Quantifying Uncertainty with Ensemble Neural Networks for Metal Oxide Spectrograms

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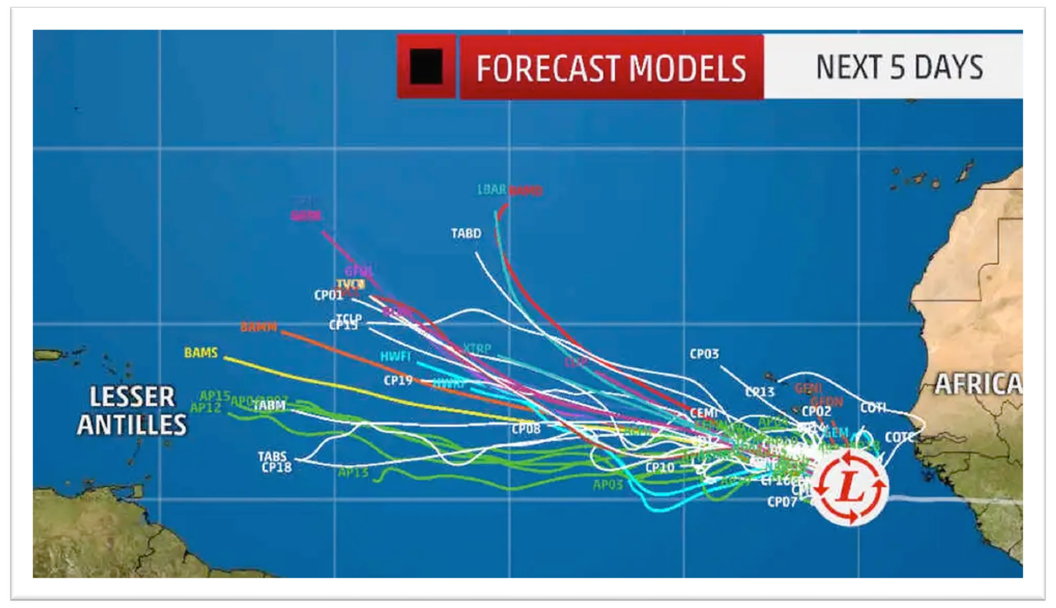
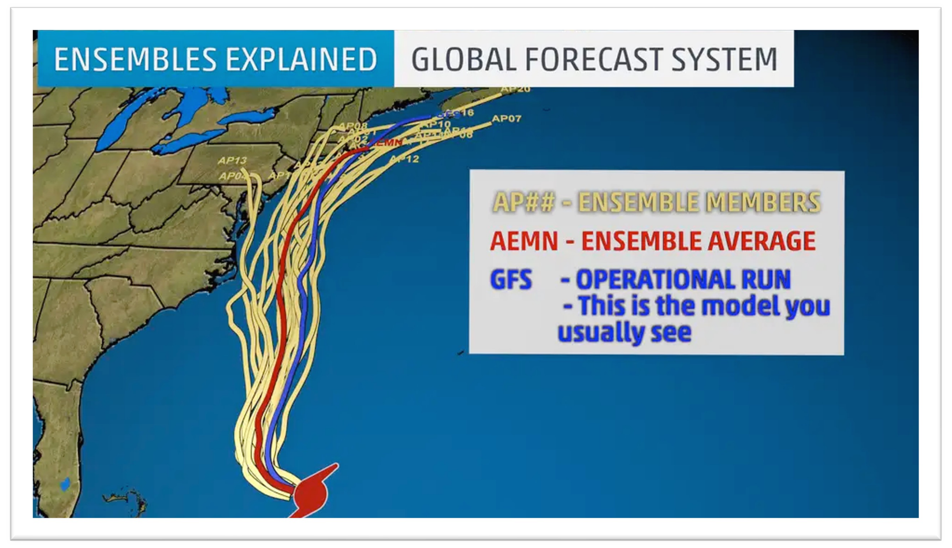
ABSTRACT

Optical absorption spectroscopy is an important characterization of materials for applications such as solar energy generation. The purpose of the study is to build an ensemble neural network for predicting metal oxide spectrograms from images of metal oxide that have been scanned. With an ensemble network, several models are trained to produce a variety of predictions. By averaging these predictions, an even more accurate prediction can be made. Furthermore, uncertainty quantification will be applied by measuring the variance between the predictions, allowing more useful statistical analysis to be done such as producing confidence intervals to determine how accurate the results are. The study was done through a quantitative empirical research method and preliminary results show that an ensemble neural network performed better on average than a base single model. Through uncertainty quantification it was also found that neural networks using this approach had little variance between models.

