

Data Mining project - part II

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1 Introduction

In the second part of the project we will use cluster analysis in connection with dimension reduction methods on *Spambase* dataset. Our goal is to assess clustering algorithms performance in differentiation between *spam* and *nonspam* types. For that we shall use *k-means*, PAM and AGNES clustering algorithms. We will also evaluate the quality of obtained results by checking separation measures of clusters built using original data and data after dimensionality reduction done with PCA algorithm. Additionally, we will also compare the results of classification performed on the former part of the project versus how the same methods will perform after applying dimensionality reduction.

2 Data preparation

To be consistent with analysis done in previous part of the project we again exclude columns that exhibit high correlation with each other. These eliminated features are *num415* and *num857*. Furthermore, we also use the same data transformations: z-score standardization and $\log(x + 0.1)$ transformation to make the explanatory variables have comparable values, as it is crucial for clustering and dimensionality reduction algorithms.

3 PCA

To be able to visualize the multidimensional data easily and reduce the noise in our data before applying the clustering algorithms, we start with performing the principal component analysis (PCA). As mentioned before, we use two data transformations, however to display an interesting behavior of the method, let us first present the outputs for non-transformed data. To visualize PCA results we will use scree plot (Figure 1) and contributions of variables to the first two principal components (Figure 2).

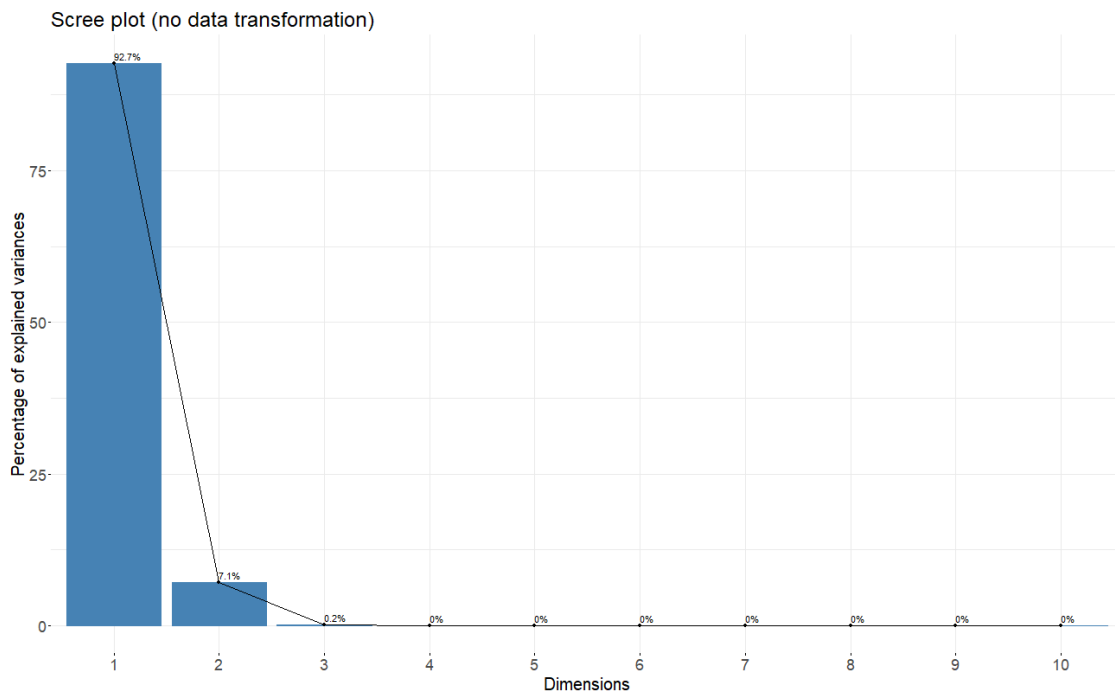


Figure 1: PCA results for original data (scree plot)

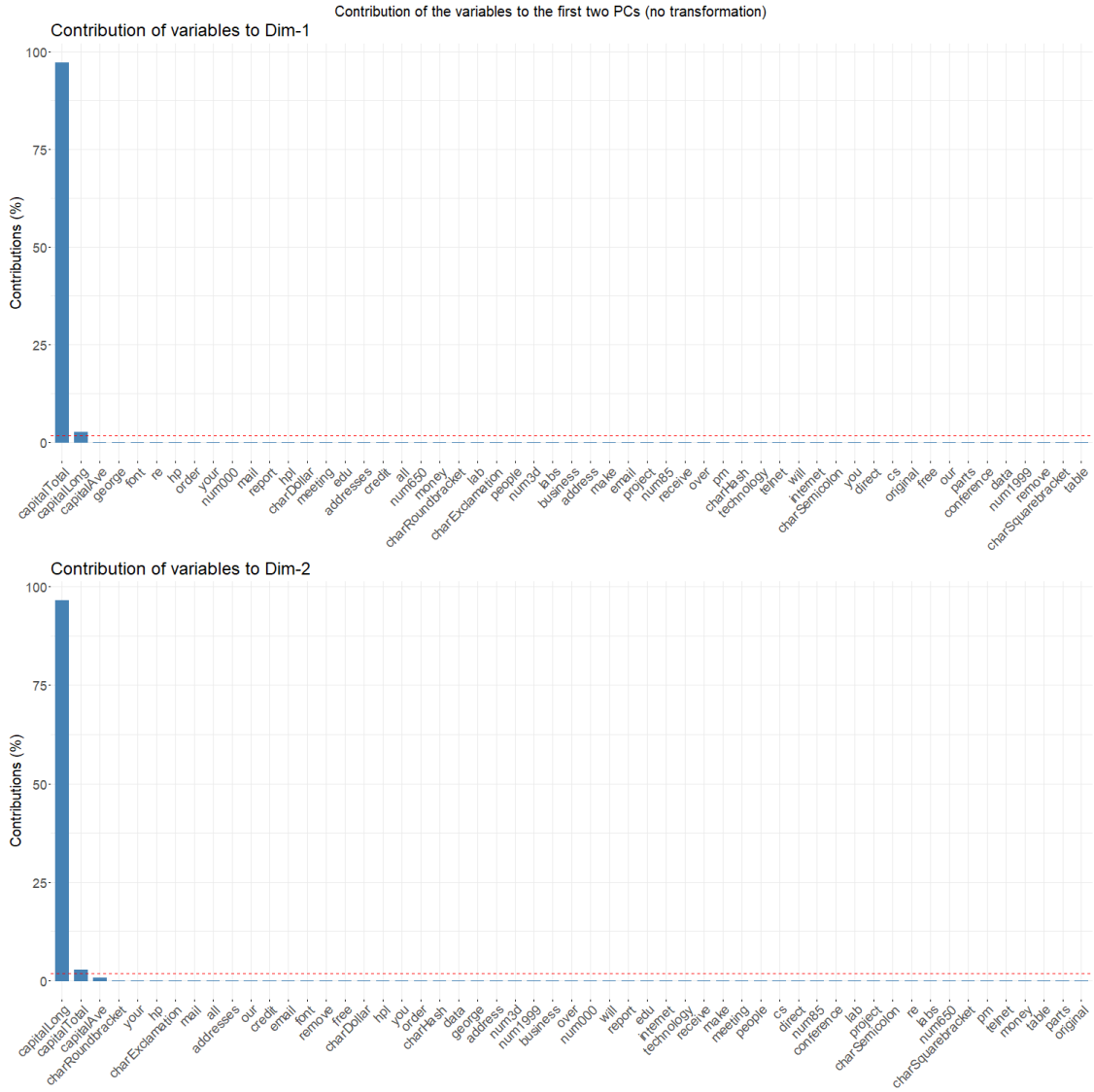


Figure 2: PCA results for original data (variable contribution plot)

As we expected, the algorithm gives poor results as only variables with highest spread are taken into consideration. In our data set most of the variables are frequencies with values in interval $[0, 100]$ and relatively low variance, and only capital letters characteristics have wider range of values. That causes the observed behavior of PCA method, which results with only 2 principal components, so in the following analyses we will use only transformed data.

Let us now check the principal components for data after z-score standardization. The screeplot is displayed on Figure 4, while the variable contribution plot can be found on Figure 4. As we anticipated, in this case we get more principal components created and also increased number of features is taken into account.

Results for log-transformed data can be seen on Figure 5 (scree plot) and Figure 6 (variable contribution plot). Here again we observe that contribution of many variables is higher than for original data. Also we see that in comparison to z-score transformed data we will probably be able to eliminate more principal components for the latter analysis.

To reduce dimensionality of our data using PCA, for both data transformations we selected a method based on feature variance. First, we compute mean standard deviation across all principal components. Second, we check which PCs display lower standard deviation than the computed mean. Finally, we reject those PCs falling below threshold – as a result, we obtain 26 principal components for z-score standardized data and 19 of them for log-transformed data. This seems like a really good reduction in dimensionality, considering that we started off with as much as 55 features!

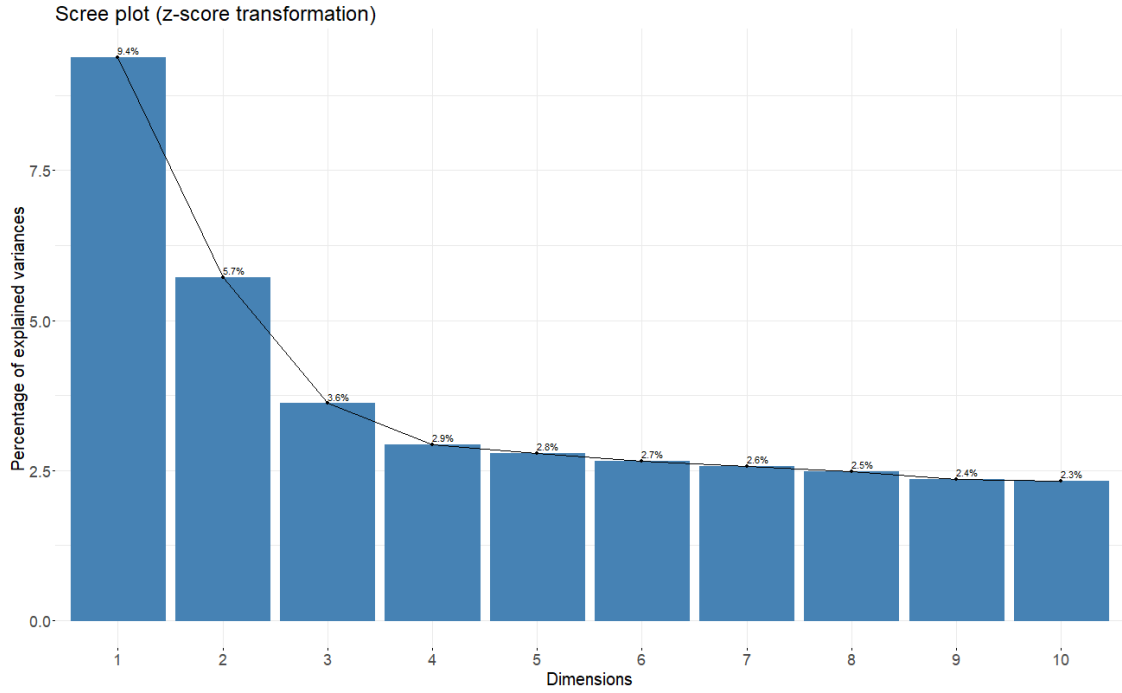


Figure 3: PCA results for standardized data (scree plot)

4 Clustering

For cluster analysis we will use k-means, PAM and AGNES algorithms for transformed *Spambase* datasets and also for datasets built using principal components extracted while performing PCA. First thing we need to do before applying the algorithms is checking the optimal number of clusters k for each of them. In case of k-means and PAM, we will do it by calculating the silhouette index, and for AGNES we will select the number of clusters by analysing the dendrogram. Given the fact that the main goal of our analysis is to check how well the clustering algorithms will be able to differentiate between spam and non-spam e-mails, we expect the optimal number of clusters to be $k = 2$, but of course we cannot eliminate other possibilities, as there might be some hidden data structures within our dataset which should not be omitted.

