

Comparison of Classification and Clustering Algorithms on Glass Dataset Using R

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```
library(caret)

## Loading required package: lattice
## Loading required package: ggplot2
library(mclust)

## Package 'mclust' version 5.4.1
## Type 'citation("mclust")' for citing this R package in publications.
library(fpc)
library(cluster)
library(clusteval)
library(factoextra)

## Welcome! Related Books: `Practical Guide To Cluster Analysis in R` at https://goo.gl/13EFCZ
library(ggplot2)
library(kmed)
library(mlbench)
```

Loading Glass Dataset

```
# attach the Glass Identification dataset to the environment
data("Glass")
# rename the dataset
dataset <- Glass
```

Partitioning Data for Validation

```
# create a list of 80% of the rows in the original dataset we can use for training
validation_index <- createDataPartition(dataset$Type, p=0.80, list=FALSE)
# select 20% of the data for validation
validation <- dataset[-validation_index,]
# use the remaining 80% of data to training and testing the models
dataset <- dataset[validation_index,]
```

Getting Insights from Data

```
# dimensions of dataset
dim(dataset)

## [1] 174 10
```

```
# list types for each attribute
sapply(dataset, class)
```

```
##           RI           Na           Mg           Al           Si           K           Ca
## "numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
##           Ba           Fe           Type
## "numeric" "numeric" "factor"
```

```
# take a peek at the first 6 rows of the data
head(dataset)
```

```
##           RI      Na      Mg      Al      Si      K      Ca      Ba      Fe      Type
## 1 1.52101 13.64 4.49 1.10 71.78 0.06 8.75 0 0.00 1
## 3 1.51618 13.53 3.55 1.54 72.99 0.39 7.78 0 0.00 1
## 4 1.51766 13.21 3.69 1.29 72.61 0.57 8.22 0 0.00 1
## 5 1.51742 13.27 3.62 1.24 73.08 0.55 8.07 0 0.00 1
## 6 1.51596 12.79 3.61 1.62 72.97 0.64 8.07 0 0.26 1
## 7 1.51743 13.30 3.60 1.14 73.09 0.58 8.17 0 0.00 1
```

```
# list the levels for the class
levels(dataset$Type)
```

```
## [1] "1" "2" "3" "5" "6" "7"
```

```
# summarize the class distribution
percentage <- prop.table(table(dataset$Type)) * 100
cbind(freq=table(dataset$Type), percentage=percentage)
```

```
##      freq percentage
## 1      56 32.183908
## 2      61 35.057471
## 3      14  8.045977
## 5      11  6.321839
## 6       8  4.597701
## 7      24 13.793103
```

```
# summarize attribute distributions
summary(dataset)
```

```
##           RI           Na           Mg           Al
## Min.      :1.511   Min.      :10.73   Min.      :0.000   Min.      :0.340
## 1st Qu.:1.517   1st Qu.:12.93   1st Qu.:2.115   1st Qu.:1.212
## Median :1.518   Median :13.30   Median :3.470   Median :1.390
## Mean      :1.518   Mean      :13.42   Mean      :2.652   Mean      :1.467
## 3rd Qu.:1.519   3rd Qu.:13.88   3rd Qu.:3.598   3rd Qu.:1.630
## Max.      :1.534   Max.      :17.38   Max.      :4.490   Max.      :3.500
##           Si           K           Ca           Ba
## Min.      :69.81   Min.      :0.0000   Min.      : 5.430   Min.      :0.0000
## 1st Qu.:72.33   1st Qu.:0.1325   1st Qu.: 8.240   1st Qu.:0.0000
## Median :72.79   Median :0.5550   Median : 8.605   Median :0.0000
## Mean      :72.63   Mean      :0.5072   Mean      : 8.952   Mean      :0.1835
## 3rd Qu.:73.08   3rd Qu.:0.6075   3rd Qu.: 9.172   3rd Qu.:0.0000
## Max.      :75.41   Max.      :6.2100   Max.      :16.190   Max.      :3.1500
##           Fe           Type
## Min.      :0.00000   1:56
## 1st Qu.:0.00000   2:61
## Median :0.00000   3:14
```

```
## Mean :0.05557 5:11
## 3rd Qu.:0.10000 6: 8
## Max. :0.37000 7:24
```

```
# split input and output
```

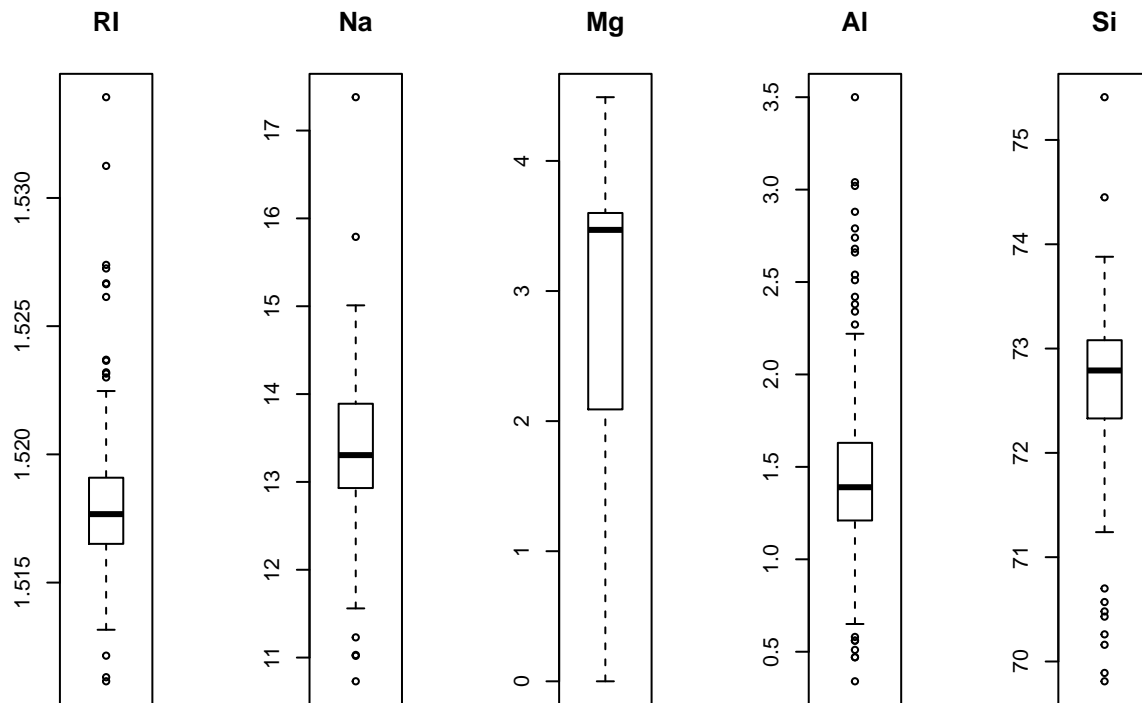
```
x <- dataset[,1:9]
```

