Ensemble Neural Networks

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1 Abstract

Neural networks are an emerging topic in the computer science industry due to their high versatility and efficiency with large data sets. The Nevada National Security Site is seeking for deep learning techniques to analyze radio graphic images of small-scale nuclear explosions in order to ensure that the United States nuclear stockpile remains safe, reliable and secure. In building a deep learning model, multiple convolutional neural network architectures are developed in parallel and combined to create an ensemble neural network. Neural networks are often referred to as a "black box algorithm" due to the uncertainty in the weights and biases applied to the model. This algorithm poses the uncertainty quantification, which is the question of how to correctly measure accuracy in a regressive convolutional neural network. The project's objective is to determine the comparative differences between the efficiency of the ensemble neural network versus each individual convolutional neural network through the uncertainty quantification. As model precision is a key aspect of machine learning, emphasis is placed on the efficiency of ensemble neural networks to produce an error bar alongside the predictions. Support for the program has been provided by the National Science Foundation (NSF) through REU Award Number DMS - 2050754.

2 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.

3 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.

4 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

5 The Data

Input: Images of metal oxides (64 x 64 Pixels, 3 RGB Channels, 179072 Samples)

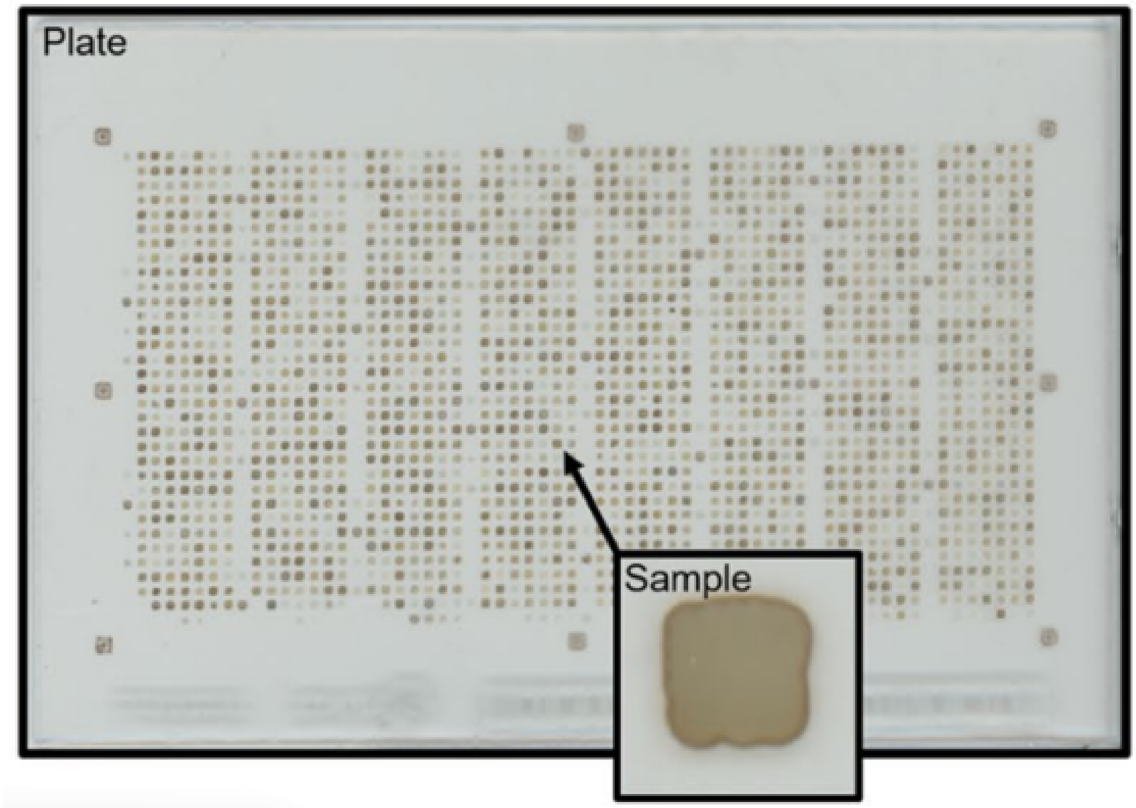
- Sample images were taken using a commercially available consumer flatbed scanner (EPSON Perfection V600) in refection configuration at 1200 dpi corresponding to a rate of 2.0 cm2 s1 or 0.019 s per sample
- All images were rescaled to 64×64 pixels via the python image library (pillow)