Let us first take a look at silhouette index values for k-means without PCA, shown on Figure 7. We see that for the z-score standardized data we should extract 2 clusters, while for the log-transformed data the optimal number of clusters is 3. The same is observed for k-means with PCA (Figure 8). Situation changes slightly in case of PAM algorithm – here, the silhouette index method picked $k = 2$ for both data transformations without PCA (Figure 9), and for PCA $k = 3$ (Figure 10).

When it comes to AGNES, the choice of the optimal number of clusters is less obvious. Looking at the dendrogram, we need to pick such k that the increase in between-cluster dissimilarity from k clusters to $k + 1$ clusters is significantly less than the increase in between-cluster dissimilarity from $k - 1$ clusters to k clusters. From Figure 11 we see that for z-score standardized data without PCA $k = 2$ would be a good choice ($k = 3$ to include outliers as separate cluster), and the same with PCA (Figure 12). For log-transformed data, both without PCA (Figure 13) and with PCA (Figure 14), the optimal number of clusters is evaluating to 3. As expected, in case of the second data transformation we don't observe any outliers detected by AGNES.

Once we have selected the optimal number of clusters k for all algorithms, we can move on to clustering. In the following subsections, we will discuss the results obtained for k-means, PAM and AGNES.

4.1 k-means

Figure 15 shows the results of clustering with k-means for z-score transformed data without PCA. We can see from this plot that cluster number 1 contains much more observations than the cluster number 2. Moreover, it looks like the nonspam class dominates in both of the clusters. We can verify this by looking at Table 1 – most observations from both classes fall into the first cluster, so this time the k-means algorithm wasn't able to differentiate well between spam and nonspam messages. What's interesting, applying PCA did not change the results much for the standardized data. Both Figure 16 and Table 2 display results almost identical to those observed in the previous case.

Situation looks quite different for the log-transformed data. Figure 17 shows cluster assignment for the no-PCA case. We see that the cluster number 3 contains mostly nonspam class, while the other two clusters consist mainly of spam, and Table 3 confirms that. Very similar situation is observed for log-transformed data with PCA. From Figure 18 we see that the cluster assignment didn't change much, except the names

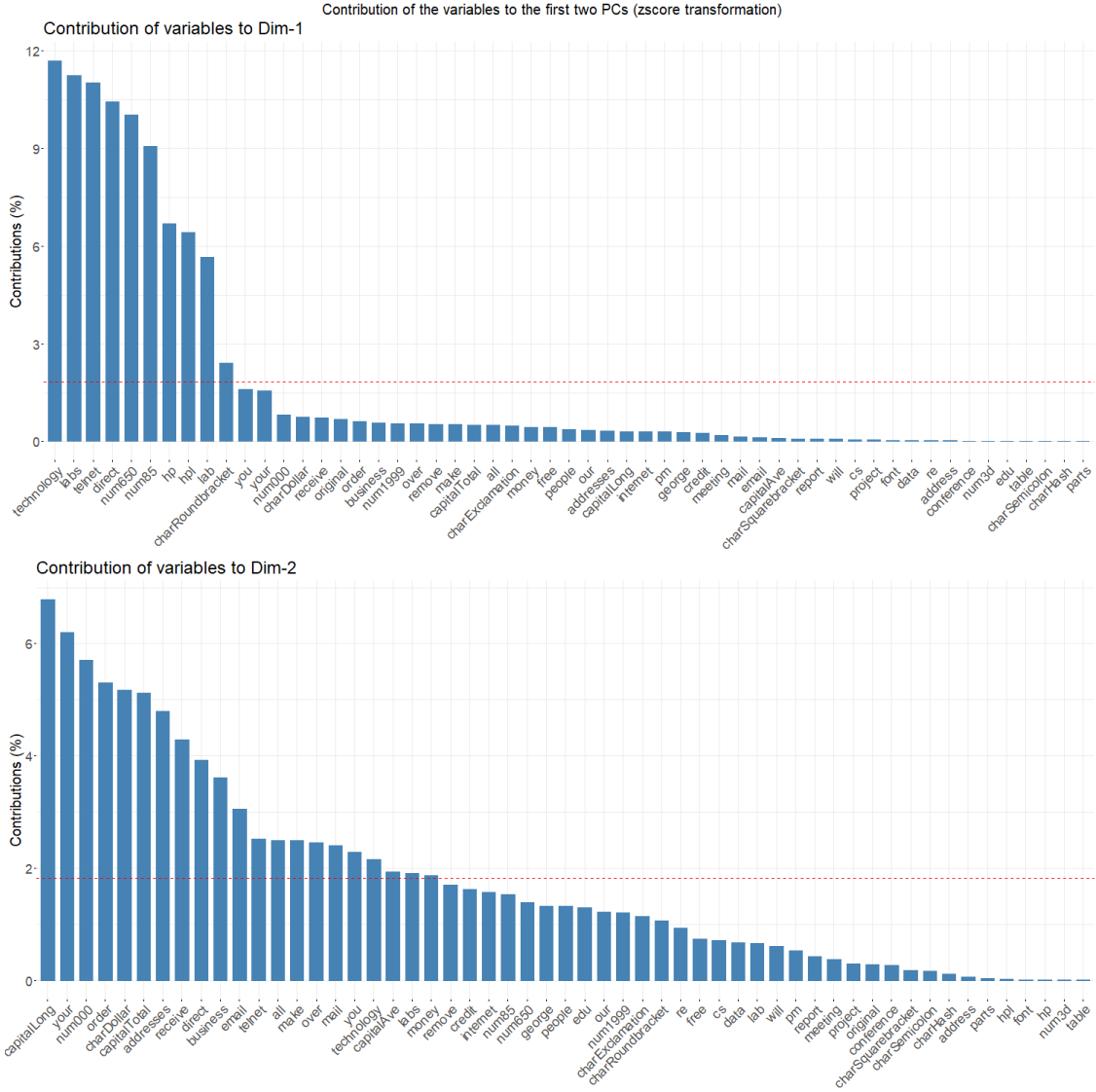


Figure 4: PCA results for standardized data (variable contribution plot)

for cluster 1 and cluster 2 are swapped. Also looking at Table 4 we can say that the proportions of classes assigned to particular clusters is almost identical as in the previous case, so again we don't observe much influence on clustering from applying PCA to our data, but we can certainly say that it is much easier for k-means to differentiate between spam and nonspam in case of log-transformation rather than for the z-score scaling.

4.2 PAM

For PAM method we again provide results for the same data transformations as for k-means. Figure 19 and Table 5 show results for standardized data. The situation, despite higher number of clusters is not significantly different that corresponding result for k-means algorithm. Clusters 2 and 3 contain almost only *nonspam* observations, but in cluster number 1 types are mixed. Let us now check the results obtained after applying PCA before PAM algorithm, that are shown on Figure 20 and Table 6. This time again the cluster number 1 contains observations with mixed types and the other cluster holds almost only *nonspam* observations.

Next, we will use data after log-transformation, first results obtained from data with original dimensionality are presented on Figure 21 and Table 7. Once again results resemble the ones obtained with k-means algorithm. In one of the clusters majority of observations are of *nonspam* type, while the opposite is for second cluster. Results of PAM clustering after PCA are presented on Figure 22 and Table 8. Here we can observe notable difference. Here the observations of different types seem to be quite well separated between two created clusters. That is the case in which we observe the best partition when comparing to external indices. It also confirms that data transformations done before clustering have high impact on the result.

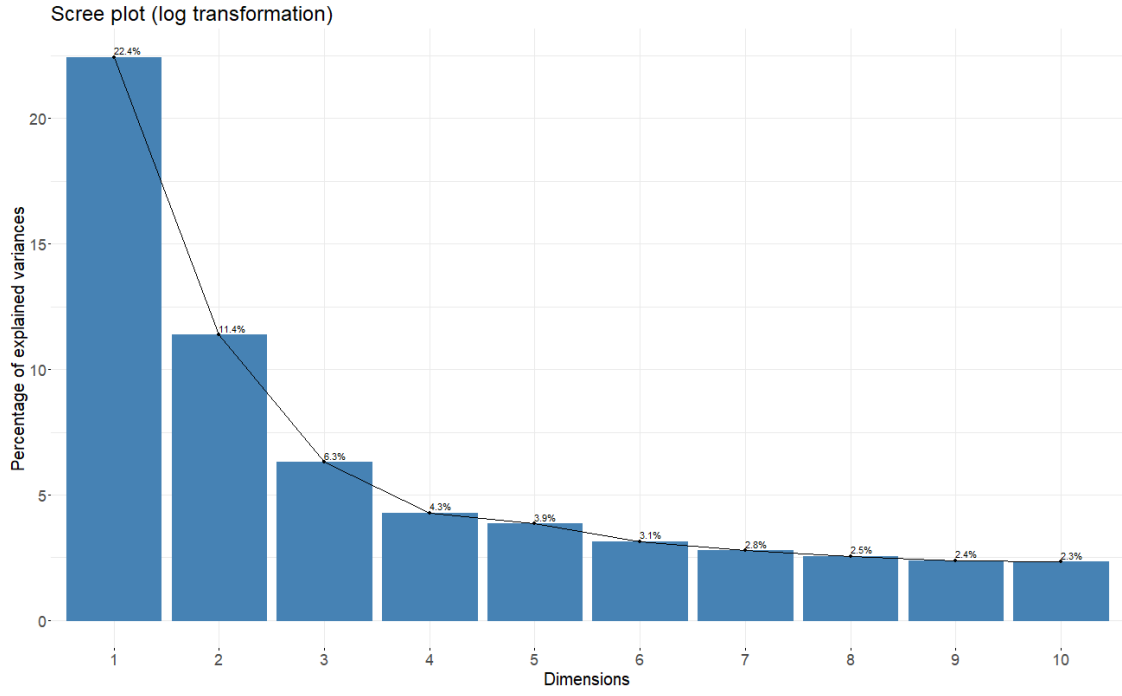


Figure 5: PCA results for log-transformed data (scree plot)

Cluster	Type	
	nonspam	spam
1	2676	1811
2	112	2

Table 1: Clustering with k-means (z-score, no PCA)

4.3 AGNES

The other type of clustering algorithm is the hierarchical clustering. We will take into consideration the agglomerative algorithm AGNES. The dendrograms were presented already in Section 4 as they were required to select the number of clusters that we want to split data to. To check how this clustering algorithm worked in case of *spam* and *nonspam* messages partition, we again provide similar plots. First for standardized data: Figure 23 and Table 9 show that all outliers placed in cluster 3 are *nonspam*. Other two clusters seem to separate two types of messages quite well, especially compared to previous results for this particular data. Let us now look, how AGNES algorithm will partition data after PCA, which is presented on Figure 24 and Table 10. Here the results are almost identical as without PCA, again one cluster contains *nonspam* outliers and the other two separate message types quite well.