```
y <- dataset[,10]
```

```
# boxplot for each attribute on one image
```

```
par(mfrow=c(1,5))
```

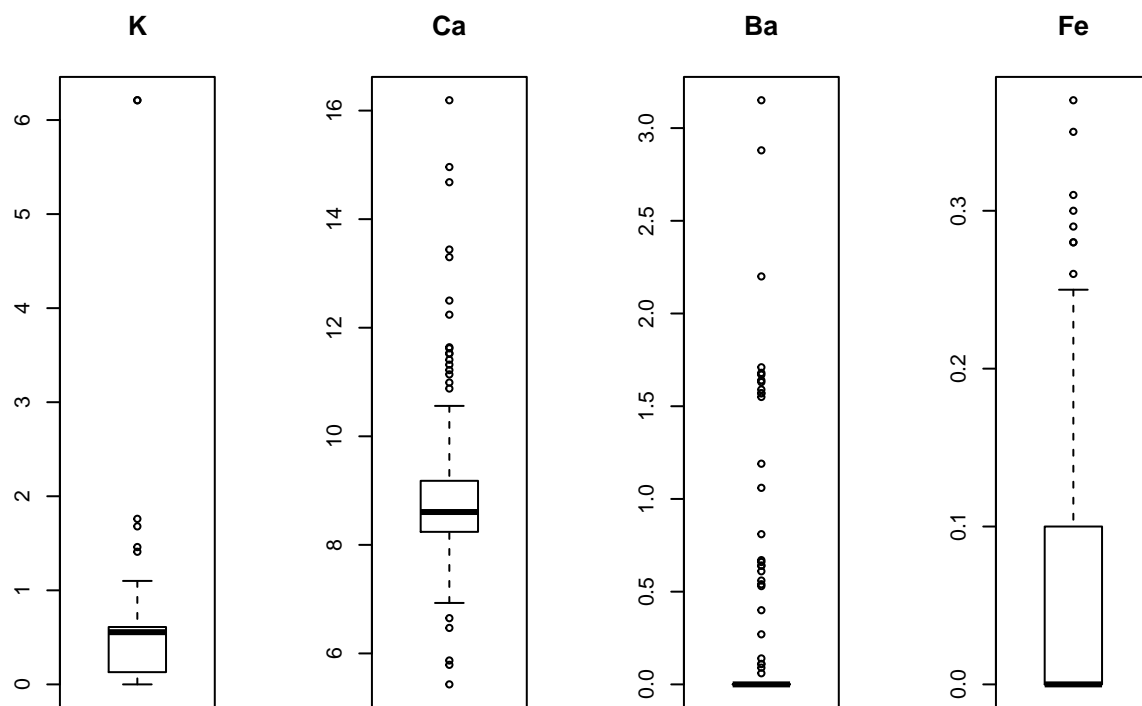
```
for(i in 1:5) {
  boxplot(x[,i], main=names(Glass)[i])
}
```



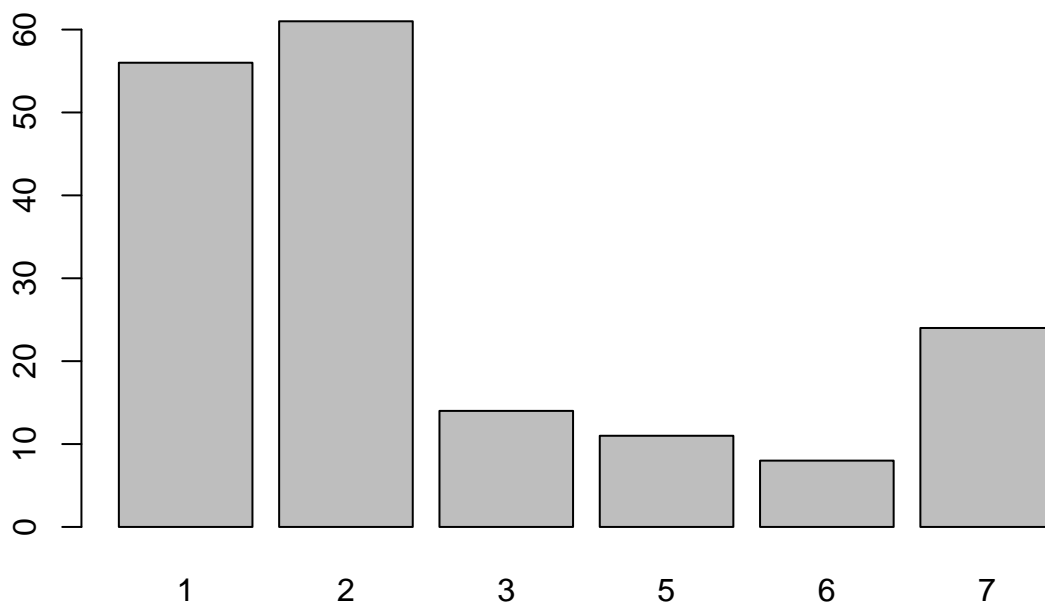
```
# boxplot for each attribute on one image
```

```
par(mfrow=c(1,4))
```

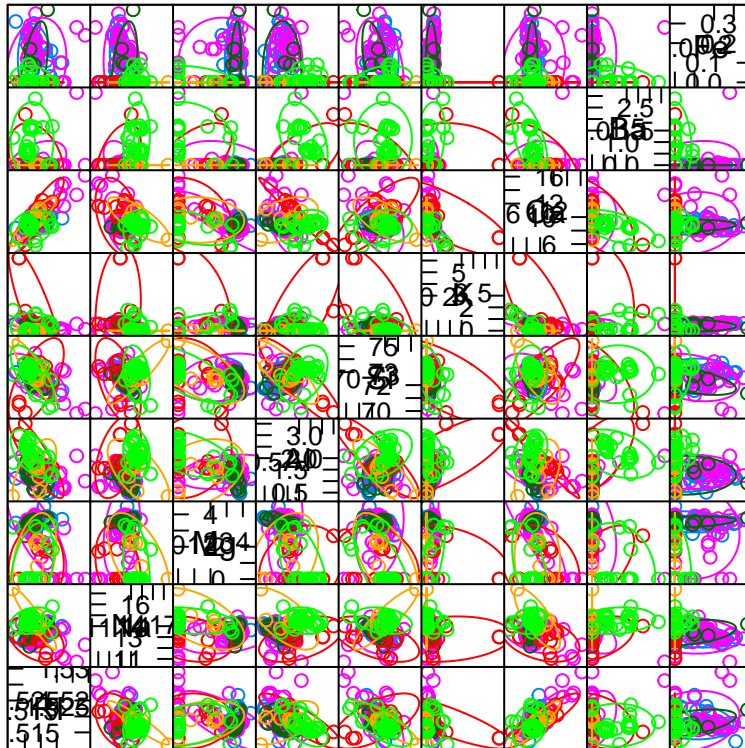
```
for(i in 6:9) {
  boxplot(x[,i], main=names(Glass)[i])
}
```



```
# barplot for class breakdown
plot(y)
```

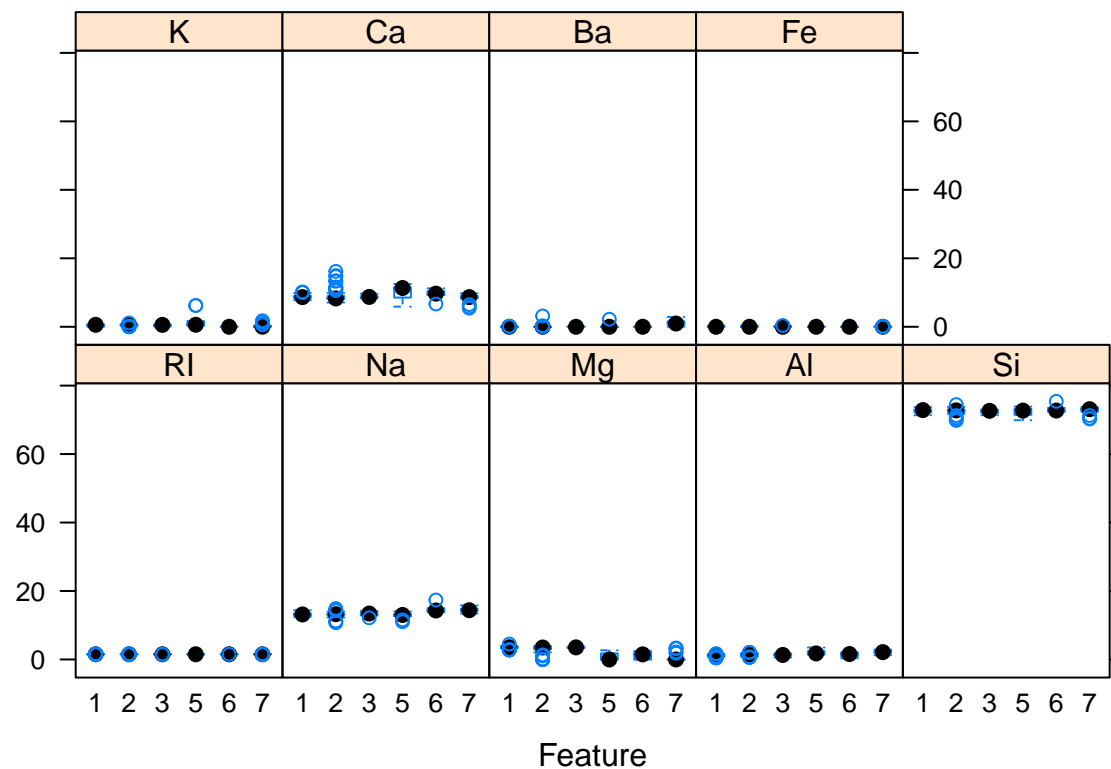


