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

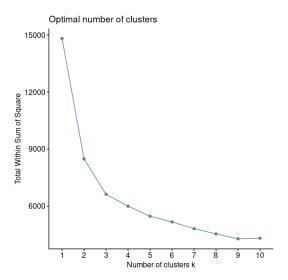


Figure 1: Elbow method plot

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 reccomended 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

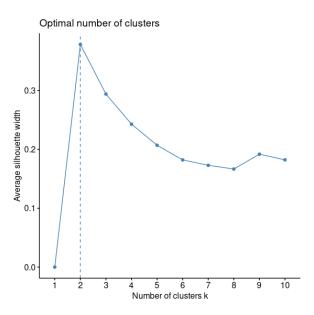


Figure 2: Gap statistics plot

The Gap statistics also uses the **WCSS** to calculate the best number of clusters to use. However, the recomended 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

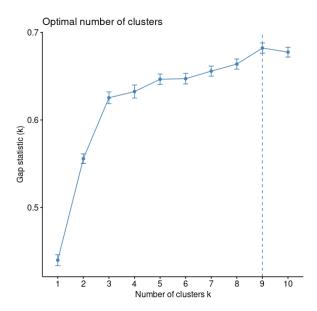


Figure 3: Sillhoutte method plot

The sillhoutte plot shows how similar a data point is to its own cluster using the **sillhuotte 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 orignal 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 3. 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

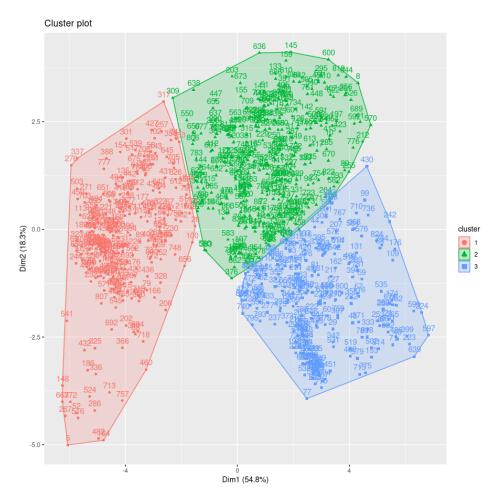


Figure 4: Clustering plot

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 **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$centers
                 D.Circ
                         Rad.Ra Pr.Axis.Ra
                                     Max.L.Ra
4
   Comp Circ
                                             Scat. Ra
5\ 1 \quad 1.1672551 \quad 1.1913560 \quad 1.2226654 \quad 1.061855474 \quad 0.2398399 \quad 0.6675158 \quad 1.3141094
\begin{smallmatrix} 6 & 2 & -0.2324797 & -0.5226347 & -0.2851558 & -0.002041173 & 0.3625937 & -0.1440161 & -0.4446806 \end{smallmatrix}
7\ 3\ -0.9361458\ -0.5569412\ -0.9224294\ -1.144132376\ -0.7654747\ -0.5198934\ -0.7984081
     Elong Pr.Axis.Rect Max.L.Rect Sc.Var.Maxis Sc.Var.maxis
                                        Ra.Gyr Skew.Maxis
                       1.2689258 1.3291991 1.0980640 -0.08461041
9 1 -1.2220251 1.3199740 1.1102132
         -0.4736786 -0.4874626
                               -0.4533218 -0.5482611 -0.66286263
10 2 0.3064563
                        -0.3936680
11 3 0.8919890
         -0.7642435 -0.5184154
                        -0.8208477
                               -0.8026391 -0.4203797 1.01716369
12 Skew.maxis Kurt.maxis Kurt.Maxis Holl.Ra
13 1 0.16667482 0.27331007 0.01515673 0.2044549
                         Holl.Ra
14 2 -0.06083852 -0.01874875 0.75780956 0.6641968
15 3 -0.09506837 -0.26903603 -1.07474720 -1.1484793
16
17 > kmeans_data$cluster
  18
 [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
20 [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
22 [165]
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
27 [370]
    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 3 1 2 3 1 1 2 3 3 1 1 2 1 3 3 1 1 1 3 3 1
32 [575]
     36 [739]
    38 [821] 2 1 2 3
40 > kmeans_data$tot.withinss
41 [1] 6624.09
43 > kmeans_data$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.

