```
library(mlbench)
 data(Glass)
 library(factoextra)
 ## Loading required package: ggplot2
 ## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
 library(dplyr)
 ## Attaching package: 'dplyr'
 ## The following objects are masked from 'package:stats':
 ##
 ##
      filter, lag
 ## The following objects are masked from 'package:base':
 ##
      intersect, setdiff, setequal, union
 ##
 library(tidyverse)
      --- Attaching packages
                                                                                                                    - tidyverse 1.3.0 ----
 ## < tibble 3.0.0 < purrr 0.3.4
 ## < tidyr 1.0.2 < stringr 1.4.0
 ## / readr 1.3.1 / forcats 0.5.0
       — Conflicts –
                                                                                                                 tidyverse_conflicts() -
 ## x dplyr::filter() masks stats::filter()
 ## x dplyr::lag() masks stats::lag()
K-means
 Glass$Type2 <- as.factor(c(rep('Window', 163), rep('Non-Window', 51)))
 glass <- Glass[,-c(10,11)]
 set.seed(42)
 wss <- function(k) {
  kmeans(glass, k, nstart = 25)$tot.withinss
```

k.values <- 1:15

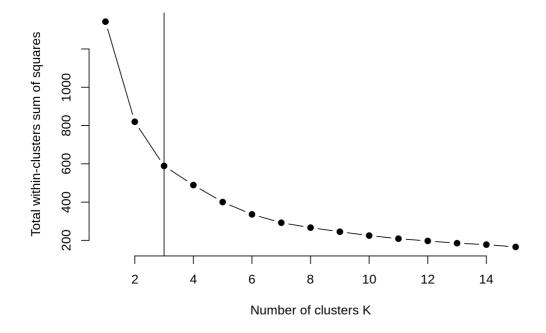
abline(v = 3)

wss\_values <-map(k.values, wss)

type="b", pch = 19, frame = FALSE, xlab="Number of clusters K",

ylab="Total within-clusters sum of squares")

plot(k.values, wss\_values,



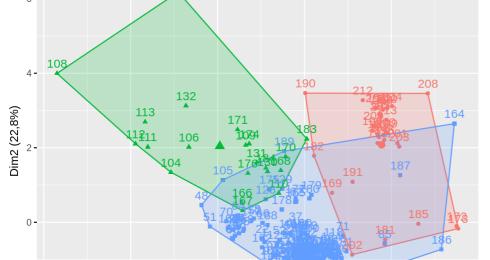
set.seed(42) km.res <- kmeans(glass,3, nstart = 25)

km.res

```
## K-means clustering with 3 clusters of sizes 31, 21, 162
##
## Cluster means:
                       Si
                                Ca
##
     RI
              Mg
                   ΑI
                            Κ
## 1 1,516358 14,45677 0,1977419 2,120968 73,12355 0,5883871 8,538387 0,88193548
## 2 1,523548 12,84524 0,4490476 1,305238 72,40524 0,2542857 12,383333 0,15000000
## 3 1,518078 13,28006 3,4501852 1,333642 72,59235 0,5110494 8,592901 0,04302469
## 1 0,01258065
## 2 0,07142857
## 3 0.06364198
## Clustering vector:
## 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
## 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
## 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60
## 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
## 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100
## 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
## 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140
## 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160
## 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180
## 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200
## 201 202 203 204 205 206 207 208 209 210 211 212 213 214
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##
## Within cluster sum of squares by cluster:
## [1] 194,4349 138,9466 255,6500
## (between_SS / total_SS = 56,1 %)
##
## Available components:
## [1] "cluster"
           "centers'
                    "totss'
                           "withinss"
                                   "tot.withinss"
## [6] "betweenss"
             "size"
                     "iter"
                           "ifault"
```

## fviz\_cluster(km.res, glass)

Cluster plot



0,0

Dim1 (27,9%)

2,5

107



-7,5

-5,0

```
##
## 1 2 3
## Non-Window 31 9 11
## Window 0 12 151
```

```
table('Glass_Type' = Glass$Type, 'Clusters' = km.res$cluster)
```

```
## Clusters
## Glass_Type 1 2 3
## 1 0 0 70
## 2 0 12 64
## 3 0 0 17
## 5 3 7 3
## 6 3 2 4
## 7 25 0 4
```

