Unsupervised Methods for OCCN

March 8, 2024

1 Unspuervised Classification Using R for Soil NanoSIMS Images

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1.1 1. Get the right version R kernel in Jupyter Notebook

1.1.1 Install necessary softwares

1. Install the latest R 4.3.1 in Windows.
2. Install Anaconda and open Anaconda Prompt from the start menu. ### Install and Adjust R kernel for Jupyter Notebook
3. Type `cd /d "your path/R/R-4.3.1"` where you installed your R. Hit return.
4. Type `cd bin`. Hit return.
5. Type `R.exe` to launch the command line R from the directory.
6. Install the package `IRkernel` which makes the newest R callable as an Jupyter kernel. Type `install.packages('IRkernel')` and hit return.
7. Type `IRkernel::installspec(name = 'Hackathon', displayname = 'R 4.3.1')` to create the latest R kernel. Both `name` and `displayname` can be changed into whatever you want.
8. Exit R and close any instances of Jupyter Notebooks you have running.
9. Launch Jupyter Notebook again and click to create a new notebook. You should find your kernel available by its display name in the drop down box. *Referenced Web* ## 2. Run a R-kernel notebook for Unsupervised Classification

[ ]:

```

```

1.1.2 Preparation for the Unsupervised Clustering

[1]:

```r
# Clear environment
rm(list=ls())
```

1.1.3 Step 1: Load all the needed stuff

1. Packages

[2]:

```r
# List out the necessary packages
pkg <- c("sp",           # Classes and Methods for Spatial Data
         "raster",       # Geographic Data Analysis and Modeling
```

```r
        #"rgdal",       # Bindings for the 'Geospatial' Data Abstraction␣
↪Library # retire this Oct -> replaced by next three
        "sf",           # Simple Features for R
        "stars",        # Spatiotemporal Arrays, Raster and Vector Data Cubes
        "terra",        # Spatial Data Analysis
        "ijtiff",       # Read and Write TIFF Images
        "lattice",      # Trellis Graphics for R
        "latticeExtra", # Extra Graphical Utilities Based on Lattice
        "ggplot2",      # Create Elegant Data Visualisations Using the Grammar␣
↪of Graphics
        "scales",       # Scale Functions for Visualization
        "cluster",      # "Finding Groups in Data": Cluster Analysis Extended␣
↪Rousseeuw et al.
        "factoextra",   # Extract and Visualize the Results of Multivariate␣
↪Data Analyses
        "gridExtra")    # Miscellaneous Functions for "Grid" Graphics

# Load packages
lapply(pkg, library, character.only = TRUE)
```

```
The legacy packages maptools, rgdal, and rgeos, underpinning the sp package,
which was just loaded, were retired in October 2023.
Please refer to R-spatial evolution reports for details, especially
https://r-spatial.org/r/2023/05/15/evolution4.html.
It may be desirable to make the sf package available;
package maintainers should consider adding sf to Suggests:.

Linking to GEOS 3.10.2, GDAL 3.4.1, PROJ 8.2.1; sf_use_s2() is TRUE

Loading required package: abind

terra 1.7.46


Attaching package: ‘ggplot2’


The following object is masked from ‘package:latticeExtra’:

    layer



Attaching package: ‘scales’


The following object is masked from ‘package:terra’:
```

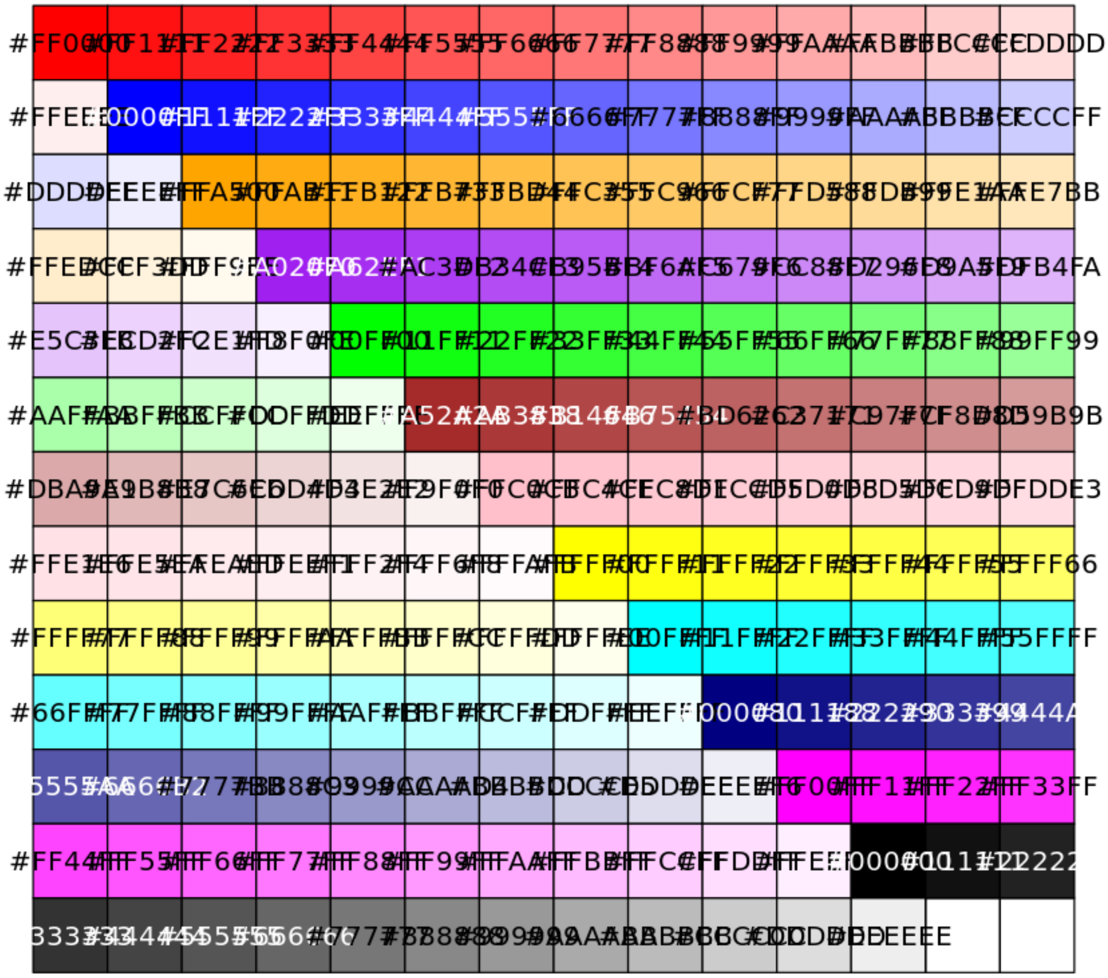
```
rescale
```

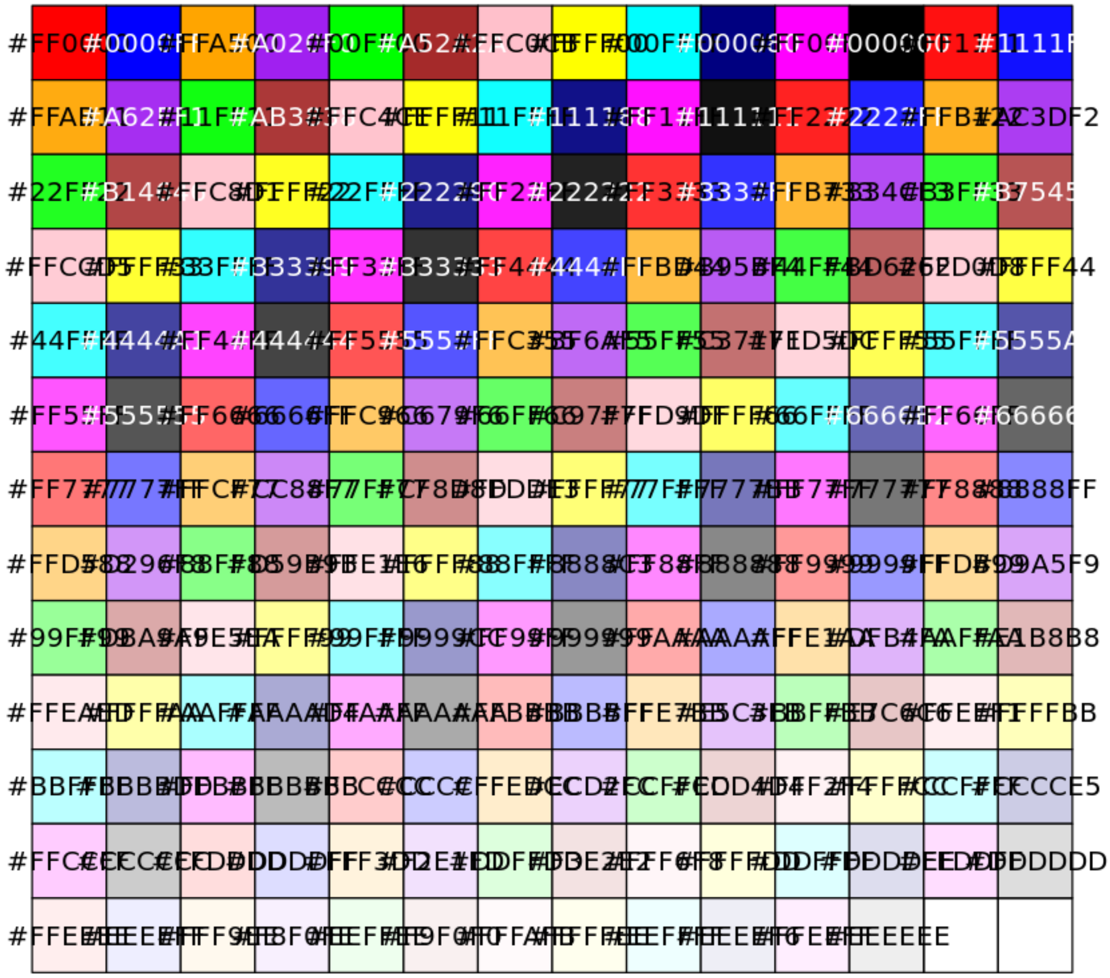
```
Welcome! Want to learn more? See two factoextra-related books at
https://goo.gl/ve3WBa
```