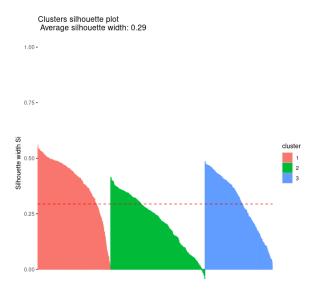


Figure 5: Sillhoutte plot

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

```
1 > eigenvalues
    \hbox{\tt [1]} \quad 9.8655415144 \quad 3.3026315672 \quad 1.2050866140 \quad 1.1255984677 \quad 0.8773731809 \quad 0.6636174794 
   [7] 0.3374343341 0.2274918343 0.1176165632 0.0871789864 0.0607683889 0.0450646831
  [13] 0.0292070985 0.0213994038 0.0150961795 0.0123913361 0.0061400710 0.0003622977
6
  > eigenvectors
                         PC1
                                       PC2
                                                    PC3
                                                                  PC4
                                                                               PC5
8 Comp
                 -0.27099550
                              0.08819711 -0.03979285 -0.142474274 -0.15979926
                                                                                     0.219704493
9 Circ
                 -0.28538005 -0.14799378 -0.19761320
                                                        0.023348077
                                                                       0.12602923 -0.019390179
                 -0.30078375
                               0.04064437
                                            0.07450874 -0.104513476
                                                                       0.07338676
                                                                                    0.000941066
10 D. Circ.
11 Rad.Ra
                 -0.27595481
                               0.19284625
                                            0.04085638
                                                         0.244080006
                                                                       -0.12620414
                                                                                    -0.153234232
                                                         0.611908838 -0.05646656 -0.599471567
12 Pr. Axis.Ra
                 -0.10790106
                               0.24598582 -0.10092681
13 Max.L.Ra
                 -0.18693783
                              0.06836380 - 0.10600156 - 0.255241647 0.70801896 - 0.255529947
```

```
-0.30925633 -0.07715243 0.10748098 0.001027495 -0.09117998 0.078463678
14 Scat.Ra
15 Elong 0.30718493 0.01853683 -0.09109269 -0.071391309 0.08547550 -0.061072204

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 
s 0.06158617 -0.50300209 0.06768991 0.125377302 -0.13879190 -0.159605991
20 Ra.Gyr
21 Skew.Maxis
22 Skew.maxis -0.03877299 0.02950349 -0.55339412 -0.517610761 -0.48274633 -0.382718195
23 Kurt.maxis -0.05921378 0.09616696 0.68221125 -0.400234808 -0.09248124 -0.471711647
24 Kurt.Maxis -0.04751059 0.50763917 -0.07208105 0.027069843 -0.17449701 0.240919678 25 Holl.Ra -0.09728514 0.50329529 -0.03870066 -0.089901222 0.12059247 0.082978199
                           PC7
                                           PC8
                                                        PC9
                                                                    PC10
                                                                                      PC11
27 Comp
                  0.25075003 -0.762917498 0.336727260 -0.17080380 0.06059915
28 Circ
                 -0.38184560 -0.084996844 0.048161956 0.14521912 -0.06103582
              0.10924250 0.307560350 0.369297550 0.09330027 0.74865950 0.13812347 0.062362314 0.159039213 -0.02487175 -0.17932432 0.06368508 -0.146618654 0.033075197 0.08677308 0.04900671
29 D.Circ
30 Rad.Ra
31 Pr.Axis.Ra
32 Max.L.Ra 0.40902849 -0.032642651 -0.227739119 -0.25103768 -0.10840290 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
36 Max.L.Rect -0.36733465 -0.241378159 -0.121107876 0.50017751 0.09455120
37 Sc. Var. Maxis 0.11234218 0.149165987 -0.129154922 -0.16972307 0.03485767
38 \ \text{Sc.Var.maxis} \quad 0.08604684 \quad 0.045421860 \ -0.102778876 \quad 0.11442449 \ -0.24325771
             -0.45586499 0.112011651 0.148879282 -0.69204782 -0.05867687 
0.11079493 -0.298664862 -0.505836049 -0.11269997 0.40780344
39 Ra. Gyr
40 Skew.Maxis
41 Skew.maxis 0.12381756 0.128361642 -0.070226350 0.07170181 -0.02036668
42 Kurt.maxis -0.31638913 -0.134628700 0.005249849 -0.04532918 -0.03440818
43 Kurt.Maxis -0.18582252 -0.098767436 -0.460060564 -0.18269431 0.16137526
44 Holl.Ra -0.18385202 -0.002257517 -0.204524578 0.01863833 0.12215130
                            PC12
                                          PC13
                                                         PC14
                                                                          PC15