Glass\$K\_means <- km.res\$cluster

#### #K-means 2 and 6

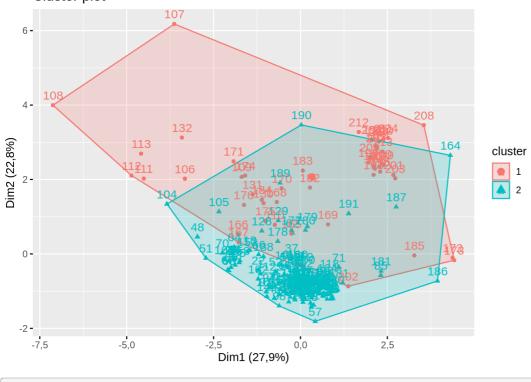
```
set.seed(42)
km.res <- kmeans(glass,2, nstart = 25)
```

#### table(Glass\$Type2, km.res\$cluster)

```
##
## 1 2
## Non-Window 39 12
## Window 11 152
```

fviz\_cluster(km.res, glass)

## Cluster plot

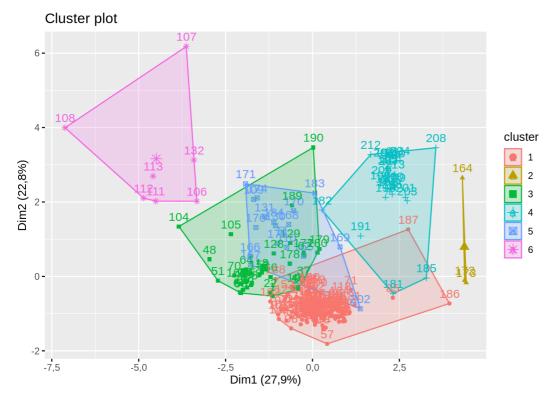


set.seed(42) km.res <- kmeans(glass, 6, nstart = 25)

table('Glass\_Type' = Glass\$Type, 'Cluster' = km.res\$cluster)

```
## Cluster
## Glass_Type 1 2 3 4 5 6
## 1 48 0 22 0 0 0
## 2 61 0 4 0 4 7
## 3 14 0 3 0 0 0
## 5 0 3 0 0 10 0
## 6 0 0 4 3 2 0
## 7 3 0 2 23 1 0
```

fviz\_cluster(km.res, glass)

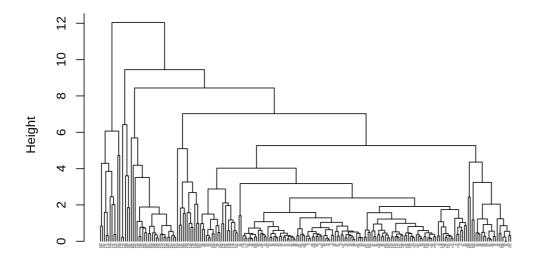


# Hierarchical clustering

```
distance <- dist(glass , method = "euclidean")
hc_comp <- hclust(distance, method = "complete")

plot(hc_comp, cex = 0.2, hang = -1)
```

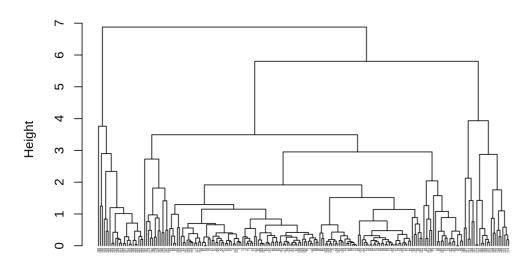
# **Cluster Dendrogram**



```
glass \leftarrow glass[,c(2,3,4)]
distance <- dist(glass, method = "euclidean")
hc_comp <- hclust(distance, method = "complete")</pre>
```

```
plot(hc\_comp, cex = 0.2, hang = -1)
```

## **Cluster Dendrogram**

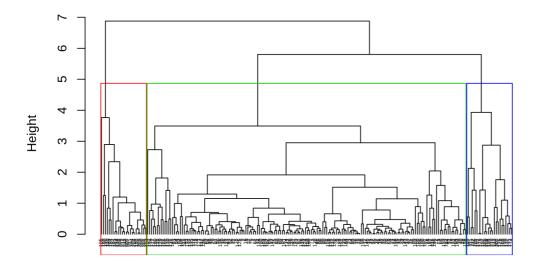


#AI,Mg, Ba

### distance hclust (\*, "complete")

```
plot(hc\_comp, cex = 0.4, hang = -1)
rect.hclust(hc\_comp, k = 3, border = 2:5)
```