Output: Spectra graph (220 Fractional Absorb Coefficients, 179072 Samples)

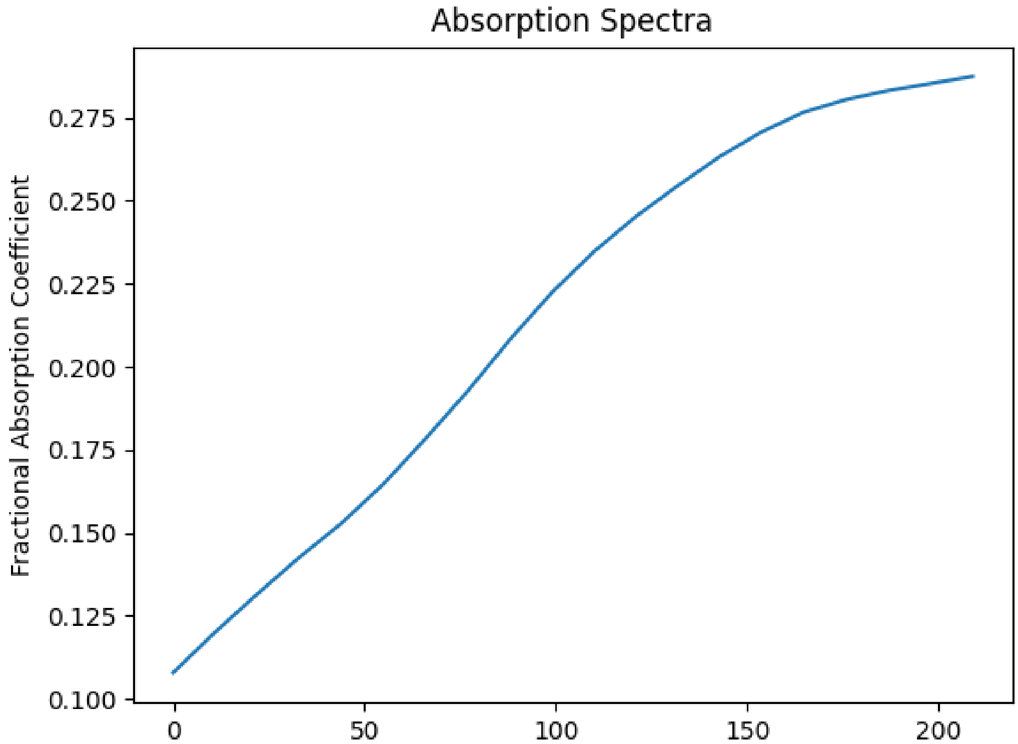
- Energy range for all spectra is 1.32 eV (left end) to 3.1 eV (right end)
- Discretize into 220 photon energies
- Optical absorption spectra were measured using an on-the-fly scanning UV-Vis dual-sphere spectrometer

An example can be seen below.

Input Images:



Output Spectra Graphs:



6 Neural Networks

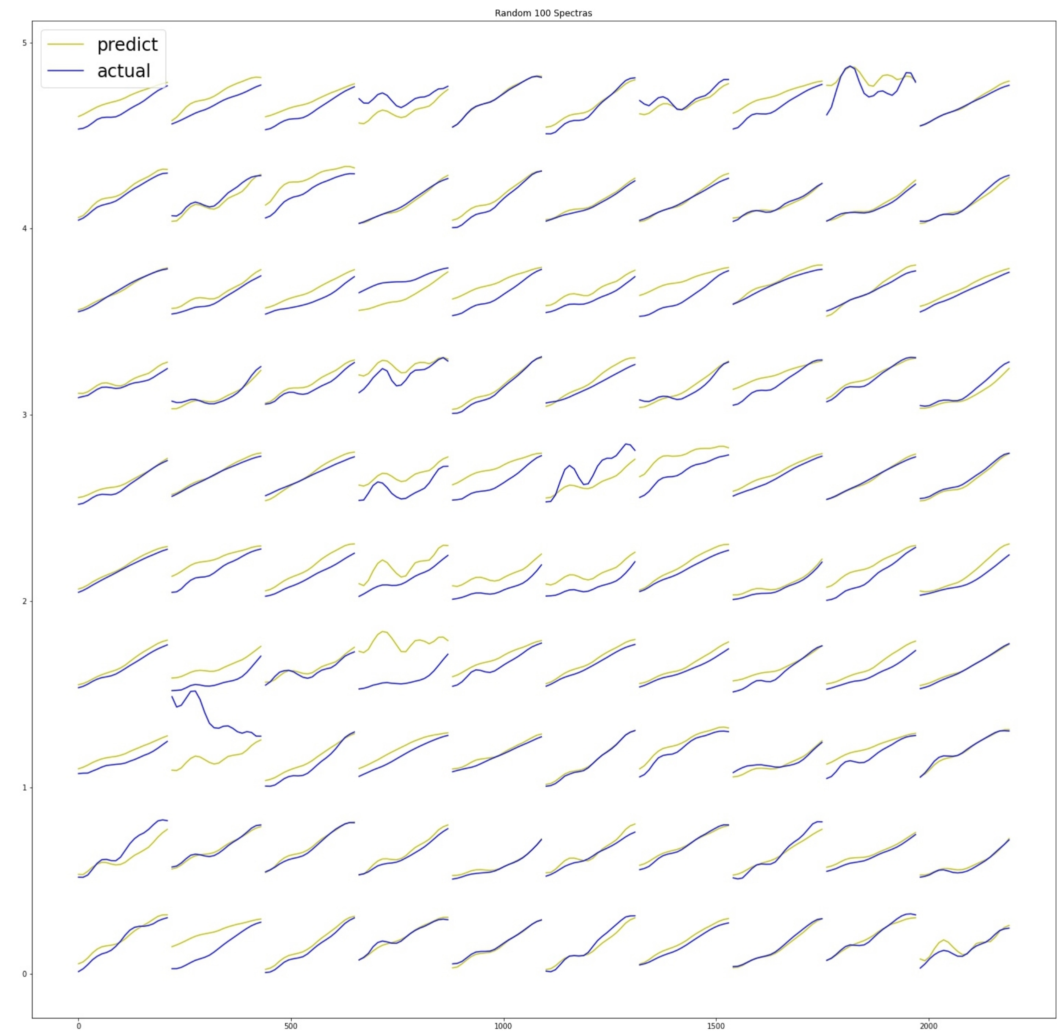
A neural network is an algorithm modeled after the network of neurons in the human brain, which, when trained, is able to identify underlying relationships in a set of data. Similarly to how we learn, it takes in training data to understand what it is looking for and then uses that to predict future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

Current Model:

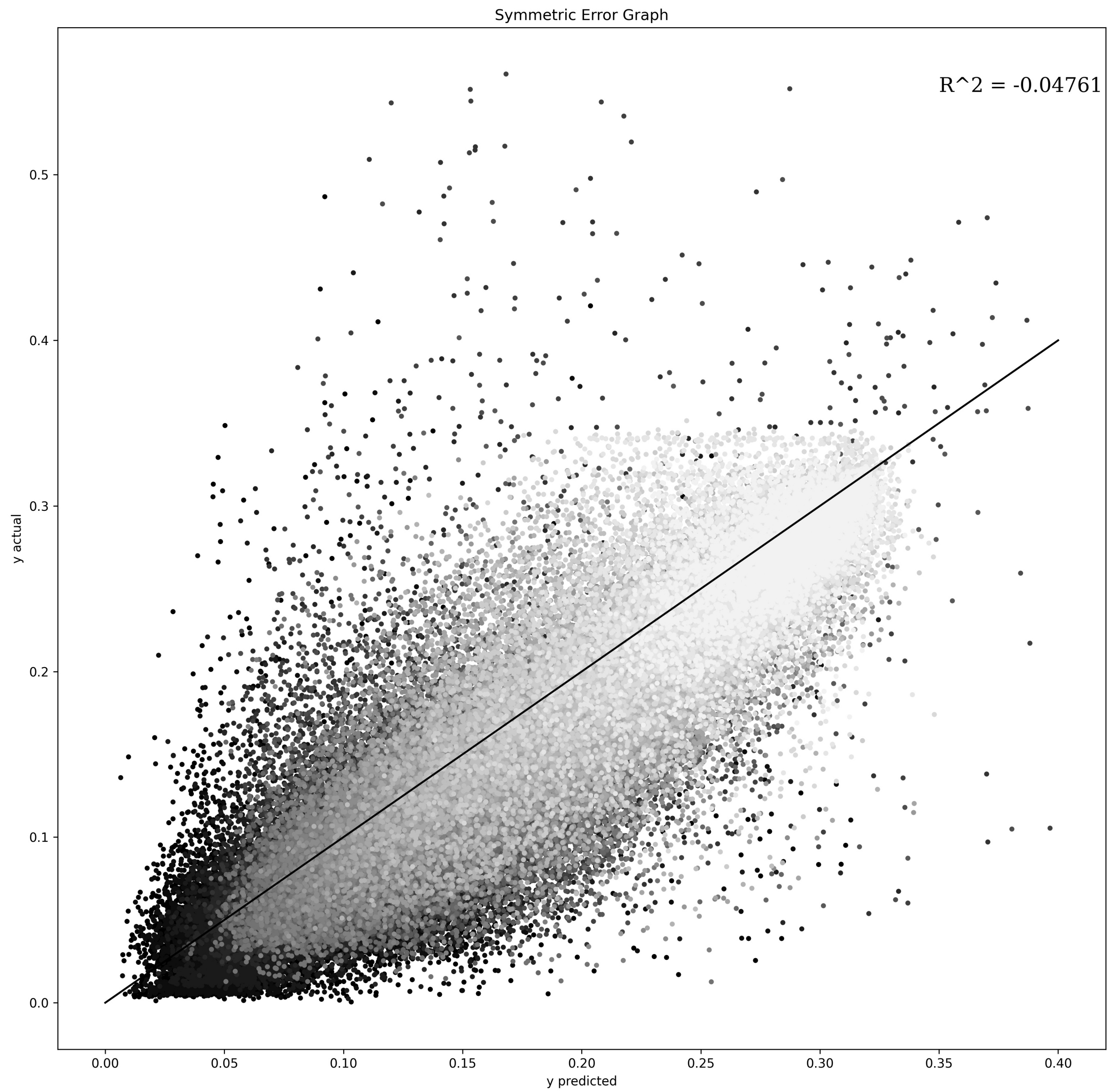
```
 Layout (type)                   Output Shape              Param #
==================================================================
 conv2d_16 (Conv2D)             (None
, 62, 62, 64)         1792

 dense_64 (Dense)               (None, 62, 62, 64)        4160

 max_pooling2d_16 (MaxPoolin     (None, 31, 31, 64)       0
 g2D)

 flatten_16 (Flatten)           (None, 61504)             0

 dense_65 (Dense)               (None, 128)               7872640

 dense_66 (Dense)               (None, 64)                8256

 dense_67 (Dense)               (None, 20)                1300

==================================================================
```