ENSEMBLED NEURAL NETWORK

Ensemble Neural network is a learning paradigm where many neural networks are jointly used to solve a problem.

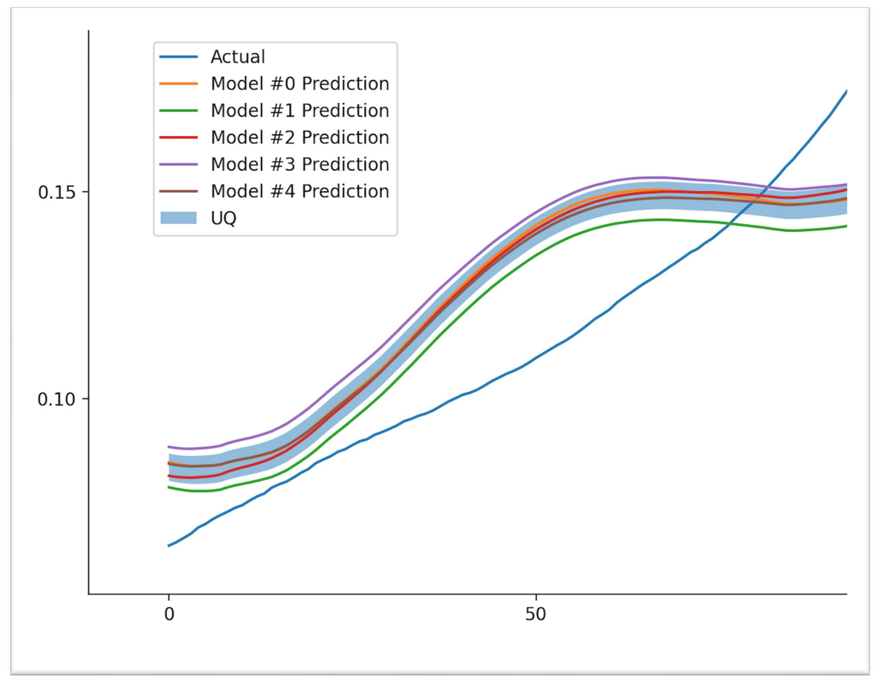


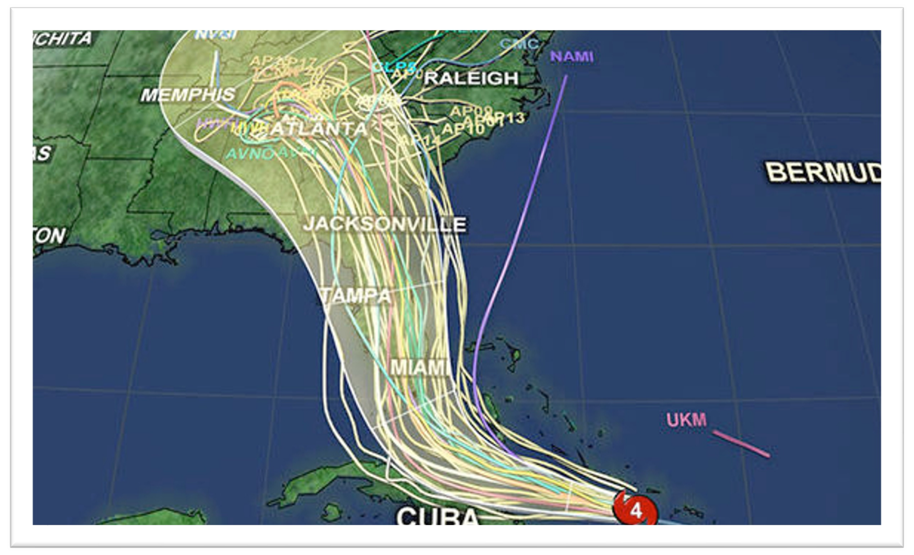


- A relatable real-world example of ensembled neural networks are hurricane predictions which are typically called spaghetti models used by meteorologist forecasters.