## **Cluster Dendrogram**



distance hclust (\*, "complete")

```
Glass$HC <- cutree(hc_comp, 3)
table('K_means' = Glass$K_means,'HC' = Glass$HC)
```

```
##
     HC
## K_means 1 2 3
     1 2 10 19
##
     2 3 14 4
##
##
     3 161 0 1
```

apply(Glass[,1:9], 2, mean)

Na

## 8,95696262 0,17504673 0,05700935

Mg

Fe

ΑI

Si

## 1,51836542 13,40785047 2,68453271 1,44490654 72,65093458 0,49705607

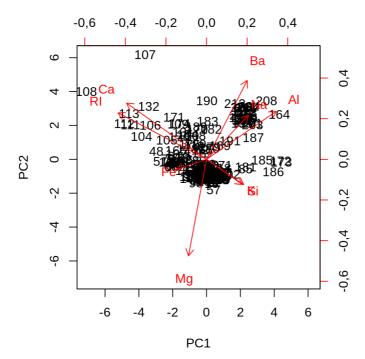
K

RI

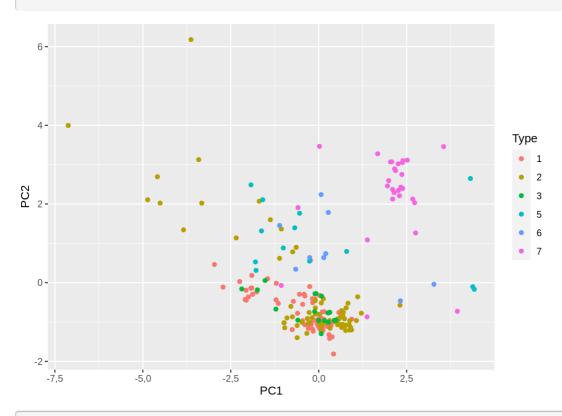
Ca

biplot(prc, scale = 0)

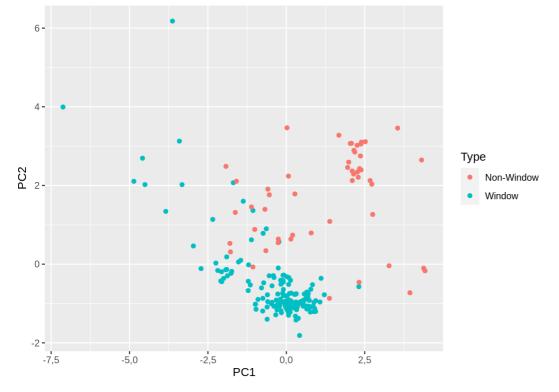
```
apply(Glass[,1:9], 2, sd)
       RI
               Na
                                       Si
                                              K
                       Mg
## 0,003036864 0,816603556 1,442407845 0,499269646 0,774545795 0,652191846
       Ca
               Ba
                       Fe
## 1,423153487 0,497219261 0,097438701
prc <- prcomp(x = Glass[,1:9], scale = TRUE)
prc
## Standard deviations (1, .., p=9):
## [1] 1,58466518 1,43180731 1,18526115 1,07604017 0,95603465 0,72638502 0,60741950
## [8] 0,25269141 0,04011007
##
## Rotation (n \times k) = (9 \times 9):
##
        PC1
                PC2
                           PC3
                                   PC4
                                             PC5
                                                      PC6
## RI -0,5451766 0,28568318 -0,0869108293 -0,14738099 0,073542700 -0,11528772
## Na 0,2581256 0,27035007 0,3849196197 -0,49124204 -0,153683304 0,55811757
## Mg -0,1108810 -0,59355826 -0,0084179590 -0,37878577 -0,123509124 -0,30818598
## AI 0,4287086 0,29521154 -0,3292371183 0,13750592 -0,014108879 0,01885731
## Si 0,2288364 -0,15509891 0,4587088382 0,65253771 -0,008500117 -0,08609797
## K 0,2193440 -0,15397013 -0,6625741197 0,03853544 0,307039842 0,24363237
## Ca -0,4923061 0,34537980 0,0009847321 0,27644322 0,188187742 0,14866937
## Ba 0,2503751 0,48470218 -0,0740547309 -0,13317545 -0,251334261 -0,65721884
## Fe -0,1858415 -0,06203879 -0,2844505524 0,23049202 -0,873264047 0,24304431
        PC7
                 PC8
                          PC9
## RI -0,08186724 -0,75221590 -0,02573194
## Na -0,14858006 -0,12769315 0,31193718
## Mg 0,20604537 -0,07689061 0,57727335
## AI 0,69923557 -0,27444105 0,19222686
## Si -0,21606658 -0,37992298 0,29807321
## K -0,50412141 -0,10981168 0,26050863
## Ca 0,09913463 0,39870468 0,57932321
## Ba -0,35178255 0,14493235 0,19822820
## Fe -0,07372136 -0,01627141 0,01466944
```



