Neural Networks Project II

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Guided by-

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Introduction

This report focuses on the same datasets as project 1. You will notice there are very few changes in data preprocessing and EDA as a result. However, this project focuses on 2L, 3L, and XL neural nets. Across the board performance of these models were better than the models used in project 1. For our pythonic neural nets, we mostly used Keras from Tensorflow due to its more streamlined implementation into datasets, although there was some use of Pytorch. Scala neural nets were optimized according to each dataset. Feel free to reach out to any of the group members listed with any questions or concerns.

Airfoil

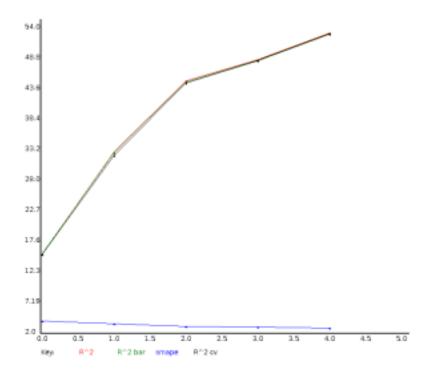
Data preprocessing:

EDA:

All data preprocessing and EDA performed for this dataset was the same as described in project 1. Please see our previous report for details. The only exception is that I found in building neural nets in Python, performance was dramatically improved when data was normalized beforehand.

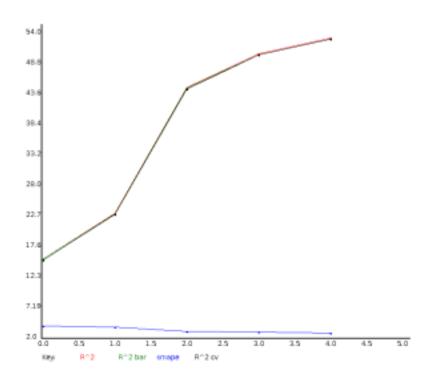
Feature Selection:

Backwards and forwards feature selection in scala show steep improvements with the addition of each feature. There seems to be no plateau as we see in the linear regression and variants in the previous project. From my understanding of how neural nets perform this makes sense. As the neural net iterates readjusting weights for each feature and through each node it will passively maximize the effectiveness of each feature's ability to predict our output. Theoretically, only features that have no relation would reduce or slow down performance.



2 layer forward selection in scala.

R^2 vs n for NeuralNet_2L_sigmoid with Backward



2 layer backward selection in scala.

Splitting Data Information:

In scala our train and test dataset was split 80-20. K-fold split was also divided into 5 and again 80-20 tnt split. Same thing for python.

Discussion of Results:

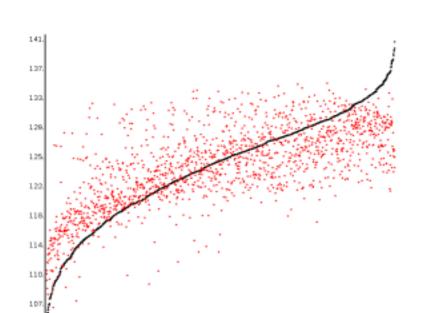
Our two layer neural nets in scala performed best using the sigmoid function. R-squared, r-squared bar, and SMAPE values were 0.533, 0.531, and 2.9 respectively. Tanh performed almost identically with r-squared, r-squared bar, and SMAPE of 0.533, 0.531, and 2.9 respectively. eLU, reLU, and IreLU all performed similarly and slightly worse than sigmoid and tanh. They contained r-squared, r-squared bar, and SMAPE values of 0.516, 0.514, and 3.0 respectively. Because of the better performance of sigmoid which is slightly simpler implementation than tanh we decided to continue 3L and XL analysis with sigmoid.

```
respectively. Because of the better performance of sigmoid which is slightly simpler
implementation than tanh we decided to continue 3L and XL analysis with sigmoid.
[info] modelName mn = NeuralNet 2L sigmoid
[info] -----
[info] hparameter hp = HyperParameter (HashMap(lambda -> (0.0
1,0.01), maxEpochs -> (400,4
00), eta -> (0.1,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))
[info] -----
[info] features fn
= Array(intercept, Fre
quency, An
gle of attack, Chord length, Free-stream velocity, Suction side displacement thickness)
[info] parameter bb = Array(b.w =
[info] MatrixD (-1.45808,
[info] -0.777800,
[info] -0.309472,
[info] -0.310131,
[info] 0.116111,
[info] -0.222863)
[info] b.b = null)
[info] -----
[info] fitMap qof =
[info] rSq -> VectorD(0.532686)
[info] rSqBar -> VectorD(0.531125)
[info] sst -> VectorD(71482.4)
[info] sse -> VectorD(33404.7)
[info] mse0 -> VectorD(22.2254)
[info] rmse -> VectorD(4.71438)
[info] mae -> VectorD(3.62733)
[info] dfm -> VectorD(5.00000)
[info] df -> VectorD(1497.00)
[info] fStat -> VectorD(341.282)
[info] aic -> VectorD(-4451.24)
[info] bic -> VectorD(-4419.35)
```

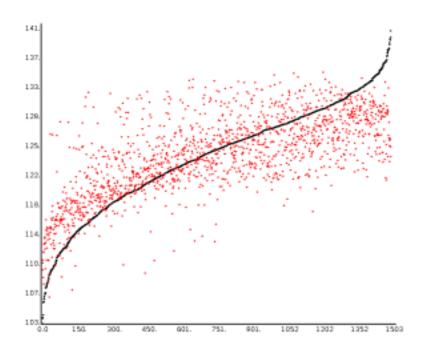
```
[info] mape -> VectorD(2.91464)
[info] smape -> VectorD(2.90617)
[info] ------
```

Table of two layer neural net summary statistics with sigmoid.

NeuralNet_2L_sigmoid: y0 black/actual vs. red/predicted

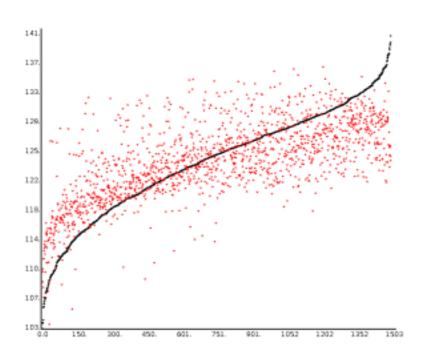


2 layer using sigmoid of actual vs predicted.



2 layer using tanh of actual vs predicted.

NeuralNet_2L_reLU: y0 black/actual vs. red/predicted



2 layer using relu of actual vs predicted values.

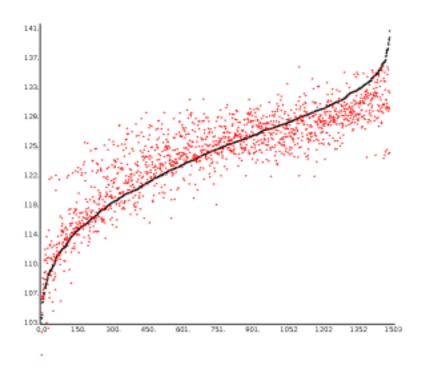
Moving over to our three layer neural net in scala we had a huge improvement in performance. Looking at our actual vs predicted values in graphs we can see predicted values are clustered much tighter around actual values. R-squared, r-squared bar, and SMAPE values improved to 0.676, 0.675, and 2.3. These values were recorded when bSize was 20 and nB was 75. When nB was reduced to 60 r-squared, r-squared bar, and SMAPE values improved to 0.783, 0.783, and 1.9 respectively.

```
[info] -----
[info] fitMap qof =
[info] rSq \rightarrow VectorD(0.675911)
[info] rSqBar -> VectorD(0.674829)
[info] sst -> VectorD(71482.4)
[info] sse -> VectorD(23166.7)
[info] mse0 -> VectorD(15.4136)
[info] rmse -> VectorD(3.92602)
[info] mae -> VectorD(2.92964)
[info] dfm -> VectorD(5.00000)
[info] df -> VectorD(1498.00)
[info] fStat -> VectorD(624.837)
[info] aic -> VectorD(-4176.21)
[info] bic -> VectorD(-4144.31)
[info] mape -> VectorD(2.35047)
[info] smape -> VectorD(2.33923)
```

Table of summary statistics of our 3 layer neural net with sigmoid.

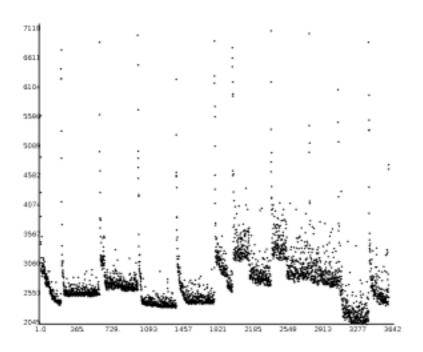
```
[info] optimize3: bSize = 20, nB = 60
[info] ending epoch = (11165.834723430013,400)
[info] rSq -> VectorD(0.783368)
[info] rSqBar -> VectorD(0.782645)
[info] sst -> VectorD(13805.5)
[info] sse -> VectorD(2990.71)
[info] mse0 -> VectorD(9.96904)
[info] rmse -> VectorD(3.15738)
[info] mae -> VectorD(2.38720)
[info] dfm -> VectorD(5.00000)
[info] df -> VectorD(1498.00)
[info] fStat -> VectorD(1083.39)
[info] aic -> VectorD(-770.942)
[info] bic -> VectorD(-748.720)
[info] mape -> VectorD(1.91188)
[info] smape -> VectorD(1.90983)
```

Table of summary statistics of our 3 layer neural net with sigmoid.



3 layer using sigmoid id of actual vs predicted values.

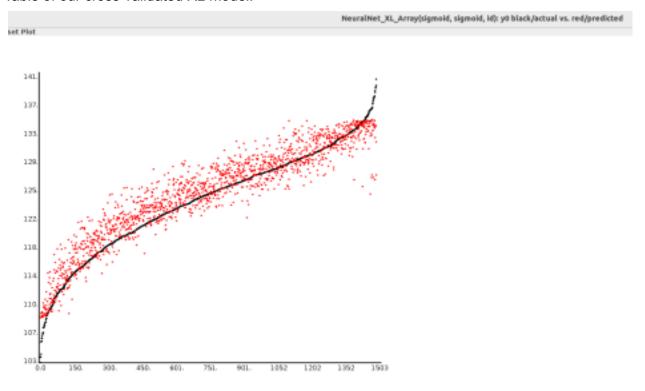
loss vs epoch NeuralNet_3L



Loss vs epoch in our 3 layer.