```
# scatterplot matrix
featurePlot(x=x, y=y, plot="ellipse")
```

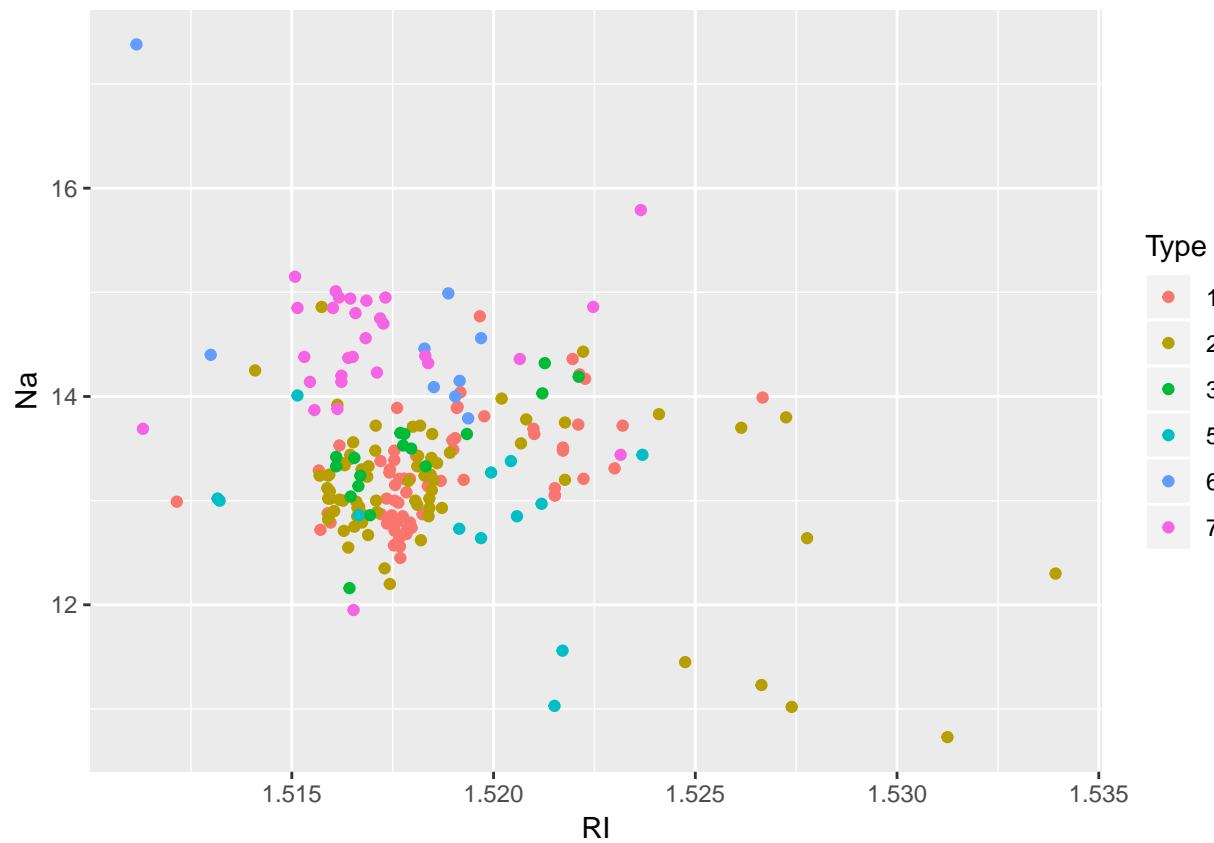


Scatter Plot Matrix

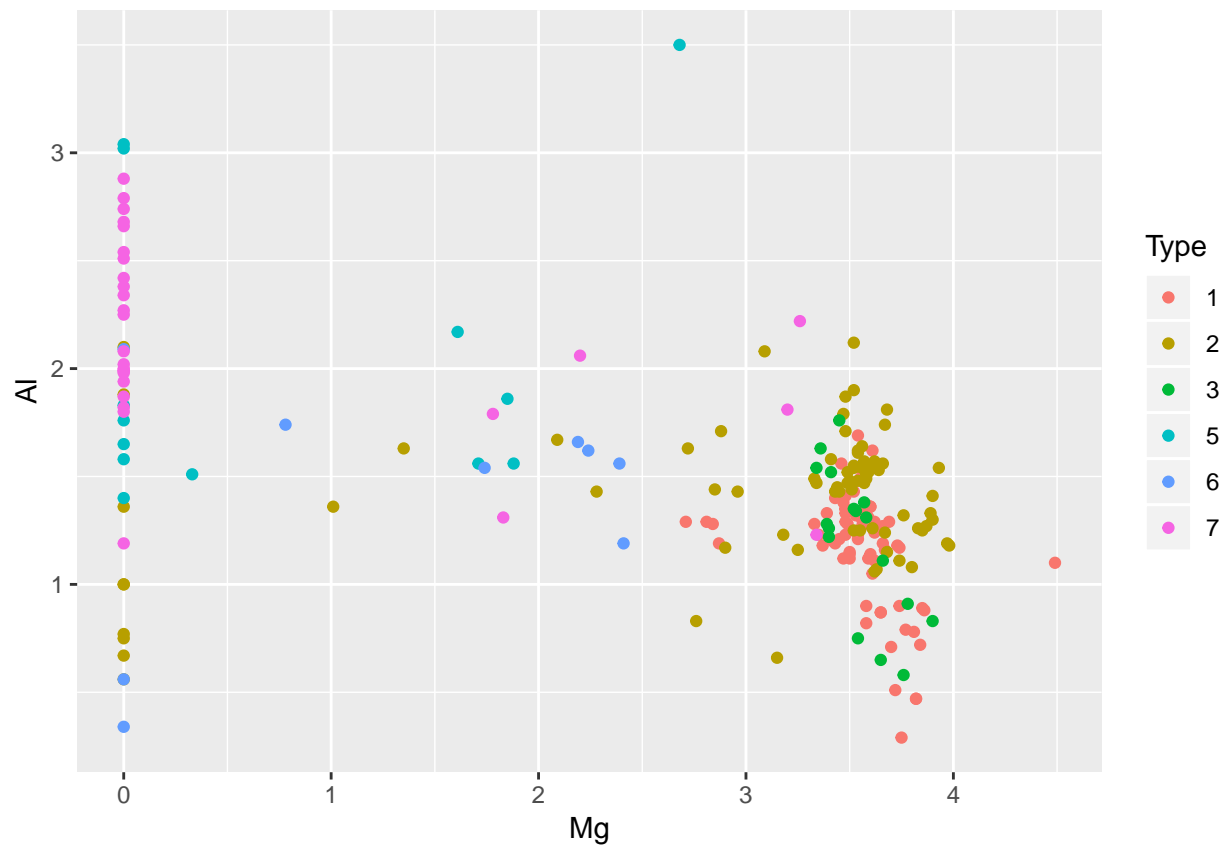
```
# box and whisker plots for each attribute
featurePlot(x=x, y=y, plot="box")
```



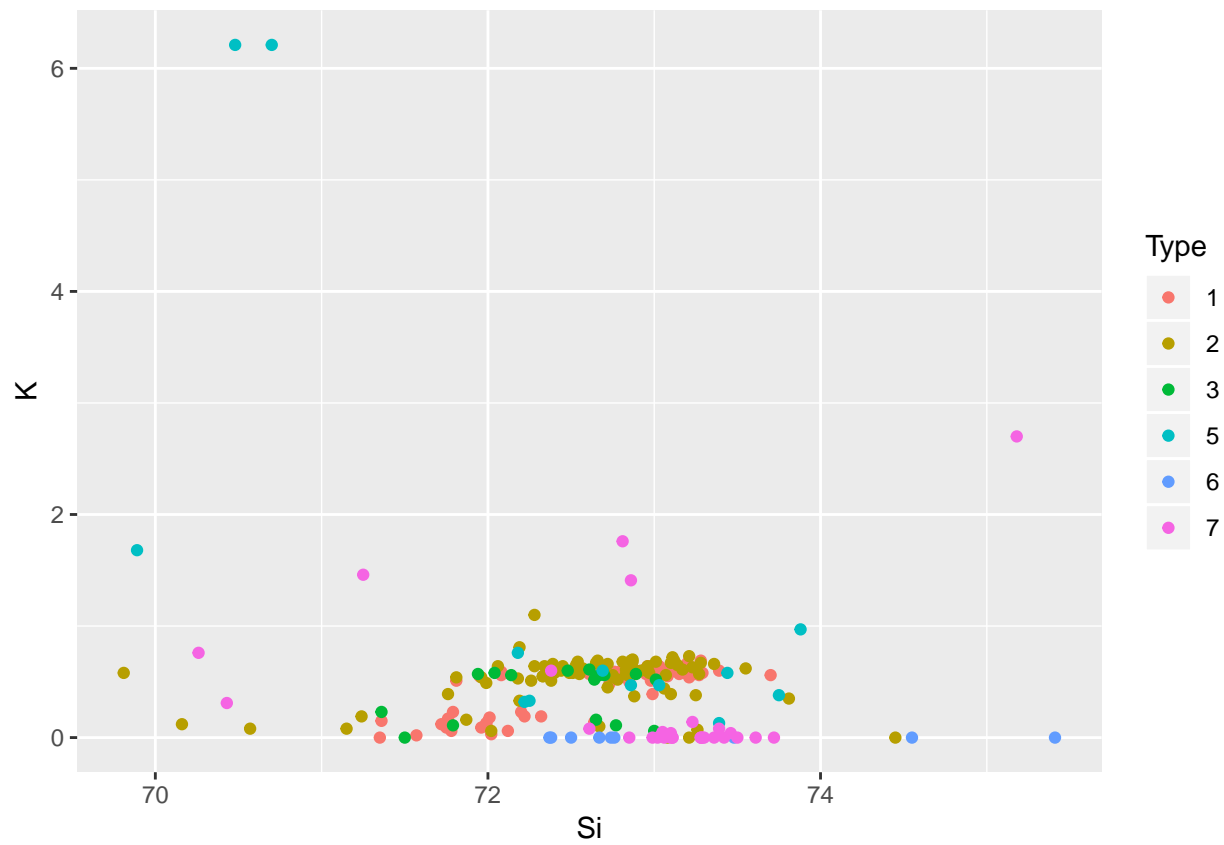
```
ggplot(Glass, aes(RI,Na, color = Type)) + geom_point()
```



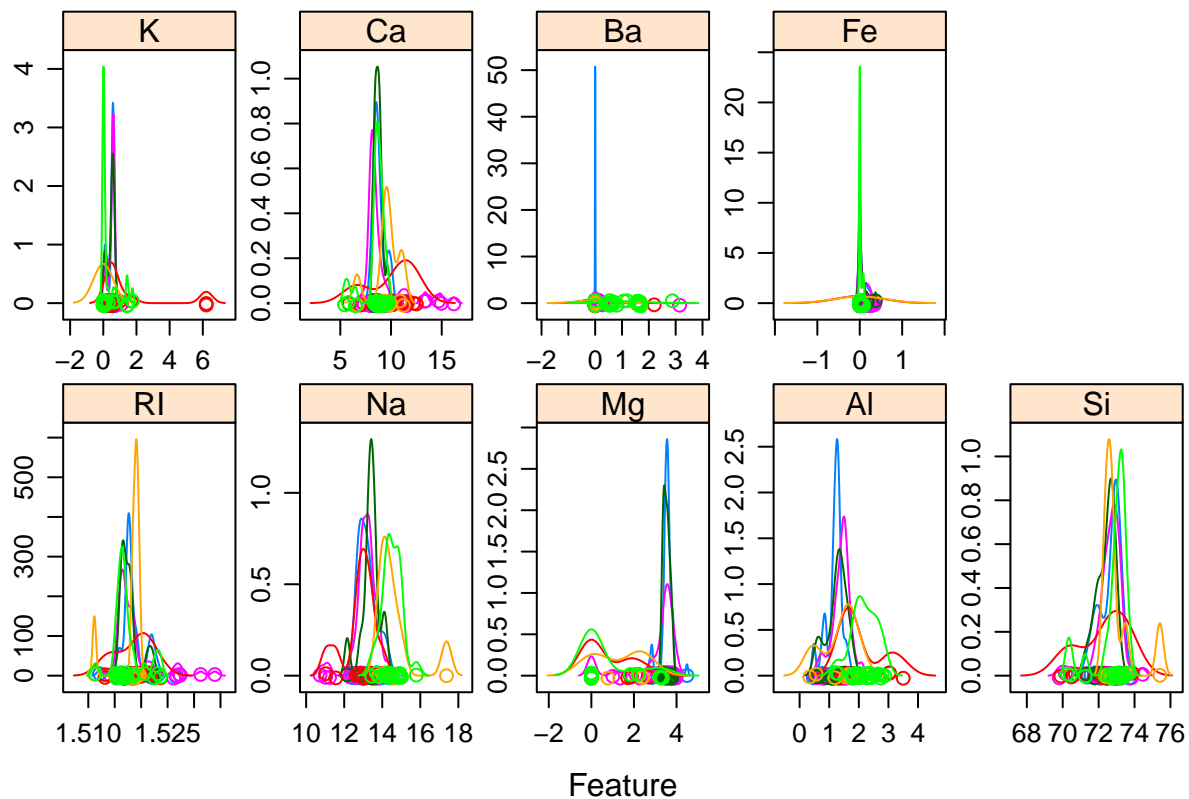
```
ggplot(Glass, aes(Mg,Al, color = Type)) + geom_point()
```