1. (a) 'sp' (b) 'stats' (c) 'graphics' (d) 'grDevices' (e) 'utils' (f) 'datasets' (g) 'methods' (h) 'base'
2. (a) 'raster' (b) 'sp' (c) 'stats' (d) 'graphics' (e) 'grDevices' (f) 'utils' (g) 'datasets' (h) 'methods' (i) 'base'
3. (a) 'sf' (b) 'raster' (c) 'sp' (d) 'stats' (e) 'graphics' (f) 'grDevices' (g) 'utils' (h) 'datasets' (i) 'methods' (j) 'base'
4. (a) 'stars' (b) 'abind' (c) 'sf' (d) 'raster' (e) 'sp' (f) 'stats' (g) 'graphics' (h) 'grDevices' (i) 'utils' (j) 'datasets' (k) 'methods' (l) 'base'
5. (a) 'terra' (b) 'stars' (c) 'abind' (d) 'sf' (e) 'raster' (f) 'sp' (g) 'stats' (h) 'graphics' (i) 'grDevices' (j) 'utils' (k) 'datasets' (l) 'methods' (m) 'base'
6. (a) 'ijtiff' (b) 'terra' (c) 'stars' (d) 'abind' (e) 'sf' (f) 'raster' (g) 'sp' (h) 'stats' (i) 'graphics' (j) 'grDevices' (k) 'utils' (l) 'datasets' (m) 'methods' (n) 'base'
7. (a) 'lattice' (b) 'ijtiff' (c) 'terra' (d) 'stars' (e) 'abind' (f) 'sf' (g) 'raster' (h) 'sp' (i) 'stats' (j) 'graphics' (k) 'grDevices' (l) 'utils' (m) 'datasets' (n) 'methods' (o) 'base'
8. (a) 'latticeExtra' (b) 'lattice' (c) 'ijtiff' (d) 'terra' (e) 'stars' (f) 'abind' (g) 'sf' (h) 'raster' (i) 'sp' (j) 'stats' (k) 'graphics' (l) 'grDevices' (m) 'utils' (n) 'datasets' (o) 'methods' (p) 'base'
9. (a) 'ggplot2' (b) 'latticeExtra' (c) 'lattice' (d) 'ijtiff' (e) 'terra' (f) 'stars' (g) 'abind' (h) 'sf' (i) 'raster' (j) 'sp' (k) 'stats' (l) 'graphics' (m) 'grDevices' (n) 'utils' (o) 'datasets' (p) 'methods' (q) 'base'
10. (a) 'scales' (b) 'ggplot2' (c) 'latticeExtra' (d) 'lattice' (e) 'ijtiff' (f) 'terra' (g) 'stars' (h) 'abind' (i) 'sf' (j) 'raster' (k) 'sp' (l) 'stats' (m) 'graphics' (n) 'grDevices' (o) 'utils' (p) 'datasets' (q) 'methods' (r) 'base'
11. (a) 'cluster' (b) 'scales' (c) 'ggplot2' (d) 'latticeExtra' (e) 'lattice' (f) 'ijtiff' (g) 'terra' (h) 'stars' (i) 'abind' (j) 'sf' (k) 'raster' (l) 'sp' (m) 'stats' (n) 'graphics' (o) 'grDevices' (p) 'utils' (q) 'datasets' (r) 'methods' (s) 'base'
12. (a) 'factoextra' (b) 'cluster' (c) 'scales' (d) 'ggplot2' (e) 'latticeExtra' (f) 'lattice' (g) 'ijtiff' (h) 'terra' (i) 'stars' (j) 'abind' (k) 'sf' (l) 'raster' (m) 'sp' (n) 'stats' (o) 'graphics' (p) 'grDevices' (q) 'utils' (r) 'datasets' (s) 'methods' (t) 'base'
13. (a) 'gridExtra' (b) 'factoextra' (c) 'cluster' (d) 'scales' (e) 'ggplot2' (f) 'latticeExtra' (g) 'lattice' (h) 'ijtiff' (i) 'terra' (j) 'stars' (k) 'abind' (l) 'sf' (m) 'raster' (n) 'sp' (o) 'stats' (p) 'graphics' (q) 'grDevices' (r) 'utils' (s) 'datasets' (t) 'methods' (u) 'base'

2. Colors

[3]:
```
# Define the base colors with 12 basic colors
base_colors <- c('red', 'blue', 'orange', 'purple', 'green', 'brown', 'pink',
                 'yellow', 'cyan',  'navy', 'magenta', 'black')

# Set the fading degree for the color palette
num_colors <- 16

# Generate the fading color palette
colors_fw <- sapply(base_colors,
                    function(color) colorRampPalette(c(color,␣
 ↪"white"))(num_colors)) # Use function to fade the basic colors

colors_f  <- colors_fw[-nrow(colors_fw),] # Exclude the white row

# Trans from DataFrame into List
colors_or <- as.vector(unlist(unlist(colors_f)))  # colors_or is a list with␣
 ↪ordered colors

colors_nor <- as.vector(unlist(unlist(t(colors_f))))  # # colors_nor is a list␣
 ↪with non-ordered colors

# Show the color palette
show_col(colors_or)
show_col(colors_nor)
```





3. Plot Settings

[4]:
```
#create a grayscale color palette for the images
greyscale_cols <- gray.colors(100,             # number of different color levels
                              start = 0.0,     # how black (0) to go
                              end = 1.0,       # how white (1) to go
                              gamma = 5,       # correction between how a digital
                              alpha = NULL)    #Null=colors are not transparent
topo <- topo.colors(100,alpha = 0.5)           #Null=colors are not transparent
```

4. Tif files

[5]:
```
# Set working directory
setwd('/tf/data/Marcus_Schiedung/dd_NanoSIMS')

# Load Tif file
Ras_original <- stack("S1_2.tif")
```

```
Warning message:
"[rast] unknown extent"
```

1.1.4 Step 2: Preprocessing on original raster

1. give the names to corresponding channels

[6]:
```
# Detailed info
Ras_name <- c('Na23', 'Mg24', 'Al27', 'K39', 'Ca40', 'Ca44','Fe56',
              'O16', 'C12', 'C13', 'CN26', 'CN27', 'Si28','Ca44O16')

names(Ras_original) <- Ras_name

Ras_original
```

```
class      : RasterStack
dimensions : 256, 256, 65536, 14  (nrow, ncol, ncell, nlayers)
resolution : 1, 1  (x, y)
extent     : 0, 256, 0, 256  (xmin, xmax, ymin, ymax)
crs        : NA
names      : Na23, Mg24, Al27, K39, Ca40, Ca44, Fe56, O16, C12, C13, CN26, CN27,
 ↪Si28, Ca44O16
```

2. Turn from a Raster brick into a dataframe

[7]:
```
# Extract coordinates from the raster brick
coords <- coordinates(Ras_original)

# Initialize an empty dataframe
Ras_df <- data.frame(x = coords[, 1], y = coords[, 2])

# Loop through each layer, extract values, and add to the dataframe
for (i in 1:nlayers(Ras_original)) {
  layer_name <- names(Ras_original[[i]])
  layer_values <- getValues(Ras_original[[i]])
  Ras_df <- cbind(Ras_df, layer_values)
  colnames(Ras_df)[i + 2] <- layer_name
}

Ras_df <- na.omit(Ras_df)

# Print the resulting dataframe
```

```r
summary(Ras_df)
```

```
Warning message:
"[rast] unknown extent"
Warning message:
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Warning message:
"[rast] unknown extent"
```

```
       x                y                Na23              Mg24
 Min.   :  0.50   Min.   :  0.50   Min.   :   0.0   Min.   :  0.00
 1st Qu.: 64.25   1st Qu.: 64.25   1st Qu.:   3.0   1st Qu.:  1.00
 Median :128.00   Median :128.00   Median :   8.0   Median :  6.00
 Mean   :128.00   Mean   :128.00   Mean   :  22.4   Mean   : 21.54
 3rd Qu.:191.75   3rd Qu.:191.75   3rd Qu.:  19.0   3rd Qu.: 26.00
 Max.   :255.50   Max.   :255.50   Max.   :3403.0   Max.   :772.00
      Al27           K39              Ca40              Ca44
 Min.   :   0   Min.   :   0.0   Min.   :  0.00   Min.   :  0.0
 1st Qu.:  50   1st Qu.:  16.0   1st Qu.:  6.00   1st Qu.:  7.0
 Median : 153   Median :  52.0   Median : 15.00   Median : 16.0
 Mean   : 382   Mean   : 325.4   Mean   : 25.86   Mean   : 30.1
 3rd Qu.: 584   3rd Qu.: 318.0   3rd Qu.: 34.00   3rd Qu.: 40.0
 Max.   :2693   Max.   :9592.0   Max.   :476.00   Max.   :436.0
      Fe56             O16             C12              C13
 Min.   :  0.00   Min.   :    0   Min.   :   0.0   Min.   :  0.00
 1st Qu.:  1.00   1st Qu.: 1733   1st Qu.: 559.4   1st Qu.: 11.75
```

```
 Median :   6.00   Median : 5482   Median :2186.2   Median : 46.48
 Mean   : 23.52   Mean   : 5516   Mean   :2099.6   Mean   : 45.13
 3rd Qu.: 26.00   3rd Qu.: 8691   3rd Qu.:3511.9   3rd Qu.: 75.00
 Max.   :690.00   Max.   :21023   Max.   :7140.4   Max.   :174.21
      CN26             CN27              Si28             Ca44O16
 Min.   :   0.0   Min.   : 0.000   Min.   :  0.000   Min.   :0.0000
 1st Qu.: 405.7   1st Qu.: 1.165   1st Qu.:  4.481   1st Qu.:0.0000
 Median : 949.7   Median : 3.438   Median : 49.748   Median :0.0000
 Mean   :1336.8   Mean   : 4.844   Mean   : 56.681   Mean   :0.1963
 3rd Qu.:1817.3   3rd Qu.: 6.734   3rd Qu.: 89.448   3rd Qu.:0.2516
 Max.   :7462.7   Max.   :33.754   Max.   :317.707   Max.   :6.7122
```