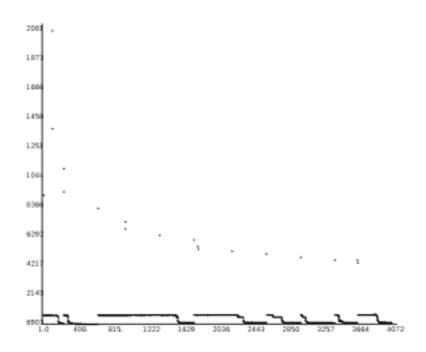
Again moving to our XL neural net we see another hike in performance. Looking at our graphs and comparing them to previous ones, we can see that our predicted values are located much more tightly around the actual values. In our cross validated model we had a mean r-squared value of 0.922, mean r-squared bar of 0.922, and mean SMAPE of 1.2. These values are a drastic improvement from our two-layer model and shows how much more accurate models can be developed with the addition of layers in scala. The only thing of concern from this model is our epoch vs loss graph. The huge drop in loss values may indicate some overfitting taking place in this model.

Table of our cross-validated XL model.



Actual vs predicted values with the use of sigmoid and id in XL neural net.

loss vs epoch NeuralNet_XL

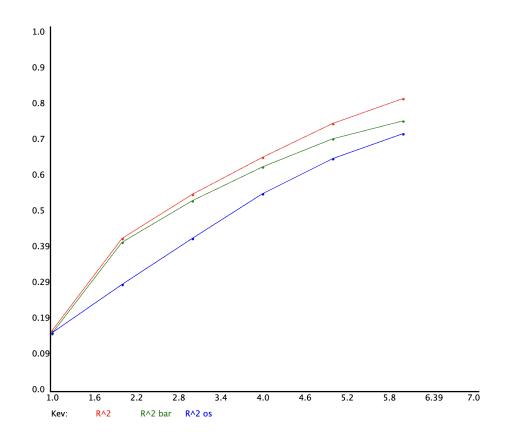


Loss vs epoch in our XL neural net.

DEBUG @ RegressionTreeRF.train: for tree6 ===

() LinkedHashMap($\mathbf{rSq} \rightarrow \mathbf{0.721805}$, rSqBar -> 1.970447, sst -> 13805.490439, sse -> 3840.613948, sde -> 3.579554, mse0 -> 12.802046, rmse -> 3.577995, mae -> 2.833136, dfm -> 386.000000, df -> -86.000000, fStat -> -0.578073, aic -> -48.005993, bic -> 1385.357825, mape -> 2.275591, smape -> 2.273016)

Random Forest Regressor



LinkedHashMap(rSq -> 0.721805, rSqBar -> 1.970447, sst -> 13805.490439, sse -> 3840.613948, sde -> 3.579554, mse0 -> 12.802046, rmse -> 3.577995, mae -> 2.833136, dfm -> 386.000000, df -> -86.000000, fStat -> -0.578073, aic -> -48.005993, bic -> 1385.357825, mape -> 2.275591, smape -> 2.273016)

Python

Note: In this report XL is 3 Hidden layer neural net.

2L layer Neural Net:

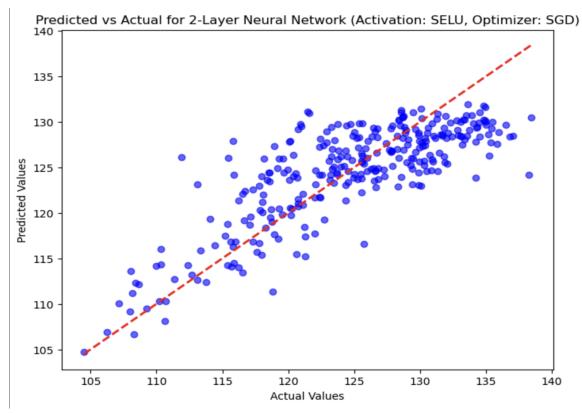
The Best performance combination was found with SELU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate: 0.0001.

Batch Size: 128. Input Layer Size:5.

Hidden Layer Size:256.

```
Testing Activation: SELU, Optimizer: SGD
training 2L net
Epoch [100/100], Loss: 18.344952
starting evaluation
5-fold cross-validation evaluation
Epoch [100/100], Loss: 16.253007
Epoch [100/100], Loss: 14.892809
Epoch [100/100], Loss: 14.435249
Epoch [100/100], Loss: 12.853898
Epoch [100/100], Loss: 12.734273
Metrics:
The best metric is Cross-validation R2.
2-Layer Neural Network:
  Best R<sup>2</sup>: 0.6960
  Best Metric: Cross-Validation R<sup>2</sup>
  Activation and Optimizer: Activation: SELU, Optimizer: SGD
  Metrics:
    In-Sample MSE: 18.644153594970703
    In-Sample RMSE: 4.317887783050537
    In-Sample R^2: 0.6026
    Validation MSE: 17.83548927307129
    Validation RMSE: 4.223208427429199
    Validation R<sup>2</sup>: 0.6440
    Cross-Validation MSE: 14.292463302612305
    Cross-Validation RMSE: 3.7420883178710938
    Cross-Validation R<sup>2</sup>: 0.6960
```



3L Layer Neural Net:

Learning Rate: 0.0001

Batch Size:128 Input Layer Size:5.

The Best performance combination was found with ReLU activation function and Stochastic Gradient Descent Optimizer.

```
Hidden Layer Size:256.

training 31 net
Epoch [100/100], Loss: 11.666045

5-fold cross-validation evaluation for 31
Epoch [100/100], Loss: 8.531790
Epoch [100/100], Loss: 7.000087
Epoch [100/100], Loss: 6.094772
Epoch [100/100], Loss: 5.181322
Epoch [100/100], Loss: 4.520917
Metrics:
```

The Best metric is 3-Layer Neural Network.

```
3-Layer Neural Network:

Best R<sup>2</sup>: 0.8630

Best Metric: Cross-Validation R<sup>2</sup>

Activation and Optimizer: Activation: ReLU, Optimizer: SGD Metrics:

In-Sample MSE: 11.668798446655273
```

In-Sample RMSE: 3.4159622192382812

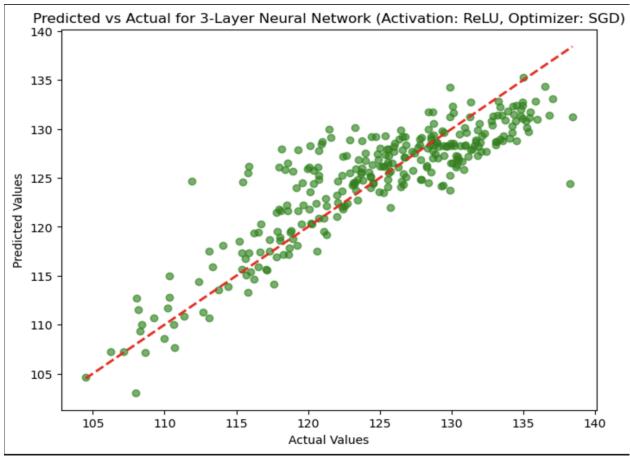
In-Sample R^2 : 0.7513

Validation MSE: 11.992977142333984 Validation RMSE: 3.463087797164917

Validation R²: 0.7606

Cross-Validation MSE: 6.4855217933654785 Cross-Validation RMSE: 2.5006473064422607

Cross-Validation R²: 0.8630



XL Neural Net:

The Best performance combination was found with SELU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate: 0.0001 Batch Size:128 Input Layer Size:5. Hidden Layer Size:256.

training Xl net

Epoch [100/100], Loss: 5.959517

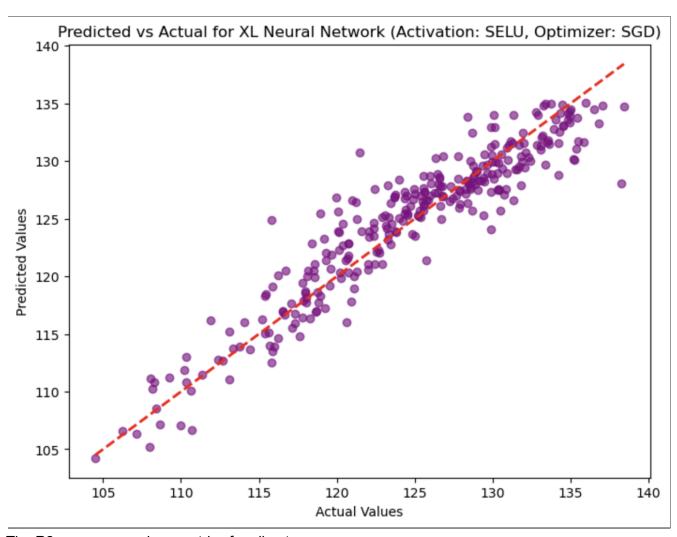
```
5-fold cross-validation evaluation for XL net Epoch [100/100], Loss: 4.222623
Epoch [100/100], Loss: 3.368778
Epoch [100/100], Loss: 2.898010
Epoch [100/100], Loss: 2.651334
Epoch [100/100], Loss: 2.429800
```

Metrics:

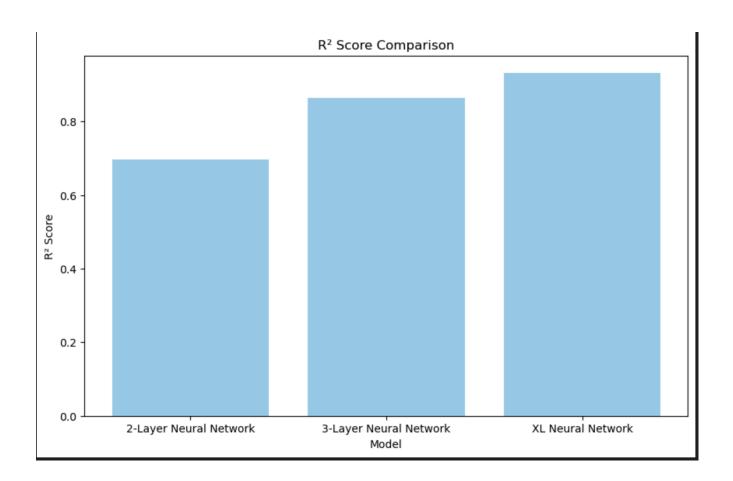
The Best metric is XLayer Neural Network.