```
ggplot(Glass, aes(Si,K, color = Type)) + geom_point()
```



```
# density plots for each attribute by class value
scales <- list(x=list(relation="free"), y=list(relation="free"))
featurePlot(x=x, y=y, plot="density", scales=scales)
```

Applying Classification Algorithms

```
# Run algorithms using 10-fold cross validation
control <- trainControl(method="cv", number=10)
metric <- "Accuracy"
```

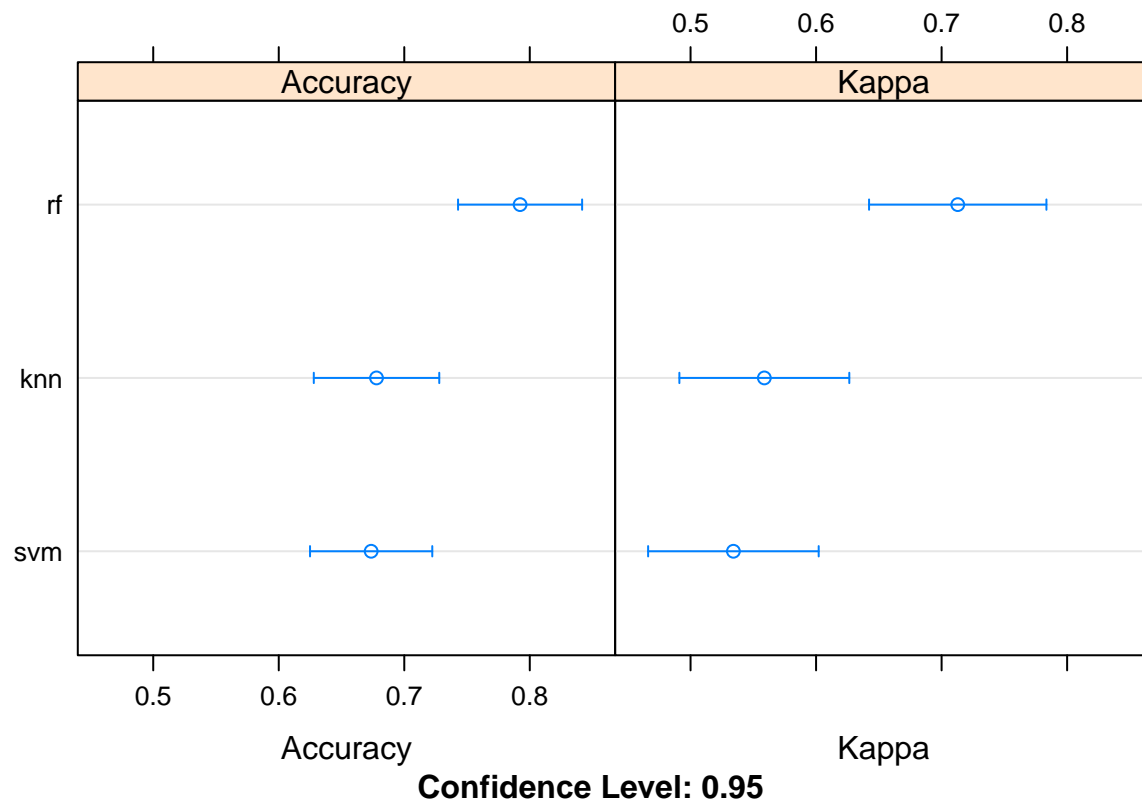
```
# kNN
set.seed(7)
fit.knn <- train(Type~., data=dataset, method="knn", metric=metric, trControl=control)
# SVM
set.seed(7)
fit.svm <- train(Type~., data=dataset, method="svmRadial", metric=metric, trControl=control)
# Random Forest
set.seed(7)
fit.rf <- train(Type~., data=dataset, method="rf", metric=metric, trControl=control)
```

Comparison of the Classification Algorithms

```
# summarize accuracy of models
results <- resamples(list(knn=fit.knn, svm=fit.svm, rf=fit.rf))
summary(results)
```

```
##
## Call:
## summary.resamples(object = results)
##
```

```
## Models: knn, svm, rf
## Number of resamples: 10
##
## Accuracy
##      Min.    1st Qu.    Median      Mean   3rd Qu.    Max. NA's
## knn 0.5789474 0.6305147 0.6764706 0.6779025 0.7331871 0.7777778    0
## svm 0.5882353 0.6315789 0.6672794 0.6736197 0.7012868 0.8235294    0
## rf  0.7058824 0.7291667 0.8009868 0.7922837 0.8374613 0.8888889    0
##
## Kappa
##      Min.    1st Qu.    Median      Mean   3rd Qu.    Max. NA's
## knn 0.4223301 0.4849092 0.5474906 0.5587690 0.6378071 0.7037037    0
## svm 0.4050000 0.4827855 0.5159344 0.5341319 0.5632360 0.7424242    0
## rf  0.5750000 0.6231361 0.7318722 0.7128649 0.7858289 0.8487395    0
# compare accuracy of models
dotplot(results)
```



Insights from the best model

```
# summarize Best Model
print(fit.rf)

## Random Forest
##
## 174 samples
## 9 predictors
## 6 classes: '1', '2', '3', '5', '6', '7'
```

```
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 157, 158, 155, 156, 158, 157, ...
## Resampling results across tuning parameters:
##
##   mtry  Accuracy   Kappa
##   2     0.7922837  0.7128649
##   5     0.7697411  0.6845109
##   9     0.7412001  0.6509035
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was mtry = 2.
# estimate skill of Random Forest on the validation dataset
predictions <- predict(fit.rf, validation)
confusionMatrix(predictions, validation$Type)