We once more compare previous results to those based on log-transformed data for which results are introduced on Figure 25 and Table 11. This time, none of three created clusters contains outliers, however once again we notice that AGNES algorithm separated *spam* and *nonspam* messages noticeably well. Let us now check if this holds also for data after PCA, for which outputs are shown on Figure 26 and Table 12. There we can see that

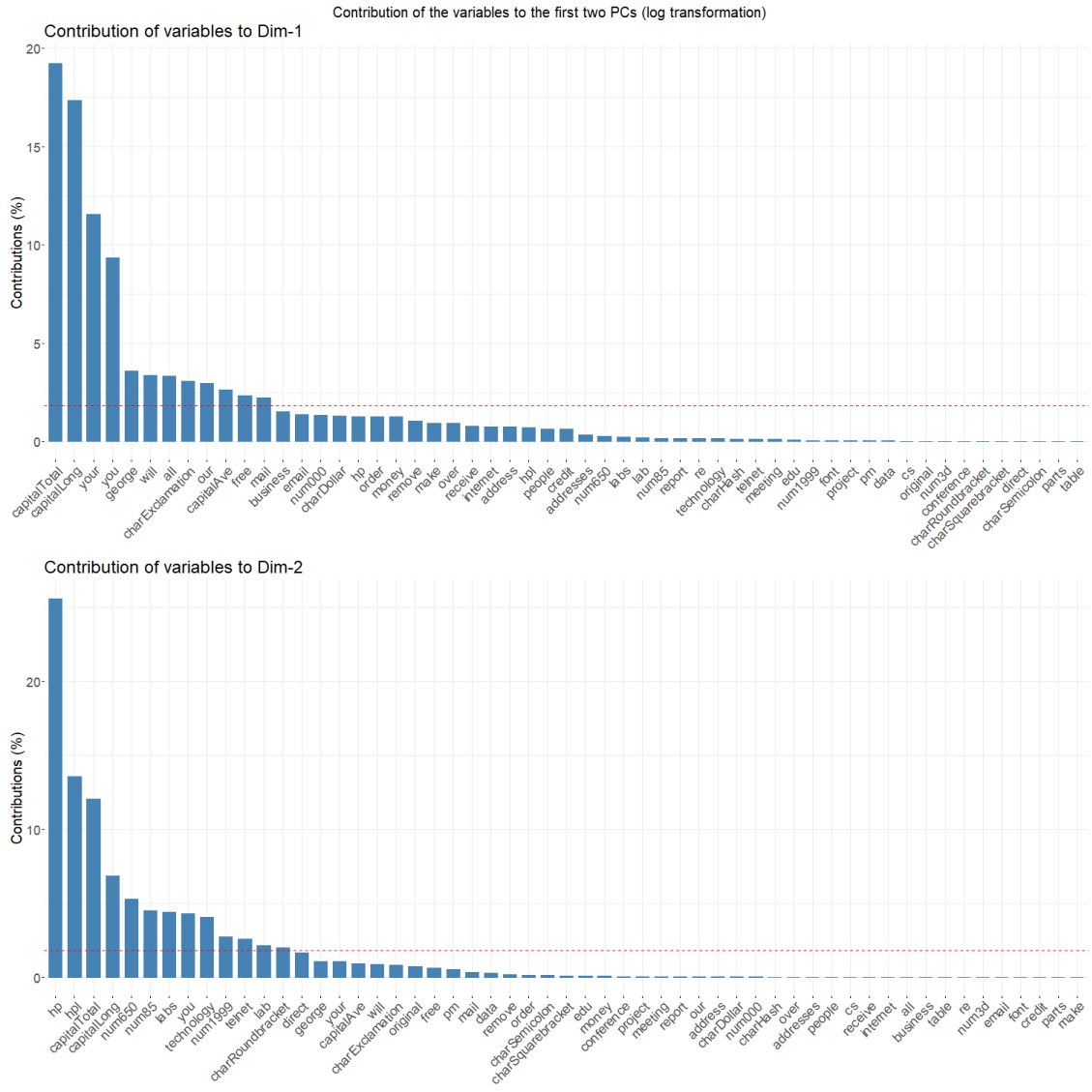


Figure 6: PCA results for log-transformed data (variable contribution plot)

Cluster	Type	
	nonspam	spam
1	2751	1813
2	37	0

Table 2: Clustering with k-means (z-score with PCA)

Cluster	Type	
	nonspam	spam
1	900	11
2	1626	326
3	262	1476

Table 3: Clustering with k-means (log, no PCA)

Cluster	Type	
	nonspam	spam
1	1628	328
2	893	11
3	267	1474

Table 4: Clustering with k-means (log with PCA)

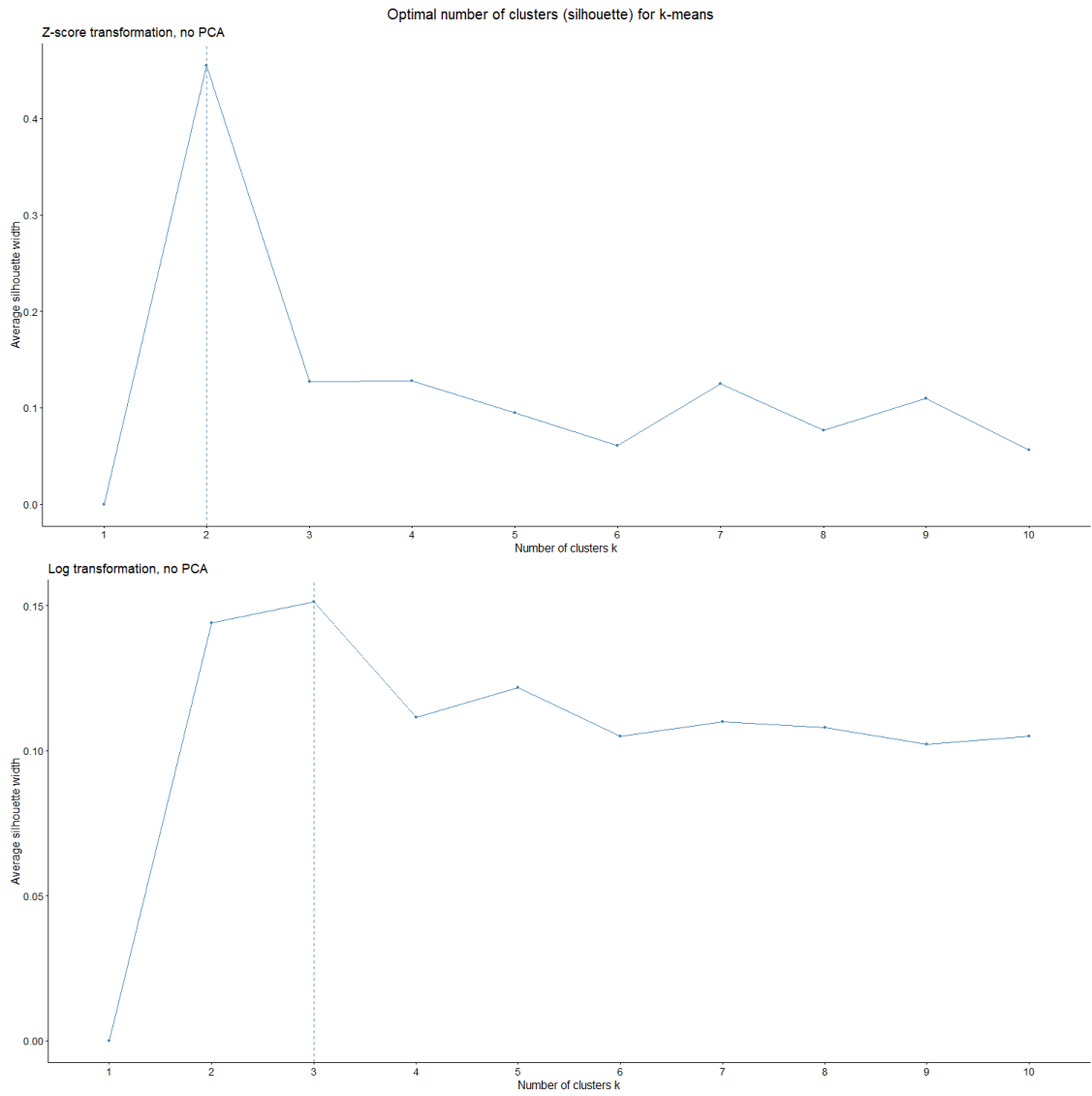


Figure 7: Number of clusters for k-means (no PCA)

Cluster	Type	
	nonspam	spam
1	2242	1810
2	421	3
2	125	0

Table 5: Clustering with PAM (z-score, no PCA)

Cluster	Type	
	nonspam	spam
1	2120	1798
2	668	15

Table 6: Clustering with PAM (z-score with PCA)

Cluster	Type	
	nonspam	spam
1	796	1558
2	1376	250
3	616	5

Table 7: Clustering with PAM (log, no PCA)