3. Use Min-Max Normalization method to scale the ion data from 0 to 1

[8]:

```
## Min-Max Normalize

#define Min-Max normalization function
min_max_norm <- function(x) {
  (x - min(x)) / (max(x) - min(x))
}
```

[9]:

```
#apply Min-Max normalization to first four columns in iris dataset
Ras_norm <- as.data.frame(lapply(Ras_df[-c(1,2)], min_max_norm))

Ras_norm$x <- Ras_df$x
Ras_norm$y <- Ras_df$y

#view first six rows of normalized iris dataset
summary(Ras_norm)
```

```
      Na23                 Mg24                Al27               K39
 Min.   :0.0000000   Min.   :0.000000   Min.   :0.00000   Min.   :0.000000
 1st Qu.:0.0008816   1st Qu.:0.001295   1st Qu.:0.01857   1st Qu.:0.001668
 Median :0.0023509   Median :0.007772   Median :0.05681   Median :0.005421
 Mean   :0.0065829   Mean   :0.027897   Mean   :0.14185   Mean   :0.033923
 3rd Qu.:0.0055833   3rd Qu.:0.033679   3rd Qu.:0.21686   3rd Qu.:0.033153
 Max.   :1.0000000   Max.   :1.000000   Max.   :1.00000   Max.   :1.000000
      Ca40              Ca44              Fe56                O16
 Min.   :0.00000   Min.   :0.00000   Min.   :0.000000   Min.   :0.00000
 1st Qu.:0.01260   1st Qu.:0.01605   1st Qu.:0.001449   1st Qu.:0.08242
 Median :0.03151   Median :0.03670   Median :0.008696   Median :0.26075
 Mean   :0.05432   Mean   :0.06905   Mean   :0.034090   Mean   :0.26238
 3rd Qu.:0.07143   3rd Qu.:0.09174   3rd Qu.:0.037681   3rd Qu.:0.41340
 Max.   :1.00000   Max.   :1.00000   Max.   :1.000000   Max.   :1.00000
      C12               C13               CN26              CN27
 Min.   :0.00000   Min.   :0.00000   Min.   :0.00000   Min.   :0.00000
 1st Qu.:0.07834   1st Qu.:0.06744   1st Qu.:0.05436   1st Qu.:0.03453
 Median :0.30618   Median :0.26678   Median :0.12726   Median :0.10185
```

```
 Mean   :0.29404   Mean   :0.25904   Mean   :0.17913   Mean   :0.14350
 3rd Qu.:0.49183   3rd Qu.:0.43051   3rd Qu.:0.24352   3rd Qu.:0.19949
 Max.   :1.00000   Max.   :1.00000   Max.   :1.00000   Max.   :1.00000
      Si28             Ca44O16              x                 y
 Min.   :0.0000   Min.   :0.00000   Min.   :  0.50   Min.   :  0.50
 1st Qu.:0.0141   1st Qu.:0.00000   1st Qu.: 64.25   1st Qu.: 64.25
 Median :0.1566   Median :0.00000   Median :128.00   Median :128.00
 Mean   :0.1784   Mean   :0.02925   Mean   :128.00   Mean   :128.00
 3rd Qu.:0.2815   3rd Qu.:0.03749   3rd Qu.:191.75   3rd Qu.:191.75
 Max.   :1.0000   Max.   :1.00000   Max.   :255.50   Max.   :255.50
```

4. Extract the ion data we are interested in

[10]:
```
# Extract Basic Channels OCCN
OCCN_names <- c("O16", "C12", "C13", "CN26", "CN27" )

Ras_OCCN <- Ras_norm[, colnames(Ras_norm) %in% OCCN_names]

# Check the detailed info in the modified raster
summary(Ras_OCCN)
```

```
      O16               C12               C13               CN26
 Min.   :0.00000   Min.   :0.00000   Min.   :0.00000   Min.   :0.00000
 1st Qu.:0.08242   1st Qu.:0.07834   1st Qu.:0.06744   1st Qu.:0.05436
 Median :0.26075   Median :0.30618   Median :0.26678   Median :0.12726
 Mean   :0.26238   Mean   :0.29404   Mean   :0.25904   Mean   :0.17913
 3rd Qu.:0.41340   3rd Qu.:0.49183   3rd Qu.:0.43051   3rd Qu.:0.24352
 Max.   :1.00000   Max.   :1.00000   Max.   :1.00000   Max.   :1.00000
      CN27
 Min.   :0.00000
 1st Qu.:0.03453
 Median :0.10185
 Mean   :0.14350
 3rd Qu.:0.19949
 Max.   :1.00000
```

1.2 Conduct K-Means Classification on the Interested Dataset

1.2.1 Step 1: Choose the Optimal K Number for this Dataset

[11]:
```
# Cleaned up the garbage
gc()
```

A matrix: 2 × 6 of type dbl

	used	(Mb)	gc trigger	(Mb)	max used	(Mb)
Ncells	2728493	145.8	4216948	225.3	4216948	225.3
Vcells	5792880	44.2	10146329	77.5	8383012	64.0

Show the elbow plot of K Means result

[12]:
```r
## Calculate the the K number for KMeans
k.max<- 70
wss_OCCN <- sapply(2:k.max, function(k){kmeans(Ras_OCCN, k, nstart=10 )$tot.
 ↪withinss})

# Plot the wss curve
plot(2:k.max, wss_OCCN, type="b", pch = 19,
     xlab="Number of clusters K",
     ylab="Total within-clusters sum of squares for OCCN")
```

```
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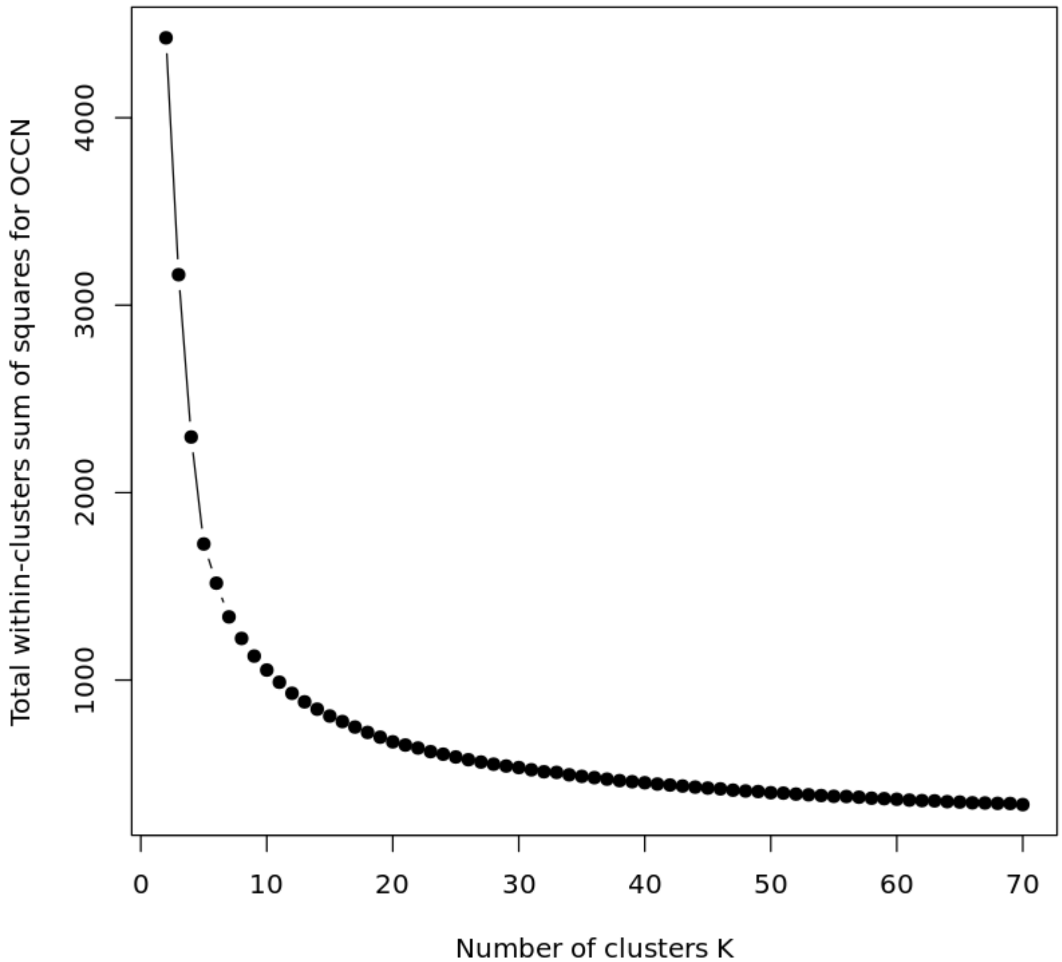
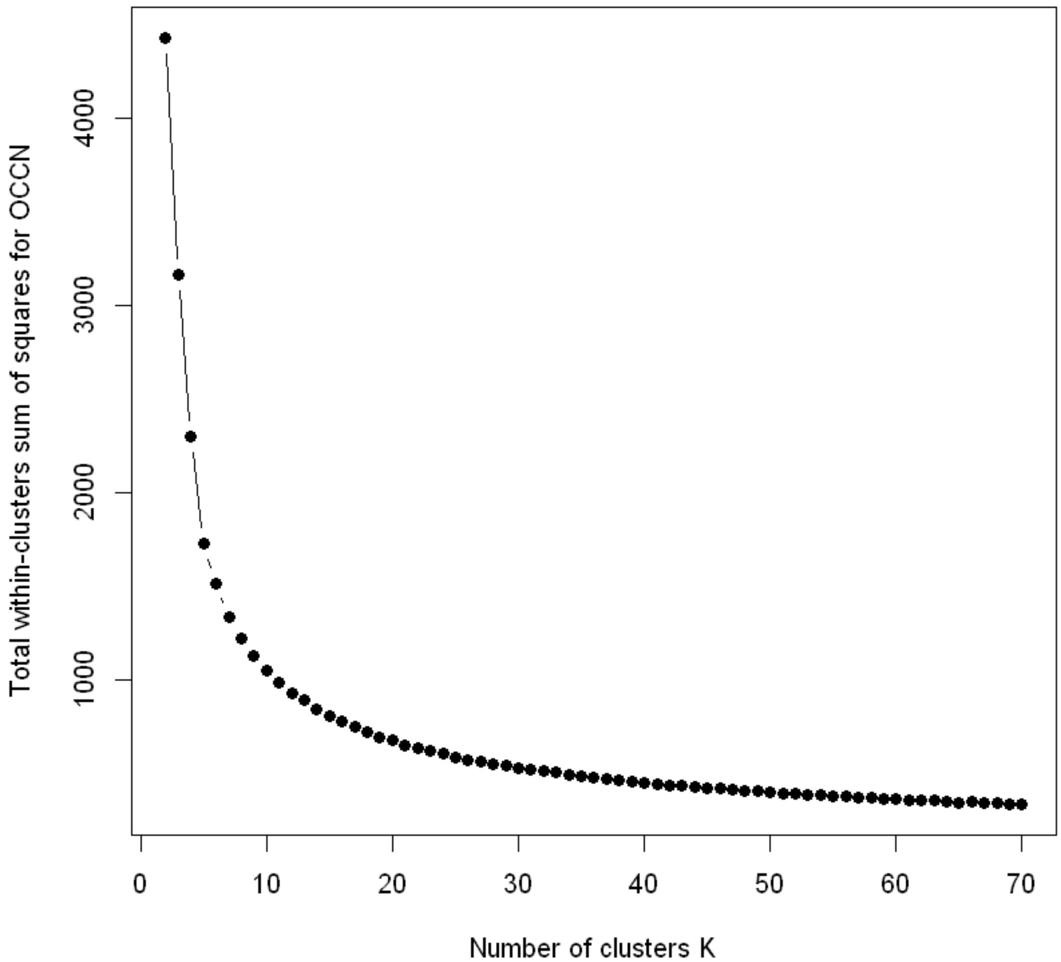

Total within-clusters sum of squares for OCCN
1000
2000
3000
4000
0
10
20
30
40
50
60
70
Number of clusters K



1.3 Step 2: Conduct K-Means Clustering with 70 Clusters

[12]:
```
# Set the number for K-means as large as possible for furter re-grouping
K <- 70

