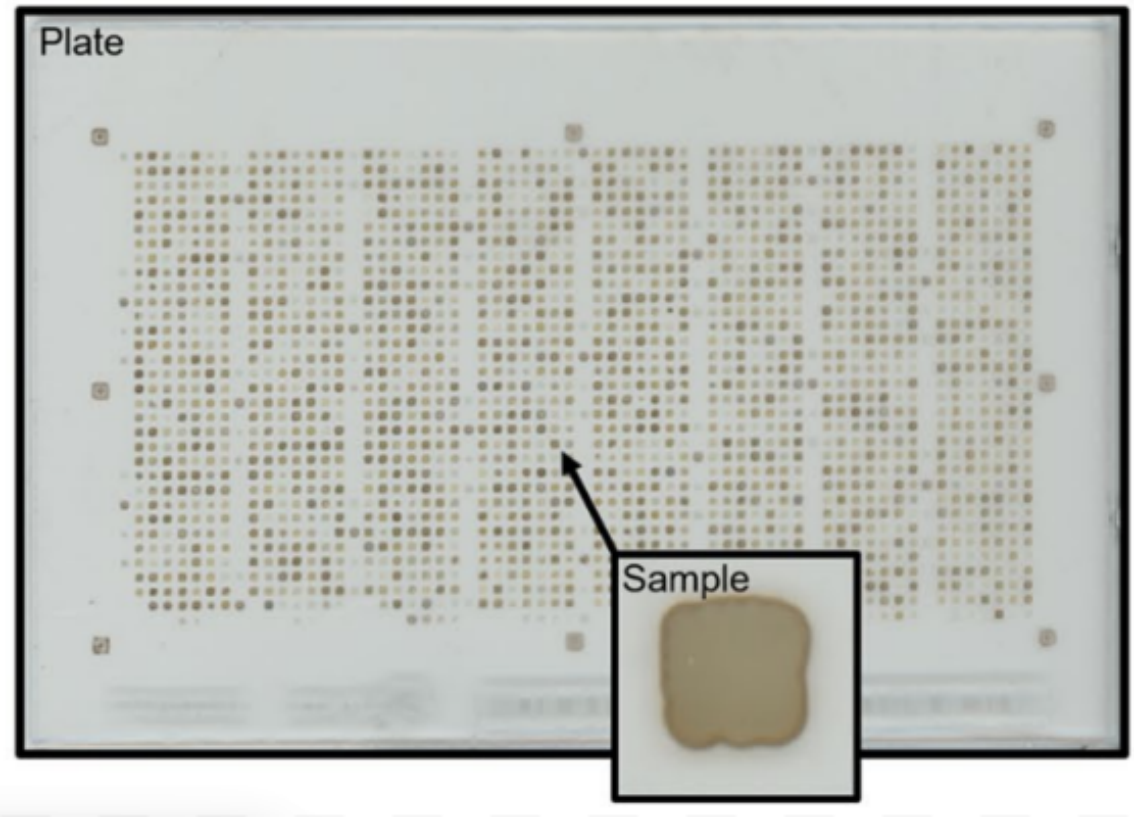
4 Purpose of Research

This algorithm is important to NNSS's nuclear weapons simulations. Current models are extremely computationally taxing even for supercomputers. By using a neural network we could lower the computation time at the cost of deep understanding that comes with all neural