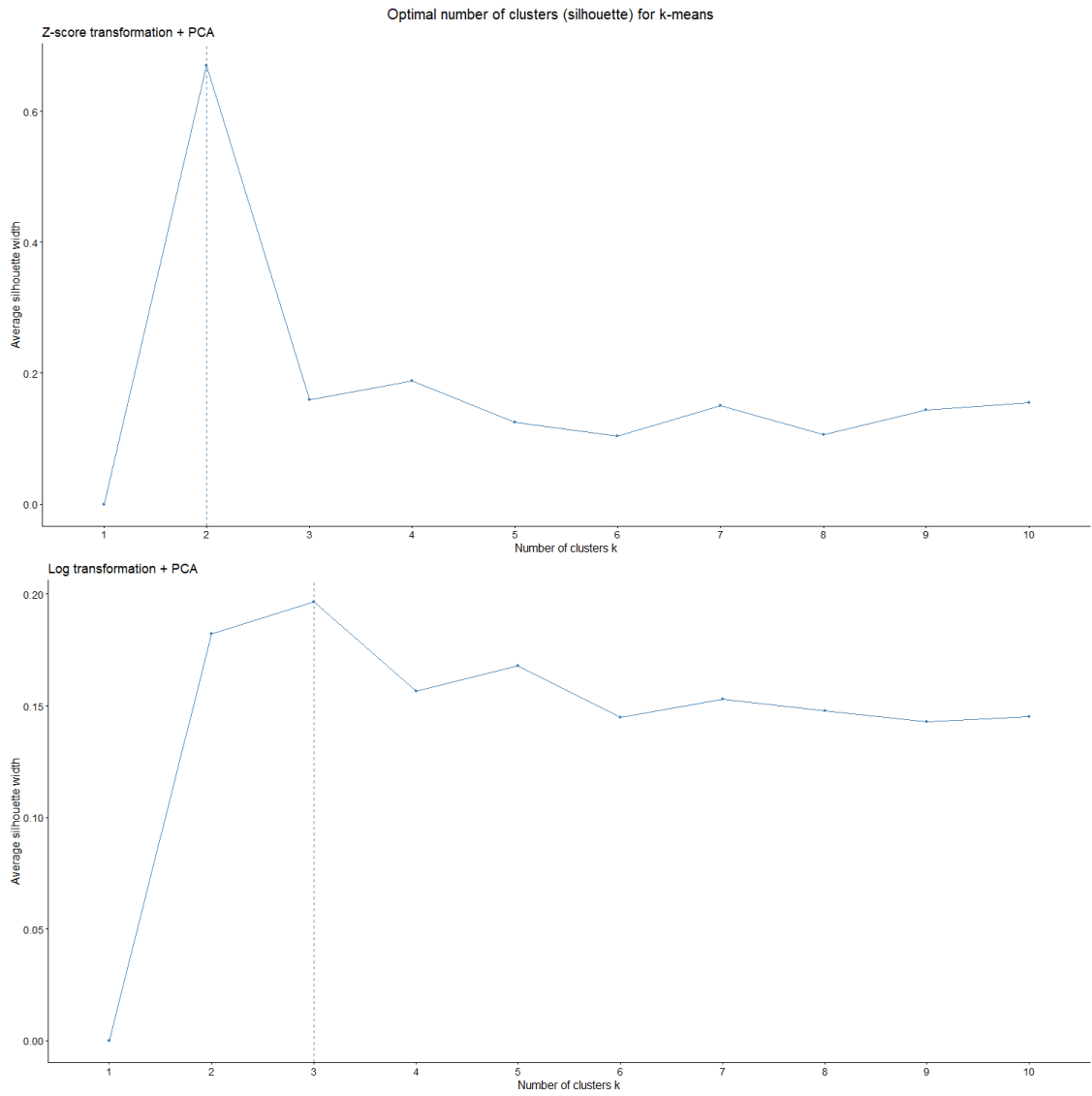


Figure 8: Number of clusters for k-means (with PCA)

Cluster	Type	
	nonspam	spam
1	203	1438
2	2585	375

Table 8: Clustering with PAM (log with PCA)

Cluster	Type	
	nonspam	spam
1	568	1445
2	2175	368
3	45	0

Table 9: Clustering with AGNES (z-score, no PCA)

Cluster	Type	
	nonspam	spam
1	2450	685
2	302	1128
3	36	0

Table 10: Clustering with AGNES (z-score with PCA)

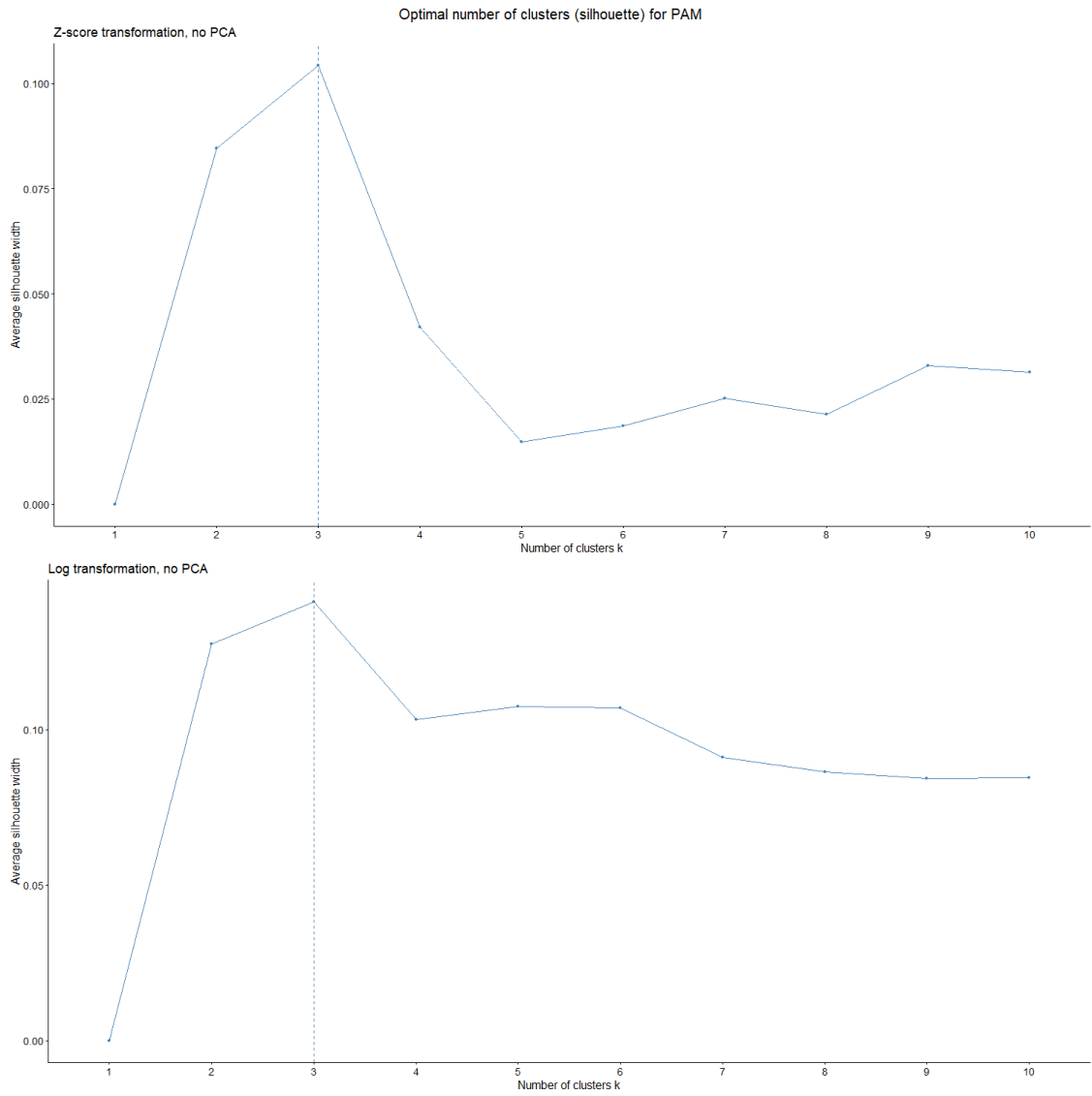


Figure 9: Number of clusters for PAM (no PCA)

Cluster	Type	
	nonspam	spam
1	117	1322
2	1672	395
3	999	96

Table 11: Clustering with AGNES (log, no PCA)

Cluster	Type	
	nonspam	spam
1	196	1436
2	1765	367
3	827	10

Table 12: Clustering with AGNES (log with PCA)

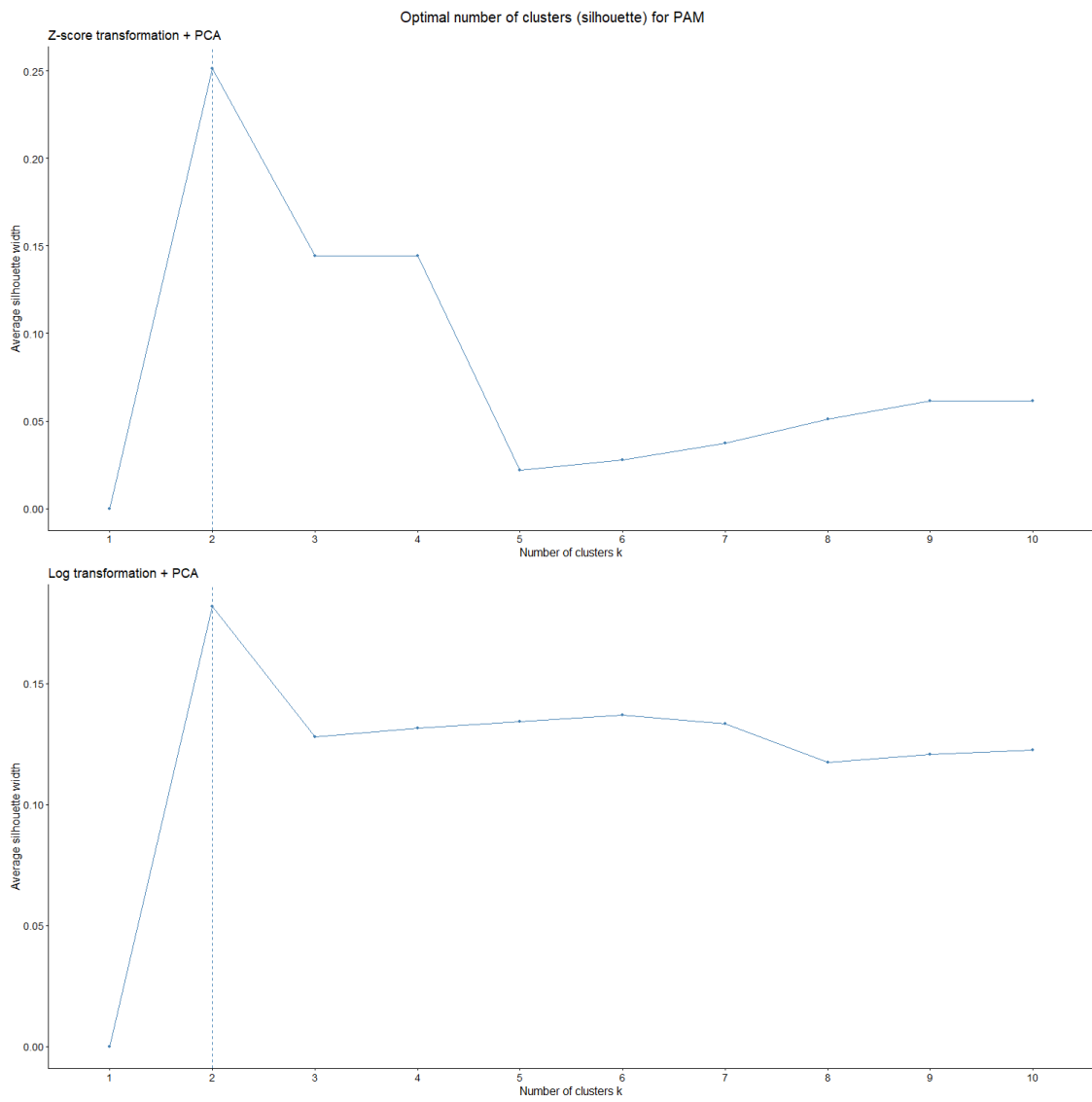


Figure 10: Number of clusters for PAM (with PCA)