Cross-Validation R²: 0.9323

```
XL Neural Network:
   Best R<sup>2</sup>: 0.9323
Best Metric: Cross-Validation R<sup>2</sup>
Activation and Optimizer: Activation: SELU, Optimizer: SGD Metrics:
   In-Sample MSE: 6.022091388702393
   In-Sample RMSE: 2.4539949893951416
   In-Sample R<sup>2</sup>: 0.8716
   Validation MSE: 5.865655422210693
   Validation RMSE: 2.4219114780426025
   Validation R<sup>2</sup>: 0.8829
   Cross-Validation MSE: 3.1851859092712402
   Cross-Validation RMSE: 1.767377495765686
```



The R2 score comparison metrics for all nets.



A **Random Forest Regressor** is initialized with 100 trees (n_estimators=100). This means the model will create 100 decision trees, each contributing to the final prediction.

The random_state=42 ensures reproducibility, meaning each run of this code will yield the same results.

```
Random Forest Test MSE : 3.2960

Random Forest Test RMSE: 1.8155

Random Forest Test R^2 : 0.9342
```

GridSearchCV is used to find the optimal hyperparameters, which can improve the model's performance.

Below is the parameter grid for searching and best combination of parameters.

```
param_grid = {
```

```
'n_estimators': [100, 200, 300],

'max_depth': [None, 10, 20, 30],

'min_samples_split': [2, 5, 10],

'min_samples_leaf': [1, 2, 4]
```

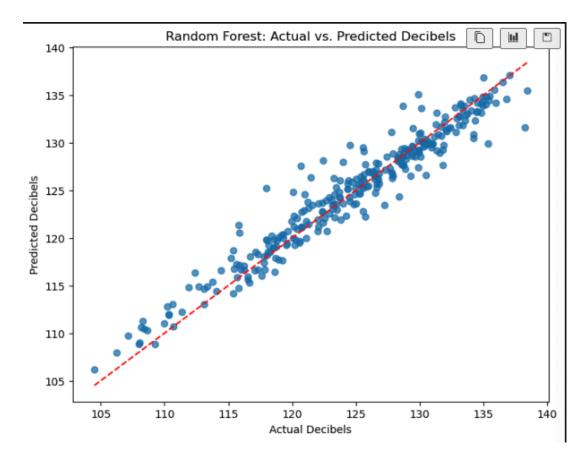
```
Best Parameters: {'max_depth': None, 'min_samples_leaf': 1,
'min_samples_split': 2, 'n_estimators': 200}

Best CV MSE: 0.9225

Best Random Forest Test MSE: 3.2967

Best Random Forest Test R2: 0.9342
```

The actual vs predicted Decibels using Random forest.



Cross Validation R2 using Random Regressor

Cross-Validated R² Scores: [0.93686281 0.92761618 0.91976964 0.92730733 0.90115417]

Average Cross-Validated R² Score: 0.9225

AutoMPG

Data preprocessing:

EDA:

All data preprocessing and EDA performed for this dataset was the same as described in project 1. Please see our previous report for details.

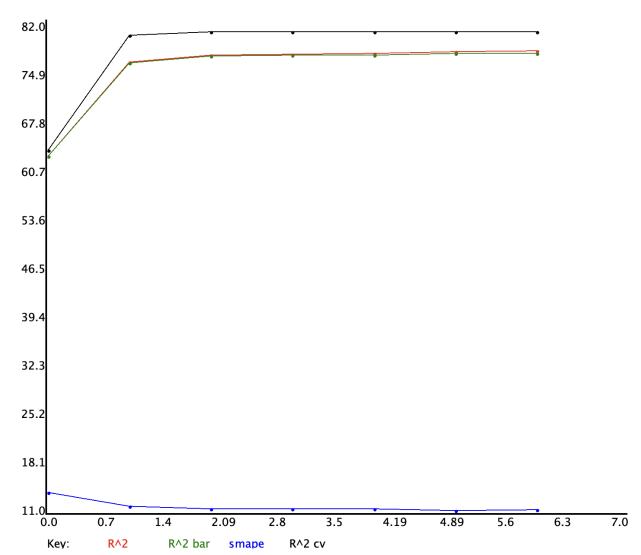
Feature Selection (Forward, Backward, Stepwise)

Neural Net 2L

When using Python, we did not do feature selection for AutoMPG as in the first project, our best performing configurations came from using all available input features. Additionally, when using Scalation, we found that the best model configurations include all input features. This saved us time greatly, as our method for finding the best model configuration when using Python was by using a random grid search.

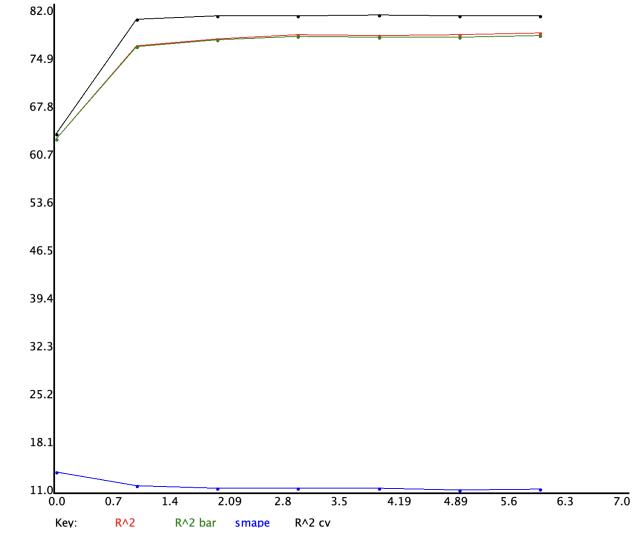
For Neural Net 2L forward selection in scala, we can see from below graph the R squared increased after second feature and doesn't vary much after that. Features were added in the following order.

Best Features: Intercept, weight, model year, horsepower, origin, displacement, cylinders, acceleration



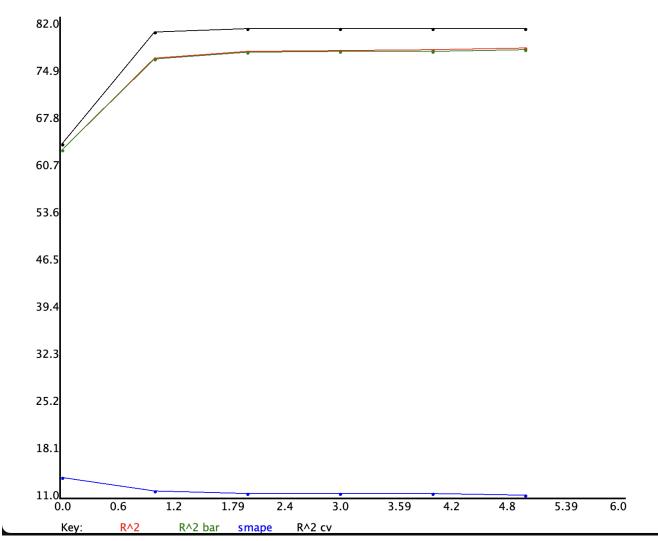
For Neural Net 2L Backward selection in scala also, we can see from below graph the R squared increased after second feature and doesn't vary much after that. Features were removed in the following order.

cylinders, acceleration, displacement, origin, horsepower, model year



For Neural Net 2L Stepwise selection in scala also, we can see from below graph the R squared increased after second feature and doesn't vary much after that. Features were removed in the following order.

Best Features: intercept, weight, model year, horsepower, origin, displacement

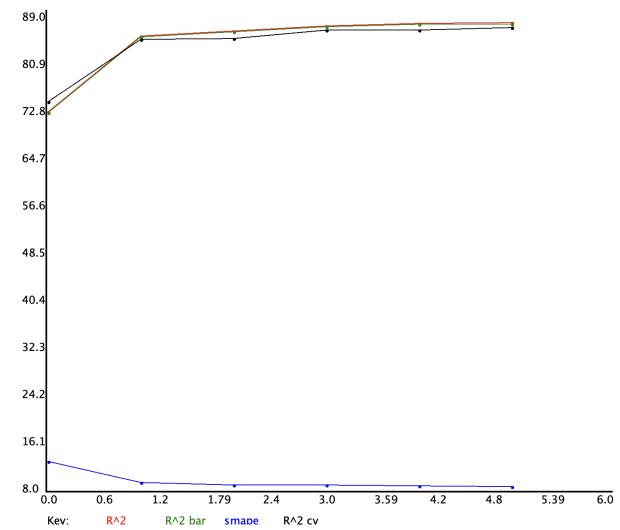


Neural Net 3L

When using Python, we did not do feature selection for AutoMPG as in the first project, our best performing configurations came from using all available input features. Additionally, when using Scalation, we found that the best model configurations include all input features.

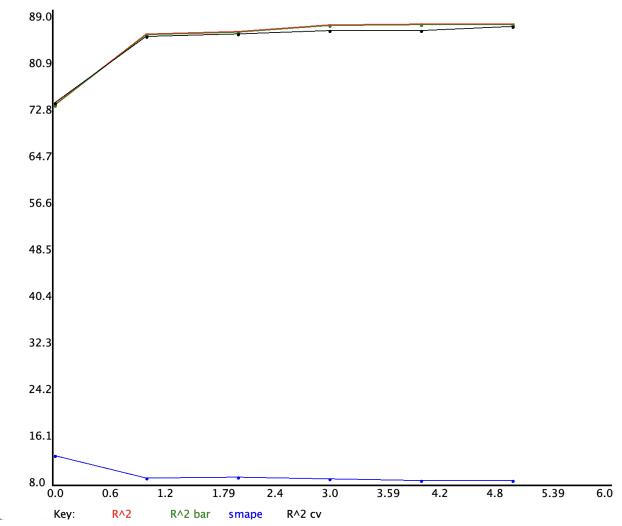
For Neural Net 3L forward selection in scala, we can see from below graph the R squared increased after second feature and slightly increases after that. Features were added in the following order.