# Conduct K-means clustering
Ras_OCCN_kmeans <- kmeans(Ras_OCCN,
                     algorithm = "Lloyd",
                     centers = K,      # the variable that determines the
 ↪number of clusters
                     iter.max = 1000,     # sets the maximum number of
 ↪iterations allowed for the k-means algorithm to converge
```

```
                    nstart = 100)      # 100 random initializations and selects␣
↪the best solution

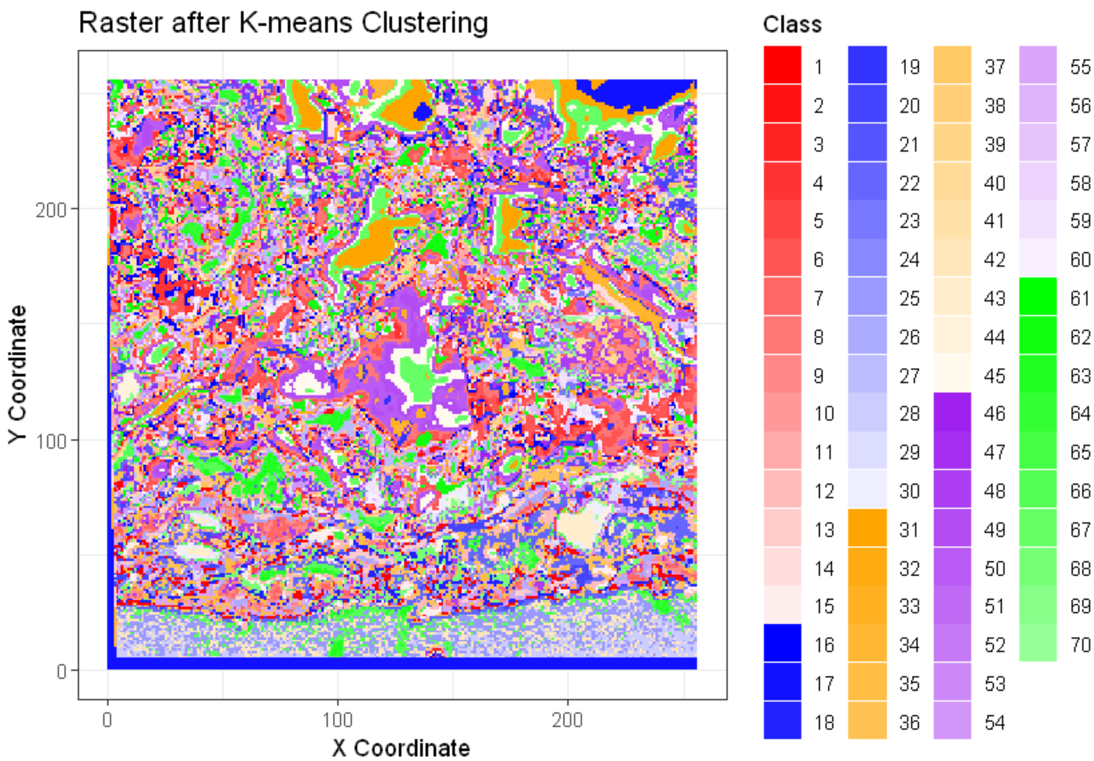
# Add cluster assigment to original data
Ras_OCCN_cluster <- cbind(Ras_OCCN,
                          class = Ras_OCCN_kmeans$cluster,
                          x = Ras_norm$x,
                          y = Ras_norm$y)

# View the clustered result
head(Ras_OCCN_cluster)
```

A data.frame: 6 × 8

	O16 <dbl>	C12 <dbl>	C13 <dbl>	CN26 <dbl>	CN27 <dbl>	class <int>	x <dbl>	y <dbl>
1	0.3261604	0.2463718	0.2524864	0.1703577	0.11622674	61	0.5	255.5
2	0.3698424	0.2496597	0.2603710	0.1712684	0.08438437	61	1.5	255.5
3	0.3898049	0.2551091	0.2613551	0.1835060	0.16330346	61	2.5	255.5
4	0.3842042	0.2504030	0.2353766	0.1878589	0.14616074	61	3.5	255.5
5	0.3673710	0.2505211	0.2146822	0.1817424	0.19765103	61	4.5	255.5
6	0.3366894	0.2856556	0.2491050	0.1995654	0.14464257	61	5.5	255.5

[14]:
```
## Plots
# Create a filled pixel plot
ggplot(Ras_OCCN_cluster, aes(x = x, y = y, fill = as.factor(class))) +
  geom_tile() +
  labs(title = "Raster after K-means Clustering", x = "X Coordinate", y = "Y␣
↪Coordinate") +
  scale_fill_manual(name = "Class", values = colors_or, guide = guide_legend())␣
↪+
  coord_fixed(ratio = 1) +  # Set aspect ratio to 1 for a squared plot
  theme_bw()
```



[ ]:
```
setwd("D:/B_6 pretest-2023 August/pic_unsuper_2")
ggsave(file = "KMeans_OCCN_pixel.png", plot = Plot_OCCN_70Cluster, width = 10,␣
 ↪height = 8, dpi = 600)
```

[15]:
```
# Create the df containg all the mean values and clusters
Ras_OCCN_clusterMean <- as.data.frame(Ras_OCCN_kmeans$centers)
Ras_OCCN_clusterMean$class <- as.factor(rownames(Ras_OCCN_clusterMean))

