Report on Partitioning Clustering and Energy Forecasting

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1 Partitioning Clustering

1.1 Pre-Processing the data

For this task we were given a vehicle xmls file containing 846 samples, with 19 different attributes including the 'Class'. However, as the goal is to perform k-means clustering on the data, an unsupervised learning algorithm, it is required to remove the 'Class' column as the model will classify the data on its own. I also removed the 'Sample' column as it will affect the next pre-processing tasks, scaling and outlier removal.

When it comes to the order, I chose to remove the outliers first as they seemed to negatively affect the clustering results if I scaled the data before removing them. To find the outliers I found the **z-score** for each of the samples and then removed any samples with a **z-score** than **3** and less than **-3**.

1.2 Finding the best k using: Nblust, Elbow method, Gap statistics and sillhoutte methods

1.2.1 Nblust

As shown below, Nbclust says the best number of clusters is 3. Considering the original number of classes is 4 I believe that this is a good result.

```
* Among all indices:
2 * 6 proposed 2 as the best number of clusters
3 * 12 proposed 3 as the best number of clusters
4 * 1 proposed 6 as the best number of clusters
5 * 1 proposed 8 as the best number of clusters
6 * 1 proposed 11 as the best number of clusters
7 * 1 proposed 12 as the best number of clusters
8 * 2 proposed 15 as the best number of clusters
9

****** Conclusion *****
11
2 * According to the majority rule, the best number of clusters is 3
```

1.2.2 Elbow Method

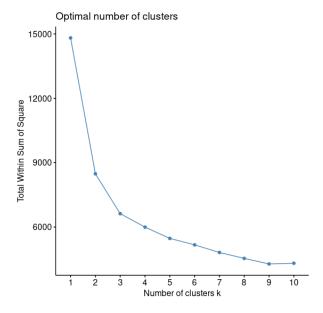


Figure 1: Elbow method plot

The Elbow method uses the WCSS(within-cluster sums of squares) which measures how close data points are in respect of their cluster centers. Based on the plot above, the recommended number of clusters is 3 as that is where the results begin to flatten out slowly indicating that increasing the clusters anymore will not result in any increase in performance.

1.2.3 Gap Statistics

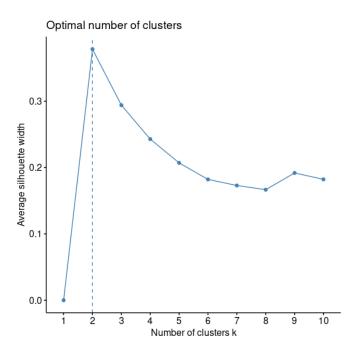


Figure 2: Gap statistics plot

The Gap statistics also uses the **WCSS** to calculate the best number of clusters to use. However, the reccomended number of clusters in this case is **2**, knowing that the original data set has **4** possible classes, we can conclude that this result is worse than what we got with the elbow method which was **3**.

1.2.4 Sillhoutte Method

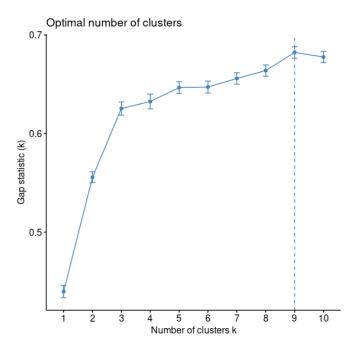


Figure 3: Sillhoutte method plot

The sillhoutte plot shows how similar a data point is to its own cluster using the **sillhoutte score**, this is a value that ranges from -1 and 1, with values closer to -1 meaning the data point should be in another cluster and the closer the value is to 1 meaning the current cluster is a good fit for the data point This is where things get interesting, based on the plot above **9** is the recommended number of clusters. This is significantly higher than any of the other results from the other evaluation methods, I made to sure to run the model several times checking if there were errors with the code, but it gave **9** as the ouput everytime. This is by far the worst result as the original data set has **4** classes

However as shown later in the report, after running the evaluation tools for the data that had **PCA** done on it. The results for the sillhoutte plot were a lot more controlled and matched the other evaluation methods as well. This led me to believe that having a data set that is too multi-demensional led to an extreme result for the sillhoutte plot.

1.3 K-means Clustering investigation

1.3.1 Discussing the K-means outputs

Using the results from the evaluation methods, I decided to go for k=3, as both **Nbclust** and the **Elbow Method** gave a result of the best k being k. Below you can see the plot made from the clustering, without looking at the output data you can see a clear distinction between the clusters where there is no overlapping

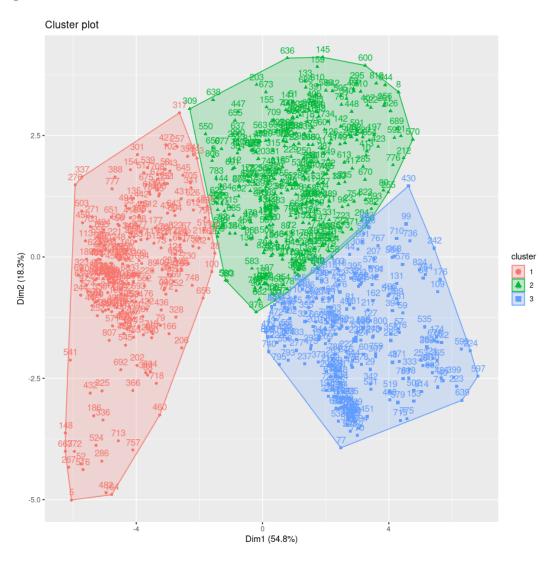


Figure 4: Clustering plot

Below are the kmeans output for the clustering attempt with k=3. You can see that the sizes of each cluster is evenly distributed which implies that the clustering did not favour or ingnore any specific cluster. The BSS(between sums of squares) in this clustering is 8189.91 while the WSS(within cluster sums of squares) is 6624.09. The ratio of the BSS and the TSS(total sums of squares) is 55.3%, this number shows how well the clusters are separated from each other where a higher value means that clusters are well separated and a lower value means the clusters are not well defined.