UNCERTAINTY QUANTIFICATION

Ensembled networks by themselves show a variety of prediction values so uncertainty quantification and variance are used to show what looks like a cone for the variance of the different model's prediction area.

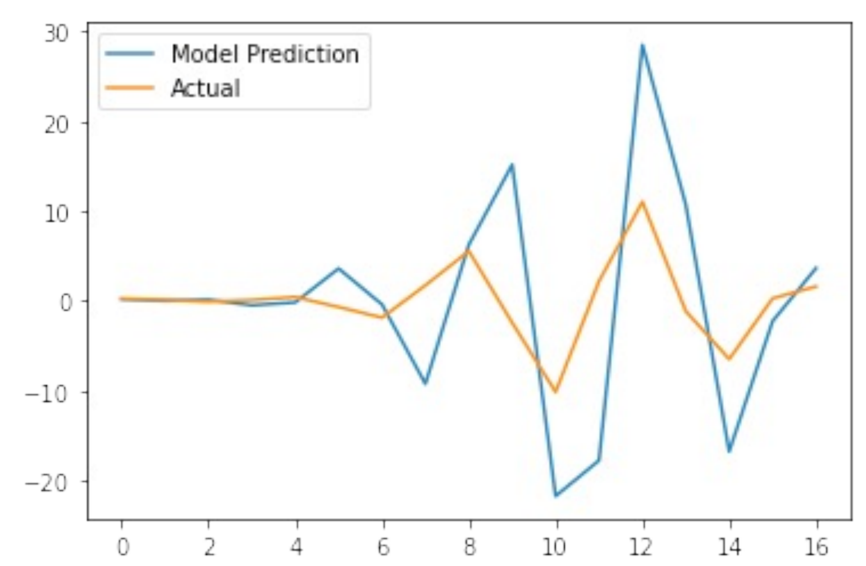




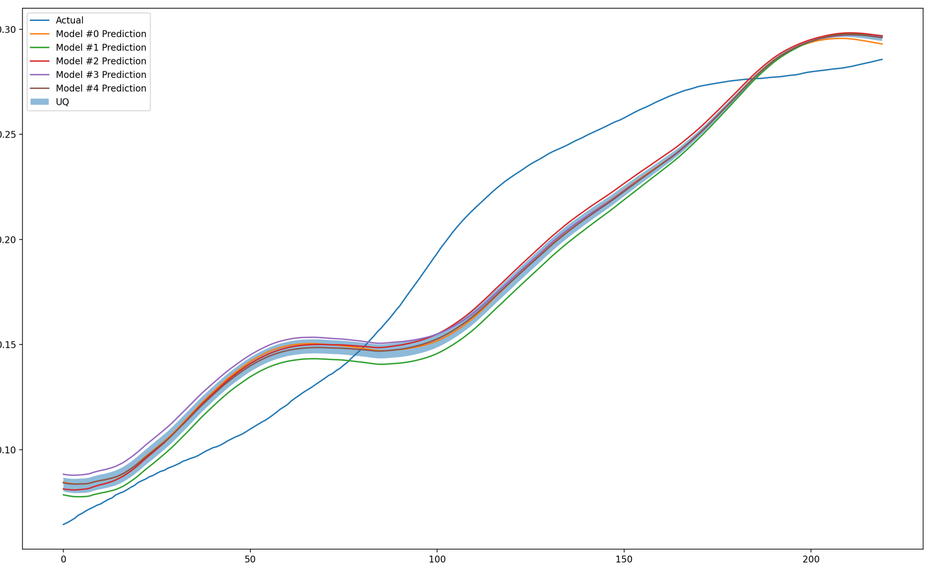
A relatable real-world example of uncertainty quantification can be seen in the cone of confusion of hurricane forecasting where many forecasted models show day by day movements.