Best Features: cylinders, model year, weight, horsepower, origin, acceleration, displacement



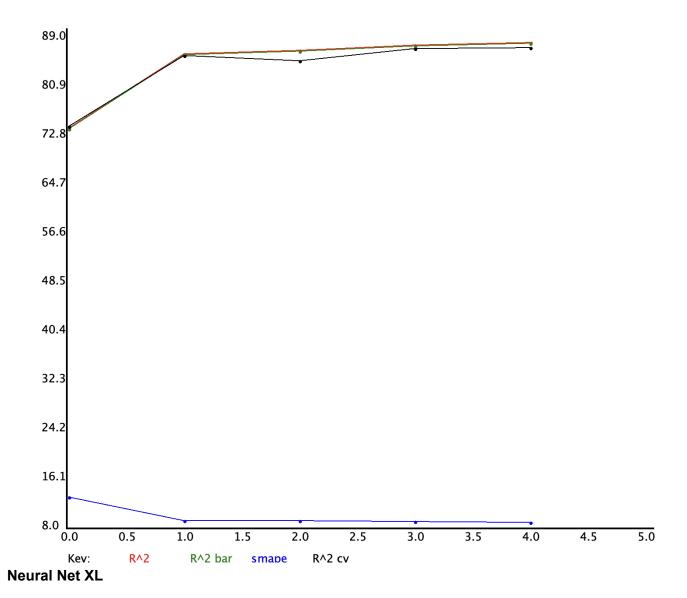
For Neural Net 3L Backward selection in scala also, we can see from below graph the R squared increased after the second feature and doesn't vary much after that. Features were removed in the following order.

displacement, horsepower, acceleration, origin, weight



For Neural Net 3L Stepwise selection in scala also, we can see from below graph the R squared increased after second feature and slightly increases after that. Features were removed in the following order.

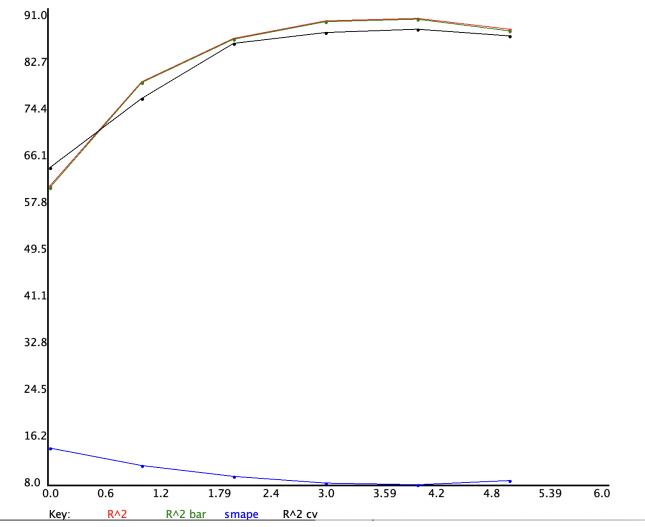
Best Features: cylinders, model year, weight, horsepower, origin, acceleration



When using Python, we did not do feature selection for AutoMPG as in the first project, our best performing configurations came from using all available input features. Additionally, when using Scalation, we found that the best model configurations include all input features.

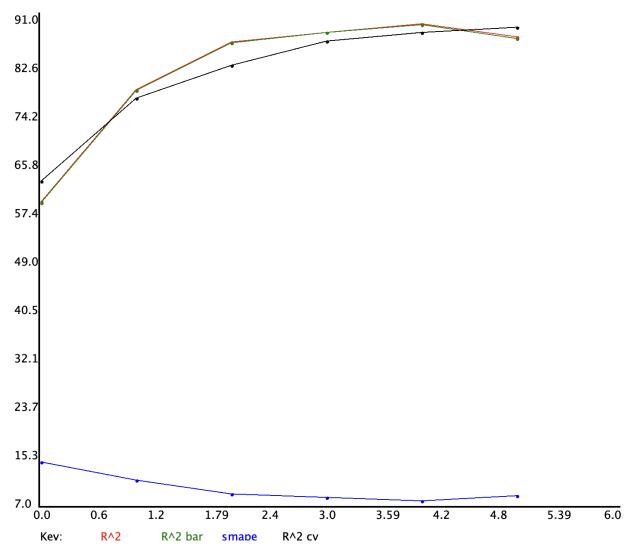
For Neural Net XL forward selection in scala, we can see from below graph the R squared increased after second feature and slightly increases after that. Features were added in the following order.

Best Features: cylinders, model year, weight, origin, acceleration, horsepower, displacement



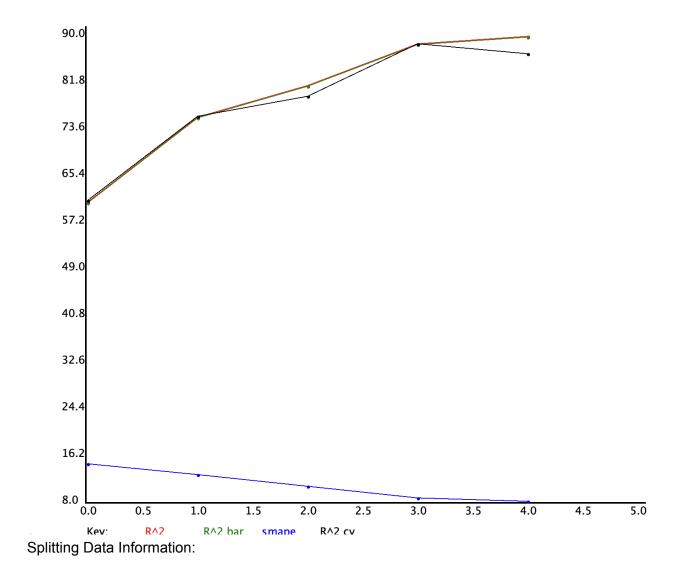
For Neural Net XL Backward selection in scala also, we can see from below graph the R squared increased after the second feature and doesn't vary much after that. Features were removed in the following order.

horsepower, displacement, origin, acceleration, weight



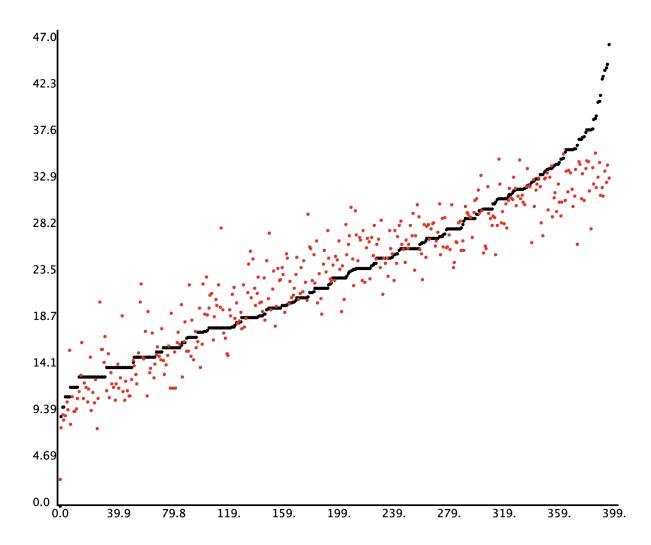
For Neural Net XL Stepwise selection in scala also, we can see from below graph the R squared increased after the second feature and slightly increased after that. Features were removed in the following order.

Best Features: cylinders, model year, weight, acceleration, origin, displacement

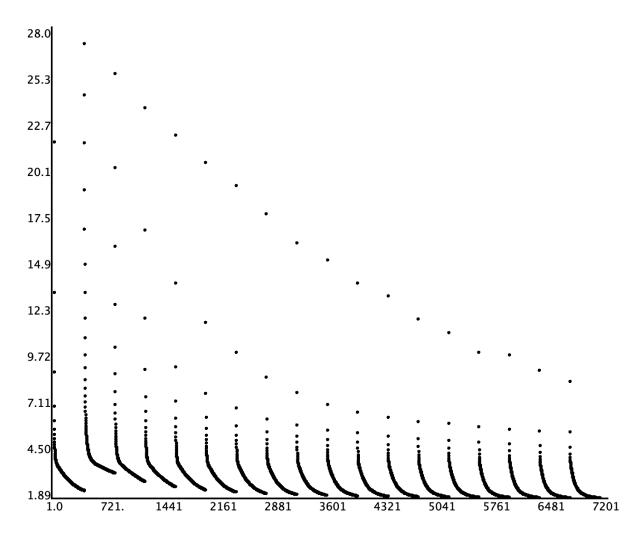


Discussion of Results:

In scala, the Neural net 2L has provided an R squared of 0.85 with an activation function sigmoid and learning rate of 0.1. Below is the y actual vs y predicted graph from Scala.



Below graph represents the loss vs epochs for the sigmoid activation on Neural net 2L.



REPORT

modelName mn = NeuralNet_2L_sigmoid

hparameter hp = HyperParameter (HashMap(lambda -> (0.01,0.01), maxEpochs -> (400,400), eta -> (0.1,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))

features fn = Array(intercept, cylinders, displacement, horsepower, weight, acceleration, model year, origin)

parameter bb = Array(b.w = MatrixD (-0.928601,

-0.00177435,

0.160674,

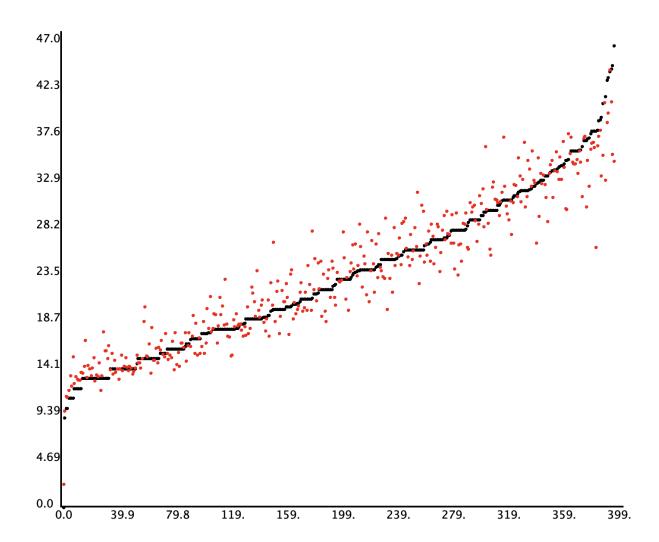
```
-0.165400,
       -0.820607,
       0.0787008,
       0.295707,
       0.0600795)
b.b = null
  fitMap qof =
               rSq -> VectorD(0.861906)
               rSqBar -> VectorD(0.859428)
               sst -> VectorD(24252.6)
               sse -> VectorD(3349.12)
               mse0 -> VectorD(8.41488)
               rmse -> VectorD(2.90084)
               mae -> VectorD(2.16566)
              dfm -> VectorD(7.00000)
               df -> VectorD(390.000)
              fStat -> VectorD(347.739)
               aic -> VectorD(-972.608)
               bic -> VectorD(-940.717)
               mape -> VectorD(9.53731)
               smape -> VectorD(9.44915)
Below is the Quality of fit table for the Neural Net 2L. This indicates the maximum R squared of
0.88.
| showQofStatTable: Statistical Table for QoF |
| name | num | min | max | mean | stdev | interval | | | | |
| rSq | 5 | 0.799 | 0.884 | 0.846 | 0.041 | 0.051 |
| rSqBar | 5 | 0.796 | 0.881 | 0.843 | 0.041 | 0.051 | | sst | 5 | 4288.643 |
5682.595 | 4683.529 | 587.830 | 730.030 | | sse | 5 | 501.613 | 882.530 |
714.605 | 174.409 | 216.599 | | mse0 | 5 | 6.350 | 11.171 | 9.046 | 2.208 |
2.742 | rmse | 5 | 2.520 | 3.342 | 2.989 | 0.378 | 0.469 |
| mae | 5 | 1.971 | 2.500 | 2.232 | 0.235 | 0.292 | | | | |
| dfm | 5 | 7.000 | 7.000 | 7.000 | 0.000 | 0.000 |
| df | 5 | 390.000 | 390.000 | 390.000 | 0.000 | 0.000 | | fStat | 5 | 221.920 |
422.671 | 327.097 | 97.341 | 120.888 | | aic | 5 | -193.189 | -170.522 |
-183.196 | 10.378 | 12.889 | | bic | 5 | -174.233 | -151.567 | -164.241 |
10.378 | 12.889 | | mape | 5 | 8.923 | 10.858 | 9.740 | 0.873 | 1.084 | |
smape | 5 | 8.856 | 10.527 | 9.701 | 0.774 | 0.961 |
```