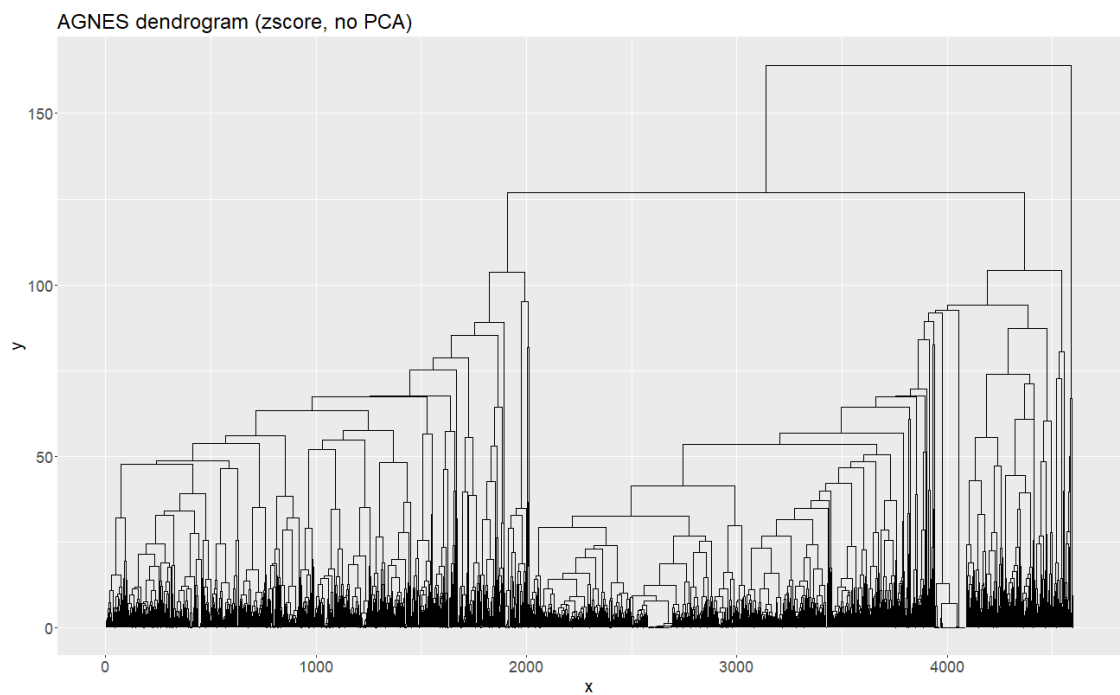


Figure 11: Number of clusters for AGNES (no PCA)

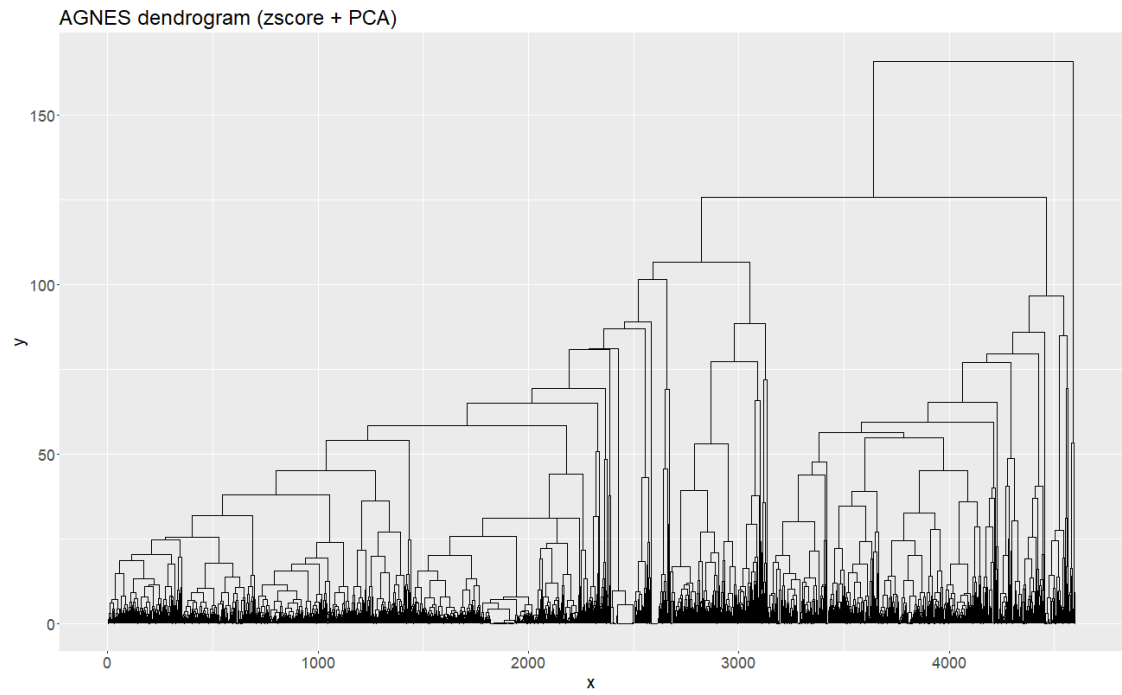


Figure 12: Number of clusters for AGNES (with PCA)

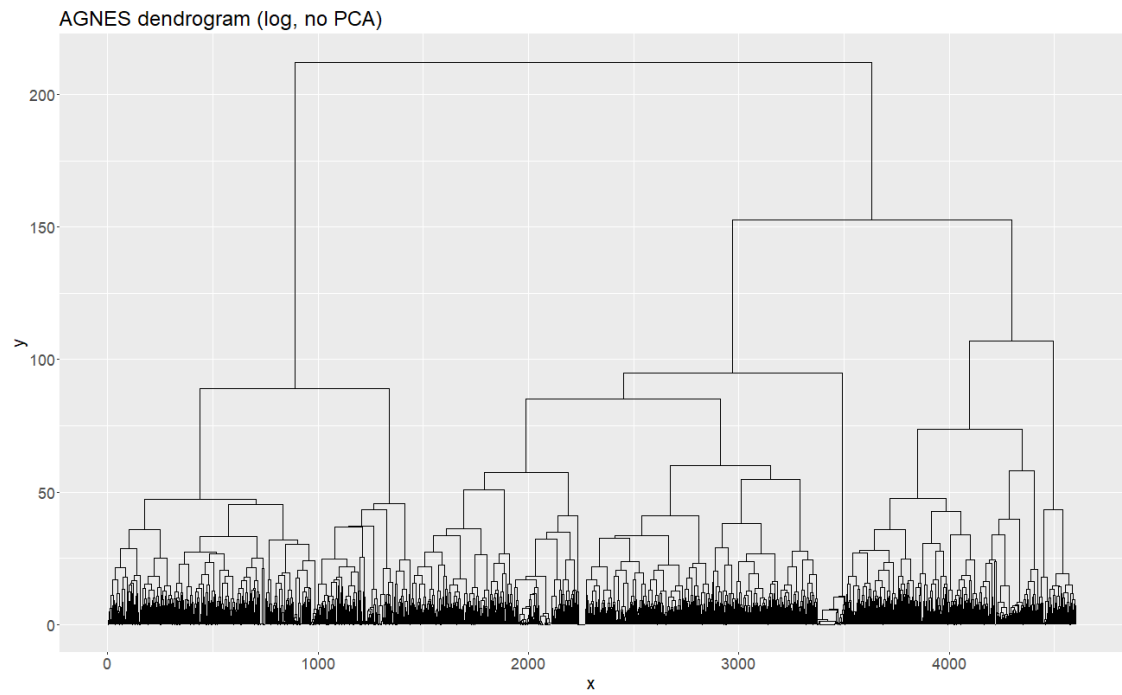


Figure 13: Number of clusters for AGNES (no PCA)

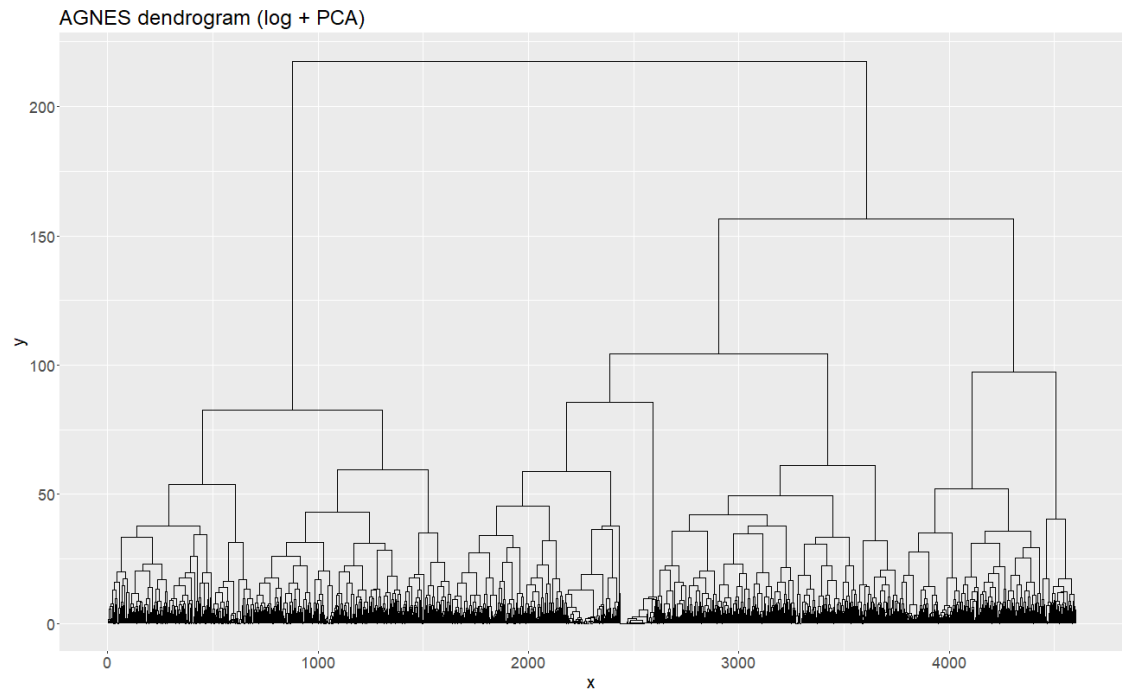


Figure 14: Number of clusters for AGNES (with PCA)

