Uncertainty Quantification in Ensemble Deep Learning

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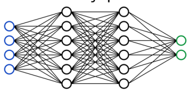
Abstract

Neural networks are an emerging topic in the computer science industry due to their high versatility and efficiency with large datasets. The Nevada National Security Site is seeking deep learning techniques to analyze radiographic images of small-scale nuclear test explosions to ensure that the United States nuclear stockpile remains safe, reliable, and secure. Neural networks are often referred to as a “black box algorithm” due to the complicated series of weights and biases that make up the model. The project’s objective is to determine the comparative differences between the predictive ability of each individual convolutional neural network versus the ensemble neural network. Additionally, we will explore how to use the ensemble model as a method of uncertainty quantification.



Nevada National Security Site

The Nevada National Security Site (NNSS) is a United States Department of Energy reservation located approximately 65 miles northwest of Las Vegas. NNSS specializes in defense nuclear nonproliferation and the pursuit of science. They cannot conduct full-scale nuclear tests, but instead conduct controlled underground experiments and computer simulations to verify that the arms are safe and usable.

Introduction

Neural networks provide the opportunity to analyze large amounts of image data to produce a regressive output quickly and cheaply. Using a set of inputs and a set of desired outputs, the network is trained and tested in order to predict the desired outputs. The network trains itself through learning patterns and correlations between data and assigning weights and biases to certain values to produce a label.

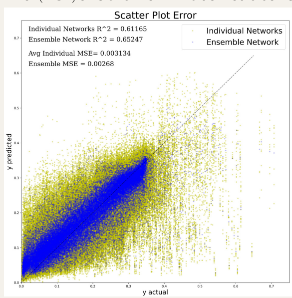
Uncertainty Quantification (UQ) is the method of using various methods to quantify and reduce the amount of uncertainty in a data set. An ensemble neural network combines multiple similar neural networks to produce a final result. These multiple outputs can be used as a method of uncertainty quantification for neural networks

DATASET

The dataset used is synthesis, optical imaging, and absorption spectroscopy data for 179072 metal oxides. The data contains 180902 64 by 64 images with their corresponding 220 point absorption spectra and chemical makeups. Some of the images are blank, leading to 179072 total samples. The color in the middle is the main contributor to the spectra, while the "coffee ring" around each sample is a result of drying and thus less important.

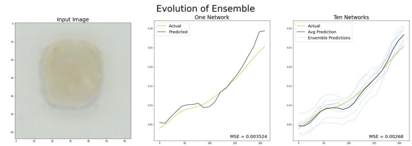
SINGLE VERSUS ENSEMBLE NETWORK ERROR

The graph below plots the actual versus the predicted value of the network. Thus the desired output is all of the points lying on the dashed y=x line. Looking at the individual(yellow) and ensemble(blue) points we can see that the ensemble points are much closer around y=x than the individual. A perfect model would have a Mean Squared Error (MSE) of 0 and the R^2 value would be 1.00 i.e. all the predictions were 100% were exactly a straight line on y=x), Thus we want to minimize MSE and maximize R^2. The figure shows we achieved a lower MSE and higher R^2 for the ensemble compared to the individual. Additionally The MSE and R^2 values of .00268 and 0.65247 respectively were acceptable values given our limitations



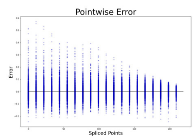
Prediction of Ensemble

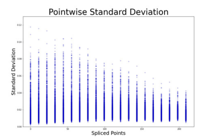
The figure gives an example output of the neural network, displaying the ensemble neural network prediction in comparison to the individual network predictions. The ensemble takes an average of each of the individual neural networks to produce a single output. Time constraints only allowed us to build an ensemble that averages all the network predictions equally, but a way to improve upon this would be to weight networks that had a lower mean squared error more significantly than networks with a high mean squared error.



Uncertainty Quantification

In the figures below we separate the data by each of the 20 points of the spectra to see the relationship between error and uncertainty. Standard deviation is measured as it is the sole factor in determining the size of the confidence interval. In both we see that the error starts out widely distributed but becomes closer as we get to the later points. This is shows that the error of the network is seemingly in proportion with the uncertainty. This is important as the error plot can only be made when the true value is known. However, if the true value is known then we have no need for a neural network. The plot of the standard deviations can be made even if the actual value is unknown as it is made from the network outputs. This will help us determine an STD cutoff for which predictions to trust and which ones to remove.





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