PRELIMINARY RESULTS

Preliminary results do not show any benefits to applying polynomial augmentation to the metal oxide dataset but further investigation is necessary to why it did not work.

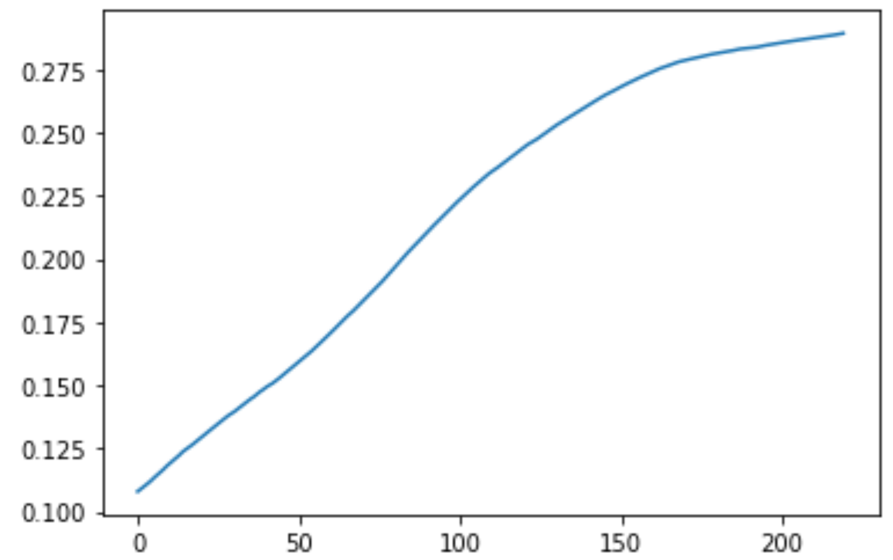


Preliminary results show that an ensemble neural network performed better on average than a base single model with little variance between the model.

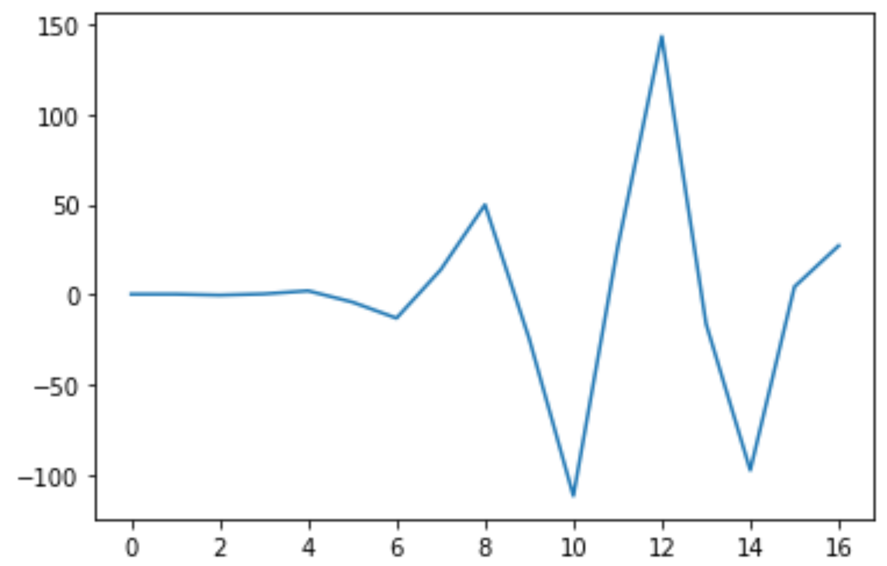


POLYNOMIAL AUGMENTATION

Using polynomial regression to change the labels from size 220 to size of 17 by using polynomial regression because the full 220 is unnecessary and computationally expensive.