To further investigate whether it was possible to get a lower **WSS** and a higher **BSS**, I run the clustering with k=2 which was the second most recommended value of k by the automated tools, I concluded that k=3 was indeed the best number of clusters as the **BSS** was higher while the the **WSS** was lower in the clustering attempt with k=2.

```
1 K-means clustering with 3 clusters of sizes 256, 331, 237
3 > kmeans_data$centers

        4
        Comp
        Circ
        D.Circ
        Rad.Ra
        Pr.Axis.Ra
        Max.L.Ra
        Scat.Ra

        5
        1
        1.1672551
        1.1913560
        1.2226654
        1.061855474
        0.2398399
        0.6675158
        1.3141094

        6
        2
        -0.2324797
        -0.5226347
        -0.2851558
        -0.002041173
        0.3625937
        -0.1440161
        -0.4446806

7\ 3\ -0.9361458\ -0.5569412\ -0.9224294\ -1.144132376\ -0.7654747\ -0.5198934\ -0.7984081
      Elong Pr. Axis. Rect Max. L. Rect Sc. Var. Maxis Sc. Var. maxis
                                              Ra.Gyr Skew.Maxis
9 1 -1.2220251
           1.3199740 1.1102132 1.2689258 1.3291991 1.0980640 -0.08461041
                                   -0.4533218 -0.5482611 -0.66286263
-0.8026391 -0.4203797 1.01716369
10 2 0.3064563
           -0.4736786 -0.4874626
                           -0.3936680
11 3 0.8919890
           -0.7642435 -0.5184154
                          -0.8208477
   Skew.maxis Kurt.maxis Kurt.Maxis
                            Holl.Ra
12
13 1 0.16667482 0.27331007 0.01515673 0.2044549
14 \ 2 \ -0.06083852 \ -0.01874875 \ 0.75780956 \ 0.6641968
15 3 -0.09506837 -0.26903603 -1.07474720 -1.1484793
16
17 > kmeans_data$cluster
  [42] 2 3 3 3 3 3 2 3 2 1 2 1 2 2 3 1 3 1 3 3 3 2 3 3 1 2 1 1 1 2 3 2 1 2 3 1 3 3 1 2 3 2
19
  [83] 2 3 2 3 1 2 1 2 3 1 3 3 1 3 2 2 3 1 1 1 3 3 2 2 2 3 3 3 2 1 1 3 2 3 3 2 2 2 3 2 2
24 [247] 2 1 2 2 1 1 3 2 2 2 1 3 3 2 2 3 3 2 2 2 1 2 3 3 1 2 2 3 3 1 3 2 2 3 1 3 3 2 2 1 2
25 [288] 1 3 2 2 1 2 2 2 3 2 1 1 1 1 1 1 2 2 1 3 3 3 2 3 1 1 3 1 2 3 1 3 2 2 2 1 1 3 1 1 3 1
29 [452] 1 3 3 1 1 2 2 1 1 1 3 1 1 2 2 3 1 1 2 2 3 3 1 2 3 1 1 2 3 3 1 1 2 1 3 3 1 1 1 3 3 1
38 [821] 2 1 2 3
39
40 > kmeans_data$tot.withinss
41 [1] 6624.09
42
43 > kmeans_data$betweenss
44 [1] 8189.91
45
46 Within cluster sum of squares by cluster:
47 [1] 2191.909 2735.763 1696.418
48 (between_SS / total_SS = 55.3 %)
```

1.3.2 Sillhoutte Plot

The sillhouette plot shows how well the clustering is taking place and it will calucalte the average distance between the clusters. In practice the plot displays how close each point in one cluster is to poins in the neighbouring clusters. The **average width score** indicates how well the samples are well clustered, it ranges from 1 to -1 where a score close to 1 means the samples are well matched to their own cluster while a score closer to -1 means the samples are poorly matched to their own clusters, and a score close to 0 means the samples are more ambiguously placed and could be in another cluster.

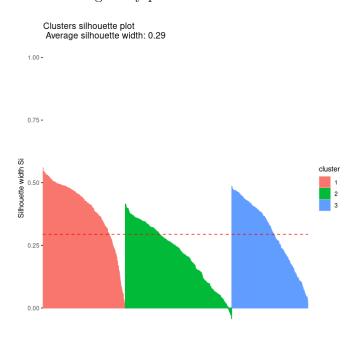


Figure 5: Sillhoutte plot

From the plot above you can see that the **average width score** is **0.29**, being a positive value we can say that the clusters are moderately accurate, but as the maxmimum score is **1** there can still be some improvements in the clustering to achieve a better **average width score**