prc\_adj <- data.frame(prc\$x, Type = Glass\$Type)
ggplot(data = prc\_adj, aes(x = PC1, y = PC2, color=Type)) +
 geom\_point()</pre>



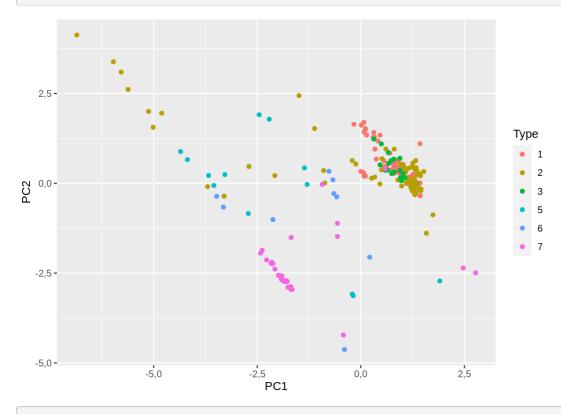
prc\_adj <- data.frame(prc\$x, Type = Glass\$Type2)
ggplot(data = prc\_adj, aes(x = PC1, y = PC2, color=Type)) +
 geom\_point()</pre>



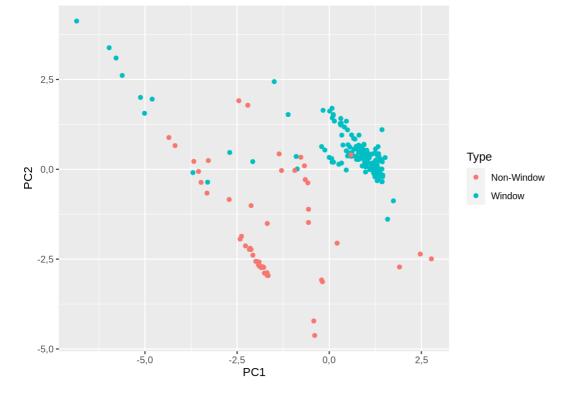
#### #Unscaled variant

```
prc_un <- prcomp(x = Glass[,1:9], scale = FALSE)
```

```
prc_adj_un <- data.frame(prc_un$x, Type = Glass$Type)
ggplot(data = prc_adj_un, aes(x = PC1, y = PC2, color=Type)) +
geom_point()</pre>
```



prc\_adj\_un <- data.frame(prc\_un\$x, Type = Glass\$Type2)
ggplot(data = prc\_adj\_un, aes(x = PC1, y = PC2, color=Type)) +
 geom\_point()</pre>



# **PVE**

```
prc_var <- prc$sdev^2
prc_pve <- prc_var / sum(prc_var)
prc_pve
```

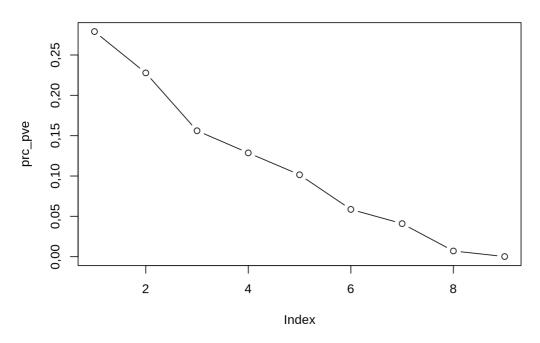
## [1] 0,2790181918 0,2277857983 0,1560937771 0,1286513829 0,1015558052 ## [6] 0,0586261325 0,0409953826 0,0070947720 0,0001787575

