ROB313 Assignment 1

Q1. Objective is to create the knn regression algorithm, knn_reg, in code. Also had to create an algorithm that can perform 5 fold cross-validation on a training dataset to estimate good K values and choose a good distance metric. This was done in one function, knn_5fold, and another function, knn_err, was created to run knn over a testing dataset and compare it to the true values to produce the RMSE of knn with its given k and distance metric.

knn_reg(xtest,xtrain,ytrain,k,l) - requires you to input k value and L (1 or 2) to specify distance metric (1=Euclidean, 2=Minkowski with p=3) as well as xtest, xtrain, and ytrain points. Will output array of y predictions for xtest.

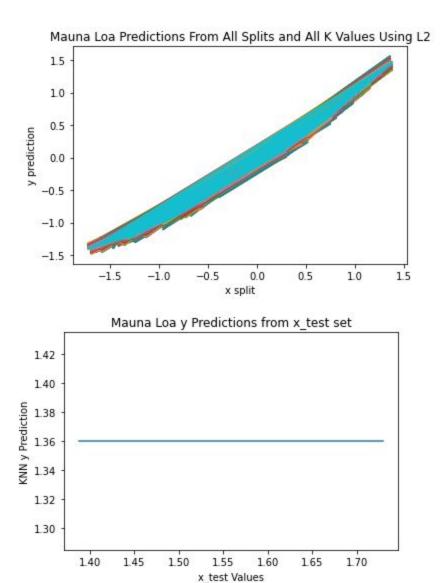
knn_5fold(xtrain,ytrain) - takes in xtrain and ytrain data sets. Performs 5 fold cross-validation on training sets and runs KNN over multiple k values and both distance metrics. Then calculates RMSE of output. Will print estimated k, L,and RMSE and return 0 on completion.

knn_err(xtest,ytest,xtrain,ytrain,k,l) - Will perform KNN, with given k and L value, on an input xtest set using input xtrain and ytrain sets then compare its predictions to the input known ytest values and then return the RMSE of the KNN with its given k and L settings.

My search procedure to estimate k and the distance metric was done by running my KNN 5 fold validation over every reasonable k ($k < \sqrt{N}$) and distance metric (L1 or L2) and calculating the RMSE of each outcome then compiling the RMSE, L, and k values into their own arrays (each had matching indices - for example the RMSE of fold 1 when k=1 and l=1 would have the same index throughout all arrays). I then used np.argmin to find the index of the lowest RMSE and thus estimate the preferred k and L combination.

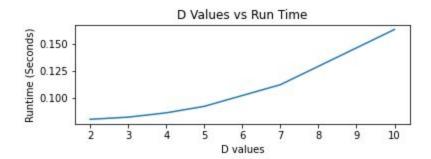
| | 5 Fold RMSE | K | L | Test RMSE |
|------------|----------------------------|----|---|------------|
| Mauna_loa | 0.00641377 | 10 | 2 | 0.06099168 |
| Rosenbrock | 0.629309131, 0.88420056 | 19 | 1 | 0.10574214 |

| D 1 00 | 0.57000000 | 07 | 4 | 0.00050704 |
|-------------|-------------|----|---|------------|
| Pumadyn32nm | 0.57328906, | 37 | 1 | 0.36359724 |
| | 0.51143701, | | | |
| | 0.54528533, | | | |
| | 0.51883375, | | | |
| | 0.53818119, | | | |
| | 0.56548371, | | | |
| | 0.55752719, | | | |
| | 0.54649141, | | | |
| | 0.53099599, | | | |
| | 0.54577932, | | | |
| | 0.57964096, | | | |
| | 0.52914075, | | | |
| | 0.53305128, | | | |
| | 0.59102843, | | | |
| | 0.5387209, | | | |
| | 0.80365903, | | | |
| | 0.56508039, | | | |
| | 0.55157636, | | | |
| | 0.52837679, | | | |
| | 0.5568946, | | | |
| | 0.54855266, | | | |
| | 0.53576814, | | | |
| | 0.56411829, | | | |
| | 0.54627673, | | | |
| | 0.52828565, | | | |
| | 0.53808016, | | | |
| | 0.53376694, | | | |
| | 0.5487159, | | | |
| | 0.53633099, | | | |
| | 0.55259372, | | | |
| | 0.52805982, | | | |
| | 0.53550876 | | | |
| | | | | |
| | | | | |



The predictions from the 5 fold validation appear to follow a similar pattern to that of the training data with an overall positive slope. The x_test values appear to give a constant prediction for the y values. This is due to the fact that every x_test value is larger than any x_train value causing every x_test value to have the same K neighbours but with different distance values to them, giving the same prediction for every point.

Q2. Create knn_reg like in Q1 but using KDTrees to compute nearest neighbours.



The performance of KNN using KDTrees is much better compared to using brute-force to find nearest neighbours. When running my brute force code with rosenbrock with d=2 and n_train=5000 it took 0.67862 seconds compared to KDTrees only taking 0.08008 seconds for rosenbrock with n_train=5000 and d=2. The KDTrees algorithm has a faster runtime and better performance compared to the brute-force approach.

Q3.