1.4 K-means Clustering with PCA

1.4.1 Creating the new dataset with PCA

Below I have known the **eigenvalues**, the **eigenvectors**, and the **cumulative score** per principle component. To make the new transformed dataset we want to use the PCs with at least a **cumulative score** of >92% I decided to use the first 6 PCs as they gave a total score of 0.94%

```
eigenvalues
   [1] 9.8655415144 3.3026315672 1.2050866140 1.1255984677 0.8773731809 0.6636174794
   [7] \quad 0.3374343341 \quad 0.2274918343 \quad 0.1176165632 \quad 0.0871789864 \quad 0.0607683889 \quad 0.0450646831
       0.0292070985 \ 0.0213994038 \ 0.0150961795 \ 0.0123913361 \ 0.0061400710
  > eigenvectors
                         PC1
                                      PC2
                                                   PC3
                                                                  PC4
                                                                               PC5
                                                                                             PC6
                              0.08819711 -0.03979285 -0.142474274 -0.15979926
                 -0.27099550
                                                                                    0.219704493
  Comp
                                           -0.19761320
  Circ
                 -0.28538005
                              -0.14799378
                                                        0.023348077
                                                                       0.12602923
                                                        -0.104513476
10 D.Circ
                 -0.30078375
                              0.04064437
                                            0.07450874
                                                                       0.07338676
                                                                                    0.000941066
11 Rad.Ra
                 -0.27595481
                              0.19284625
                                            0.04085638
                                                         0.244080006 -0.12620414 -0.153234232
12 Pr.Axis.Ra
                 -0.10790106
                              0.24598582 -0.10092681
                                                        0.611908838 -0.05646656 -0.599471567
13 Max. I. . Ra
                 -0.18693783
                              0.06836380 -0.10600156 -0.255241647
                                                                       0.70801896 -0.255529947
                                           0.10748098
  Scat.Ra
                 -0.30925633 -0.07715243
                                                        0.001027495 -0.09117998
```

```
0.30718493 0.01853683 -0.09109269 -0.071391309 0.08547550 -0.061072204
15 Elong
16 Pr.Axis.Rect -0.30618660 -0.09004872 0.10605368 -0.025003047 -0.08566679 0.087748728
17 Max.L.Rect -0.27419519 -0.13582051 -0.20286313 -0.052151262 0.25259264 -0.012583332
18 Sc.Var.Maxis -0.30244511 -0.07264590 0.13477043 0.057153180 -0.15616630 0.103440122
19 Sc. Var. maxis -0.30676191 -0.08004640 0.10787776 0.004398469 -0.12508727 0.106371087
               -0.25860012 \ -0.21823056 \ -0.21386460 \ \ 0.068595328 \ \ 0.01184258 \ -0.063754044
20 Ra.Gyr
               21 Skew.Maxis
22 Skew.maxis
               -0.05921378 0.09616696 0.68221125 -0.400234808 -0.09248124 -0.471711647
23 Kurt.maxis
                -0.04751059 \quad 0.50763917 \quad -0.07208105 \quad 0.027069843 \quad -0.17449701 \quad 0.240919678
24 Kurt.Maxis
25 Holl.Ra
               -0.09728514 \quad 0.50329529 \quad -0.03870066 \quad -0.089901222 \quad 0.12059247 \quad 0.082978199
26
                       PC7
                                     PC8
                                                  PC9
                                                             PC10
27 Comp
                0.25075003 -0.762917498 0.336727260 -0.17080380 0.06059915
                -0.38184560 -0.084996844 0.048161956 0.14521912 -0.06103582
28 Circ
29 D.Circ
               0.10924250 0.307560350 0.369297550 0.09330027 0.74865950
                30 Rad.Ra
31 Pr.Axis.Ra
                0.40902849 -0.032642651 -0.227739119 -0.25103768 -0.10840290
32 Max.L.Ra
33 Scat.Ra
                0.09891112 0.092046874 -0.128654451 0.10439303 -0.14948976
34 Elong
                -0.10476915 -0.225039791 0.263923313 0.02991565 -0.09895280
35 Pr.Axis.Rect 0.09681861 0.043426157 -0.071150433 0.18287483 -0.26837448
               -0.36733465 \ -0.241378159 \ -0.121107876 \ 0.50017751 \ 0.09455120
36 Max.L.Rect
37 Sc. Var. Maxis 0.11234218 0.149165987 -0.129154922 -0.16972307 0.03485767
38 Sc. Var. maxis 0.08604684 0.045421860 -0.102778876 0.11442449 -0.24325771
39 Ra.Gyr
               -0.45586499 0.112011651 0.148879282 -0.69204782 -0.05867687
               0.11079493 -0.298664862 -0.505836049 -0.11269997 0.40780344
0.12381756 0.128361642 -0.070226350 0.07170181 -0.02036668
40 Skew.Maxis
41 Skew.maxis
42 Kurt.maxis
               -0.31638913 -0.134628700 0.005249849 -0.04532918 -0.03440818
               -0.18582252 -0.098767436 -0.460060564 -0.18269431 0.16137526
43 Kurt.Maxis
44 Holl.Ra
               -0.18385202 \ -0.002257517 \ -0.204524578 \ 0.01863833 \ 0.12215130
                       PC12
                                 PC13
                                              PC14
                                                            PC15
45
                                                                             PC16
46 Comp
                0.016236215 -0.15538799 -0.084941797 -0.009893937
                                                                     0.014731452
                -0.108002512 -0.02379761 0.200359434 -0.411699600 0.633197650
47 Circ
48 D.Circ
               -0.148278795 \quad 0.02028449 \quad 0.782962301 \quad -0.002680653 \quad -0.262185162
49 Rad.Ra
                50 Pr.Axis.Ra
                                                                     0.091207086
51 Max.L.Ra
                                                                     0.023924621
               0.114239242 -0.02130040 -0.070286104 -0.106776285 0.005784063
52 Scat.Ra
53 Elong
                0.155162263 0.75286275 0.157069120 0.228858568 0.132825704
54 Pr.Axis.Rect 0.272369519 0.30540490 -0.201563990 -0.167283715 -0.290260077
55 Max.L.Rect -0.201414962 -0.03380300 -0.013996509 0.370105120 -0.376075706
56 Sc. Var. Maxis -0.228758252 0.06412845 -0.026516516 0.694529334 0.411479615
57 Sc. Var. maxis 0.177853616 0.28399252 -0.085543400 -0.046373620 0.145074045
58 Ra.Gyr
             0.153739469 0.03885792 -0.107040664 0.039303314 -0.249704673
               0.220683275 0.09807688 0.277643886 -0.073168084 -0.021263745
0.001322677 -0.01515260 0.002919287 0.032651291 0.017641831
59 Skew.Maxis
60 Skew.maxis
61 Kurt.maxis
               -0.087563183 -0.01891627 -0.022107399 -0.022609384 0.002337621
62 Kurt.Maxis
                -0.385070902 0.34206081 -0.073483280 -0.224113793 -0.089715206
63 Holl.Ra
               0.697685477 -0.19114605 0.188619261 0.198088827 0.123427696
                         PC17
                                       PC18
64
                0.0022871138 -0.0001888306
65 Comp
                0.1935606420 0.0189798203
66 Circ
67 D.Circ
                -0.0338082604 -0.0095717960
68 Rad.Ra
                0.0060687302 -0.0275176970
69 Pr.Axis.Ra
                -0.0091405437 0.0177603416
70 Max.L.Ra
                -0.0048404910 -0.0083581152
                -0.3857289906 0.7909901632
71 Scat. Ra
72 Elong
                -0.0570308312 0.2237899607
73 Pr.Axis.Rect 0.6548967453 -0.0151607986
74 Max.L.Rect -0.1025905067 -0.0266527364
75 Sc.Var.Maxis 0.2336432149 0.0416825198
76 Sc. Var. maxis -0.5542304543 -0.5644496563
            -0.0737884732 0.0031786081
77 Ra.Gyr
78 Skew.Maxis
               0.0234042984 -0.0068080750
79 Skew.maxis
                0.0046042860 -0.0030669415
                -0.0007617607 -0.0075237217
80 Kurt.maxis
                -0.0118304320 0.0341259519
81 Kurt.Maxis
                 0.0432842111 -0.0094922864
83
84
85 > summary(pca_data)
```

```
86 Importance of components:
                             PC1
                                    PC2
                                             PC3
                                                     PC4
                                                             PC5
                                                                     PC6
                                                                              PC7
                                                                                      PC8
87
                          3.1409 1.8173 1.09776 1.06094 0.93668 0.81463
                                                                         0.58089 0.47696
88
  Standard deviation
89 Proportion of Variance 0.5481 0.1835 0.06695 0.06253 0.04874 0.03687 0.01875 0.01264
90
  Cumulative Proportion 0.5481 0.7316 0.79851 0.86105 0.90979 0.94666 0.96540 0.97804
91
                              PC9
                                     PC10
                                             PC11
                                                     PC12
                                                             PC13
                                                                     PC14
                                                                              PC15
                          0.34295 0.29526 0.24651 0.2123 0.17090 0.14629 0.12287 0.11132
92
  Standard deviation
  Proportion of Variance 0.00653 0.00484 0.00338 0.0025 0.00162 0.00119 0.00084 0.00069
94
  Cumulative Proportion 0.98458 0.98942 0.99280 0.9953 0.99692 0.99811 0.99895 0.99964
95
                             PC17
96 Standard deviation
                          0.07836 0.01903
97 Proportion of Variance 0.00034 0.00002
  Cumulative Proportion 0.99998 1.00000
```

1.5 Finding the best k for PCA dataset using: Nblust, Elbow method, Gap statistics and sillhoutte methods

1.5.1 Nblust

The results for **Nbclust** while using the newly made dataset using **PCA** were not different from the original k-means clustering attempt using the original dataset. Nbclust still says the best number of clusters is **3**.

```
* Among all indices:

* 7 proposed 2 as the best number of clusters

* 10 proposed 3 as the best number of clusters

* 1 proposed 4 as the best number of clusters

* 2 proposed 6 as the best number of clusters

* 2 proposed 9 as the best number of clusters

* 2 proposed 15 as the best number of clusters

* 2 proposed 15 as the best number of clusters

* 3 ****** Conclusion ******

* According to the majority rule, the best number of clusters is 3
```

1.5.2 Elbow Method

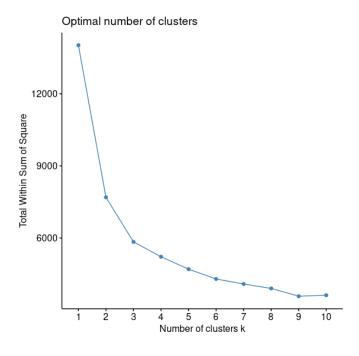


Figure 6: Elbow method plot

The **elbow method** is not showing new reults and also says the reccomended number of clusters is still **3**.