head(Ras_OCCN_clusterMean)
```

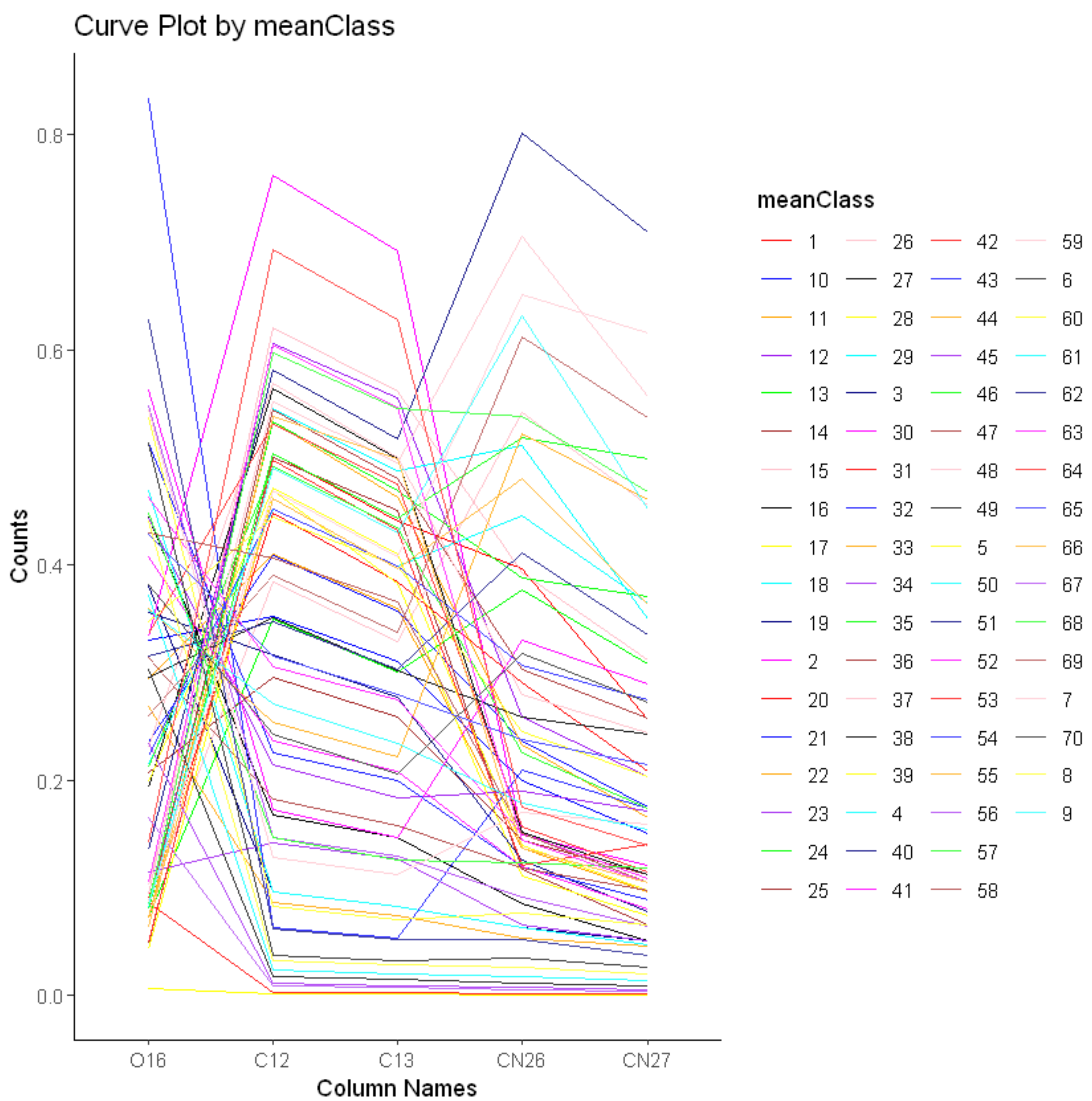
A data.frame: 6 × 6

	O16 <dbl>	C12 <dbl>	C13 <dbl>	CN26 <dbl>	CN27 <dbl>	class <fct>
1	0.0799946	0.50324781	0.44042678	0.39610196	0.25607846	1
2	0.3332785	0.76192110	0.69186000	0.14963650	0.12112609	2
3	0.3559697	0.31630688	0.27703542	0.12596410	0.07810824	3
4	0.4692743	0.09682117	0.08345702	0.06319495	0.04720071	4
5	0.3477244	0.44405965	0.39919035	0.24572208	0.20366407	5
6	0.5129381	0.03777648	0.03201914	0.03502878	0.02591258	6

1.3.1 Step 3: Check the Mean Classes Curve of each ions' counts

[17]:
```
# Create a long-format dataframe for plotting
plot_OCCN_clusterMean <- reshape2::melt(Ras_OCCN_clusterMean, id.vars = "class")

# Create a plot
ggplot(plot_OCCN_clusterMean, aes(x = variable, y = value, color = class, group
 ↪= class)) +
  geom_line() +
  labs(title = "Curve Plot by meanClass", x = "Column Names", y = "Counts") +
  scale_color_manual(values = colors_nor, name = "meanClass") +
  theme_classic()
```



[ ]:
```
ggsave(file = "KMeans_OCCN_curve.png", plot = Plot_OCCN_70Curves, width = 14,␣
↪height = 8, dpi = 600)
```

1.4 Re-Group the K-Means results using Hierarchical Clustering

1.4.1 Step 1: Choose the Optimal number for these K-Means results

[18]:
```
#define linkage methods
m <- c( "average", "single", "complete", "ward")
names(m) <- c( "average", "single", "complete", "ward")

#function to compute agglomerative coefficient
ac_OCCN <- function(x) {
```

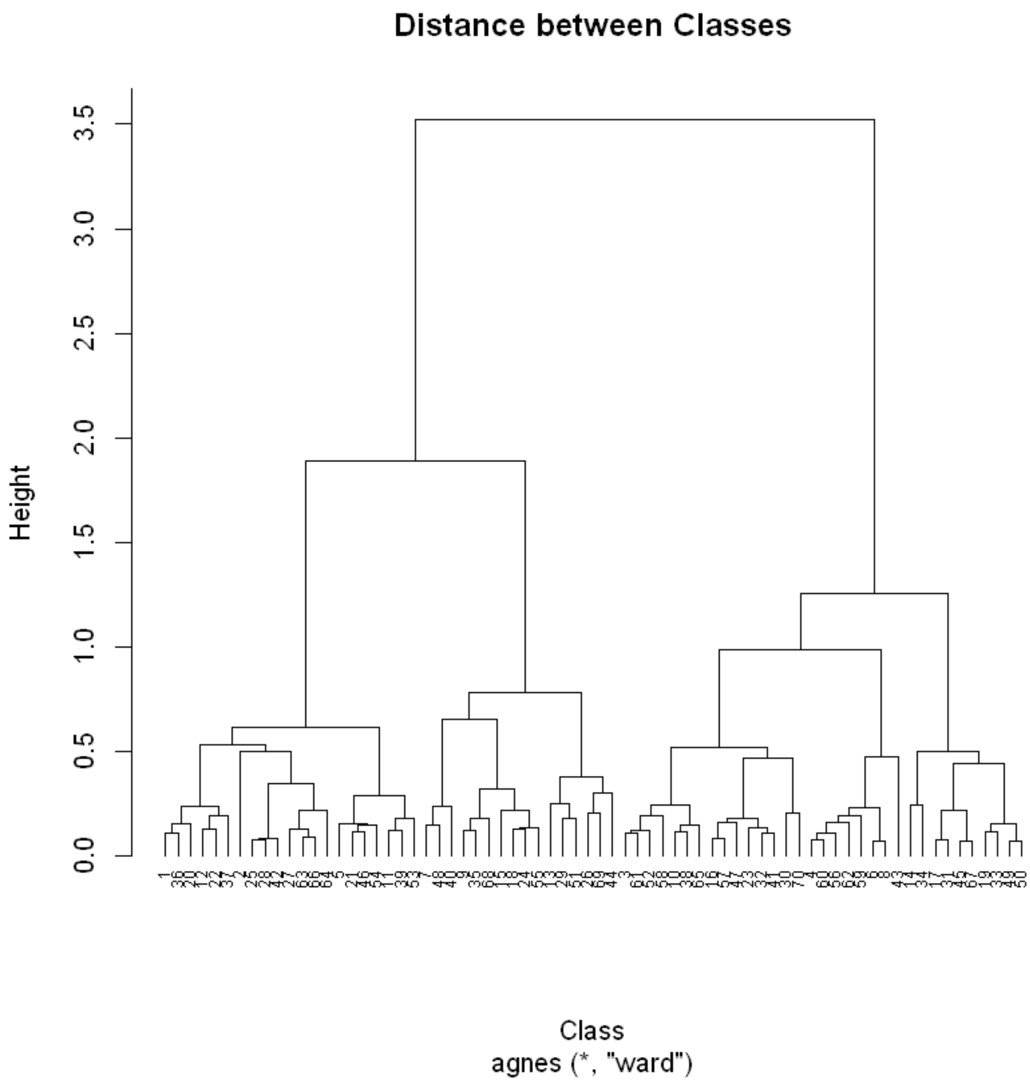
```
  agnes(Ras_OCCN_clusterMean[,-ncol(Ras_OCCN_clusterMean)], method = x)$ac
}

#calculate agglomerative coefficient for each clustering linkage method
coefficients_OCCN <- sapply(m, ac_OCCN)

# Find the method with the largest coefficient
best_OCCN_method <- names(coefficients_OCCN)[which.max(coefficients_OCCN)]
```

[19]:
```
#perform hierarchical clustering using Ward's minimum variance
clust_OCCN <- agnes(Ras_OCCN_clusterMean[,-ncol(Ras_OCCN_clusterMean)], method␣
↪= best_OCCN_method)