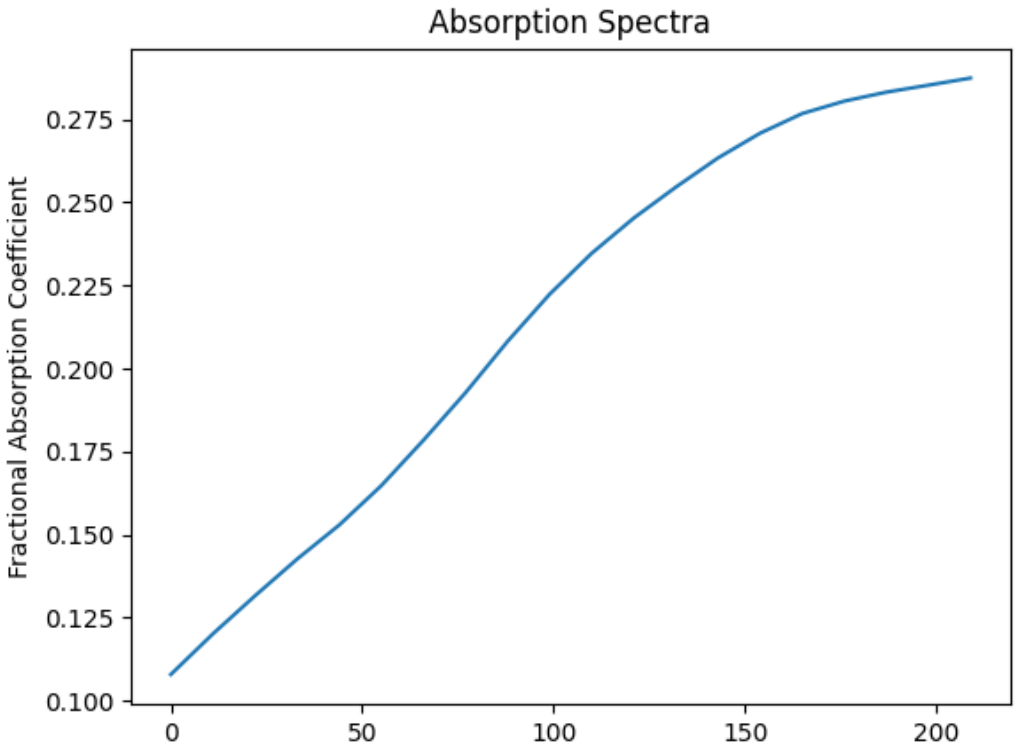
networks. Once this is achieved, our work will also find ways around the “black box” nature of neural networks and put predictive errors on our results.

5 The Data

As was mentioned previously, for this project, the input data is 181,000 images of metal oxides. An example can be seen below.

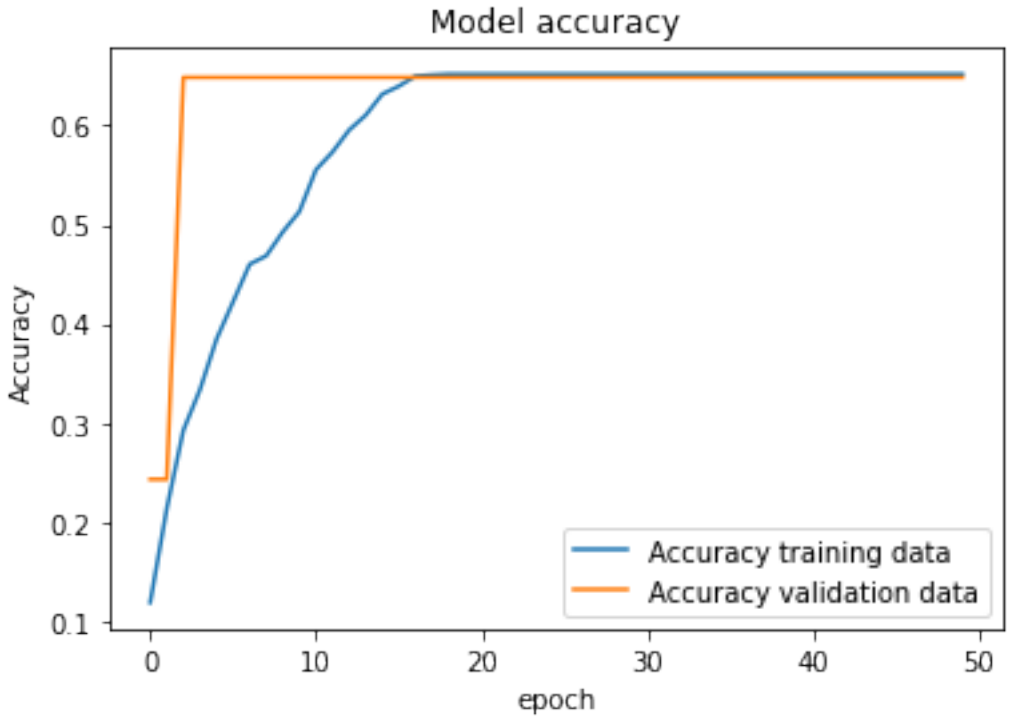


The data is stored in a 64 x 64 x 3 array. This means each image is 64 by 64 pixels with 3 channels corresponding to the RGB values of each pixel. The interesting data lies in the center of the image as coffee ring that forms around the oxide is a result of hardening and is not useful. For each oxide there is a spectra graph with 220 points. An example is shown below.



6 Progress

We currently have a semi-working neural network, but it still needs a lot of work. The code took about 3 hours to run and thus we ran out of time to do any concrete testing on the results. Our plan is to put several test points in and see if the graph created is what we expect. Next, we want to investigate the strange graph that came from our epoch history graph.



As can be seen the accuracy validation data follows a straight line rather than a curve. Finally, we want to change some settings in the neural network and see if changing the number of neurons, layers, etc lead to a higher accuracy.