1.5.3 Gap Statistics

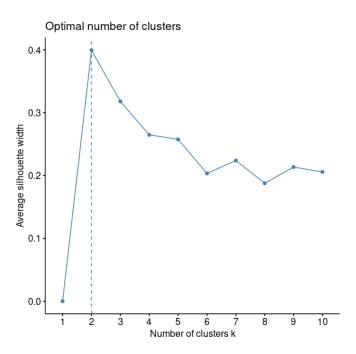


Figure 7: Gap statistics plot

The gap statistics also still says the reccomended number of clusters is still 2.

1.5.4 Sillhoutte Method

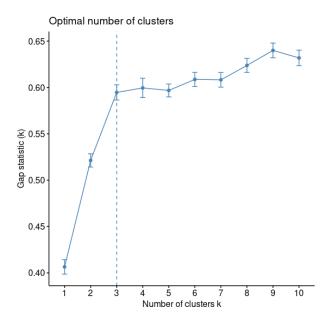


Figure 8: Sillhoutte method plot

As stated previously, the **sillhoutte plot** for the data that had **PCA** done to it gives a more reasonable result for the recomended number of clusters, this being **3**.

1.6 K-means Clustering Investigation with PCA

1.6.1 Discussing the K-means outputs

The most recomended number of clusters is still 3, however this time as the data has been passed through **PCA**, the clustering is significantly different compared to the attempt done with the original data. As shown in the plot below, this time there is a lot more of overlapping especially with cluster 1 and 2. This is not ideal as we want each cluster to have a clear distance from the other ones.

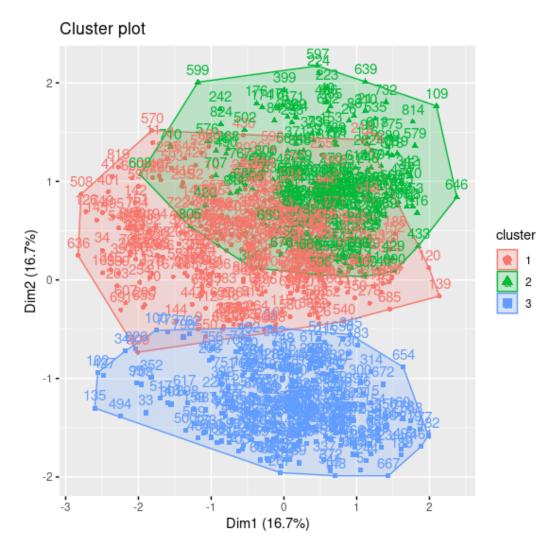


Figure 9: Clustering plot

I have put below the kmeans output for the clustering attempt using the data passed through **PCA**. I am still using **k=3** as Nbclust, elbow method and the sillhoutte plot all had an output of 3 as the best number of clusters. The **BSS** in this clustering is **8183.617** while the **WSS** is **5840.179**. The ratio of the **BSS** and the **TSS** is **58.4%**. By running **PCA** on the data, we were able to improve our results especially for the **WSS** as this time it is a lot lower than the original attempt.

```
K-means clustering with 3 clusters of sizes 332, 236, 256

kmeans_pca_data$centers
```

```
PC4
         PC2
               PC3
                          PC5
4
    PC1
7 3 4.082068 0.3618108 -0.08402257 0.1035711 0.101921914 -0.08108694
9 > kmeans_pca_data$cluster
 10
11 2
12 [42] 1 2 2 2 2 1 2 1 3 1 3 1 1 2 3 2 3 2 2 2 1 2 2 3 1 3 3 3 1 2 1 3 1 2 3 2 2 3 1 2
13 1
14 [83] 1 2 1 2 3 1 3 1 2 3 2 2 3 2 1 1 2 3 3 3 2 2 1 1 1 2 2 2 1 3 3 2 1 2 2 1 1 1 2 1
15 1
\begin{smallmatrix} 16 \end{smallmatrix} \ [124] \ 3\ 3\ 1\ 2\ 3\ 2\ 1\ 2\ 1\ 1\ 2\ 3\ 2\ 1\ 3\ 1\ 1\ 1\ 1\ 3\ 1\ 1\ 3\ 1\ 3\ 1\ 2\ 1\ 1\ 2\ 3\ 1\ 1\ 3\ 3\ 1\ 3\ 2\ 2\ 3
17 3
19 1
21 1
22 [247] 1 3 1 1 3 3 2 1 1 1 3 2 2 1 1 2 2 1 1 1 3 1 2 2 3 1 1 2 2 3 2 1 1 2 3 2 1 1 1 3
23 1
24 [288] 3 2 1 1 3 1 1 1 2 1 3 3 3 3 3 2 1 3 2 2 2 1 2 3 3 2 3 1 2 3 2 1 1 1 3 3 2 3 3 2
25 3
27 2
29 1
31 2
32 [452] 3 2 2 3 3 1 1 3 3 3 2 3 3 1 1 2 3 3 1 1 2 2 3 1 2 3 3 1 2 3 3 1 3 2 2 3 3 3 2 2
33 3
35 1
37 3
39 3
41 3
43 3
45 2
47 1
49 1
50 [821] 1 3 1 2
51
52 > kmeans_pca_data$tot.withinss
53 [1] 5840.179
54
55 > kmeans_pca_data$betweenss
56 [1] 8183.617
57
58 Within cluster sum of squares by cluster:
59 [1] 2415.343 1461.091 1963.745
60 (between_SS / total_SS = 58.4 %)
```

1.6.2 Sillhoutte Plot

From the plot below you can see that the **average width score** this time is **0.32**, this is an increase of **0.03** as in the original attempt the score was **0.29**. Again, this is not the best result as the maximum is score **1**, but

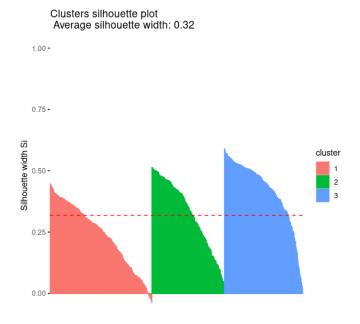


Figure 10: Sillhoutte plot

1.6.3 Calinski Harabasz index

This is a measure of the optimal number of clusters, the value can range between 0 and infinity where higher values means a better clustering. For the k-means model with a k of 3 the score received is 575.2178.