                  0.016236215 -0.15538799 -0.084941797 -0.009893937 0.014731452
46 Comp
47 Circ
                  -0.108002512 \ -0.02379761 \ \ 0.200359434 \ -0.411699600 \ \ 0.633197650
48 D.Circ
                  0.027236923 \quad 0.23107314 \quad -0.032038645 \quad -0.128176485 \quad -0.032941366
                 -0.148278795 0.02028449 0.782962301 -0.002680653 -0.262185162
0.061511729 0.03176897 -0.360686574 0.022171363 0.091207086
49 Rad.Ra
50 Pr.Axis.Ra
                  -0.103284857 0.09369549 -0.004005999 -0.047699349 0.023924621
51 Max.L.Ra
52 Scat.Ra
                 0.114239242 -0.02130040 -0.070286104 -0.106776285 0.005784063
53 Elong
                   0.155162263 \quad 0.75286275 \quad 0.157069120 \quad 0.228858568 \quad 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
              0.153739469 0.03885792 -0.107040664 0.039303314 -0.249704673

s 0.220683275 0.09807688 0.277643886 -0.073168084 -0.021263745

s 0.001322677 -0.01515260 0.002919287 0.032651291 0.017641831
58 Ra.Gyr
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
             -0.0338082604 -0.0095717960
67 D.Circ
68 Rad.Ra
                   0.0060687302 -0.0275176970
                  69 Pr.Axis.Ra
70 Max.L.Ra
                  -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.Gvr
                   0.0234042984 -0.0068080750
0.0046042860 -0.0030669415
78 Skew.Maxis
79 Skew.maxis
80 Kurt.maxis -0.0007617607 -0.0075237217
81 Kurt.Maxis -0.0118304320 0.0341259519
                  0.0432842111 -0.0094922864
82 Holl.Ra
83
84
```

```
85 > summary(pca_data)
86 Importance of components:
                             PC1
                                    PC2
                                             PC3
                                                     PC4
                                                              PC5
                          3.1409 1.8173 1.09776 1.06094 0.93668 0.81463 0.58089 0.47696
  Standard deviation
88
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
                              PC9
                                      PC10
                                              PC11
                                                     PC12
                                                              PC13
                                                                      PC14
                                                                              PC15
91
92 Standard deviation
                          0.34295 \ 0.29526 \ 0.24651 \ 0.2123 \ 0.17090 \ 0.14629 \ 0.12287 \ 0.11132
93 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
                             PC17
                                      PC18
96 Standard deviation
                          0.07836 0.01903
97 Proportion of Variance 0.00034 0.00002
98 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**.

1.5.2 Elbow Method

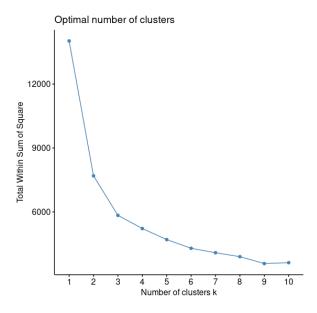


Figure 6: Elbow method plot

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

1.5.3 Gap Statistics

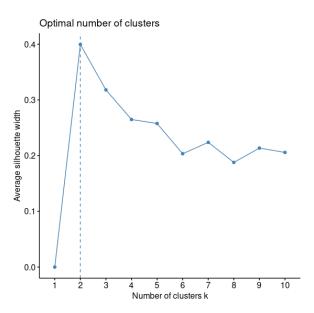


Figure 7: Gap statistics plot

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

1.5.4 Sillhoutte Method

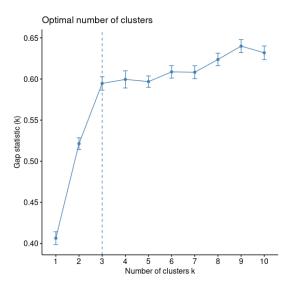


Figure 8: Sillhoutte method plot

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 reccomended 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.

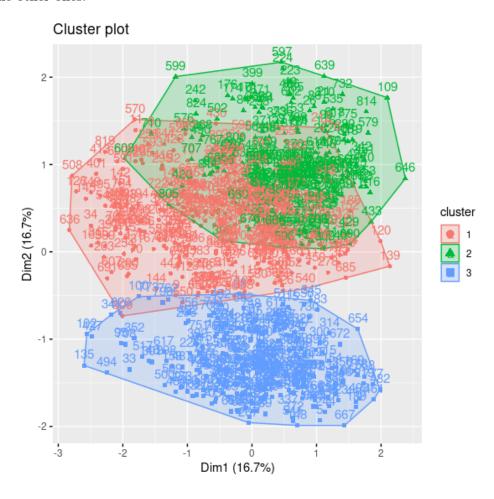


Figure 9: Clustering plot

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$centers
        PC1
                    PC2
                                 PC3
  -1.078026
             -1.5110695
                         0.04723636
                                    -0.1754898
                                                 0.009380699
                                                              -0.01659038
  -2.911460
             1.7332691
                         0.02469198
                                      0.1345272
                                                -0.123755941
                                                               0.11129772
   4.082068
             0.3618108
                        -0.08402257
                                      0.1035711
                                                 0.101921914
                                                              -0.08108694
> kmeans_pca_data$cluster
```

```
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 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
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 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

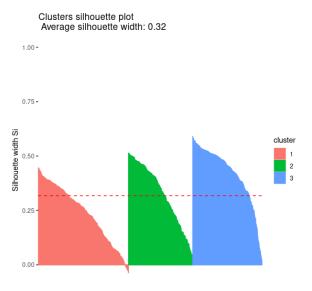


Figure 10: Sillhoutte plot

2 Energy Forecasting

A code