The activation function selection done in scala has given the best results with sigmoid function. Below are the results for this run.

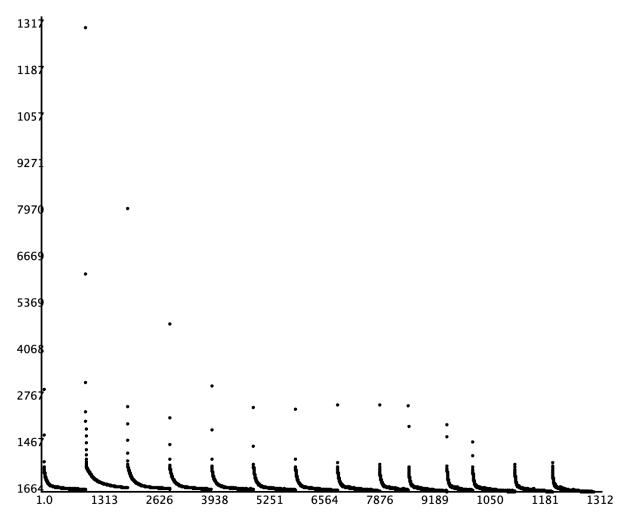
```
REPORT
  modelName mn = NeuralNet 2L sigmoid
  hparameter hp = HyperParameter (HashMap(lambda -> (0.01,0.01), maxEpochs ->
(400,400), eta -> (0.1,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))
_____
  features fn = Array(intercept, cylinders, displacement, horsepower, weight, acceleration,
model year, origin)
  parameter bb = Array(b.w =
MatrixD (-1.05371,
      0.0372628.
      0.104693,
      -0.288520,
      -0.758932.
      0.0230306.
      0.291694,
      0.0586901)
b.b = null
             _____
  fitMap qof =
             rSq \rightarrow VectorD(0.863092)
             rSqBar -> VectorD(0.860635)
            sst -> VectorD(24252.6)
            sse -> VectorD(3320.37)
             mse0 -> VectorD(8.34263)
             rmse -> VectorD(2.88836)
             mae -> VectorD(2.15410)
            dfm -> VectorD(7.00000)
            df -> VectorD(390.000)
            fStat -> VectorD(351.233)
            aic -> VectorD(-970.893)
             bic -> VectorD(-939.001)
             mape -> VectorD(9.49008)
            smape -> VectorD(9.44301)
```

Neural Net 3L

In scala, the Neural net 3L has provided an R squared of 0.93 with an activation function



Below is the loss vs epochs graph for this run.



REPORT

modelName mn = NeuralNet_3L_sigmoid_id

hparameter hp = HyperParameter (HashMap(lambda -> (0.01,0.01), maxEpochs -> (1000,400), eta -> (0.01,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))

features fn = Array(cylinders, displacement, horsepower, weight, acceleration, model year, origin)

parameter bb = Array(b.w =

MatrixD (1.86321, 1.04372, -1.06053, 1.01585, -1.12428, -0.771175, 1.24719, -0.504893, 0.776952, 0.409431, -1.34338, 0.0319128, -0.310463, 0.829072, 0.902026,

```
2.83590, -0.316080, -0.290286, 0.290362, 0.129741, 1.76084, 2.23738, 0.763239,
1.54982, -1.82092, -0.993986, -0.952304, 0.282476, -2.23941, 0.0682018,
       -0.681312, 0.382190, 0.118804, -1.42275, -0.247070, -0.274539, -2.04907,
-0.220625, -2.57749, -0.931825, -1.98981, -0.221887, -0.441380, -1.30239, -1.51540,
       -1.68630, -2.50444, -1.78127, -0.341761, -2.24155, -3.04670, -3.05008, 1.92765,
-2.98440, -1.15817, -2.03586, 0.987056, -1.98405, -0.754865, -0.00317017,
       2.95935, 0.610676, -0.856629, 0.765101, -0.854784, 1.44259, 0.140657, 2.01778,
-1.42050, -1.86556, -0.0582271, -0.120732, -1.20351, -1.49345, 1.52713,
       3.98199, -0.938310, 0.0366900, -1.95391, 0.147727, 2.40450, 3.43409, 1.47676,
-0.460450, 0.0101855, -2.75515, 4.36123, 1.34455, -0.529500, -2.62039,
       2.65680, 0.366207, 0.457576, -1.94836, 0.680804, 0.306730, 3.14585, -3.28973,
-1.90143, 2.65097, -1.45560, -1.05770, 0.562446, 1.74775, -2.32025)
b.b = VectorD(-3.86386, -3.52830, -2.43722, 0.958187, -2.67221, -4.68682,
-3.27569, 0.444117, -0.492185, -0.185390, -2.56153, -2.22970, -1.55157,
-0.0941967, 1.08257), b.w =
MatrixD (5.16147,
       3.48298,
       2.64462,
       2.46878,
       3.01807,
       4.34762,
       5.34847.
       3.56074,
       3.44188,
       2.91350,
       3.29997,
       4.02907,
       2.80294,
       2.85156,
       3.20587)
b.b = VectorD(0.427617))
  fitMap qof =
              rSq -> VectorD(0.934239)
              rSqBar -> VectorD(0.933062)
              sst -> VectorD(24252.6)
              sse -> VectorD(1594.86)
              mse0 -> VectorD(4.00720)
              rmse -> VectorD(2.00180)
              mae -> VectorD(1.48301)
             dfm -> VectorD(7.00000)
              df -> VectorD(391.000)
             fStat -> VectorD(793.544)
              aic -> VectorD(-824.968)
```

```
bic -> VectorD(-793.076)
mape -> VectorD(6.46087)
smape -> VectorD(6.41443)
```

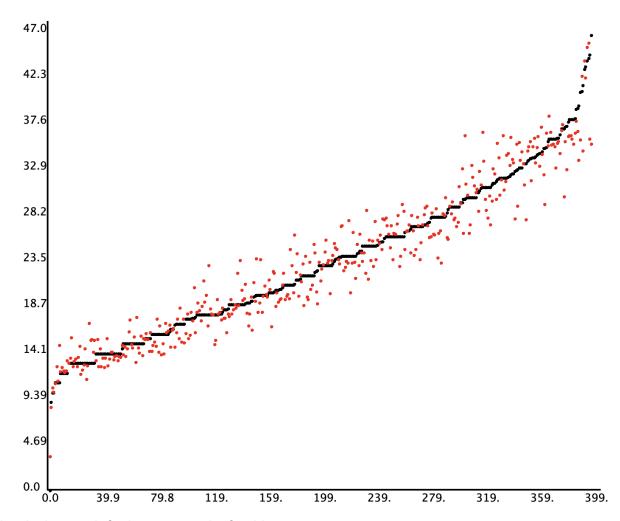
While trying the best activation functions, I have figured the tanh has worked best on the Nueral net 3L and provided a R squared of 0.94. Below are the results for this run.

```
REPORT
  modelName mn = NeuralNet 3L tanh id
  hparameter hp = HyperParameter (HashMap(lambda -> (0.01,0.01), maxEpochs ->
(400,400), eta -> (0.01,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))
  features fn = Array(cylinders, displacement, horsepower, weight, acceleration, model year,
origin)
  parameter bb = Array(b.w =
MatrixD (1.12379, 0.346883, -2.17898, -1.61364, -0.0165722, -0.373094, -0.505182,
-2.49079, -0.614917, 1.69633, 0.431740, -0.364007, 1.28345, -1.05168, -0.0928464,
       0.184795, 1.17822, -0.609622, -0.432550, 1.98675, 1.90807, 2.63954, -2.13823,
0.462415, -1.14164, -0.213652, 1.25847, 1.01828, -2.12493, 1.21956,
       1.39385, 0.427880, 1.47574, -0.146241, -1.06876, 0.601788, 0.118321, 0.582375,
-2.42572, -1.73644, 1.82587, 0.785387, -0.697205, 1.70771, -1.55954,
       1.38219, 0.178048, 1.31951, 1.40874, 1.02822, -0.942454, 0.817721, 2.74497,
1.32609, 1.80583, 1.94591, 0.383129, 0.628785, 1.95933, 2.82338,
       2.53010, 1.19676, -0.367348, -0.719374, 1.15945, -2.43225, 0.290985, -2.53699,
0.983692, 0.892733, 1.09385, 2.00865, 0.583003, -0.430222, 0.280728,
       -0.367345, 0.141374, -0.0868986, 3.96117, 1.07572, 2.19330, 0.720679,
-2.53318, -2.84328, -3.54975, 0.151685, -0.495712, 0.642296, -2.58630, -0.266640,
       2.03063, 1.36688, -0.0952498, -1.55941, 2.09952, 1.60832, -0.496280, -2.00329,
-2.59268, -0.0407647, -1.04554, 1.52022, 1.28049, -2.80735, -0.210231)
b.b = VectorD(-0.886440, -1.68170, -2.06313, -1.52923, -2.05185, -2.95208,
0.321919, 3.31634, 0.747109, 3.44173, 2.46616, -1.92458, -2.27060, 1.98430,
3.05937), b.w =
MatrixD (-2.61953,
       -3.64281,
       -3.24084
       2.02752,
       -2.39243
       -3.04218,
       -2.70361,
       -4.29510,
```