2 Energy Forecasting

2.1 Type of input variables used for electricity load forecasting

2.2 Normalising the data

Before beginning the training of the neural networks I normalised the I/O matrices. This is an essential step because it helps to improve the performance and training speed of the model. It also improves the stability of the model as outliers will not have as heavy of an influence in the models output, it also increases the rate of convergence as the model will be working with values in a smaller range allowing it to find the optimal weights faster.

2.3 Evaluating the models using: RMSE, MAE, MAPE. sMAPE

RMSE(Root Mean Square Error) is calculated using the following formula:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}}$$

The formula uses the square root of the mean of the squared differences between the predicted and the actual values to tell us how far the predictions are on average from the actual values where a smaller **RMSE** means the model is predicting well and a bigger **RMSE** means the model is not predicting the data well. The downside here is that it is more sensitive to outliers as they can influence sum of squared errors. Another issue is that it can be affected by differences in scale between variables, if one has values in a much larger range than another it will be emphasised more.

MAE(Mean Absolute Error) is calculated using the following formula:

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

This uses the average of the absolute difference between each predicted and actual value to tell us how far the predictions are on average from the actual values where a smaller **MAE** means the model is predicting well and a bigger **MAE** means the model is not predicting the data well. The downside here is that as it takes in the absolute error it will treat all errors equally so whether they are positive or negative it will not matter. Unlike **RMSE**, **MAE** is not as sensitive to outliers so it will not reflect the effect outliers have in the model prediction, which makes it a less accurate evaluation tool if the data still has outliers.

MAPE(Mean Absolute Percentage Error) is calculated using the following formula:

$$MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{y_i} \right| \times 100\%$$

This uses the absolute difference between predicted and actual value, it then divides the difference by the actual value and the result is expressed as a percentage in the end. This tells us how far the predictions are on average from the actual values where a smaller **MAPE** means the model is predicting well and a bigger **MAPE** means the model is not predicting the data well. This is useful when the scale of the data varies a lot, it is also commonly used as it provides the result in percentages which is easier to understand. The problem with this metric is that it can put more emphasis on large errors and less emphasis on smaller errors, it is also does not work as well when the actual value is equal to or close to **0**. In such cases it can be expected to receive a very large **MAPE** result or even for it to be undefined.

sMAPE(Symmetric Mean Absolute Percentage Error) is calculated using the following formula:

$$SMAPE = \frac{1}{n} \sum_{i=1}^{n} \frac{|y_i - \hat{y}_i|}{(|y_i| + |\hat{y}_i|)/2} \times 100\%$$

This measures the average of the absolute percentage difference between predicted and actual value, it then divides the difference by the sum of the absolute predicted and actual values. In situations where the actual values are equal to or close to **0**, **sMAPE** is preferred as it handles them better compared to **MAPE**.

2.4 Evaluating the results

When it came to the actual training of the neural network models I focused on a few parameters to change the output of the models, these being: the input I/O matrices, the layers and number of nodes per layer and whether the output is linear or not. I did not change the activation function as the difference in output was negligible in my attempts at training the models, so I chose to not include it as a parameter and just used the default one that comes with the **neuralnet()** function, the logistic activation function.

I made 5 different input delayed I/O matrices and made sure to train at least 2 models with each matrix, the first with 1 hidden layer while the second with 2 hidden layers.

Table 1: Comparison table

Model	RMSE	MAE	MAPE	sMAPE	Description
NN_1	0.1152572	0.0921373	0.1859476	0.1818735	I/O matrix: t-2, t-1, t, t+1
					layers: 1x8
					linear output: TRUE
NN_2	0.11671855	0.09510258	0.18712046	0.18152017	I/O matrix: t-7, t-1, t+1
					layers: 2x6-4
					linear output: FALSE
NN_3	0.11274105	0.08804056	0.16946062	0.17188169	I/O matrix: t-7, t-2, t-1, t+1
					layers: 1x5
					linear output: TRUE
NN_4	0.1368248	0.1034995	0.2027808	0.2093880	I/O matrix: t-7, t-4, t-3, t-2, t-1, t,
					t+1
					layers: 2x12-6
					linear output: FALSE
NN_5	0.11566742	0.09362933	0.19071920	0.18508842	I/O matrix: t-1, t, t+1
					layers: 1x4
					linear output: TRUE
NN_6	0.11586446	0.08959127	0.17309226	0.17616521	I/O matrix: t-7, t-2, t-1, t+1
					layers: 1x6
					linear output: TRUE
NN_7	0.11679370	0.09541529	0.18768615	0.18188354	I/O matrix: t-7, t-1, t+1
					layers: 1x4
					linear output: FALSE
NN_8	0.1111209	0.0878771	0.1782428	0.1735545	I/O matrix: t-2, t-1, t, t+1
					layers: 2x7-3
					linear output: FALSE
NN_9	0.11686106	0.09053119	0.17770444	0.17620528	I/O matrix: t-7, t-4, t-3, t-2, t-1, t,
					t+1
					layers: 1x10
					linear output: TRUE
NN_10	0.11076446	0.09087368	0.18499380	0.17967582	I/O matrix: t-1, t, t+1
					layers: 2x4-2
					linear output: FALSE
NN_11	0.10991593	0.08468949	0.16530730	0.16681759	I/O matrix: t-7, t-2, t-1, t+1
					layers: 2x5-3
					linear output: FALSE
NN_12	0.1324693	0.1046402	0.1981125	0.2063737	I/O matrix: t-7, t-4, t-3, t-2, t-1, t,
					t+1
					layers: 2x6-2
					linear output: TRUE

From the table above you can see that the results for the different models are not too different from each other. After looking at the results I found that the best 1-layer NN is NN_3 while the best 2-layer NN is NN_11 . I am basing this decision on the scores achieved for the evaluation metrics, I tried to find the total number of weights but it did not calculate properly as it showed 2 and 3 for all models. Another

observation made from the table above is that both NN_3 and NN_11 have the period t-7 in their input matrix. As suggested by the specification it appears that the t-7 period does indeed hold more influence on the prediction made by the model.

2.5 NN training with the NARX approach

With the **NARX** approach we also have to consider the input vectors from the **18th** and **19th** hour columns. My expectations were that with a more varied amount of data it would lead to better results when it comes to NN training.

I made 4 different I/O matrices which ranged from t to t-4 and included t-7 for some of the I/O matrices.

2.5.1 Evaluating the results in the NARX approach

Below you can see the results from this training attempt, as you can see this models performed better than the ones trained with the AR approach.