## Confusion Matrix and Statistics
##
##           Reference
## Prediction  1  2  3  5  6  7
##           1 14  3  2  0  0  0
##           2  0 11  1  1  0  1
##           3  0  0  0  0  0  0
##           5  0  1  0  1  0  0
##           6  0  0  0  0  1  0
##           7  0  0  0  0  0  4
##
## Overall Statistics
##
##           Accuracy : 0.775
##           95% CI : (0.6155, 0.8916)
##       No Information Rate : 0.375
##       P-Value [Acc > NIR] : 2.97e-07
##
##           Kappa : 0.6724
##   McNemar's Test P-Value : NA
##
## Statistics by Class:
##
##           Class: 1 Class: 2 Class: 3 Class: 5 Class: 6 Class: 7
## Sensitivity          1.0000   0.7333   0.000   0.5000   1.000   0.8000
## Specificity          0.8077   0.8800   1.000   0.9737   1.000   1.0000
## Pos Pred Value       0.7368   0.7857   NaN     0.5000   1.000   1.0000
## Neg Pred Value       1.0000   0.8462   0.925   0.9737   1.000   0.9722
## Prevalence           0.3500   0.3750   0.075   0.0500   0.025   0.1250
## Detection Rate       0.3500   0.2750   0.000   0.0250   0.025   0.1000
## Detection Prevalence 0.4750   0.3500   0.000   0.0500   0.025   0.1000
## Balanced Accuracy     0.9038   0.8067   0.500   0.7368   1.000   0.9000
```

Applying Clustering Algorithms

```
# K-means
set.seed(20)
fit.kmeans <- kmeans(Glass[, 1:9], 7, nstart = 20)
# Hierarchical Agglomerative
set.seed(20)
d <- dist(Glass[,1:9], method = "euclidean") # distance matrix
fit.ha <- hclust(d, method="ward.D")
# K-Medoids Clustering
num <- as.matrix(Glass[,1:9])
mrwdist <- distNumeric(num, method = "mrw")
fit.kmedoids <- fastkmed(mrwdist, ncluster = 7, iterate = 50)
```

Getting insights from Hierarchical Agglomerative Clustering

```
# Cut tree into 4 groups
sub_grp <- cutree(fit.ha, k = 7)

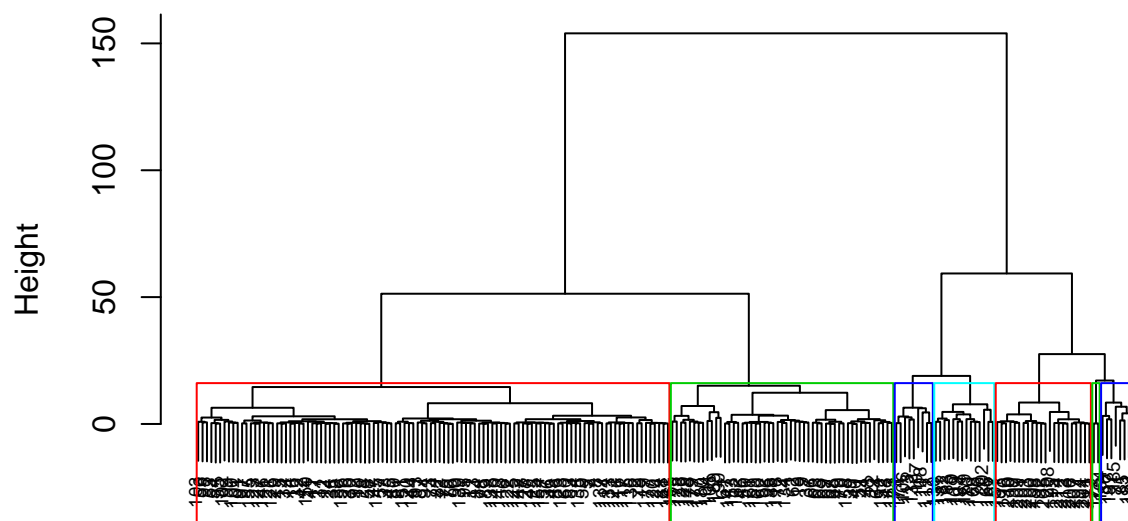
# Number of members in each cluster
table(sub_grp)

## sub_grp
##   1   2   3   4   5   6   7
## 51 108   8   9  14   2  22

## sub_grp

plot(fit.ha, cex = 0.6)
rect.hclust(fit.ha, k = 7, border = 2:5)
```

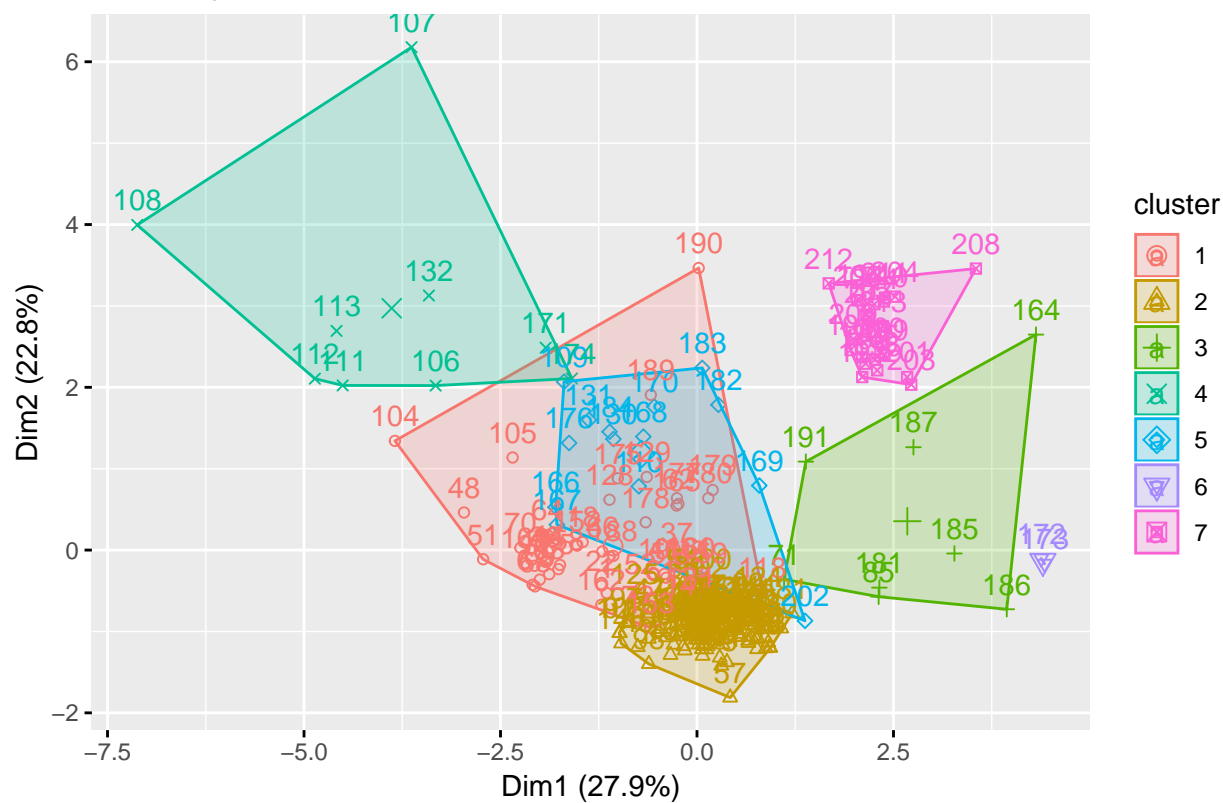
Cluster Dendrogram



d
hclust (*, "ward.D")