7 Current Progress

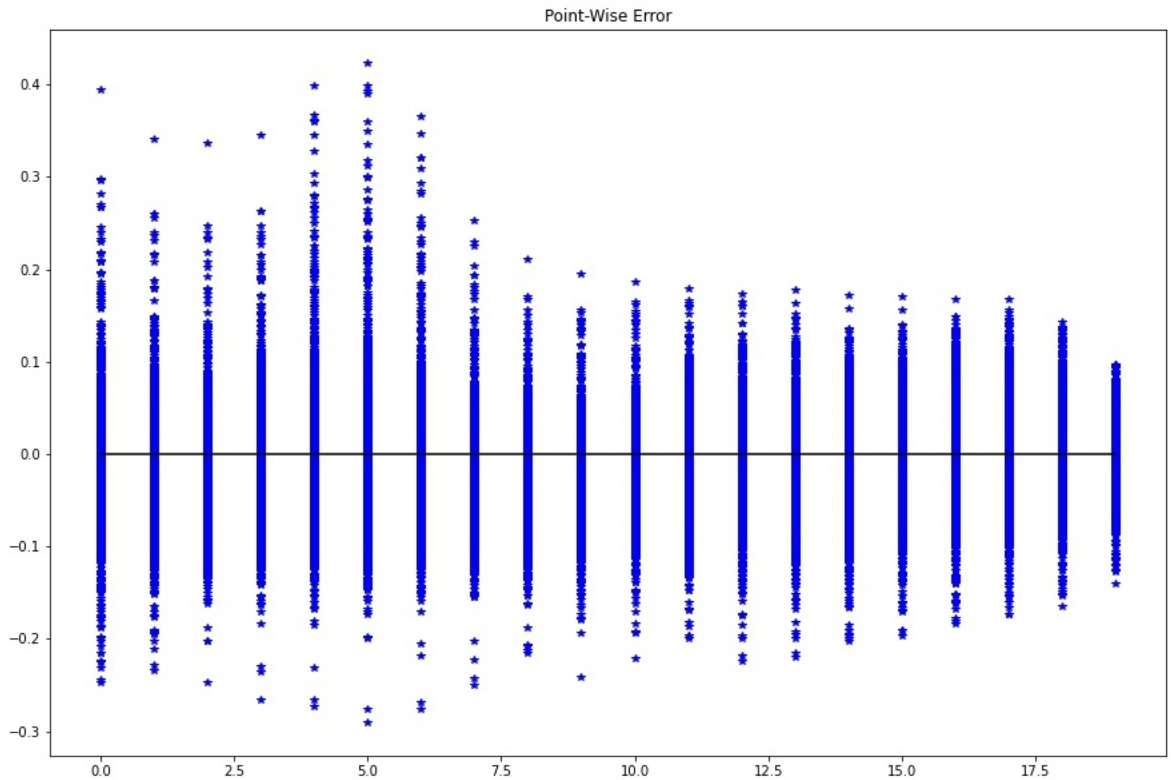
To increase the accuracy of our predictions, we have made an ensemble neural network consisting of 5 networks all using the architecture from above. Since the networks all start with random weights they produce slightly different predictions despite training on the same data and architecture. Once the 5 networks are trained their outputs are geometrically averaged for the final prediction of the ensemble. The most recent model produced the following results.



Obviously the graphs produced are not exactly correct. To compare the predictions a symmetric error graph was created. In this graph the predicted value is on the x axis and the actual value is on the y axis for all of the validation data. Thus the desired area for the points to be on is near y=x. Points above the curve means the prediction was under-approximated and vice versa.



This plot is useful as the spread helps us see which ensembles are better. The R^2 in the corner is a measure of the linearity of the graph. As that approaches 1 the points should get closer to y=x. This specific graph shows that our points are being consistently under-approximated. This is further reinforced by the following point-wise error graph. This plots the error at each of the 20 output points individually to see whether the error is consistent across all points or focused on certain ones



From this we can see that the error is largely found in the first 5th, 6th, and 7th points. More research must be conducted to figure out how to remedy this.

8 Next Steps

1. Fix the inaccuracies in the neural network
2. Create metrics that the final neural network will have to meet
3. Create detailed reasons for each of the choices we made in the network i.e. epochs, batch size, error method, etc
4. Start research on the uncertainty quantification