Table 2: Comparison table for NARX approach

Model	RMSE	MAE	MAPE	sMAPE	Description
NN_1	0.09954752	0.08211452	0.16860201	0.15971510	I/O matrix: 18(t-2), 19(t-1), 19(t),
					20(t+1)
					layers: 1x8
					linear output: TRUE
NN_2	0.10163645	0.08423843	0.15945130	0.16691218	I/O matrix: 20(t-7), 19(t-7), 18(t-
					4), 20(t-2), 19(t), 20(t+1)
					layers: 2x10-4
					linear output: FALSE
NN_3	0.10463934	0.08856077	0.18183779	0.17094784	I/O matrix: 18(t-7), 20(t-4), 19(t),
					20(t), 20(t+1)
					layers: 2x8-3
					linear output: TRUE
NN_4	0.09084888	0.07564465	0.15531772	0.14718595	I/O matrix: 18(t-4), 19(t), 20(t+1)
					layers: 1x6
					linear output: FALSE
NN_5	0.11171708	0.09121835	0.17266331	0.18359165	I/O matrix: 20(t-7), 19(t-7), 18(t-
					4), 20(t-2), 19(t), 20(t+1)
					layers: 1x12
					linear output: TRUE

It seems that by using the other hours to train the model, it was able to make a better prediction across all the evaluation metrics. What seems to affect the accuracy of the model is the I/O matrix used as the input, in the AR approach training the t-7 period led to the models performing better than others, but in this case models with I/O matrices with that period did not perform the best. Instead it was NN_11 which had inputs from the periods 18(t-4), 19(t), 20(t+1).

A Code for Partitioning clustering

Listing 1: My R script

¹ library("readxl")

```
2 library("ggplot2")
3 library("dplyr")
4 # Reading in the vehicle.xlsx file
5 data <- read_excel("~/Documents/rcw/data/vehicles.xlsx")</pre>
6 #removing the class and sample column as we do not need it for the k means clustering.
7 data <- subset(data, select = -c(Samples, Class))</pre>
8 str(data)
9 #making sure there are no null values in the data set before checking for outliers.
10 sum(is.na(data))
12 #using the boxplot to visually show the outliers
13 boxplot(data)
14 #use the sapply function to find the z-score for all the samples to then determine the outliers.
15 #I am creating a new column for the z-score for each of the samples,
16 #this makes it easier to remove the outliers.
17 data$zscore <- sapply(data, function(data) (data-mean(data))/sd(data))
18 #just double checking the dimensions of the original data set before removing outliers.
19 dim(data)
20 head(data$zscore)
22 #creating a new table that does not contain the outliers,
23 #anything that has a z-score lower than 3 and more than -3.
24 no_outliers <- data[!rowSums(abs(data$zscore) > 3), ]
26 #checking the maximum and minimum z-score to make sure the previous step worked as planned.
27 max(no_outliers$zscore)
28 min(no_outliers$zscore)
_{29} #new dimension of the new table, it is now 824 x 19 instead of 846 x 19
30 dim(no_outliers)
31
32 #this is just visually compare the original data set with the newly made one
33 boxplot(data)
34 boxplot(no_outliers)
36 #now removing the z-score column as it will change the result of the clustering
37 no_outliers <- subset(no_outliers, select = -c(zscore))
38 #scaling the data using the built-in scale function in R,
39 #I am also making a new dataframe to make comparisons easier.
40 no_outliers_normalised <- as.data.frame(scale(no_outliers))
41 #making sure the data was normalised properly
42 no_outliers$Rad.Ra
43 no_outliers_normalised$Rad.Ra
44
45 #using automated tools to determine the best number of cluster centers
46 library("NbClust")
47 library ("factoextra")
48 library("cluster")
49 library("fpc")
51 #Nbclust
52 NbClust(no_outliers_normalised, distance = "euclidean", method = "kmeans", index="all")
53 #Elbow method
54 fviz_nbclust(no_outliers_normalised, kmeans, method='wss')
55 #Silhouette method
56 fviz_nbclust(no_outliers_normalised, kmeans, method='silhouette')
57 #Gap Stastics
58 fviz_nbclust(no_outliers_normalised, kmeans, method='gap_stat')
60 #performing kmeans clustering using the most favoured "k" from the automated methods used above.
61 kmeans_data <- kmeans(no_outliers_normalised, centers = 3, nstart = 10)
62 fviz_cluster(kmeans_data, data = no_outliers_normalised)
63
64 data_cluster <- data.frame(no_outliers_normalised, cluster = as.factor(kmeans_data$cluster))
65 head(data_cluster)
66
67 #showing the kmeans output
68 kmeans_data
69 #showing the within cluser summs of squares(WSS) and the between cluster sums of squares (BSS)
70 kmeans_data$centers
71 kmeans_data$tot.withinss
72 kmeans_data$betweenss
```

```
73 #showing the silhouette plot for the clustering
74 kmeans data$cluster
75 silhouette <- silhouette(kmeans_data$cluster, dist(no_outliers_normalised))
76 fviz_silhouette(silhouette)
78 #applying PCA to the dataset to reduce dimensionality.
79 #this is the scaled dataset without the outliers
80 head(no_outliers_normalised)
81 pca_data <- prcomp(no_outliers_normalised, center = TRUE, scale = TRUE)</pre>
82 eigenvalues <- pca_data$sdev^2
83 eigenvectors <- pca_data$rotation
84 eigenvalues
85 eigenvectors
86 summary(pca_data)
88 #making a new dataset with only the first 6 PCA as the cumulative proportion for them is > 92\%
89 transformed_data <- as.data.frame(-pca_data$x[,1:6])
90 head(transformed_data)
_{91} #new dimension is 824\ x 6, thus reducing the attributes by 3 times.
92 dim(pca data$x)
93 dim(transformed_data)
95 #applying the same 4 automated tools to find the new favoured k for the clustring
96 #Nbclust
97 NbClust(transformed_data, distance = "euclidean", method = "kmeans", index="all")
98 #Elbow method
99 fviz_nbclust(transformed_data, kmeans, method='wss')
100 #Silhouette method
101 fviz_nbclust(transformed_data, kmeans, method='silhouette')
102 #Gap Stastics
103 fviz_nbclust(transformed_data, kmeans, method='gap_stat')
105\ \mbox{\#performing kmeans} clustering using the new dataset
106 #performing kmeans clustering using the most favoured "k" from the automated methods used above.
107 kmeans_pca_data <- kmeans(transformed_data, centers = 3, nstart = 10)
108 fviz_cluster(kmeans_pca_data, data = transformed_data)
110 data_cluster <- data.frame(transformed_data, cluster = as.factor(kmeans_pca_data$cluster))
111 head(data_cluster)
112
113 #showing the kmeans output
114 kmeans_pca_data
115 #showing the within cluser summs of squares(WSS) and the between cluster sums of squares (BSS)
116 kmeans_pca_data$centers
117 kmeans_pca_data$tot.withinss
118 kmeans_pca_data$betweenss
119 #showing the silhouette plot for the clustering
120 kmeans_pca_data$cluster
121 silhouette <- silhouette(kmeans_pca_data $cluster, dist(transformed_data))
122 fviz_silhouette(silhouette)
124 #using the calinski-harabasz index
125 calinhara(transformed_data, kmeans_pca_data$cluster)
```