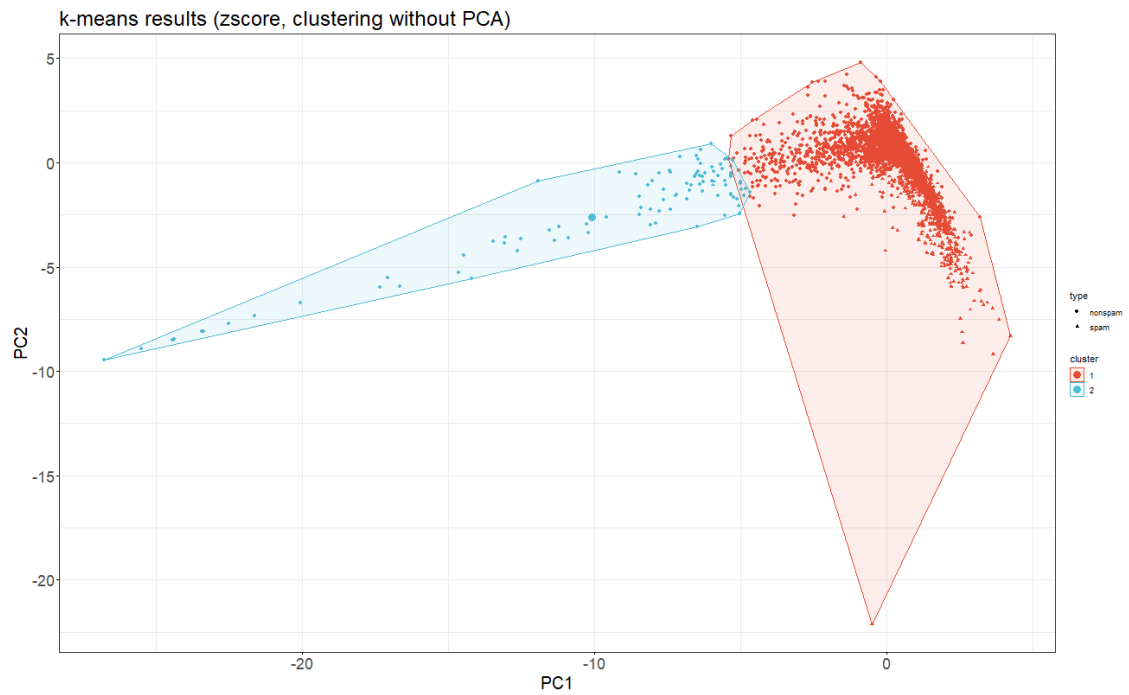


Figure 15: Clustering with k-means (z-score, no PCA)

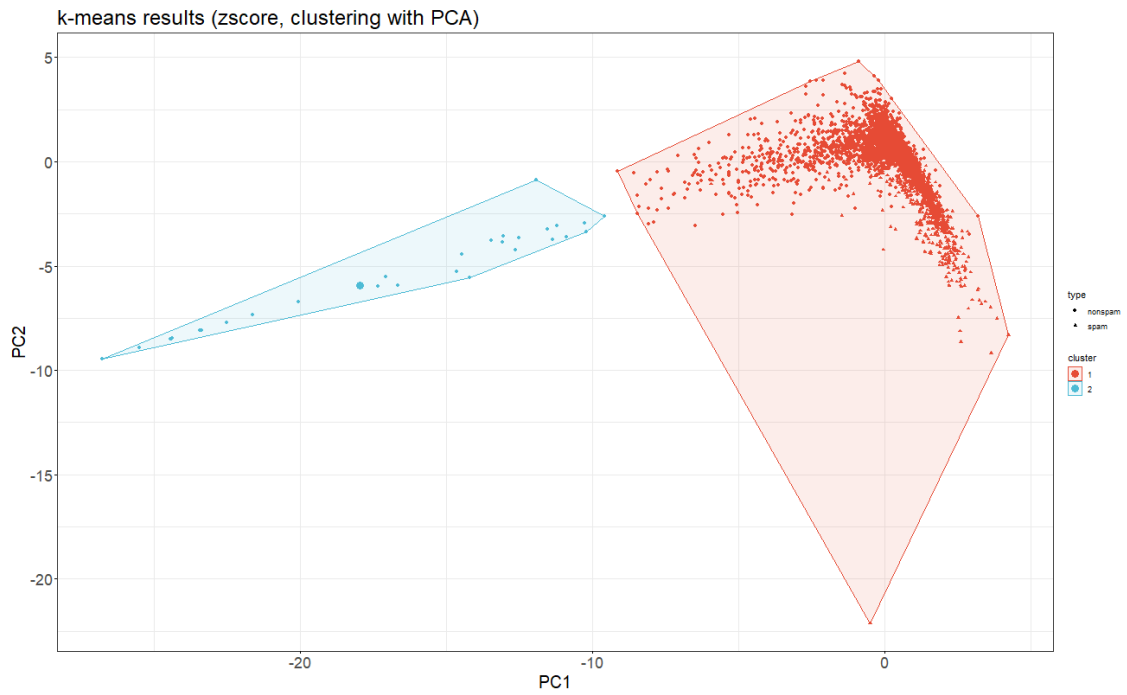


Figure 16: Clustering with k-means (z-score with PCA)

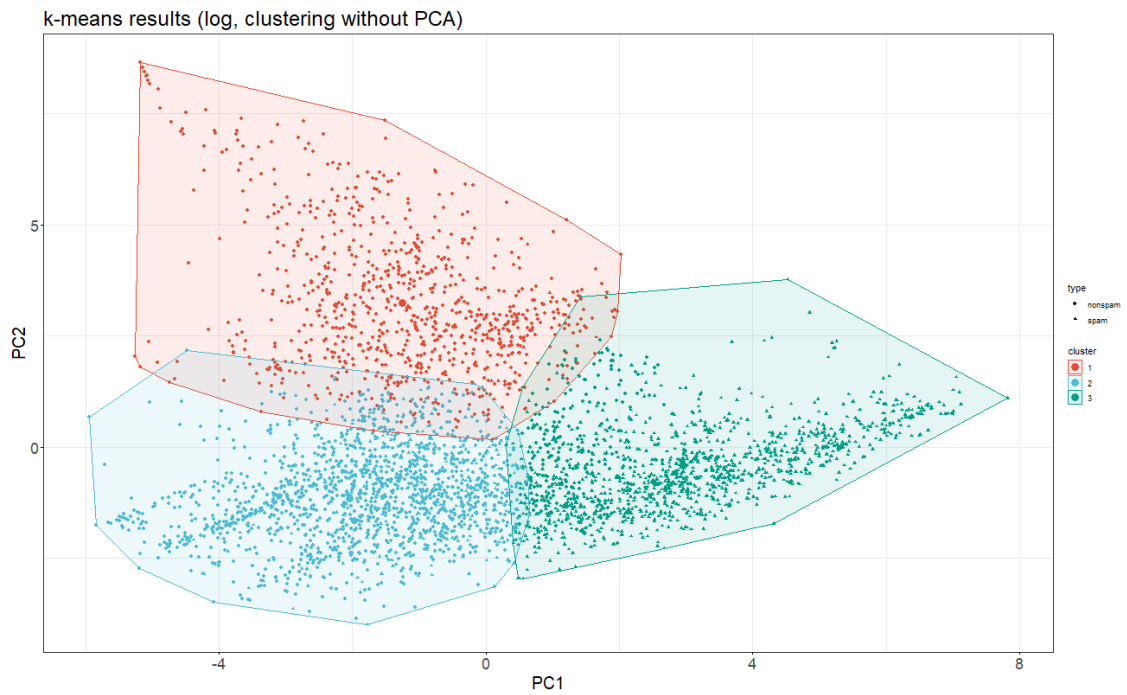


Figure 17: Clustering with k-means (log, no PCA)

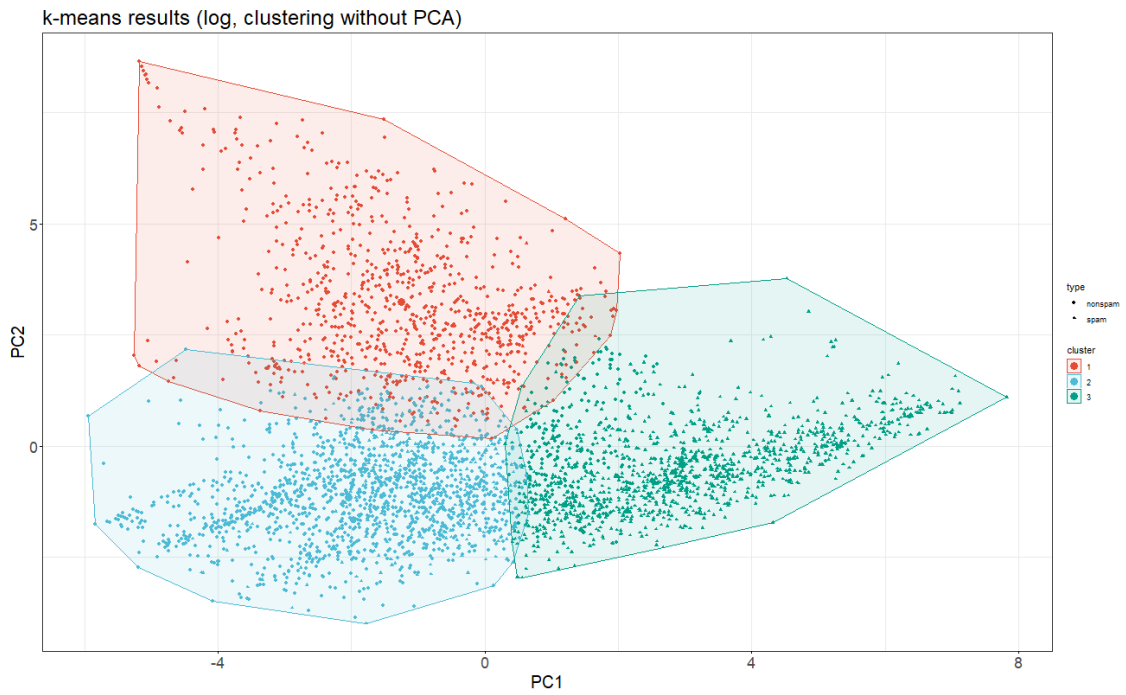


Figure 18: Clustering with k-means (log with PCA)