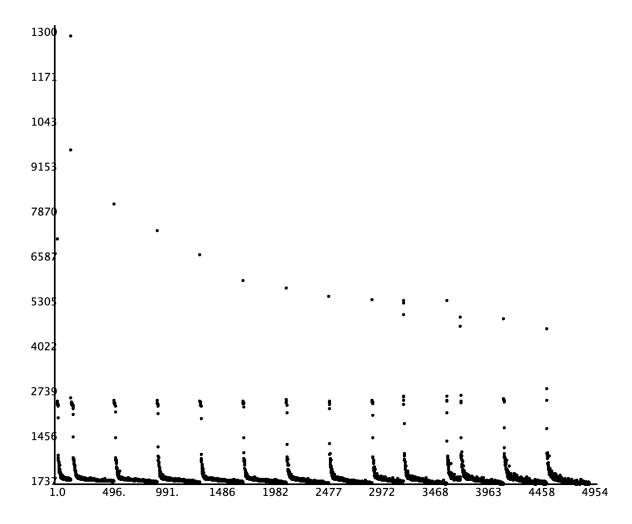
```
3.72968,
      -2.38708,
      -2.25280,
      -4.18851,
      -3.71806,
      -3.72346,
      -2.24047)
b.b = VectorD(7.00842))
 fitMap qof =
             rSq -> VectorD(0.948194)
             rSqBar -> VectorD(0.947266)
             sst -> VectorD(24252.6)
             sse -> VectorD(1256.43)
             mse0 -> VectorD(3.15687)
             rmse -> VectorD(1.77676)
             mae -> VectorD(1.31662)
             dfm -> VectorD(7.00000)
             df -> VectorD(391.000)
             fStat -> VectorD(1022.34)
             aic -> VectorD(-777.519)
             bic -> VectorD(-745.627)
             mape -> VectorD(5.75821)
             smape -> VectorD(5.66119)
```

Neural Net XL

In scala, the Neural net XL has provided an R squared of 0.93 with an activation function sigmoid and learning rate of 0.1. Below is the y actual vs y predicted graph from Scala.



Below is the graph for loss vs epochs for this run.



Below results are obtained for Neural net XL with sigmoid, tanh, reLU, id as activation functions and learning rate 0.1.

fitMap qof =

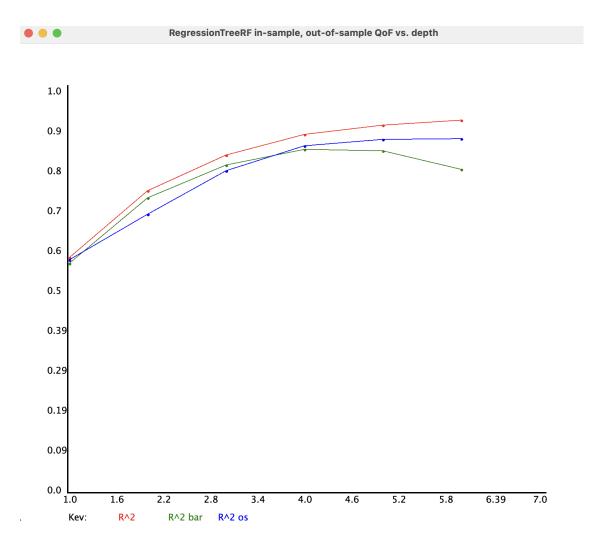
```
rSqBar -> VectorD(0.934673)
              sst -> VectorD(24252.6)
              sse -> VectorD(1556.49)
              mse0 -> VectorD(3.91077)
              rmse -> VectorD(1.97757)
              mae -> VectorD(1.46390)
              dfm -> VectorD(7.00000)
              df -> VectorD(391.000)
              fStat -> VectorD(814.486)
              aic -> VectorD(-820.149)
              bic -> VectorD(-788.258)
              mape -> VectorD(6.29490)
              smape -> VectorD(6.31131)
While searching the activation features, we have found the best results with tanh, tanh, id as the
activation functions. This provided a R squared of 0.97 and adjusted R squared of 0.97. This
REPORT
  modelName mn = NeuralNet_XL_Array(tanh, tanh, id)
  hparameter hp = HyperParameter (HashMap(lambda -> (0.01,0.01), maxEpochs ->
(400,400), eta -> (0.01,0.1), nu -> (0.9,0.9), upLimit -> (4,4), beta -> (0.9,0.9), bSize -> (20,20)))
  features fn = Array(cylinders, displacement, horsepower, weight, acceleration, model year,
origin)
  fitMap qof =
              rSq \rightarrow VectorD(0.970755)
              rSqBar -> VectorD(0.970231)
              sst -> VectorD(24252.6)
              sse -> VectorD(709.268)
              mse0 -> VectorD(1.78208)
              rmse -> VectorD(1.33495)
              mae -> VectorD(0.974232)
              dfm -> VectorD(7.00000)
              df -> VectorD(391.000)
              fStat -> VectorD(1854.11)
              aic -> VectorD(-663.716)
              bic -> VectorD(-631.825)
              mape -> VectorD(4.16925)
              smape -> VectorD(4.15652)
```

rSq -> VectorD(0.935822)

DEBUG @ RegressionTreeRF.train: for tree6 === ()

LinkedHashMap($\mathbf{rSq} \rightarrow \mathbf{0.887677}$, rSqBar -> 1.049025, sst -> 4980.717468, sse -> 559.448162, sde -> 2.677726, mse0 -> 7.081622, rmse -> 2.661132, mae -> 1.962935, dfm -> 260.000000, df -> -181.000000, fStat -> -5.501642, aic -> 325.519226, bic -> 943.945115, mape -> 8.356778, smape -> 8.331557)

Random Forest Regressor



LinkedHashMap(rSq -> 0.887677, rSqBar -> 1.049025, sst -> 4980.717468, sse -> 559.448162, sde -> 2.677726, mse0 -> 7.081622, rmse -> 2.661132, mae -> 1.962935, dfm -> 260.000000, df -> -181.000000, fStat -> -5.501642, aic -> 325.519226, bic -> 943.945115, mape -> 8.356778, smape -> 8.331557)

Python:

2L Neural Net:

The Best performance combination was found with Tanh activation function and Stochastic Gradient Descent Optimizer.

```
Learning Rate:0.001
Batch Size:32
Hidden Layer Size:128
Input Size:8
```

```
training 2L net Epoch [100/100], Loss: 6.147181 cross validation of 2L net 5-fold cross-validation evaluation Epoch [100/100], Loss: 5.320034 Epoch [100/100], Loss: 4.774090 Epoch [100/100], Loss: 4.298034 Epoch [100/100], Loss: 3.893799 Epoch [100/100], Loss: 3.546644
```

Metrics:

The best performance was found with Cross-Validation.

```
2-Layer Neural Network:

Best R<sup>2</sup>: 0.9277

Best Metric: Cross-Validation R<sup>2</sup>

Activation and Optimizer: Activation: Tanh, Optimizer: SGD Metrics:

In-Sample MSE: 6.1132707595825195

In-Sample RMSE: 2.4725029468536377

In-Sample R<sup>2</sup>: 0.9025

Validation MSE: 4.470783233642578

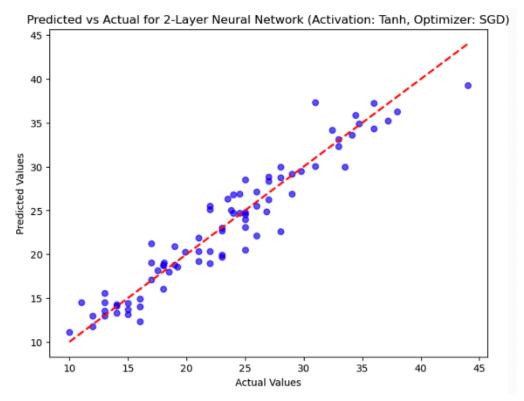
Validation RMSE: 2.114422559738159

Validation R<sup>2</sup>: 0.9168

Cross-Validation MSE: 4.506539821624756

Cross-Validation RMSE: 2.0948846340179443

Cross-Validation R<sup>2</sup>: 0.9277
```



3L Neural Net:

The Best performance combination was found with ReLU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate:0.001 Batch Size:32

Hidden Layer Size:128

Input Size:8

training 31 net Epoch [100/100], Loss: 5.104767 cross validation of 3L net 5-fold cross-validation evaluation Epoch [100/100], Loss: 3.874587 Epoch [100/100], Loss: 3.002533 Epoch [100/100], Loss: 2.314301 Epoch [100/100], Loss: 1.900708 Epoch [100/100], Loss: 1.578532

Metrics:

The best performance metric is Cross-validation.

```
3-Layer Neural Network: Best R^2: 0.9568 Best Metric: Cross-Validation R^2 Activation and Optimizer: Activation: ReLU, Optimizer: SGD
```

Metrics:

In-Sample MSE: 5.085403919219971
In-Sample RMSE: 2.2550840377807617

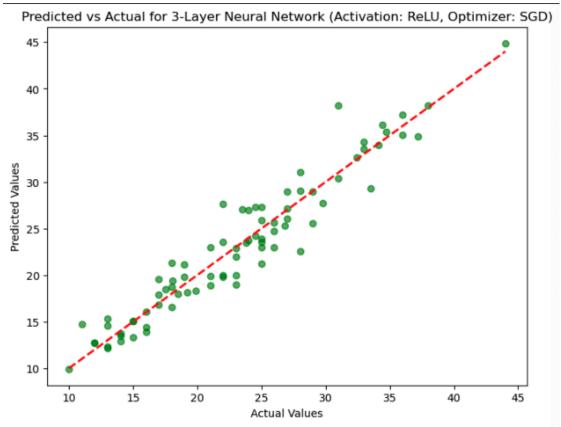
In-Sample R^2 : 0.9189

Validation MSE: 4.543299198150635 Validation RMSE: 2.1315016746520996

Validation R^2 : 0.9155

Cross-Validation MSE: 2.7511565685272217 Cross-Validation RMSE: 1.5926520824432373

Cross-Validation R²: 0.9568



XL Neural Net:

The Best performance combination was found with ReLU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate: 0.001 Batch Size: 32

Hidden Layer Size:128

Input Size:8

training Xl net

Epoch [100/100], Loss: 3.467718

cross validation of XL net

5-fold cross-validation evaluation

```
Epoch [100/100], Loss: 2.015366
Epoch [100/100], Loss: 1.341067
Epoch [100/100], Loss: 1.007442
Epoch [100/100], Loss: 0.782131
Epoch [100/100], Loss: 0.623834
```

Metrics:

The best performance was found with Cross-Validation.