#produce dendrogram
pltree(clust_OCCN, cex = 0.6, hang = -1,
       xlab = "Class", main = 'Distance between Classes')
```



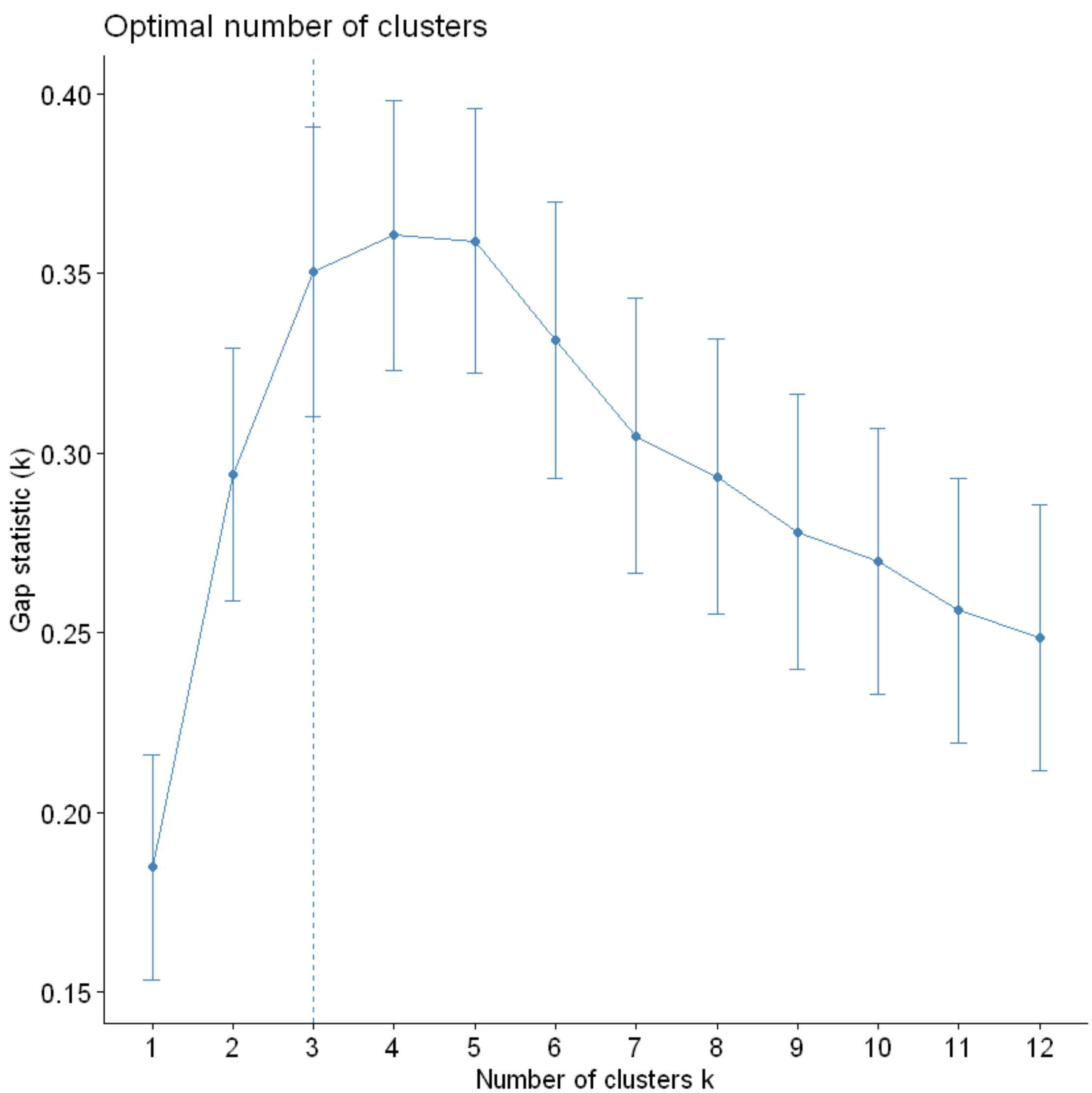
[20]:

```
### Pick the best regroup number
#calculate gap statistic for each number of clusters (up to 12 clusters)
gap_OCCN_stat <- clusGap(Ras_OCCN_clusterMean[,-ncol(Ras_OCCN_clusterMean)], FUN = hcut,
                    nstart = 25, K.max = 12, B = 50)

#produce plot of clusters vs. gap statistic
fviz_gap_stat(gap_OCCN_stat)

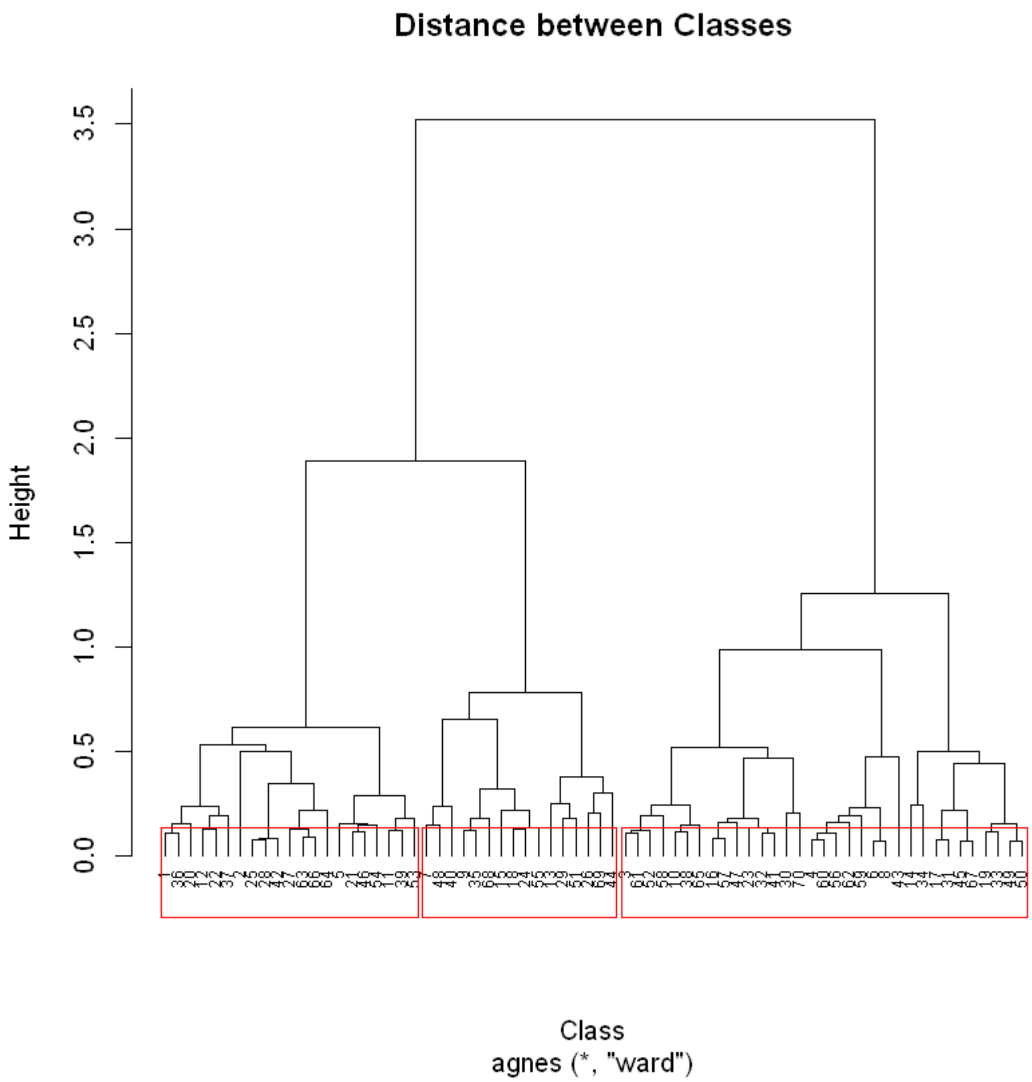
###problem here
num_OCCN_gr <- with(gap_OCCN_stat,maxSE(Tab[,"gap"],Tab[,"SE.sim"]))

Ras_OCCN_groups <- cutree(clust_OCCN, k=num_OCCN_gr)
```



[21]:
```
#produce dendrogram
pltree(clust_OCCN, cex = 0.6, hang = -1,
       xlab = "Class", main = 'Distance between Classes')

# Add rectangles to highlight clusters
rect.hclust(clust_OCCN, k = num_OCCN_gr, border = "red")
```



1.4.2 Step 2: Combine the K-Means and Hierarchical results together

[22]:
```
#find number of observations in each cluster
table(Ras_OCCN_groups)

#append cluster labels to original data
Ras_OCCN_regroup <- cbind(Ras_OCCN_clusterMean, regroup = Ras_OCCN_groups)

#display first six rows of final data
head(Ras_OCCN_regroup)
```

```
Ras_OCCN_groups
 1  2  3
```

21 33 16

A data.frame: 6 × 7

	O16 <dbl>	C12 <dbl>	C13 <dbl>	CN26 <dbl>	CN27 <dbl>	class <fct>	regroup <int>
1	0.0799946	0.50324781	0.44042678	0.39610196	0.25607846	1	1
2	0.3332785	0.76192110	0.69186000	0.14963650	0.12112609	2	1
3	0.3559697	0.31630688	0.27703542	0.12596410	0.07810824	3	2
4	0.4692743	0.09682117	0.08345702	0.06319495	0.04720071	4	2
5	0.3477244	0.44405965	0.39919035	0.24572208	0.20366407	5	1
6	0.5129381	0.03777648	0.03201914	0.03502878	0.02591258	6	2

[23]:
```
### Generate the Regroup df
gr_OCCN_cl <- as.data.frame(table(Ras_OCCN_groups))
gr_OCCN_cl
```

A data.frame: 3 × 2

Ras_OCCN_groups <fct>	Freq <int>
1	21
2	33
3	16

[24]:
```
## Create suitable color list
# Initialize an empty list to store color palettes
color_palettes <- list()

# Iterate through each row in the dataframe
for (i in 1:nrow(gr_OCCN_cl)) {
  gr_bcolor <- base_colors[i]
  gr_color_w <- sapply(gr_bcolor,
                   function(color) colorRampPalette(c(color,␣
↪"white"))(gr_OCCN_cl$Freq[i] + 1))
  gr_color <- gr_color_w[-nrow(gr_color_w), ]
  color_palettes[[i]] <- gr_color
}

