Mayna Nguyen

Project Report

Introduction

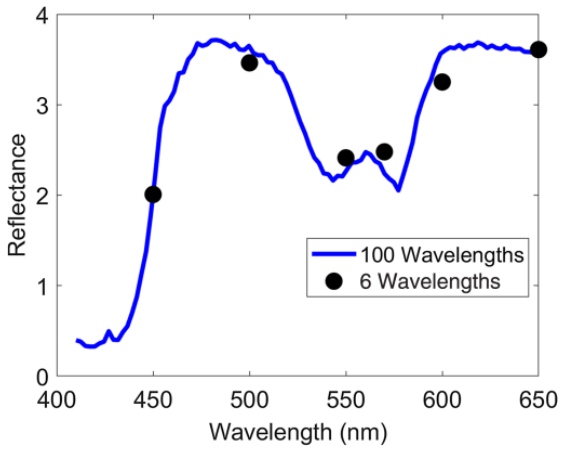
The topic of this project is on using diffuse reflectance spectroscopy (DRS) as an optical technique to extract optical properties and physiological parameters. This topic is interesting especially in the field of biomedical engineering because DRS is a noninvasive method where you shine light on tissue such as skin and the light that is collected back after scattering can determine how much scattering and absorption is in a specific area of tissue. This can be extremely useful in medical diagnosis of diseases such as skin cancer, breast cancer, cervical cancer, and so on. If fewer wavelengths of data could be used for DRS, then a cheaper device can be used, making for an easier transition to the clinic. This project is original work and is an extension of my recent paper from undergrad, "Machine learning to extract physiological parameters from multispectral diffuse reflectance spectroscopy" published in the Journal of Biomedical Optics.

Problem definition

This paper explores using machine learning methods to see if fewer wavelengths of data could be used to extract optical properties/physiological parameters. The main idea was to explore different machine learning methods to see if the accuracy and speed were advantageous, with the point of the paper being not on the algorithms themselves but seeing if machine learning could be sufficient for fewer wavelengths. The R package H2O with default parameters was used so there was not an understanding of the parameters of each model. The results turned out to be good enough to show that machine learning could be accurate enough, but there is room for improvement, optimization, and more testing. For this project, the tools we learned in class to were used to build the models in python to understand better what these models are doing, how they work, what parameters are used to adjust the model, and to further optimize the deep learning neural network model that was the most accurate in the paper.

Methods

The data set for this project is 100,000 spectra from 10 linearly spaced values of 5 different parameters: blood volume fraction (BVF), reduced scattering coefficient (μ_s' or musp), scattering exponent (B), melanin (Mel), and oxygen saturation (O2). These spectra are scaled to be at 6 different wavelengths using a weighted average, so there are 6 reflectance values for each spectrum for a total of 100,000 spectra, which are split randomly into a 70% training set and 30% test set.



Mayna Nguyen

Following the models used in the paper, random forest (RF), gradient boosting machine (GBM), generalized linear model (GLM), and deep learning/neural network (DL) models were built in python. The sklearn package was used for the RF, GBM, and GLM models and the pytorch package was used for the DL model.

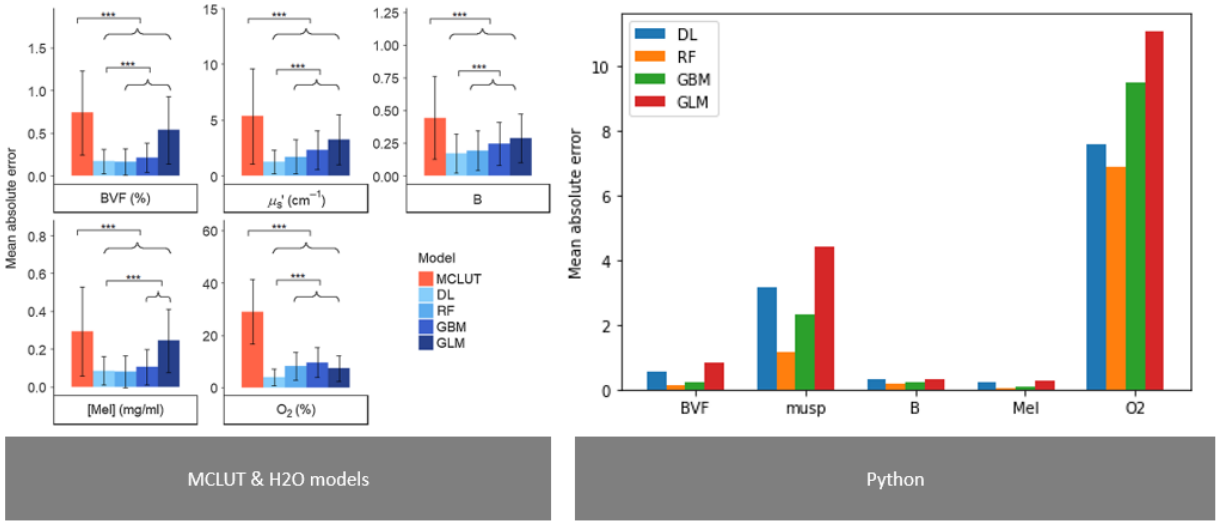
Next, the neural net model parameters were adjusted for optimization. This was all done in pytorch and a new neural network with a different parameter was tested to see what parameters best optimize the network. The original neural network was built to reflect H2O's default deep learning model of a 2-layer neural network with a rectifier (ReLU) activation, Adam optimizer, and MSE loss function. The following parameters were changed one parameter at a time to see if they would optimize the model: tanh activation function, SGD optimizer, L1 loss function, and a 3-layer network.

