Ensemble Deep Learning: Neural Networks

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Introduction

Embry-Riddle Aeronautical University's Research Experience for Undergraduates program (REU) is partnering with the Nevada National Security Site (NNSS) with funding from the National Science Foundation (NSF) in order to develop methods for quantifying and understanding uncertainty in the accuracy of neural network algorithms. The REU students will use publicly available datasets to develop a neural network, and will also create an ensemble with some uncertainty quantification (UQ) approach, such as Monte Carlo (MC) dropout, in order to better comprehend the results of the neural network and the uncertainty factor of their accuracy (Adams & Lund, 2022).

Background

The NNSS, formerly known as the Nevada Test Site (NTS), is a part of the United States Department of Energy (DOE). Their complex is larger than the state of Rhode Island and focuses mainly on Defense Nuclear Nonproliferation and Stewardship Science & Experimentation. Although there are many divisions within the NNSS, REU students will be working directly with the Weapons' Program, whose goal is to ensure the United States' nuclear stockpile remains safe, secure, and effective. In order to do this, they conduct classified nuclear experiments, high-tech computer modeling, and detailed engineering analysis according to their website, (*About the NNSS*, n.d.). At the U1a underground facility high energy tests are conducted so that radiographers can capture high resolution images of the explosions and interpret if things are working the way that they should be. This is where neural networks are widely used. There are thousands of images to sort through and interpret, and there is a lot of post processing to complete to learn anything from the images, so therefore neural networks are used to speed up the process and essentially extract the truth. But when using neural networks to determine if nuclear weapons are working as they should, a high amount of accuracy is needed since the safety of our nation depends on these tests. Without accurate error bars on these neural networks' predictions, detrimental explosions or mishaps could occur because of a slightly off uncertainty value. Therefore, it is necessary to research implementation methods for better quantifying uncertainty levels in neural networks.

Scope of the Problem

Neural networks are computer algorithms modeled after the neuron connections in a human brain and are used to detect relationships and patterns in large sets of data to better understand it. They consist of an input layer, multiple hidden layers, and an output layer. Given some input data a neural network will go through multiple different layers and pathways until it decides on the most likely output value. In essence, neural networks can be used as a type of prediction model. But no prediction model has 100 percent accuracy all the time; there is always some error. A widely used example of how neural networks can have high uncertainty is as follows. Say you have a neural network that takes in images and gives an output of whether they are a cat or a dog, but then you input an image of a zebra. The neural network will still predict this image as either a cat or a dog because it has not been trained to recognize zebras as an output, and therefore has a high uncertainty value and subsequent error bar for that specific image. Learning how to accurately quantify the level of uncertainty in neural networks by accounting for situations like these is what the REU students will be focusing on for the duration of their research.

Uncertainty Quantification (UQ) is the science of using various methods to quantify and reduce the amount of uncertainty in a data set. An ensemble neural network combines multiple similar but individual neural networks to decide on the most likely cumulative output based on each networks individual results. An ensemble is a type of UQ approach because it adds more checks to the neural network to ensure it is as certain as possible about its output value. REU students will attempt to implement an ensemble neural network for their selected dataset alongside another UQ approach to see how low the uncertainty factor in the accuracy can get without overtraining the network. Students will decide on their specific UQ approach individually, and combine individual efforts to develop the best neural network possible.

Data Visualization/Description

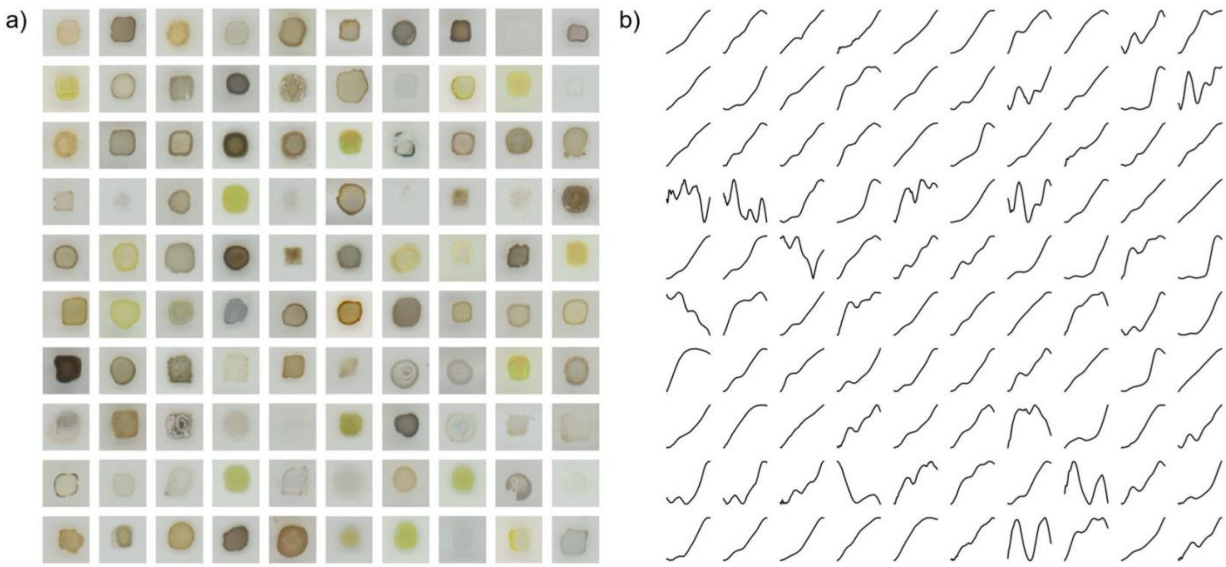
The selected data set is JCAP images and absorption spectra for 179072 metal oxides, and is provided by the US DOE and described by Figure 1, (Gregoire et al., 2018). Inputs are characterized as images and outputs are characterized as spectra. There are 220 output values for each input. Images were taken using a consumer flatbed scanner and scaled to 64 x 64 pixels. The colored imaging in the center is the printed material, whereas the coffee-ring-like structure on the outer edge is due to drying of the printed solutions and you can see these different structures in numerous images within Figure 2. All of the absorption spectra were measured using a dual sphere spectrometer, and represents 220 photon energies between the 1.31 to 3.1 eV energy range. The reported outputs are “fractional optical absorbance, which is the product of the absorptions coefficient and effective material thickness,” (Stein et al., 2019). These are represented by the graphed line data in Figure 2.

Figure 1:

Dataset	Content Description	Data Range	Data Size	Physical Units	Method
Images	Sample images	0–1 for every channel	(64,64,3,180902)	Color values for RGB	platebead scanner
spectra	fractional optical absorbance spectrum	0–ca. 0.5	(220,180902)	fractional absorb. coefficient	dual-sphere optical spectrometer

Description of JCAP Dataset. Note that images are normalized between zero and one, and are routed through three channels (RGB), (Stein et al., 2019).

Figure 2:



Correlation of input images and there corresponding output spectra line graph, (Stein et al., 2019).

References

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