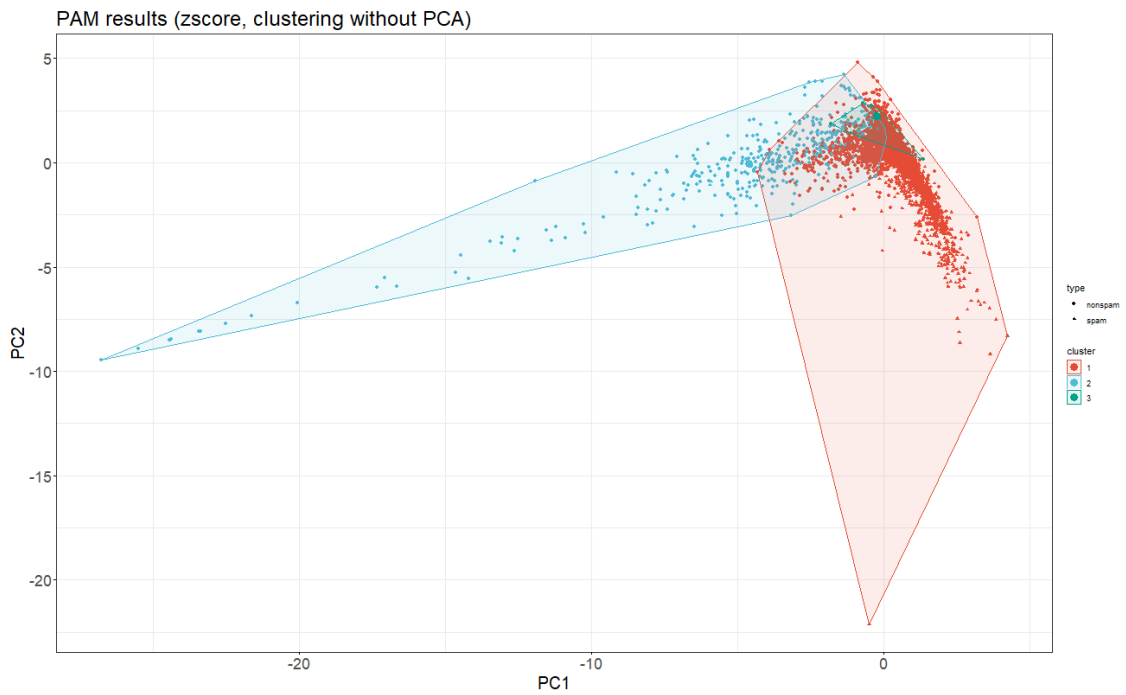


Figure 19: Clustering with PAM (z-score, no PCA)

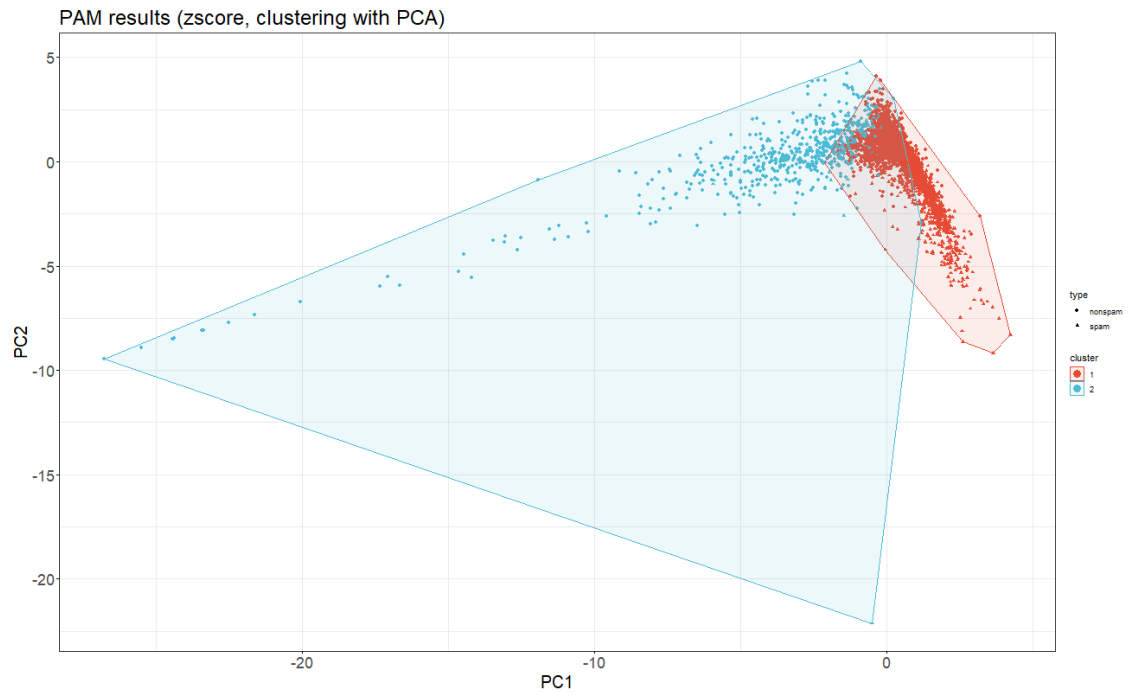


Figure 20: Clustering with PAM (z-score with PCA)

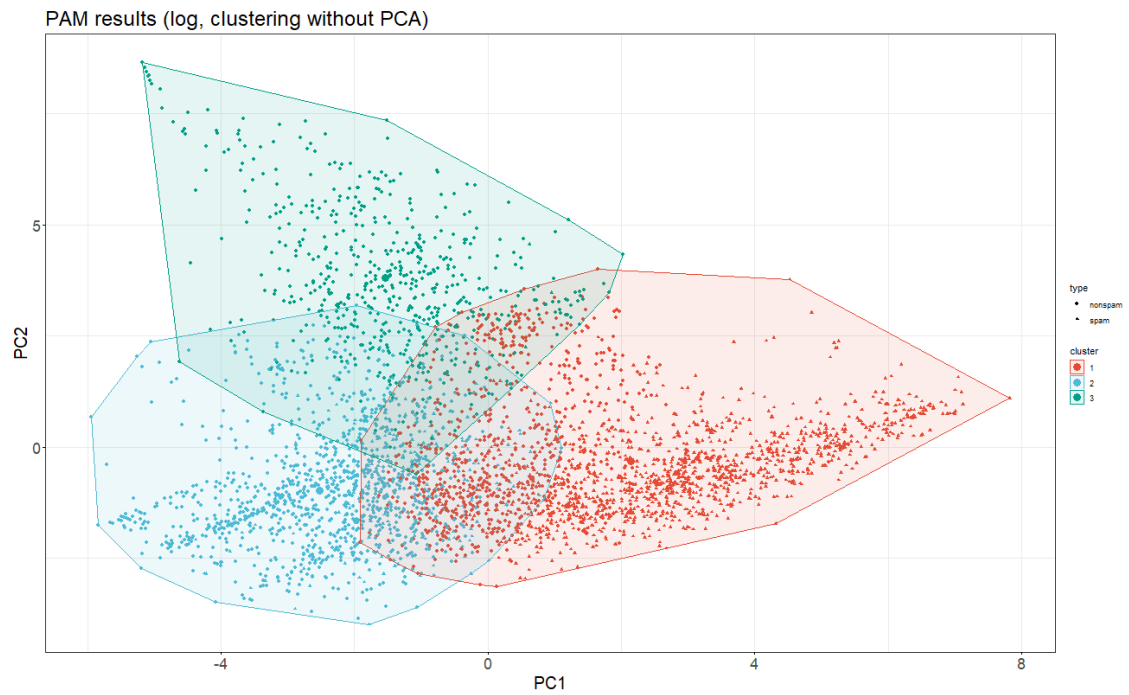


Figure 21: Clustering with PAM (log, no PCA)

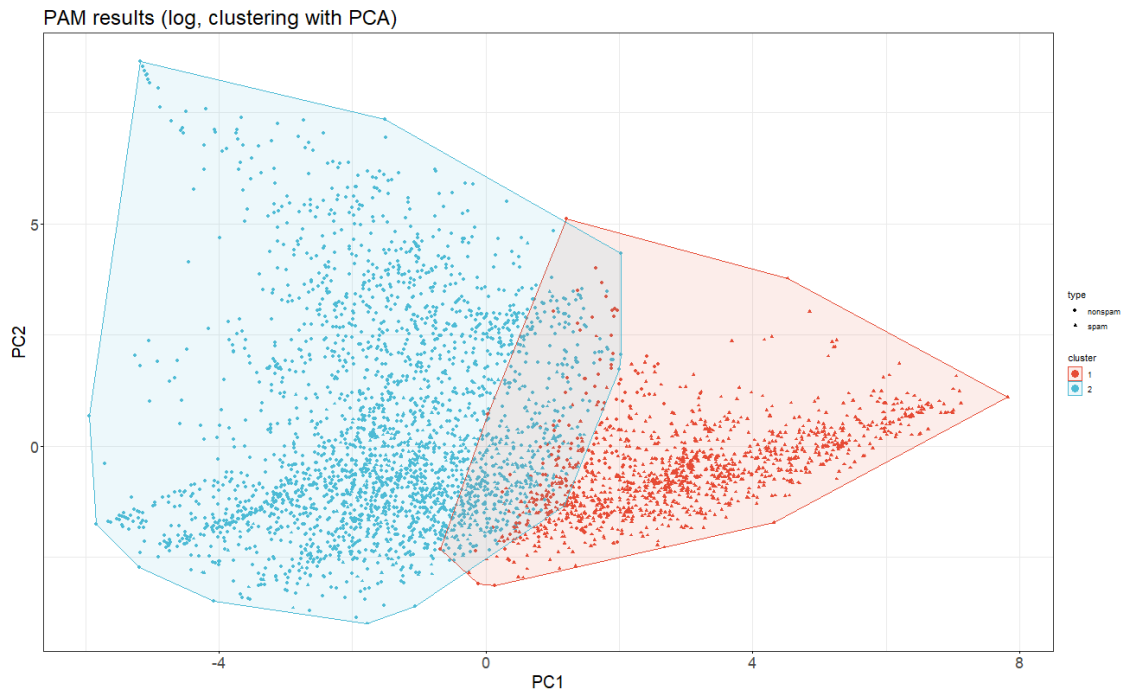


Figure 22: Clustering with PAM (log with PCA)