```
fviz_cluster(list(data = Glass[,1:9], cluster = sub_grp))
```

Cluster plot

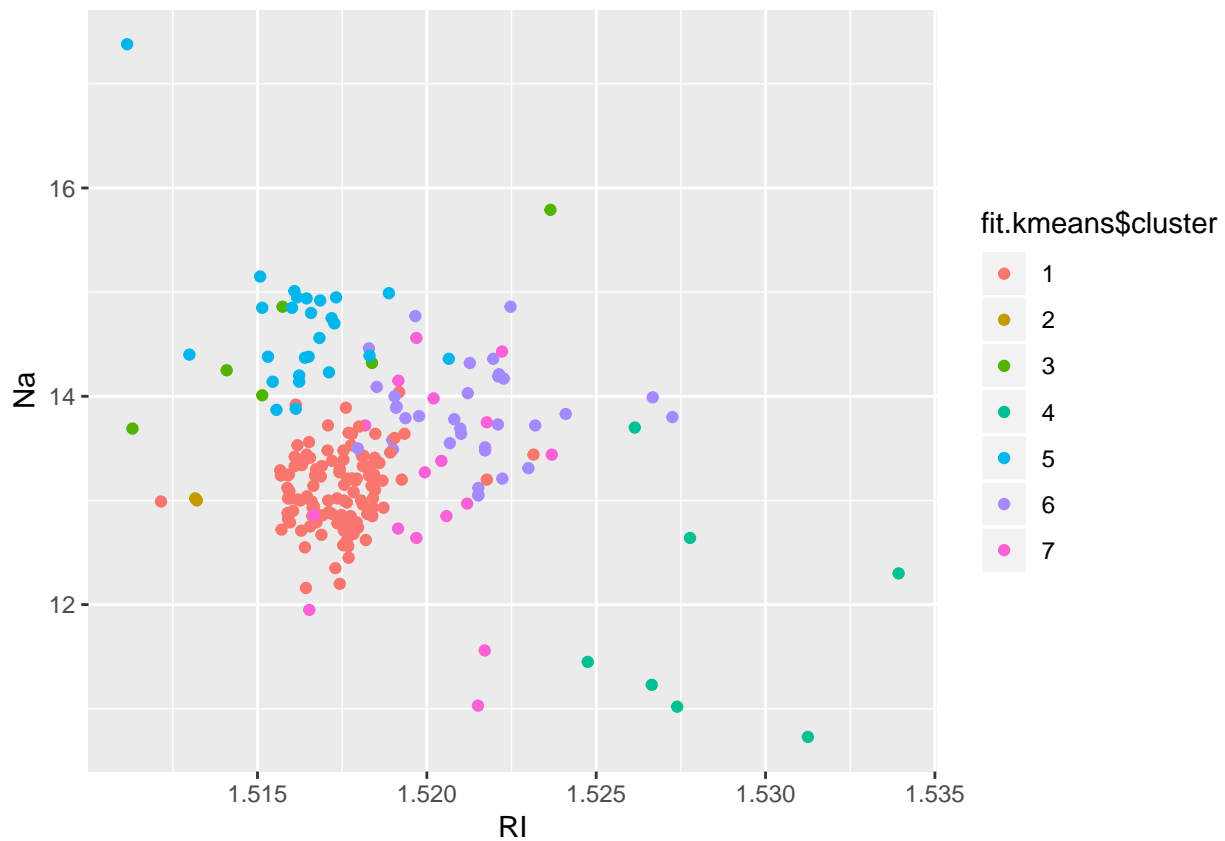


Getting insights from K-Means Clustering

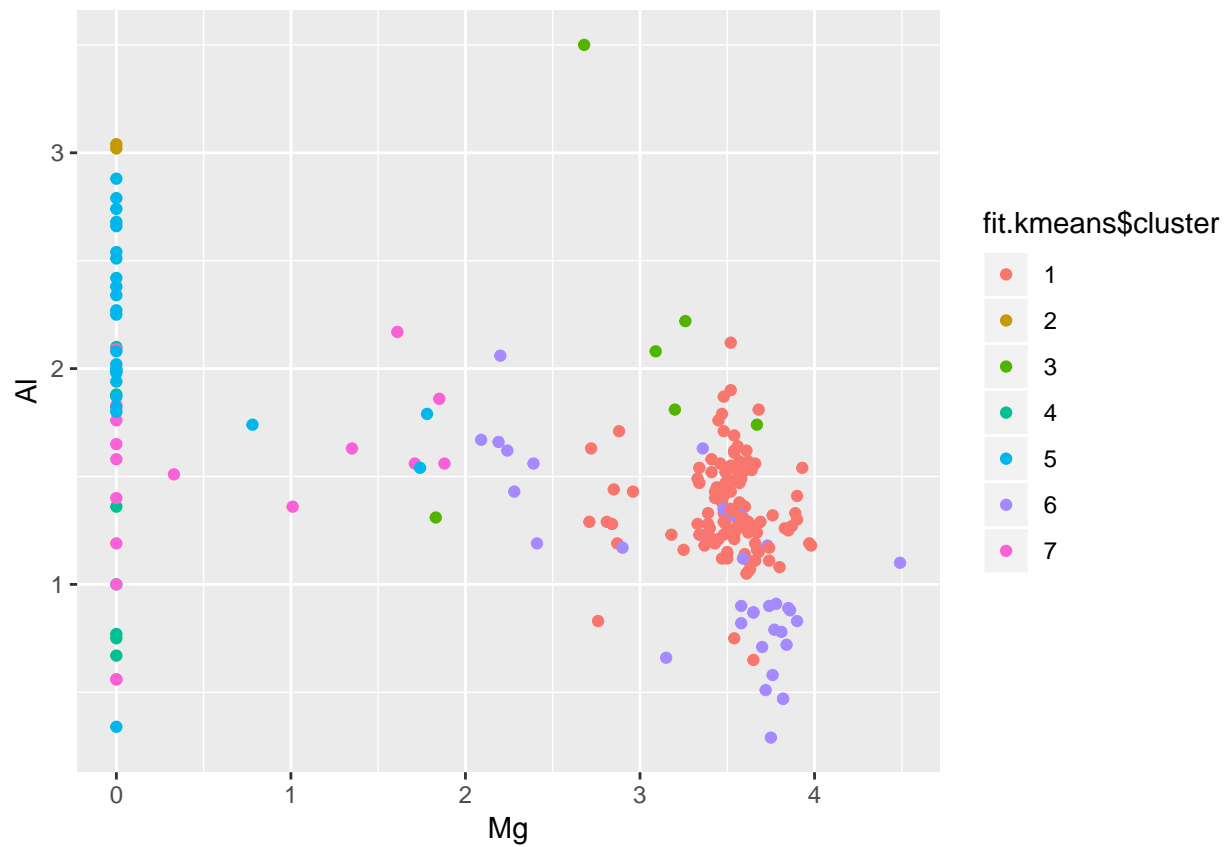
```
table(fit.kmeans$cluster, Glass$Type)
```

```
##  
##      1  2  3  5  6  7  
##  1 48 59 13  0  0  1  
##  2  0  0  0  2  0  0  
##  3  0  2  0  1  0  3  
##  4  0  7  0  0  0  0  
##  5  0  0  0  0  3 23  
##  6 22  4  4  0  4  1  
##  7  0  4  0 10  2  1
```

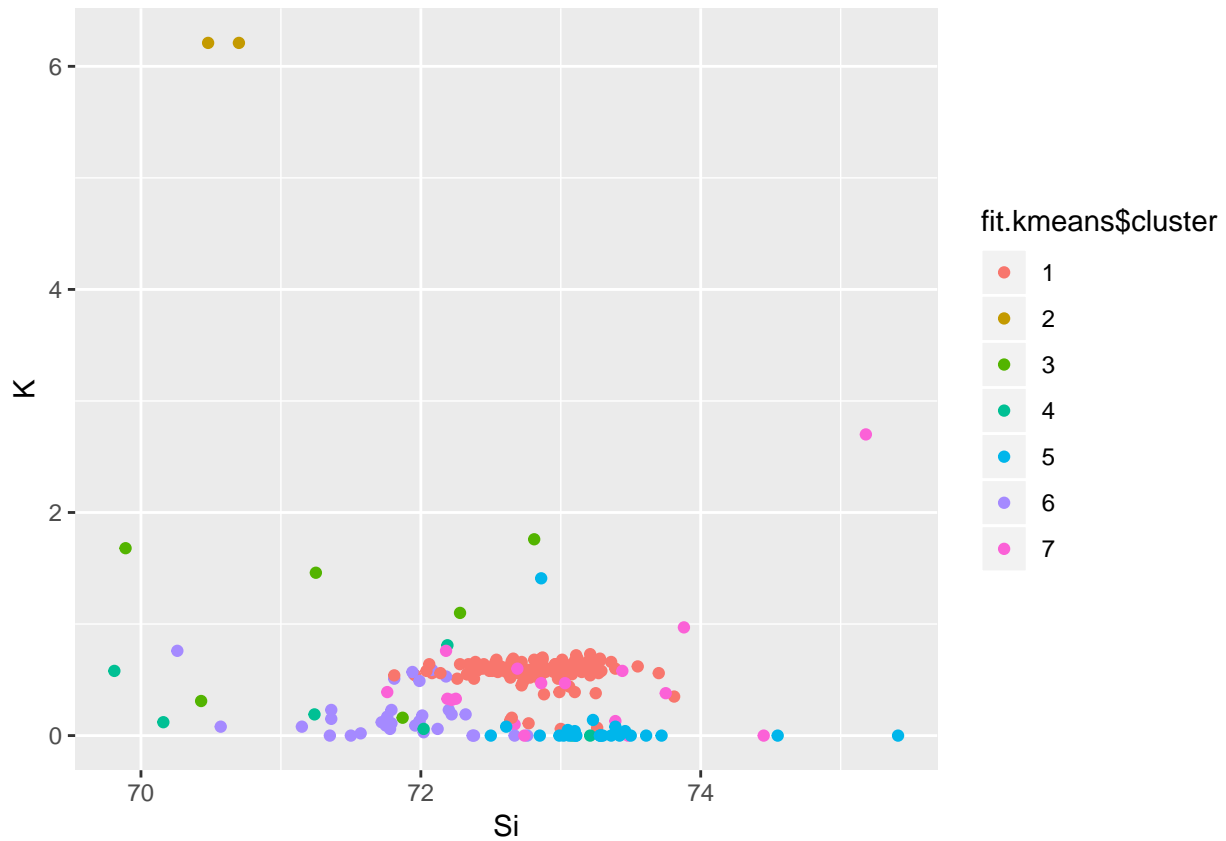
```
fit.kmeans$cluster <- as.factor(fit.kmeans$cluster)  
ggplot(Glass, aes(RI, Na, color = fit.kmeans$cluster)) + geom_point()
```