XL Neural Network:

Best R²: 0.9818

Best Metric: Cross-Validation R²

Activation and Optimizer: Activation: ReLU, Optimizer: SGD Metrics:

In-Sample MSE: 3.450523853302002

In-Sample RMSE: 1.8575586080551147

In-Sample R²: 0.9450

Validation MSE: 5.17495059967041

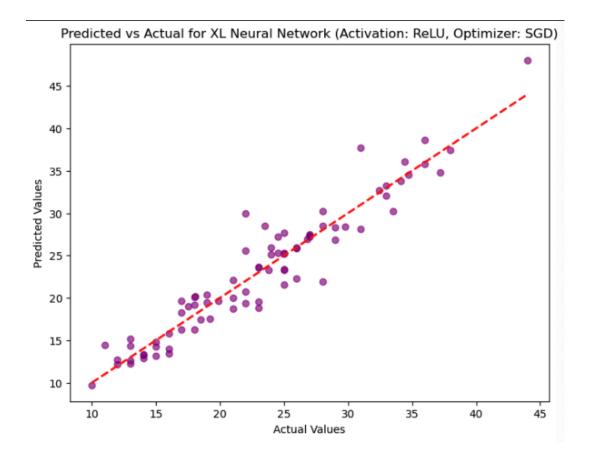
Validation RMSE: 2.2748517990112305

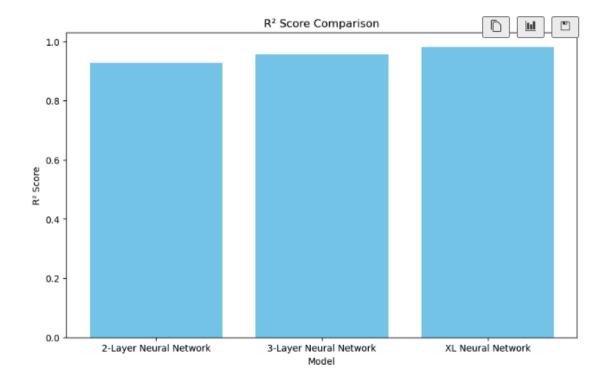
Validation R²: 0.9038

Cross-Validation MSE: 1.1483126878738403

Cross-Validation RMSE: 1.0151135921478271

Cross-Validation R²: 0.9818





A **Random Forest Regressor** is initialized with 100 trees (n_estimators=100). This means the model will create 100 decision trees, each contributing to the final prediction.

The random_state=42 ensures reproducibility, meaning each run of this code will yield the same results.

```
Random Forest Test MSE: 4.5168
Random Forest Test RMSE: 2.1253
Random Forest Test R<sup>2</sup>: 0.9160
```

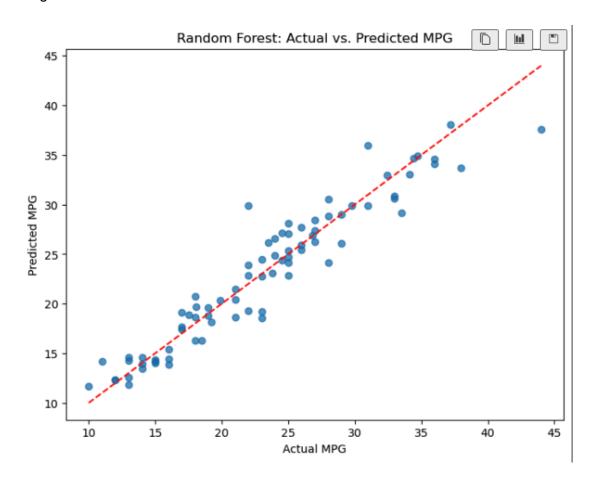
GridSearchCV is used to find the optimal hyperparameters, which can improve the model's performance

Below is the parameter grid for searching and best combination of parameters.

```
param_grid = {
'n_estimators': [100, 200, 300],
'max_depth': [None, 10, 20, 30],
'min_samples_split': [2, 5, 10],
'min_samples_leaf': [1, 2, 4]
```

```
Best Parameters: {'max_depth': None, 'min_samples_leaf': 1,
'min_samples_split': 2, 'n_estimators': 200}
Best CV MSE: 0.8527
Best Random Forest Test MSE: 4.6478
```

Below is the graph for actual vs predicted values using Random Forest Regressor.



The Cross Validation scores are:

Cross-Validated R^2 Scores: [0.89809161 0.86080208 0.84204864 0.77571794 0.88691443]

Average Cross-Validated R² Score: 0.8527

Seoul Bike Data

Data Preprocessing Dataset does not have any identifier columns, Null values,

hence no imputations are done. However, the dataset contains 3 categorical columns (Seasons, Holiday and Functioning day), these are converted into categorical codes. The Hour column is converted into categorical by cutting into Morning, afternoon, evening and night.

```
Rented Bike Count int64

Hour int64

Temperature(°C) float64

Humidity(%) int64

Wind speed (m/s) float64

Visibility (10m) int64

Dew point temperature(°C) float64

Solar Radiation (MJ/m2) float64

Rainfall(mm) float64

Snowfall (cm) float64

Seasons int32

Holiday int32

Functioning Day int32

hourOfDay int32

dtype: object
```

The outliers in the dataset are checked by Z scores outlier detection method. We have found below outliers for snowfall, rainfall, wind speed, however these scenarios occur rarely but they are a part of realistic data and hence we need not remove these as outliers.

When we have checked the variance and covariance, we observed the covariance Dew Point Temperature with Rented Bike count is close to 0, also Dew point temperature and Temperature are having high collinear values, hence the dew point temperature will be removed during model creation. Also, the date column is dropped as it needs to be converted to timeseries to use in our models.

Variance

Rented Bike Count 416021.733390 Temperature(°C) 142.678850 Humidity(%) 414.627875 Wind speed (m/s) 1.073918 Visibility (10m) 370027.323001 Dew point temperature(°C) 170.573247 Solar Radiation (MJ/m2) 0.754720 Rainfall(mm) 1.272819

Snowfall (cm) 0.190747

Seasons 1.241906

Holiday 0.046888

Functioning Day 0.032545

hourOfDay 2.833657

Rented Bike Count Temperature(°C) Humidity(%)

Rented Bike Count 416021.73339 4149.257754 -2623.853782 Temperature(°C) 4149.257754 142.67885 38.763038 Humidity(%)

-2623.853782 38.763038 414.627875 Wind speed (m/s) 80.950203

-0.448739 -7.10454 Visibility (10m) 78187.849382 252.817084

-6726.950421 Dew point temperature(°C) 3199.299111 142.400017

142.782065 Solar Radiation (MJ/m2) 146.717508 3.668334 -8.171237

Rainfall(mm) -89.558657 0.677602 5.430677

Snowfall (cm) -39.946114 -1.139387 0.962098

Seasons 258.539368 7.874302 4.294195 Holiday -10.103104

-0.144665 -0.221685

Functioning Day 23.730746 -0.10811 -0.076408 hourOfDay

343.54972 3.120162 -11.464437

Wind speed (m/s) Visibility (10m)

Rented Bike Count 80.950203 78187.849382 Temperature(°C) -0.448739 252.817084 Humidity(%) -7.10454 -6726.950421 Wind speed (m/s) 1.073918 108.11466 Visibility (10m) 108.11466 370027.323001 Dew point temperature(°C) -2.388639 -1403.253586 Solar Radiation (MJ/m2) 0.29914 79.130141

Rainfall(mm) -0.023002

-115.040313

Snowfall (cm) -0.001609 -32.330842

Seasons -0.19267

75.906527

Holiday 0.005165

4.185096

Functioning Day 0.000942 -2.853224

hourOfDay 0.607215 86.007307

Dew point temperature(°C) Solar Radiation(MJ/m2)

Rented Bike Count 3199.299111 146.717508 Temperature(°C)

142.400017 3.668334 Humidity(%) 142.782065 -8.171237 Wind speed

(m/s) -2.388639 0.29914 Visibility (10m) -1403.253586 79.130141 Dew

point temperature(°C) 170.573247 1.070865 Solar Radiation (MJ/m2)

1.070865 0.75472

Rainfall(mm)

1.85062 -0.072813

Snowfall (cm) -0.860668 -0.027432 Seasons 8.476852 0.091664

Holiday -0.188799 -0.000955 Functioning Day -0.124492

-0.001201 hourOfDay -0.380226 0.6462

Rainfall(mm) Snowfall (cm) Seasons Holiday

Rented Bike Count -89.558657 -39.946114 258.539368 10.103104 Temperature(°C) 0.677602 -1.139387 7.874302 -0.144665 Humidity(%) 5.430677 0.962098 4.294195 -0.221685 Wind speed (m/s) -0.023002 -0.001609 -0.19267 0.005165 Visibility (10m) -115.040313 -32.330842 75.906527 4.185096

Dew point temperature(°C) 1.85062 -0.860668 8.476852 -0.188799 Solar Radiation (MJ/m2) -0.072813 -0.027432 0.091664 -0.000955

Rainfall(mm) 1.272819 0.004188 0.042059 -0.003486

Snowfall (cm) 0.004188 0.190747 -0.070796 -0.001191 Seasons 0.042059 -0.070796 1.241906 -0.013903

Holiday -0.003486 -0.001191 -0.013903 0.046888 -0.001079

Functioning Day 0.000418 0.002528 -0.039421

hourOfDay 0.028514 -0.005217 -0.0 -0.0 Functioning Day hourOfDay

Rented Bike Count 23.730746 343.54972

Temperature(°C)

-0.10811 3.120162

Humidity(%) -0.076408 -11.464437

Wind speed (m/s)

0.000942 0.607215

Visibility (10m) -2.853224 86.007307 Dew point temperature(°C) -0.124492 -0.380226 Solar Radiation (MJ/m2) -0.001201 0.6462 Rainfall(mm) 0.000418 0.028514 Snowfall (cm) 0.002528 -0.005217 Seasons -0.039421 -0.0 Holiday -0.001079 -0.0 Functioning Day 0.032545 0.001085 hourOfDay 0.001085 2.833657

feature VIF

0 Rented Bike Count 4.385017

1 Temperature(°C) 46.418062

2 Humidity(%) 22.407409

3 Wind speed (m/s) 4.866986

4 Visibility (10m) 9.719935

5 Dew point temperature(°C) 25.000918 6 Solar

Radiation (MJ/m2) 3.020596

7 Rainfall(mm) 1.108003

8 Snowfall (cm) 1.123911

9 Seasons 5.117387

10 Holiday 1.063033

11 Functioning Day 32.796315

12 hourOfDay 2.625944

<u>Exploratory Data Analysis S</u>catterplots and histograms are generated using matplotlib for each column present in the dataset. Most of the columns are continuous apart from a few variables such as Snowfall, Rainfall and categorical variables such as Seasons, Holiday and Functioning day.