# Create a named list of color palettes
colors_OCCN_list <- setNames(color_palettes, gr_OCCN_cl$groups)                ␣
↪
colors_OCCN_list[[1]]
```

1. '#FF0000' 2. '#FF0C0C' 3. '#FF1818' 4. '#FF2424' 5. '#FF3030' 6. '#FF3C3C' 7. '#FF4848' 8. '#FF5555' 9. '#FF6161' 10. '#FF6D6D' 11. '#FF7979' 12. '#FF8585' 13. '#FF9191' 14. '#FF9D9D' 15. '#FFAAAA' 16. '#FFB6B6' 17. '#FFC2C2' 18. '#FFCECE' 19. '#FFDADA' 20. '#FFE6E6' 21. '#FFF2F2'

1.4.3 Step 3: Visualize the Regrouped Clustering Curves

[25]:
```
## Plot the regroup plot
# Create a grid layout
cols <- 3  # Number of columns in the grid
rows <- ceiling(num_OCCN_gr / cols)  # Number of rows in the grid
```

[26]:
```
# Create a function to draw curve plots for each group
draw_curve_plot <- function(data, group) {
  # Filter data for the current group
  group_data <- subset(data, group == regroup)

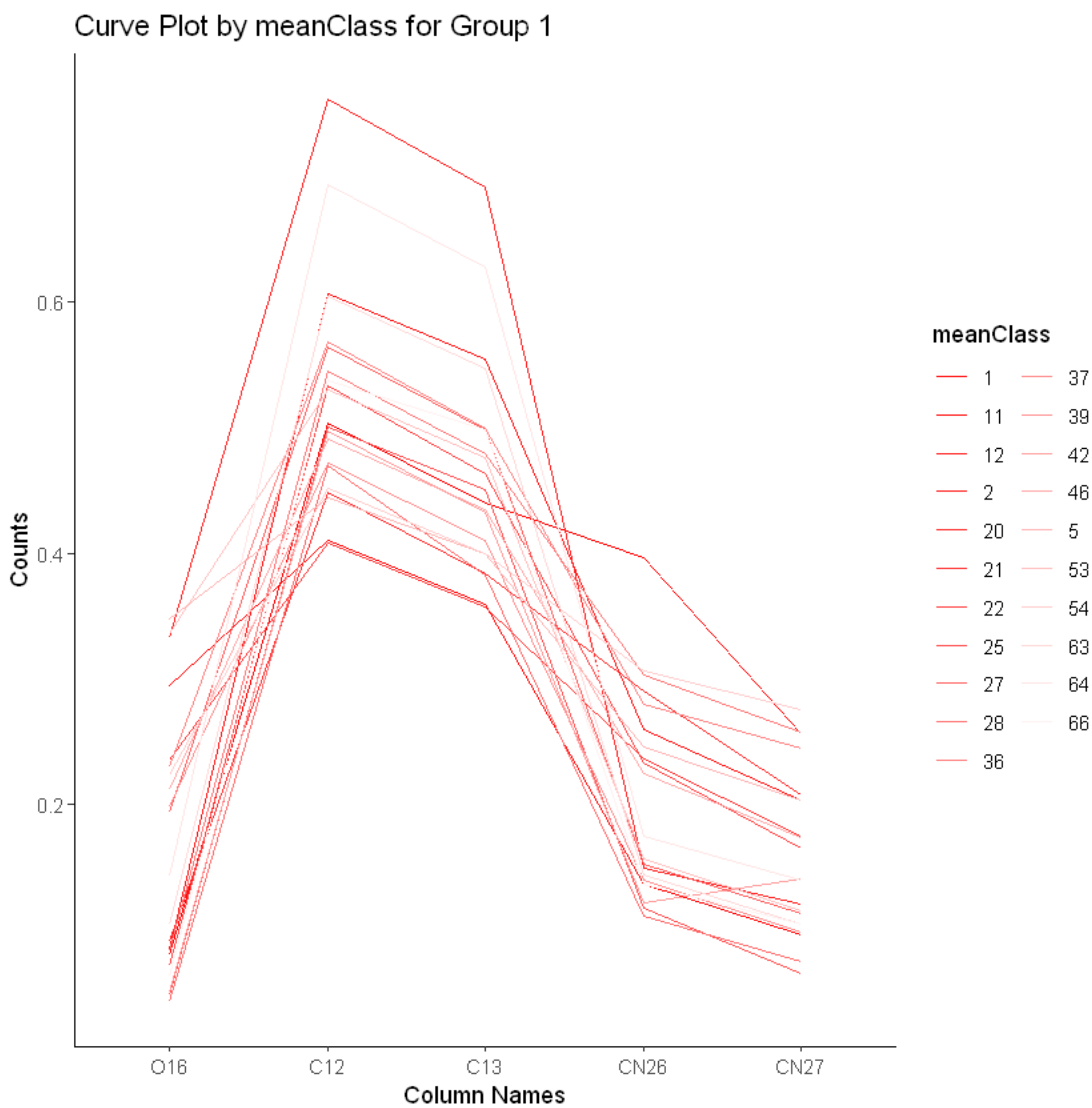
  # Create a long-format dataframe for plotting
  plot_data <- reshape2::melt(group_data, id.vars = c("class", "regroup"))

  # Create a plot for the current group
  p <- ggplot(plot_data, aes(x = variable, y = value, color = class, group =␣
↪class)) +
    geom_line() +
    labs(title = paste("Curve Plot by meanClass for Group", group),
         x = "Column Names", y = "Counts") +
    scale_color_manual(values = colors_OCCN_list[[as.numeric(group)]], name =␣
↪"meanClass")+
    theme_classic()