```
fit.kmeans$cluster <- as.factor(fit.kmeans$cluster)  
ggplot(Glass, aes(Mg, Al, color = fit.kmeans$cluster)) + geom_point()
```

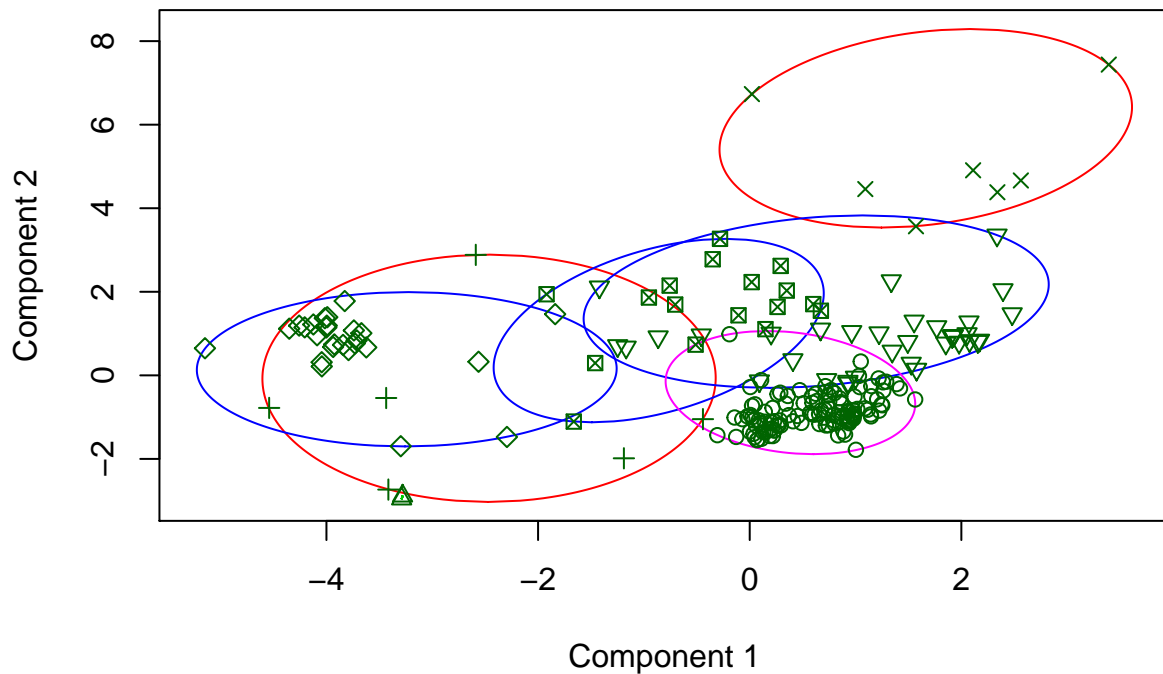


```
fit.kmeans$cluster <- as.factor(fit.kmeans$cluster)
ggplot(Glass, aes(Si, K, color = fit.kmeans$cluster)) + geom_point()
```



```
clusplot(Glass, fit.kmeans$cluster, color=TRUE, shade=FALSE, labels=7, lines=0)
```

CLUSPLOT(Glass)



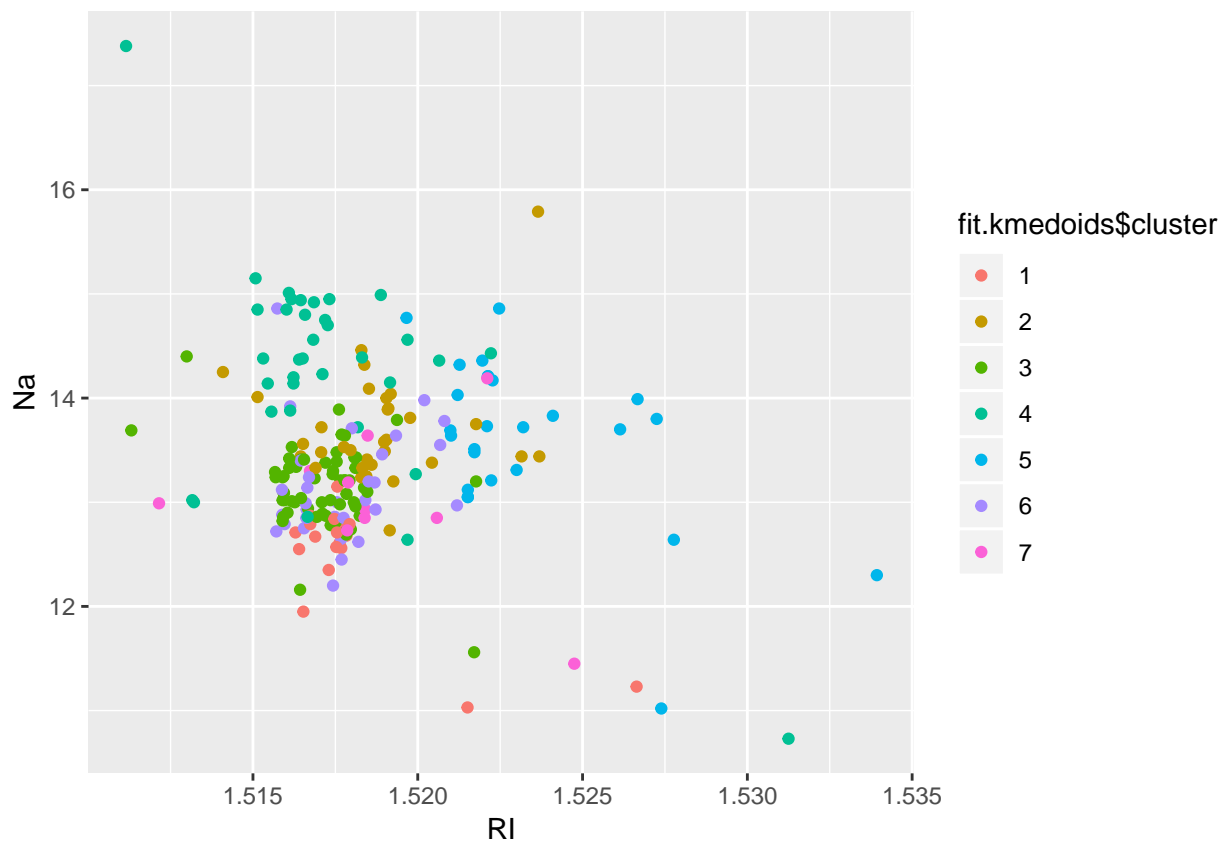
These two components explain 53.37 % of the point variability.

Getting insights from K-Medoids Clustering

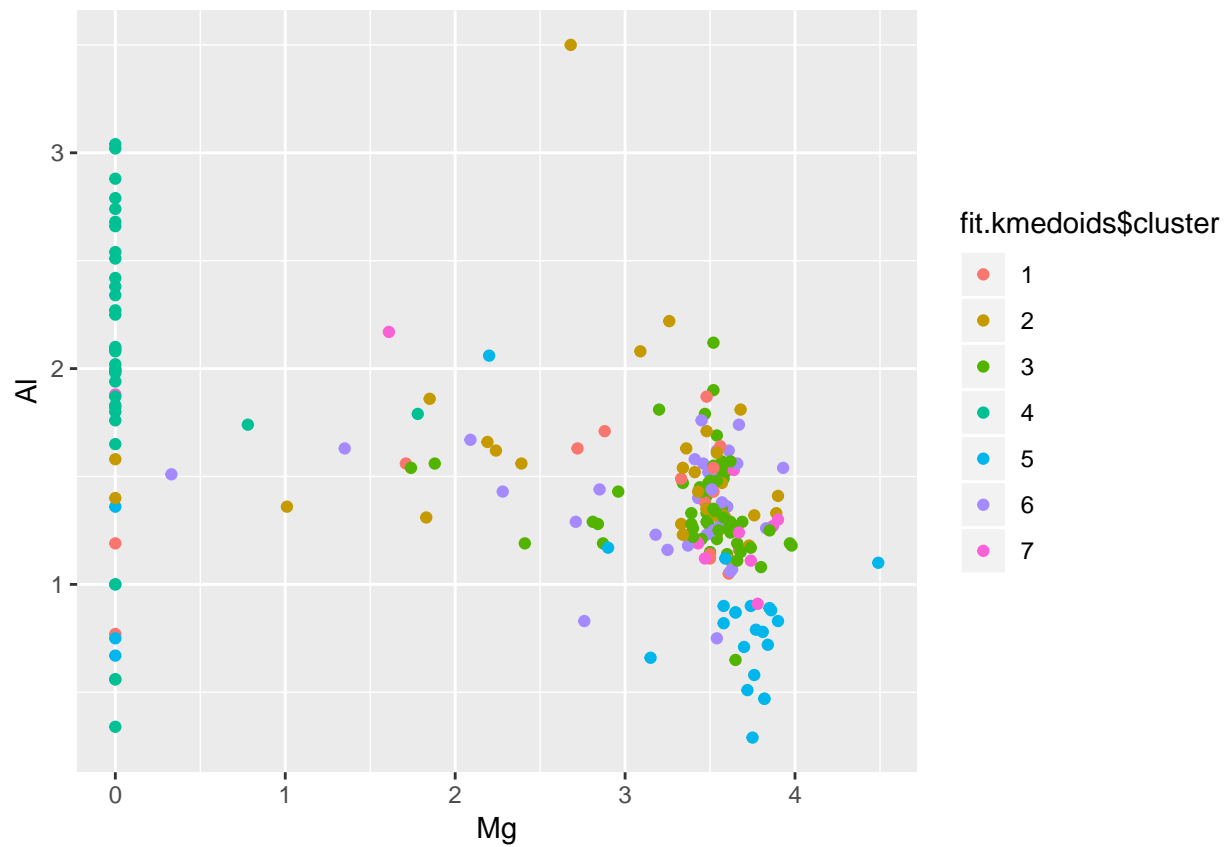
```
table(fit.kmedoids$cluster, Glass[,10])
```