When we use the describe() function on the dataset, we can see the mean of Rainfall, snowfall is close to 0, but the Rented bike count covariance with these columns is high, hence we will include these columns in our models.

DEBUG @ RegressionTreeRF.train: for tree6 ===

LinkedHashMap(**rSq -> 0.962847**, rSqBar -> 0.952032, sst -> 11138737787.460625, sse -> 413837637.347054, sde -> 486.147147, mse0 -> 236208.697116, rmse -> 486.013063, mae -> 343.342250, dfm -> 395.000000, df -> 1357.000000, fStat -> 89.031978, aic -> -12542.468462, bic ->

-10376.937206, mape -> Infinity, smape -> 17.193500)

Python:

2L Neural Net:

Learning Rate:1e-5
Batch Size:4096

Hidden Layer Size:512

The Best performance combination was found with ReLU activation function and Stochastic Gradient Descent Optimizer.

Input Size:11

training 2L net

Epoch [100/100], Loss: 151656.843750
5-fold cross-validation evaluation for 2L net

Epoch [100/100], Loss: 145072.476562

Epoch [100/100], Loss: 141301.726562

Epoch [100/100], Loss: 141973.593750

Epoch [100/100], Loss: 139124.375000

Epoch [100/100], Loss: 137281.640625

Metrics:

The best performance was found with Cross Validation.

Best Performance for Each Neural Network:

```
2-Layer Neural Network:

Best R<sup>2</sup>: 0.6602

Activation and Optimizer: Activation: ReLU, Optimizer: SGD Metrics:

In-Sample MSE: 151686.234375

In-Sample RMSE: 389.46917724609375

In-Sample R<sup>2</sup>: 0.6352

Validation MSE: 149774.140625

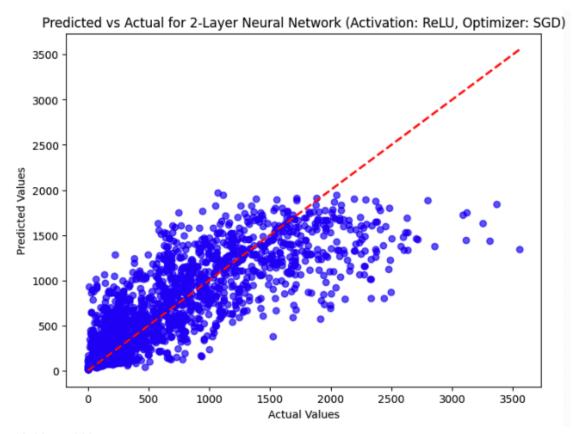
Validation RMSE: 387.00665283203125

Validation R<sup>2</sup>: 0.6405

Cross-Validation MSE: 141125.546875

Cross-Validation RMSE: 375.6151428222656

Cross-Validation R<sup>2</sup>: 0.6602
```



3L Neural Net:

The Best performance combination was found with SELU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate:1e-5 Batch Size:4096 Hidden Layer Size:512 Input Size:11

training 31 net Epoch [100/100], Loss: 90142.054688 5-fold cross-validation evaluation Epoch [100/100], Loss: 75487.250000 Epoch [100/100], Loss: 68721.410156 Epoch [100/100], Loss: 64444.488281 Epoch [100/100], Loss: 61178.160156 Epoch [100/100], Loss: 59334.775391

Metrics:

The best metric was found with Cross validation.

```
3-Layer Neural Network: Best R^2: 0.8425 Activation and Optimizer: Activation: SELU, Optimizer: SGD
```

Metrics:

In-Sample MSE: 90175.5234375

In-Sample RMSE: 300.2923889160156

In-Sample R^2 : 0.7831

Validation MSE: 94231.7421875

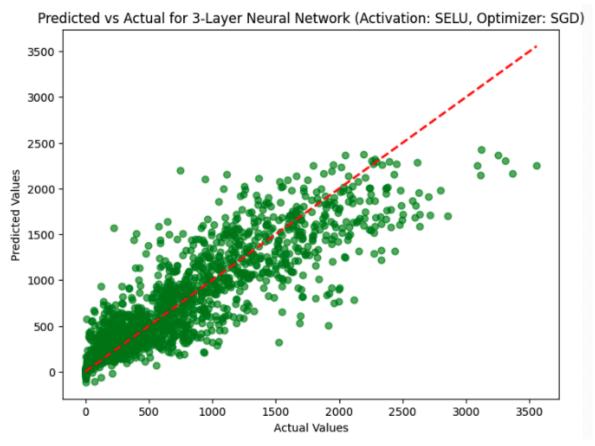
Validation RMSE: 306.9718933105469

Validation R²: 0.7738

Cross-Validation MSE: 65384.8125

Cross-Validation RMSE: 255.5073699951172

Cross-Validation R²: 0.8425



XL Neural Net:

The Best performance combination was found with SELU activation function and Stochastic Gradient Descent Optimizer.

Learning Rate:1e-5 Batch Size:4096 Hidden Layer Size:512 Input Size:11

training Xl net

Epoch [100/100], Loss: 73971.078125

5-fold cross-validation evaluation Epoch [100/100], Loss: 60883.871094 Epoch [100/100], Loss: 55344.636719 Epoch [100/100], Loss: 51475.718750 Epoch [100/100], Loss: 47158.734375 Epoch [100/100], Loss: 43589.261719

Metrics:

The best metric was found with Cross validation.

XL Neural Network:

Best R^2 : 0.8753

Activation and Optimizer: Activation: SELU, Optimizer: SGD

Metrics:

In-Sample MSE: 74270.4140625

In-Sample RMSE: 272.5260009765625

In-Sample R^2 : 0.8214

Validation MSE: 79367.546875

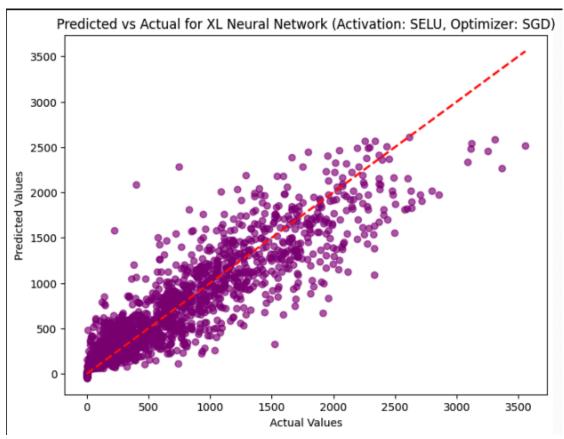
Validation RMSE: 281.72247314453125

Validation R²: 0.8095

Cross-Validation MSE: 51764.8515625

Cross-Validation RMSE: 227.0684814453125

Cross-Validation R²: 0.8753



A **Random Forest Regressor** is initialized with 100 trees (n_estimators=100). This means the model will create 100 decision trees, each contributing to the final prediction.

The random_state=42 ensures reproducibility, meaning each run of this code will yield the same results.

```
Random Forest Test MSE : 76185.7484 Random Forest Test RMSE: 276.0177 Random Forest Test R^2 : 0.8171
```

GridSearchCV is used to find the optimal hyperparameters, which can improve the model's performance

Below is the parameter grid for searching and best combination of parameters.

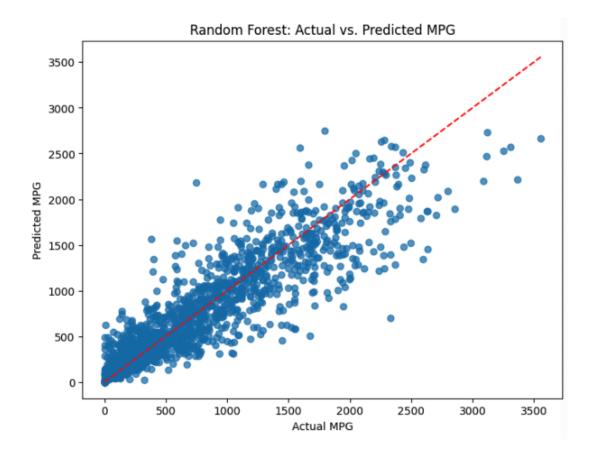
```
param_grid = {
'n_estimators': [100, 200, 300],
'max_depth': [None, 10, 20, 30],
'min_samples_split': [2, 5, 10],
'min_samples_leaf': [1, 2, 4]

Best Parameters: { 'max_depth': None, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 100}

Best CV MSE: 0.8283

Best Random Forest Test MSE: 76185.7484
```

Below is the Random Forest Regressor graph:



The Cross validation scores are:

Cross-Validated R² Scores: [0.81055458 0.83807724 0.82366025 0.84661243 0.82267248]

Average Cross-Validated R² Score: 0.8283

Feature Selection:

Feature Selection has been included in the code for all forward, backward and stepwise.

Bonus 1: Feature Selection - Implemented for all three datasets.

Note: As discussed with the professor and agreed on implementing Feature selection for AutoMPG would be fine. Whereas we implemented for all three however provided results for only Airfoil and AutoMPG here.

Bonus 2: Random Forest Regressor

It has been implemented in both Scala and Python and results has been reported here.

Tabular representation of results:

Dataset Model	AirFoil		AutoMPG		SeoulBike	
	Scala	Python	Scala	Python	Scala	Python
2 Layer Network	0.533	0.6960	0.822	0.9277	0.692	0.6602
3 Layer Network	0.805	0.8630	0.924	0.9568	0.861	0.8425
X Layer Network	0.913	0.9323	0.928	0.9818	0.867	0.8753
RF Regressor	0.820	0.9342	0.933	0.9160	0.962	0.8283