  return(p)
}
```

[32]:
```
# Loop through each group and draw the curve plot
group_OCCN_list <- unique(Ras_OCCN_regroup$regroup)
plot_OCCN_list <- lapply(group_OCCN_list, draw_curve_plot, data =␣
↪Ras_OCCN_regroup)
```

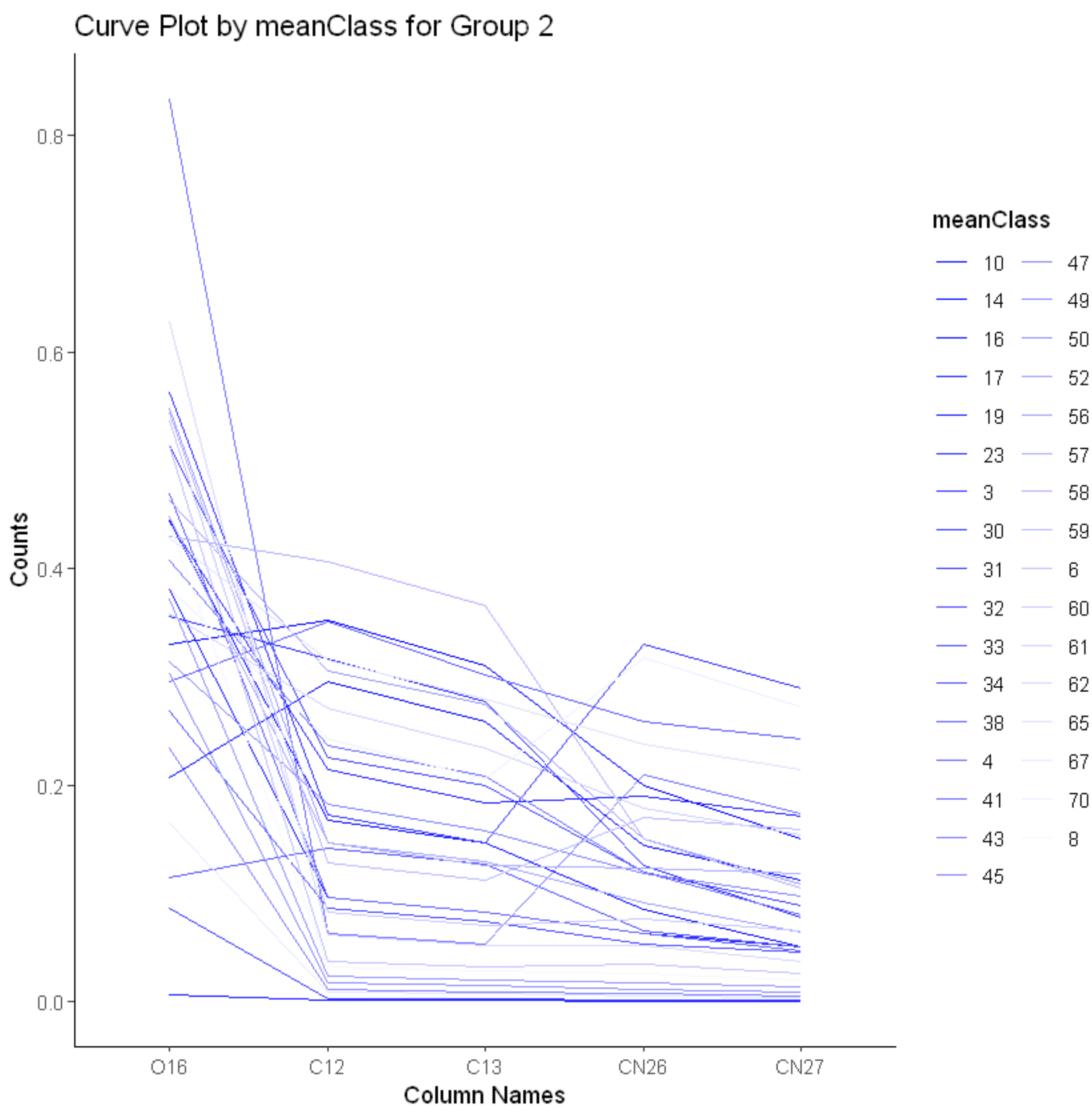
[28]:
```
plot_OCCN_list
```

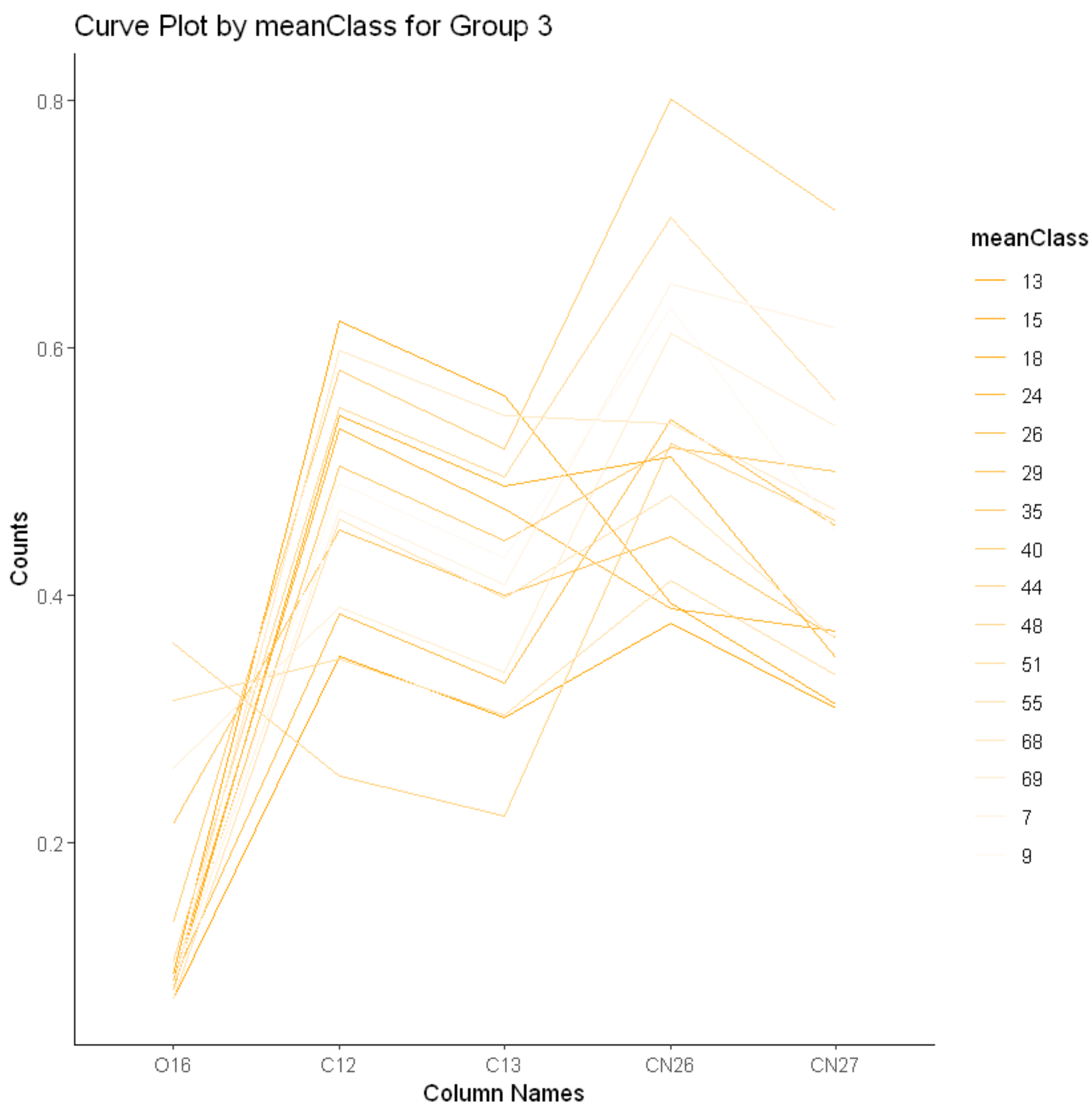

Curve Plot by meanClass for Group 1
Counts
0.6
0.4
0.2
O16
C12
C13
CN26
CN27
Column Names
meanClass
1
11
12
2
20
21
22
25
27
28
36
37
39
42
46
5
53
54
63
64
66

[[1]]

[[2]]

[[3]]


Curve Plot by meanClass for Group 2
Counts
0.8
0.6
0.4
0.2
0.0
O16
C12
C13
CN26
CN27
Column Names
meanClass
10
14
16
17
19
23
3
30
31
32
33
34
38
4
41
43
45
47
49
50
52
56
57
58
59
6
60
61
62
65
67
70
8



[ ]:
```
ggsave(file = "KMeans_OCCN_regroup_curve.png", plot = grid_OCCN, width = 18,␣
  ↪height = 8, dpi = 600)
```

1.4.4 Step 4: Visualize the Regrouped plot

[29]:
```
## Assign regroup result into df
# Assign group information from df1 to df2 based on common class numbers
Ras_OCCN_cluster$regroup <-␣
  ↪Ras_OCCN_regroup$regroup[match(Ras_OCCN_cluster$class,␣
  ↪Ras_OCCN_regroup$class)]

# Split regroup
```

```
split_OCCN_df <- split(Ras_OCCN_cluster, Ras_OCCN_cluster$regroup)
```

[30]:
```
# Create a list to store modified data frames
colored_OCCN_dfs <- list()

# Loop through the list of dataframes and assign colors sequentially
for (i in as.numeric(names(split_OCCN_df))) {
  df <- split_OCCN_df[[i]]
  colors <- colors_OCCN_list[[i]]

  # Step 1: Already done in the loop
  # Step 2: Get unique levels of 'class' column
  level_df <- levels(as.factor(df$class))

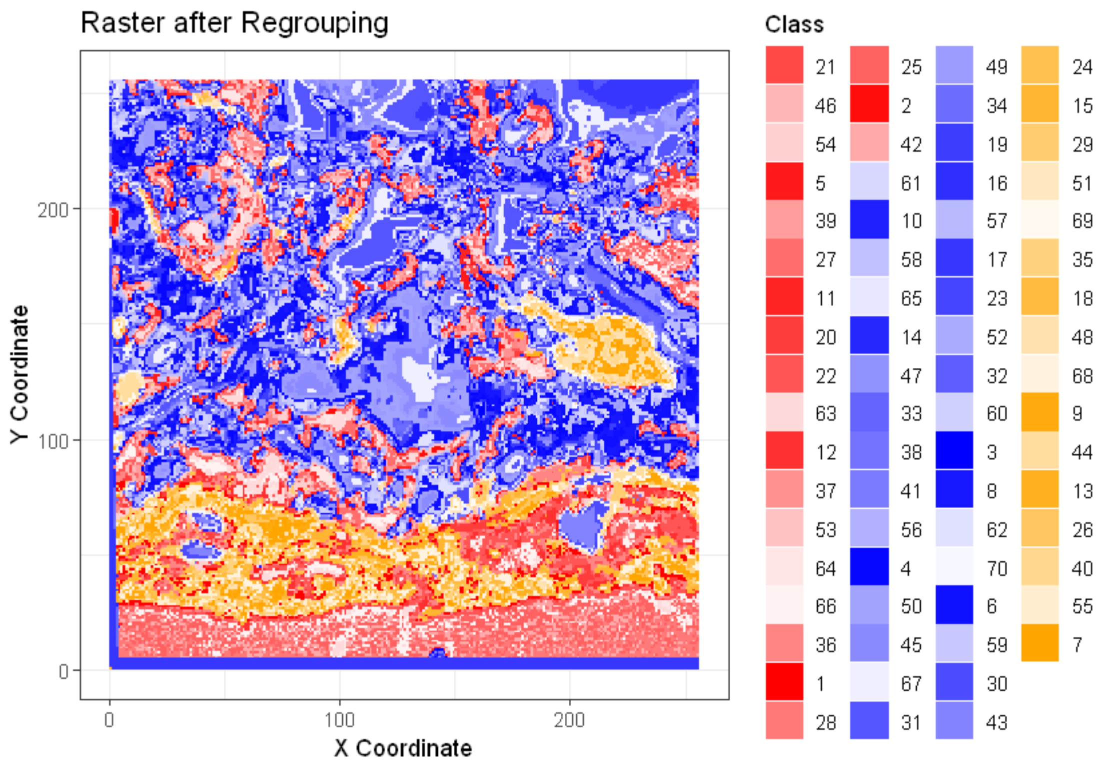
  # Step 3: Assign colors based on matching levels
  for (m in 1:length(df$class)) {
    for (n in 1:length(level_df)) {
      if (df$class[m] == level_df[n]) {
        df$color[m] <- colors[n]
        break  # No need to continue checking once matched
      }
    }
  }
  colored_OCCN_dfs[[i]] <- df
}

Ras_OCCN_re_col <- do.call(rbind, colored_OCCN_dfs)
```

[31]:
```
# Create a filled pixel plot

Ras_OCCN_re_col$class <- factor(Ras_OCCN_re_col$class)
Ras_OCCN_re_col$regroup <- factor(Ras_OCCN_re_col$regroup)

ggplot(Ras_OCCN_re_col, aes(x = x, y = y, fill = Ras_OCCN_re_col$class)) +
  geom_tile() +
  labs(title = "Raster after Regrouping",
       x = "X Coordinate", y = "Y Coordinate",
       fill = "Class") +
  scale_fill_manual(values = Ras_OCCN_re_col$color,
                    breaks = Ras_OCCN_re_col$class,
                    labels = Ras_OCCN_re_col$class) +
  coord_fixed(ratio = 1) +
  geom_rect(xmin = 0, xmax = 1, ymin = 0, ymax = 1) +
  theme(legend.position = "right") +
  theme_bw()
```



Raster after Regrouping
Y Coordinate
X Coordinate
0
100
200
Class
21
46
54
5
39
27
11
20
22
63
12
37
53
64
66
36
1
28
25
2
42
61
10
58
65
14
47
33
38
41
56
4
50
45
67
31
49
34
19
16
57
17
23
52
32
60
3
8
62
70
6
59
30
43
24
15
29
51
69
35
18
48
68
9
44
13
26
40
55
7