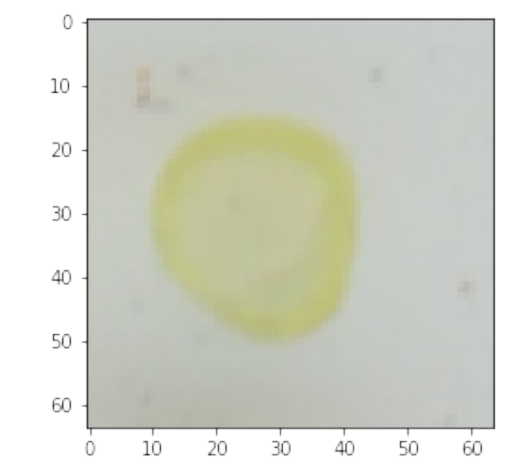


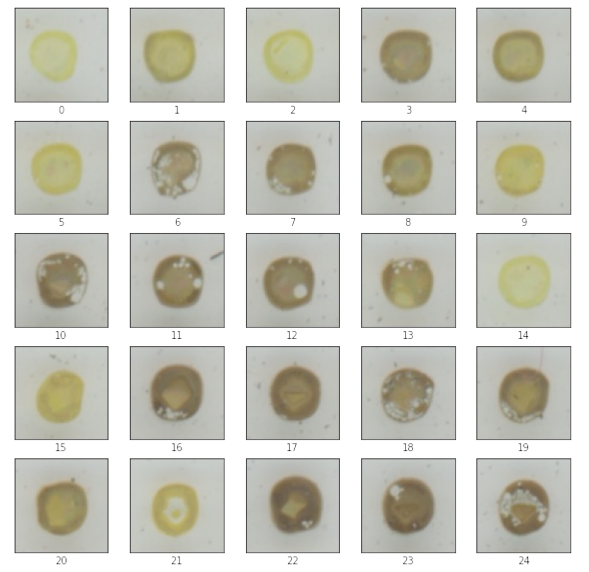
With polynomial regression reduces the data points from the original 220 to 17 datapoints which can be seen in the image to the right



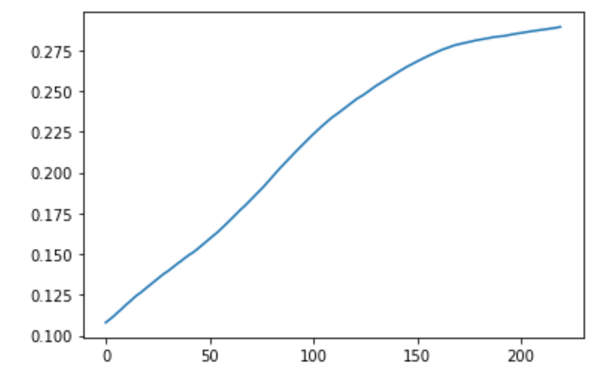
DATASET

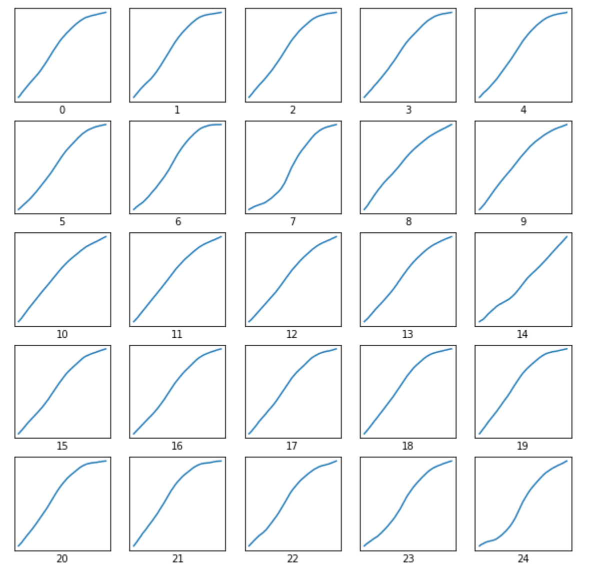
- **CALTECH JCAP images and absorption spectra for 179072 metal oxides was used for the experiments.** bit.ly/3v9itPk





Input – 64px,64px,3 layers





Output – 220 data point spectrogram