 $cumsum(prc\_pve)$ 

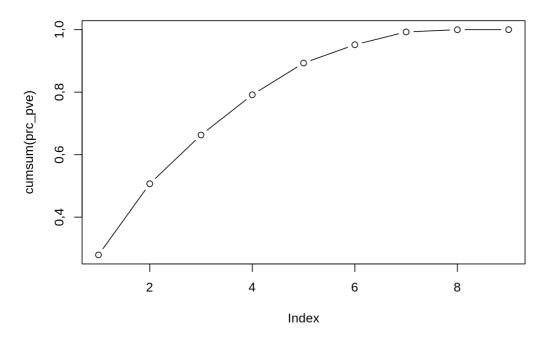
## [1] 0,2790182 0,5068040 0,6628978 0,7915492 0,8931050 0,9517311 0,9927265 ## [8] 0,9998212 1,0000000

plot(prc\_pve, type = "b", main = "Proportion of Variance Explained")

# **Proportion of Variance Explained**



# **Cumulative Proportion of Variance Explained**



# K-means

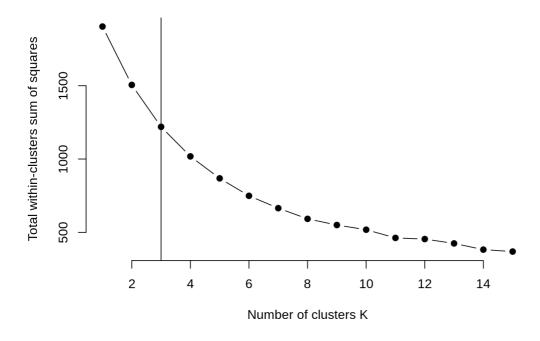
```
prc <- prc$x[,1:7]
set.seed(42)

wss <- function(k) {
   kmeans(prc, k, nstart = 25)$tot.withinss
}

k.values <- 1:15
   wss_values <-map(k.values, wss)

plot(k.values, wss_values,
   type="b", pch = 19, frame = FALSE,
        xlab="Number of clusters K",
   ylab="Total within-clusters sum of squares")

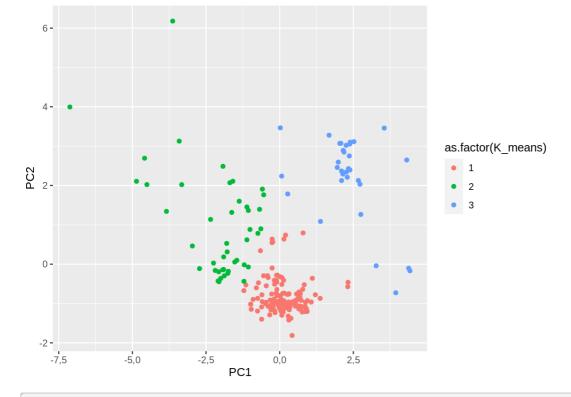
abline(v = 3)
```



```
set.seed(42)
km.res <- kmeans(prc,3, nstart = 25)
```

```
## K-means clustering with 3 clusters of sizes 137, 45, 32
## Cluster means:
    PC1 PC2
                   PC3
##
                         PC4
                                PC5
                                      PC6
## 1 0,1414358 -0,8325299 0,008226861 0,07806163 -0,01529622 -0,1052881
## 2 -2,1058788 0,9684670 -0,082629603 -0,17190774 0,14847033 0,2518977
## 3 2,3558700 2,2023619 0,080976631 -0,09245609 -0,14329946 0,0965335
      PC7
## 1 0,07344303
## 2 -0,12911682
## 3 -0,13285745
##
## Clustering vector:
## 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
    ## 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
## 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2
## 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60
## 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
## 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100
## 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120
## 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140
## 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160
## 1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1 2 1 1
## 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180
## 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200
## 201 202 203 204 205 206 207 208 209 210 211 212 213 214
## 3 1 3 3 3 3 3 3 3 3 3 3 3 3
## Within cluster sum of squares by cluster:
## [1] 331,3635 455,9302 432,1088
## (between_SS / total_SS = 35,9 %)
## Available components:
## [1] "cluster" "centers"
                            "withinss" "tot.withinss"
                    "totss"
## [6] "betweenss" "size"
                     "iter"
                            "ifault"
```

```
df <- as.data.frame(prc)
df$K_means <- km.res$cluster
ggplot(df,aes(x=PC1,y=PC2,color= as.factor(K_means))) + geom_point()
```



```
table('Glass_Type' = Glass$Type, 'Cluster' = km.res$cluster)
```

```
## Cluster
## Glass_Type 1 2 3
## 1 54 16 0
## 2 61 15 0
## 3 14 3 0
## 5 2 8 3
## 6 5 1 3
## 7 1 2 26
```

```
table('Glass_Type' = Glass$Type2, 'Cluster' = km.res$cluster)
```