The mean absolute error and mean absolute percent error were both calculated. The mean absolute percent error is important to compare to errors in prior biomedical studies of optical properties, which are typically less than 10%. The mean absolute error is presented due to the variability in errors that are caused by dividing by very small parameter values.

A couple of other approaches were also attempted but the results are not presented here, as they resulted in larger errors than the original neural network. After the activation function was changed to tanh, this change was fixed for the rest of the changes. Also, a model with the tanh, SGD optimizer, and L1 loss function was tested to see if all the changes resulted in an even more optimized model, but this did not work. Instead, the models used and presented below are the original neural network but with just one parameter and the activation function changed.

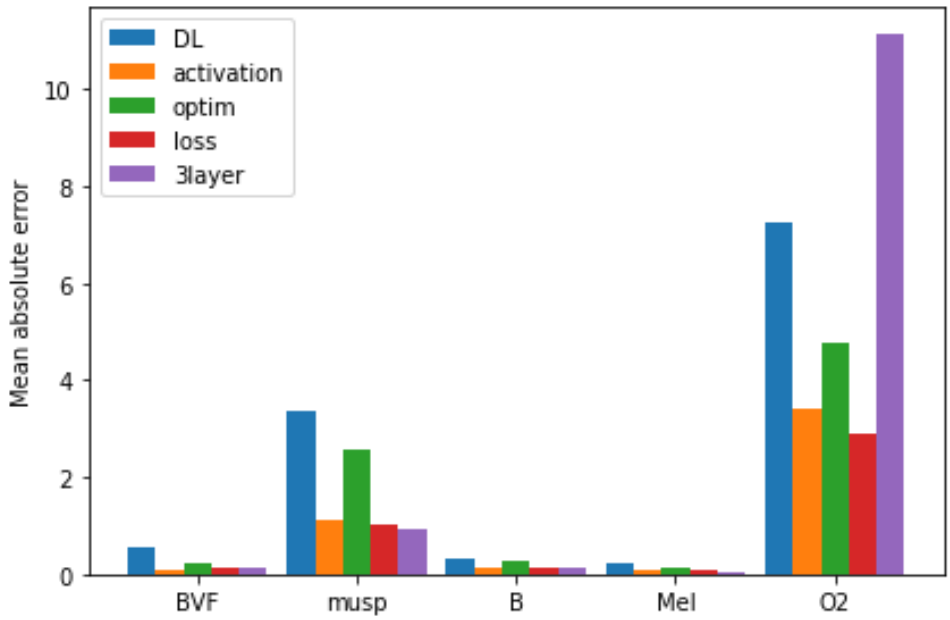
This project only used the sklearn and pytorch packages, which were used in the class previously, so no installation of other packages is necessary. To run the code, open the jupyter notebook and run the cells in order to load the packages, error calculations, data, and then models and the subsequent testing code cells. The models are in order: random forest, gradient boosting machine, generalized linear model, and 2-layer neural network. There is then a cell to plot the absolute error of each model. Then the optimized parameter neural network models by parameter follow, along with a cell to plot the errors from those models.

Results



Mayna Nguyen

Compared to the Monte Carlo Lookup Table (MCLUT) model, all the machine learning methods in H2O and in python perform better for extracting physiological parameters. The model results for RF, GBM, and GLM were very similar to their respective H2O model. The DL model seemed to have higher errors than the H2O version, but this is fine as it will be optimized further.



Overall, each change decreased the error except for the 3-layer network. The 3-layer network is more accurate for every parameter except for O2. The changed loss function to L1 loss seems to have the least error in general, although the tanh activation is also pretty similar. Because of this, the mean absolute percent errors of the L1 loss change are as follows: 5.01% for BVF, 5.32% for musp (μ_s'), 7.10% for B, 8.13% for Mel, and 3.76% for O2. This is an improvement from the H2O deep learning errors of 5.15% for BVF, 6.88% for musp, 9.81% for B, 9.91% for Mel, and 4.61% for O2.

Machine learning can extract physiological parameters from only 6 wavelengths of data better than Monte Carlo methods. Optimization of parameters (activation function, optimizer, loss function) for the neural network lowered errors from the default H2O Deep Learning model. An optimized model will hopefully provide better results for when testing with actual measurements. Overall, an optimized deep learning model will provide better accuracy when extracting physiological parameters for aiding in the diagnosis of skin cancer with diffuse reflectance spectroscopy and will be more compelling for a physician to use a device like this in the clinic.

Github repository: https://github.com/maynanguyen/PHYS8100-Project