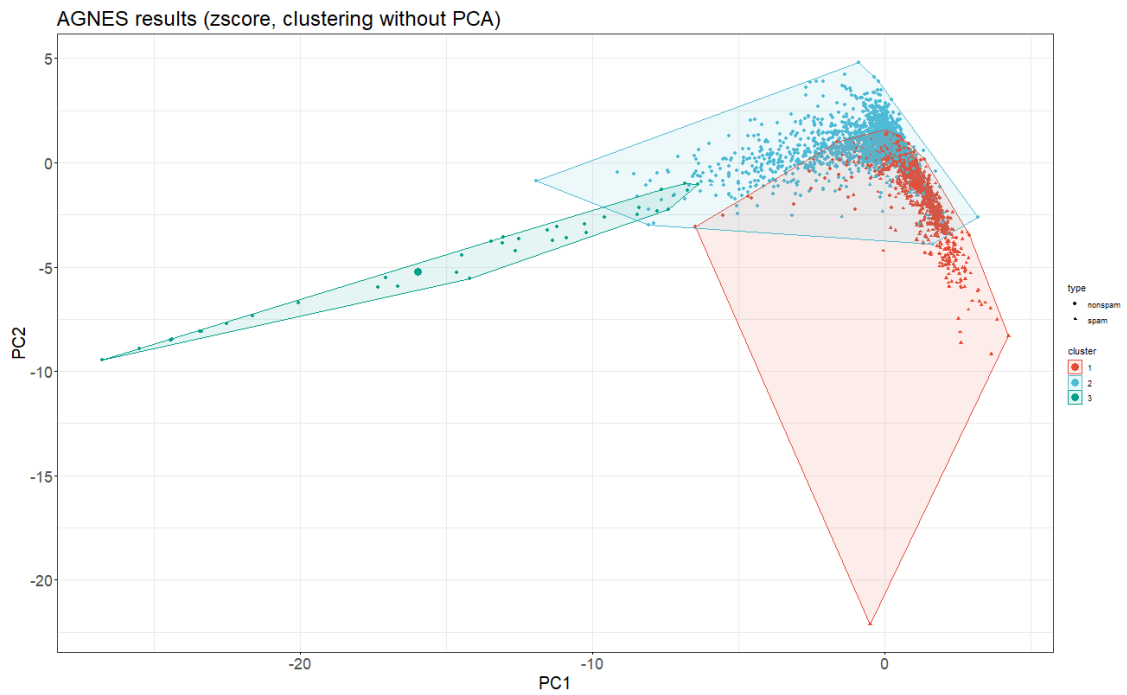


Figure 23: Clustering with AGNES (z-score, no PCA)

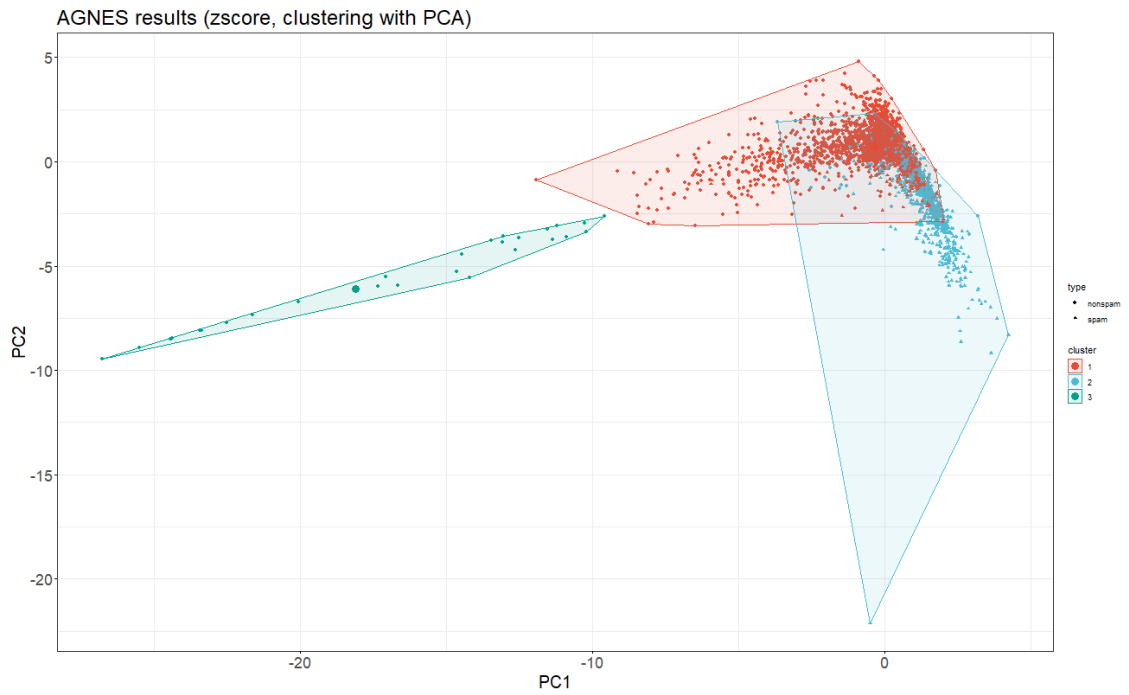


Figure 24: Clustering with AGNES (z-score with PCA)

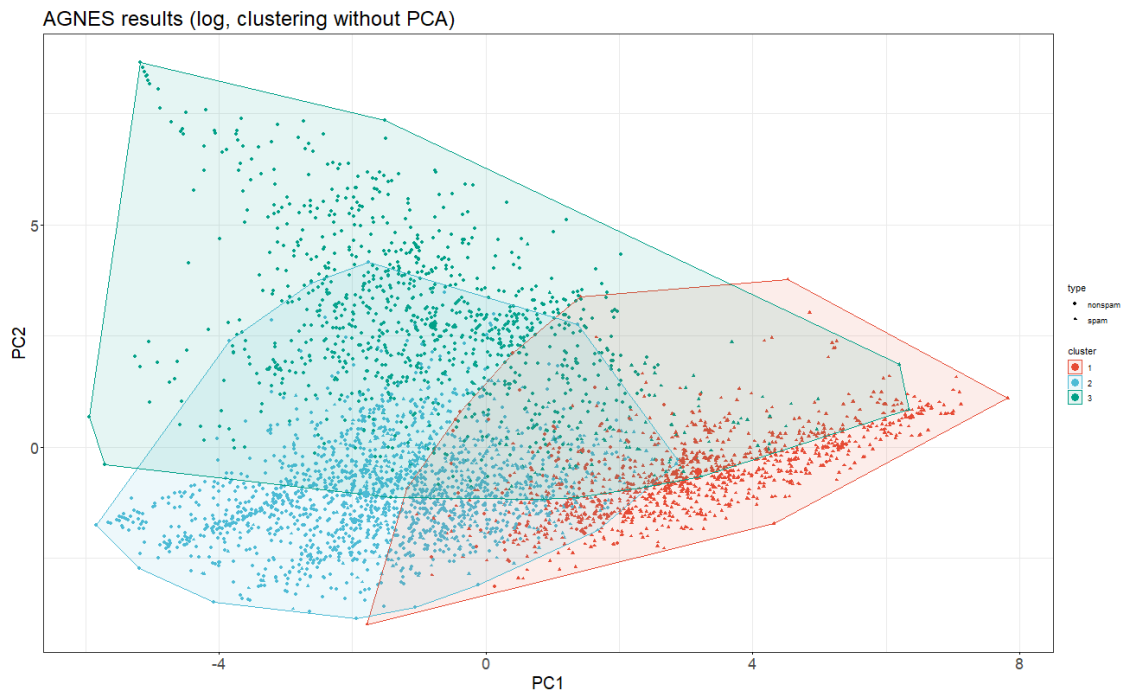


Figure 25: Clustering with AGNES (log, no PCA)

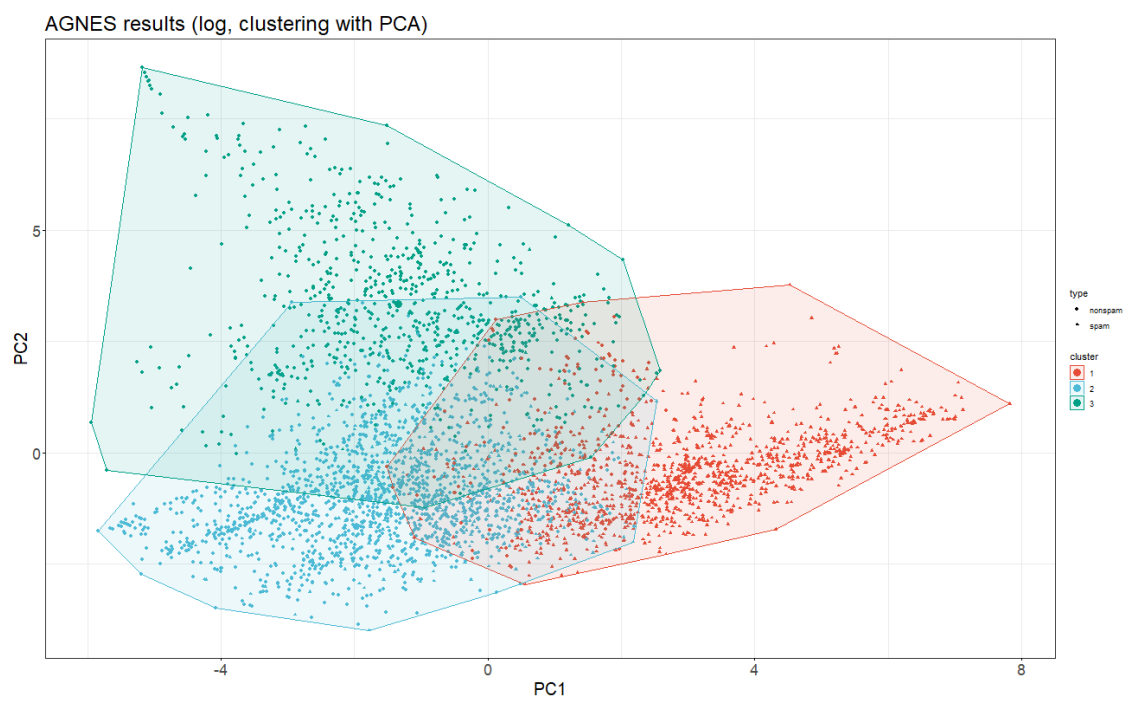


Figure 26: Clustering with AGNES (log with PCA)