B Code for Energy forecasting

Listing 2: My R script

```
library("readxl")
library("dplyr")
library("neuralnet")
library("Metrics")

data <- read_excel("~/Documents/rcw/data/uow_consumption.xlsx")

#renaming the columns as they have weird names by default
names(data)[2] <- '18:00'
names(data)[3] <- '19:00'
names(data)[4] <- '20:00'
head(data)</pre>
```

```
14\ \mbox{\#getting} the 20:00 column only as it is our focus
input_data <- subset(data, select = c('20:00'))</pre>
16 input_data
18 #normalising the data
19 normalize <- function(x) {</pre>
20 return((x - min(x)) / (max(x) - min(x)))
21 }
23\ \mbox{\#normalizing} data before creating the delayed input I/O matrices
24 normalized_input_data <- as.data.frame(lapply(input_data, normalize))
25 normalized_input_data
26 head(normalized_input_data)
27 #function to create the time delayed input variables I/O matrices
28 create_time_lagged_data <- function(data, lag_values, name) {</pre>
29
       #this lets me specify the time lag and it will bind the time delayed column
30
       #to the orginal dataset orginal
       #which acts as the column for the predicted column, as it has no lag
31
       time_lagged_data <- cbind(lapply(lag_values, function(x) lag(data, x)), data)
33
       # Remove rows with missing values
34
       time_lagged_data <- time_lagged_data[complete.cases(time_lagged_data),]
35
       #Raname the data with the relevant names
       names(time_lagged_data) <- name</pre>
36
       return(time_lagged_data)
37
38 }
39
40 # Create different versions of the time-lagged data
41 time_lagged_data_1 <- create_time_lagged_data(normalized_input_data,
42
                                                 c(3,2,1),
                                                 c("previous2", "previous1", "current", "predicted"))
43
44
  time_lagged_data_2 <- create_time_lagged_data(normalized_input_data,</pre>
                                                 c(8, 2),
45
46
                                                 c("previous7", "previous1", "predicted"))
47 time_lagged_data_3 <- create_time_lagged_data(normalized_input_data,
                                                 c(8, 5:1),
48
                                                  c("previous7", "previous4", "previous3", "previous2",
49
                                                      "previous1", "current", "predicted"))
51 time_lagged_data_4 <- create_time_lagged_data(normalized_input_data,
                                                 c(8, 3, 1),
                                                 c("previous7", "previous2", "current", "predicted"))
53
54 time_lagged_data_5 <- create_time_lagged_data(normalized_input_data,
                                                 c(2.1).
55
                                                  c("previous1", "current", "predicted"))
57
58 # Define a function to make training the nn models easier
59
  train_neuralnet <- function(data, layers, linear_output) {</pre>
60
61
       #creating the training and testing batches for the nn, keeping the training sample to 380.
       train_data <- data[1:380,]</pre>
62
       test_data <- data[381:nrow(data),]</pre>
63
64
       #making the nn using the neuralnet function.
65
       nn <- neuralnet(predicted ~ .,
66
67
                        data = train_data,
68
                        hidden = layers,
                        linear.output = linear_output)
69
70
71
       # calculating the total number of weights in the neural network
72
       #I was not able to get the weights to show properly as it was giving an
       #output of 2 and 3 for all models
73
       total_weights <- sum(sapply(nn$weights, length))</pre>
74
75
76
       predicted <- predict(nn, newdata = test_data)</pre>
77
       actual <- test_data$predicted</pre>
       #using the RMSE, MAE, MAPE and SMAPE to evaluate the models,
78
       #It is also saved into a list which makes it easy to view all results
79
       metrics <- c("RMSE" = rmse(actual, predicted),</pre>
81
                  "MAE" = mae(actual, predicted),
                   "MAPE" = mape(actual, predicted);
82
                  "SMAPE" = smape(actual, predicted),
83
```

```
"Total Weights" = total_weights)
84
85
       #plotting for visual representation
        # plot(nn)
86
        return(metrics)
87
88 }
89
90 #I am making a list that holds all the parameters I will be using to train each of the 15 models
91 #So for example any values at index 1 of the different keys of the nn_parameters list
92 #will be used to train nn_1, index 2 for nn_2 and so on.
93 nn_parameters <- list()
94 #specifying the data to be used to train the model
95 nn_parameters$data <- list(time_lagged_data_1,#nn1
96
                            time_lagged_data_2,
                            time_lagged_data_4,
                                                     #nn3
97
98
                            time_lagged_data_3,
                                                     #nn4
gg
                            time_lagged_data_5,
                                                     #nn5
100
                            time_lagged_data_4,
                                                      #nn6
                            time_lagged_data_2,
                                                     #nn7
                                                     #nn8
                            time_lagged_data_1,
                                                     #nn9
                            time_lagged_data_3,
                                                     #nn10
                            time_lagged_data_5,
                            time_lagged_data_4,
                                                      #nn11
106
                            time_lagged_data_3)
                                                     #nn12
108 #specifying the number of layers and nodes per layer
109 nn_parameters$layers <- list(c(8),</pre>
                                             #nn1
                                  c(6,4),
111
                                  c(5),
                                             #nn3
112
                                  c(12,6),
                                             #nn4
113
                                  c(4),
                                             #nn5
                                  c(6),
                                             #nn6
114
                                  c(4),
                                             #nn7
                                  c(7,3),
                                             #nn8
116
117
                                  c(10),
                                             #nn9
118
                                  c(4,2),
                                             #nn10
                                  c(5,3),
                                             #nn11
119
120
                                  c(6,2))
                                             #nn12
121
122 #specifying if the output should be linear or not
123 nn_parameters$linear_output <- list(TRUE, #nn1</pre>
124
                                           FALSE, #nn2
                                           TRUE, #nn3
                                           FALSE, #nn4
126
                                           TRUE, #nn5
127
                                          TRUE, #nn6
FALSE, #nn7
128
129
                                          FALSE, #nn8
130
                                          TRUE, #nn9
131
                                          FALSE, #nn10
                                           FALSE, #nn11
                                           TRUE) #nn12
134
135
136
137 nn_parameters
138
139 #this is the training loop, it makes use of the nn_parameters list made above,
140 #it makes it easy to train a variety of models and experimenting with parameters
141 #I made an empty list which I use to store the model outputs after each loop.