```
##  
##      1  2  3  5  6  7  
##  1  9  7  0  1  0  1  
##  2  8 11  3  4  3  3  
##  3 24 25  8  1  2  1  
##  4  0  3  0  5  4 23  
##  5 17  6  2  0  0  1  
##  6 10 18  3  1  0  0  
##  7  2  6  1  1  0  0
```

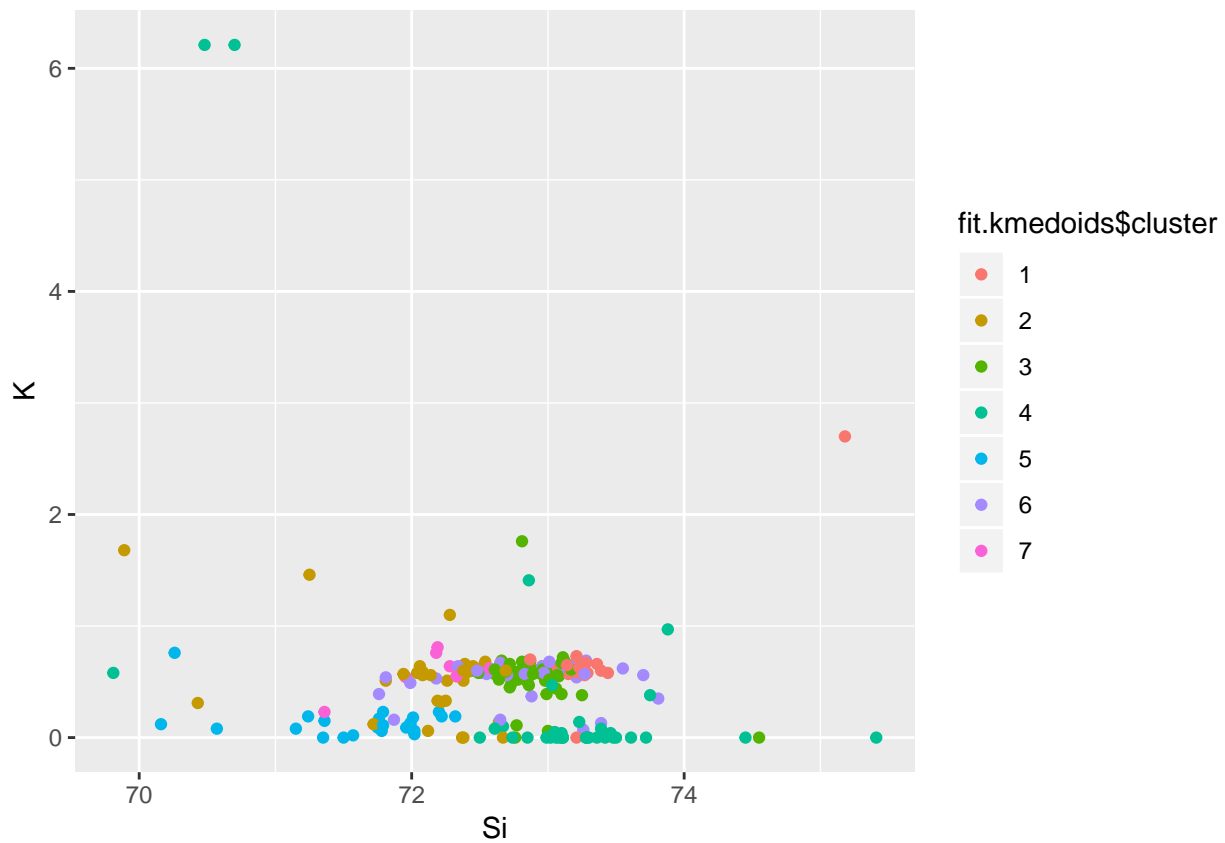
```
fit.kmedoids$cluster <- as.factor(fit.kmedoids$cluster)  
ggplot(Glass, aes(RI, Na, color = fit.kmedoids$cluster)) + geom_point()
```



```
fit.kmedoids$cluster <- as.factor(fit.kmedoids$cluster)  
ggplot(Glass, aes(Mg, Al, color = fit.kmedoids$cluster)) + geom_point()
```

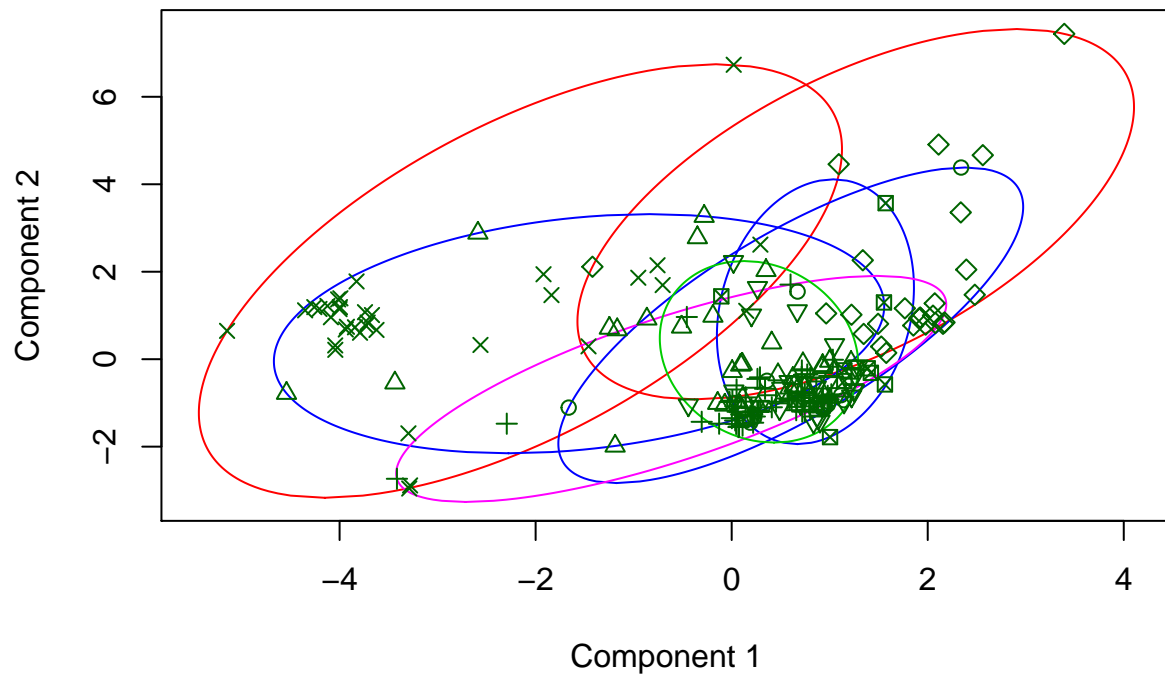


```
fit.kmedoids$cluster <- as.factor(fit.kmedoids$cluster)
ggplot(Glass, aes(Si, K, color = fit.kmedoids$cluster)) + geom_point()
```



```
clusplot(Glass, fit.kmedoids$cluster, color=TRUE, shade=FALSE, labels=7, lines=0)
```

CLUSPLOT(Glass)



These two components explain 53.37 % of the point variability.

Conclusion

With better accuracy and kappa measures, Random Forest has outperformed other competitors on Glass Dataset while Hierarchical Agglomerative Clustering is the winner when compared with K-Means and K-Medoids Clustering on Glass Dataset as it has clustered data better evident from the Cluster Plot and Cluster Dendrogram.