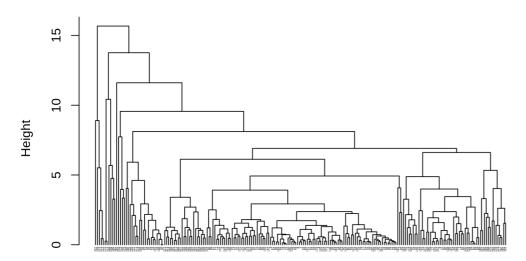
```
## Cluster
## Glass_Type 1 2 3
## Non-Window 8 11 32
## Window 129 34 0
```

# Hierarchical clustering

```
distance <- dist(prc, method = "euclidean")
hc_comp <- hclust(distance, method = "complete")
```

```
plot(hc_comp, cex = 0.2, hang = -1)
```

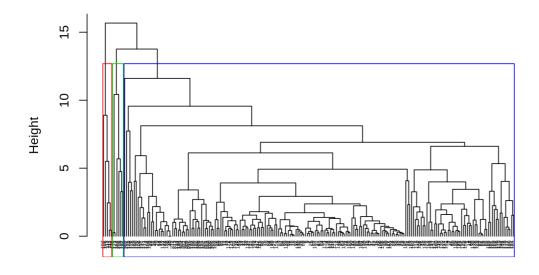
# **Cluster Dendrogram**



distance hclust (\*, "complete")

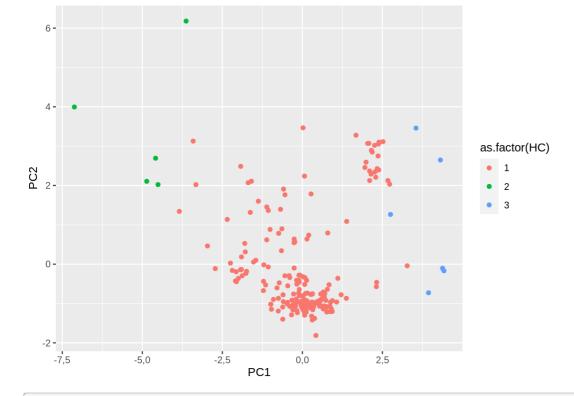
```
plot(hc_comp, cex = 0.4, hang = -1)
rect.hclust(hc_comp, k = 3, border = 2:5)
```

# **Cluster Dendrogram**



distance hclust (\*, "complete")

```
\label{eq:comp_def} \begin{split} & \texttt{df\$HC} <- \texttt{cutree}(\texttt{hc\_comp}, 3) \\ & \texttt{ggplot}(\texttt{df}, \texttt{aes}(\texttt{x=PC1}, \texttt{y=PC2}, \texttt{color=} \texttt{ as.factor}(\texttt{HC}))) + \texttt{geom\_point}() \end{split}
```



### table('Glass\_Type' = Glass\$Type, 'Cluster' = km.res\$cluster)

```
## Cluster
## Glass_Type 1 2 3
## 1 54 16 0
## 2 61 15 0
## 3 14 3 0
## 5 2 8 3
## 6 5 1 3
## 7 1 2 26
```

#### table('Glass\_Type' = Glass\$Type2, 'Cluster' = km.res\$cluster)

```
## Cluster
## Glass_Type 1 2 3
## Non-Window 8 11 32
## Window 129 34 0
```

### $table('K_means' = df$K_means, 'HC' = df$HC)$

```
## HC

## K_means 1 2 3

## 1137 0 0

## 2 40 5 0

## 3 26 0 6
```