142 nn_output <- list()
143 for (i in 1:length(nn_parameters$data)) {
144
        #using my custom function to make the models and save the results for the evaluation metrics
        nn_output[[i]] <- train_neuralnet(nn_parameters$data[[i]];</pre>
145
146
                                             nn_parameters$layers[[i]],
147
                                             nn_parameters$linear_output[[i]])
       #renaming the keys in the list to make it easier to extract results
148
       names(nn_output)[i] <- paste0("nn_", i)</pre>
149
150 }
152 nn_output
154 #using the NARX approach to include the 18\,\mathrm{th} and 19\,\mathrm{th} hour attributes
```

```
155 narx_input_data <- subset(data, select = c("18:00", "19:00", "20:00"))
156 head(narx_input_data)
158 # narx_create_time_lagged_data <- function(target_data, data, lag_values) {
159 #
         time_lagged_data <- cbind(lapply(lag_values, function(x) lag(data, x)), target_data)</pre>
160 #
         # Remove rows with missing values
161 #
         # time_lagged_data <- time_lagged_data[complete.cases(time_lagged_data),]</pre>
162 #
         #Raname the data with the relevant names
         # names(time_lagged_data) <- name</pre>
163 #
164 #
         return(time_lagged_data)
165 # }
166
167 #Above I tried to make a similar function to make the time lagged data,
_{
m 168} #as 18th and 19th hour need to be accounted for I struggled to find a solution.
169 #So instead I just manually made the time lagged data for the narx approach as the actual result
170 #I was at least able to use the nn training function and loop with some minor tweaking.
171
172 # normalizing data before creating the delayed input I/O matrices
173 narx_normalized_input_data <- as.data.frame(lapply(narx_input_data, normalize))
174 head(narx_normalized_input_data)
175 #I had to rename the columns as after normalizing the data they changed for some reason
176 names(narx_normalized_input_data) <- c("18:00", "19:00", "20:00")
177
178 #begging to manually make the I/O matrices
179 narx_time_lagged_data_1 <- cbind(previous2_18= lag(narx_normalized_input_data$"18:00", 3),
                              previous1_19 = lag(narx_normalized_input_data$"19:00", 2),
180
181
                              current_19 = lag(narx_normalized_input_data$"19:00", 1),
                              predicted = narx_normalized_input_data$"20:00")
182
183
184 narx_time_lagged_data_1 <- narx_time_lagged_data_1[complete.cases(narx_time_lagged_data_1),]
185
186
   narx_time_lagged_data_2 <- cbind(previous7_20= lag(narx_normalized_input_data$"20:00", 8),</pre>
                               previous7_19 = lag(narx_normalized_input_data$"19:00", 8),
187
188
                              previous4_18 = lag(narx_normalized_input_data$"18:00", 5),
                              previous2_20 = lag(narx_normalized_input_data$"20:00", 3),
189
                              current_19 = lag(narx_normalized_input_data$"19:00", 1),
190
                              predicted = narx_normalized_input_data$"20:00")
191
193 narx_time_lagged_data_2 <- narx_time_lagged_data_2[complete.cases(narx_time_lagged_data_2),]
194
195 narx_time_lagged_data_3 <- cbind(previous4_18= lag(narx_normalized_input_data$"18:00", 5),
196
                               current_19 = lag(narx_normalized_input_data$"19:00", 1),
                              predicted = narx_normalized_input_data$"20:00")
197
198
199 narx_time_lagged_data_3 <- narx_time_lagged_data_3[complete.cases(narx_time_lagged_data_3),]
200
201
   narx_time_lagged_data_4 <- cbind(previous7_18 = lag(narx_normalized_input_data$"18:00", 8),
                               previous4_20 = lag(narx_normalized_input_data$"20:00", 5),
202
203
                               current_19 = lag(narx_normalized_input_data$"19:00", 1),
                               current_20 = lag(narx_normalized_input_data$"20:00", 1),
204
                              predicted = narx_normalized_input_data$"20:00")
205
206
207 narx_time_lagged_data_4 <- narx_time_lagged_data_4 [complete.cases(narx_time_lagged_data_4),]
208
209
210 #for the NARX approach I am only making 5 models to see if there is any difference in outputs
211 #So for example any values at index 1 of the different keys of the nn_parameters list will b
212 #e used to train nn_1, index 2 for nn_2 and so on.
213 narx_nn_parameters <- list()</pre>
214 #specifying the data to be used to train the model
215 narx_nn_parameters$data <- list(narx_time_lagged_data_1,#nn1</pre>
216
                           narx_time_lagged_data_2,
                                                         #nn2
217
                           narx_time_lagged_data_4,
                                                         #nn3
                                                         #nn4
218
                           narx_time_lagged_data_3,
219
                           narx_time_lagged_data_2)
                                                         #nn5
220
221 #specifying the number of layers and nodes per layer
222 narx_nn_parameters$layers <- list(c(8), #nn1</pre>
223
                                c(10,4),
                                             #nn2
224
                                c(8,3),
                                             #nn3
225
                                c(6),
                                             #nn4
```

```
c(12))
226
                                              #nn5
227
228 #specifying if the output should be linear or not
229 narx_nn_parameters$linear_output <- list(TRUE, #nn1
230
                                          FALSE, #nn2
                                          TRUE, #nn3
FALSE, #nn4
231
232
233
                                          TRUE) #nn5
234
235 #I was getting an error saying "$ is invalid for atmoic vectors" when running this function.
236 #After quite a while I found out that the test data was being turned into an atomic vector
237 #and needed to be accessed using the [] instead of \$\,.
238 #R error messages aren't the greatest which made finding the issue even more challening.
239 train_neuralnet <- function(data, layers, linear_output) {</pre>
240
241
        #creating the training and testing batches for the nn, keeping the training sample to 380.
242
        train_data <- data[1:380,]
        test_data <- data[381:nrow(data),]</pre>
243
244
245
        #making the nn using the neuralnet function.
       nn <- neuralnet(predicted ~ .,
246
                         data = train_data,
247
248
                         hidden = layers,
                         linear.output = linear_output)
249
250
251
       #code for the total weights does not seem to be working
252
        total_weights <- sum(sapply(nn$weights, length))</pre>
253
       predicted <- predict(nn, newdata = test_data)</pre>
       #this is where the error was happening.
254
        actual <- test_data[1]
       #using the RMSE, MAE, MAPE and SMAPE to evaluate the models,
256
257
        #It is also saved into a list which makes it easy to view all results
       metrics <- c("RMSE" = rmse(actual, predicted),</pre>
258
                   "MAE" = mae(actual, predicted),
259
                   "MAPE" = mape(actual, predicted)
260
                   "SMAPE" = smape(actual, predicted),
261
                    "Total Weights" = total_weights)
262
       #plotting for visual representation
263
        # plot(nn)
264
265
       return(metrics)
266 }
267
268 narx_nn_output <- list()
269 for (i in 1:length(narx_nn_parameters$data)) {
270
        narx_nn_output[[i]] <- train_neuralnet(narx_nn_parameters$data[[i]],
271
                                                  narx_nn_parameters$layers[[i]],
272
                                                  narx_nn_parameters$linear_output[[i]])
        #renaming the keys in the list to make it easier to compare results
273
274
        names(narx_nn_output)[i] <- paste0("nn_", i)</pre>
275 }
277 narx_nn_output
```