# Feature Space Diagrams in R

Testing the methods on Epileptic Seizure Recognition Dataset

John Erickson

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#### Introduction

This is a first effort to implement "feature space diagrams" in R, inspired by https://towardsdatascience.com/escape-the-correlation-matrix-into-feature-space-4d71c51f25e5

```
#library(devtools)
#install_github("vqv/ggbiplot")
library(ggbiplot)
library(lessR)
library(Hmisc)
library(corrplot)
library(gplots)
library(igraph)
library(tidyverse)
library(ggrepel)
library(shiny)
library(plotly)
library(ggrepel)
```

#### Workflow

Our workflow is generally as described in the original post:

- Generate the correlation matrix
- Take the absolute value of correlation matrix and subtract each value from 1. The result is a distance matrix.
- Use PCA to reduce our NxN matrix to Nx2.
- Plot each feature's location using the two principal components.
- Use Feature Agglomeration to generate feature clusters.
- Color each feature by its cluster.
- Draw lines to represent relationships of at least r = 0.7 (or user's choosing)

### Data Load

```
# TODO: User uploads data
# Load data
#boston <- read.csv("boston.csv", header = TRUE, fileEncoding="latin1")
#WDBC <- read.csv("WDBC.csv", header = TRUE, fileEncoding="latin1")
esr <- read.csv("EpilepticSeizureRecognition.csv", header = TRUE, fileEncoding="latin1")
# Ensure we have a matrix
#mydata <- na.omit(as.matrix(boston))</pre>
```

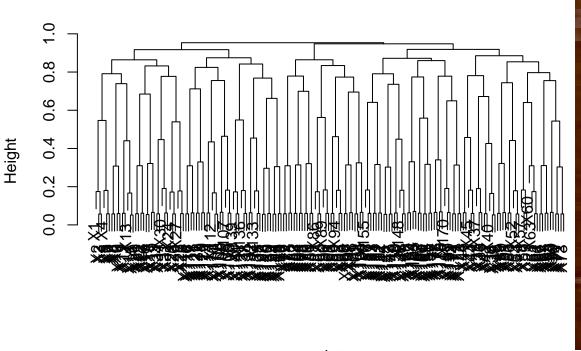
```
mydata <- na.omit(as.matrix(esr[,2:179]))
#mydata <- as.matrix(mtcars[,c(1:7,10,11)])</pre>
```

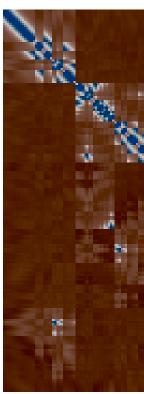
### **Initial Correlation Matrix**

```
# Simple correlation matrix calculation
# TODO: user chooses method
#mydata.cor <- cor(mydata, method = c("pearson"), use = "complete.obs")
#mydata.cor <- cor(mydata, method = c("kendall"), use = "complete.obs")
mydata.cor <- cor(mydata, method = c("spearman"), use = "complete.obs")

# # Optional
# corrplot(mydata.cor)
#
# palette <- colorRampPalette(c("green", "white", "red")) (20)
# heatmap.2(x = mydata.cor, col = palette, symm = TRUE)

# Reorder correlation matrix based on: https://rdrr.io/cran/lessR/man/corReorder.html
mydata.cor.ro <- corReorder(mydata.cor)</pre>
```





dst hclust (\*, "complete")

### **Distance Matrix Calculation**

Correlation can often be used as a distance metric for hierarchical clustering; see e.g. this discussion.

We're using the dist() function to provide a number of different distance options (default is euclidean distance).

```
# # Simplistic distance matrix (Absolute value et.al.)
# mydata.cor.ro.1 <- abs(mydata.cor.ro) - 1

# Distance Matrix via: https://stat.ethz.ch/R-manual/R-devel/library/stats/html/dist.html
mydata.dist <- dist(mydata.cor.ro, upper = TRUE, method = "manhattan")
mydata.dist.sym <- as.matrix(mydata.dist )</pre>
```

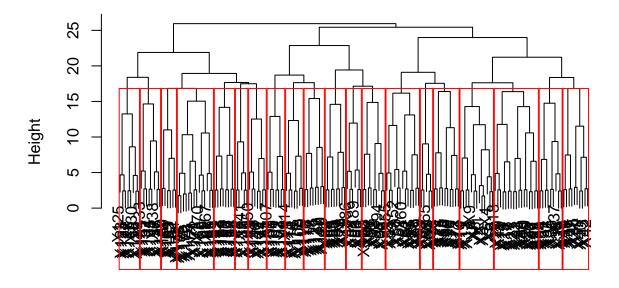
## Hiearchical/Agglomerative Clustering (NEW)

```
# See eg:
# * https://metudatascience.github.io/datascience/clustering.html
# * https://uc-r.github.io/hc_clustering

# Distance calculated above
mydata.hclust <- hclust(mydata.dist)
plot(mydata.hclust)

# NOTE! These clusters are in numerical order, not feature order!
mydata.hclust.groups <- cutree(mydata.hclust, k=20) # Usually 3 is used for mtcars demos
rect.hclust(mydata.hclust, k=20, border="red")</pre>
```

# **Cluster Dendrogram**



mydata.dist hclust (\*, "complete")

## PCA on Distance Matrix

```
# PCA
#mydata.dist.sym.pca <- prcomp(mydata.dist.sym,scale=TRUE)
mydata.dist.sym.pca <- prcomp(mydata.dist.sym) # Un-scaled gives results closer to source article</pre>
```

```
# Plottable version:
mydata.dist.sym.pca.plot <- as.data.frame(mydata.dist.sym.pca$x[,1:2])</pre>
```

## Finding the Clusters

Write the cluster assignments and the feature names into the PCA data frame.

```
# Pull out our clusters (calculated)
mydata.dist.sym.pca.plot$cluster <- as.factor(mydata.hclust.groups)
mydata.dist.sym.pca.plot$name <- rownames(mydata.cor.ro)</pre>
```

## Finding the Graph!

This is the hard part...

```
# Determine connectivity!
# This selects the nodes (features) we want to connect
threshold <- 5.5
selector <- ((abs(mydata.dist.sym) <= threshold ) * 1) # Filter out lines greater than threshold distan
for (i in 1:length(mydata.dist.sym.pca.plot$cluster)) {selector[,i] <- selector[,i] * as.numeric(mydata</pre>
diag(selector) <- 0
filtered <- abs(mydata.dist.sym)</pre>
filtered[ filtered <= threshold ] <- 0</pre>
# Get the function for re-scaling the line weights
# Line thicknesses will automatically range from 1-10
range \leftarrow c(1,10)
domain <- c(min(filtered[filtered > 0]),max(filtered))
line.lm <- lm(range~domain)</pre>
adjust <- function(x){</pre>
  # stupid lm trick to scale
    line.lm$coefficients[[2]] * x + line.lm$coefficients[[1]]
 }
# Repeat selector matrix, this time for strength of relationships
# Select the nodes (features) we want to connect
thickness <- ((abs(mydata.dist.sym) <= threshold ) * 1) # Filter out lines greater than threshold dista
diag(thickness) <- 0 # remove diagonal</pre>
# Use distances as thicknesses for the arcs we're keeping
for (i in 1:length(mydata.dist.sym.pca.plot$cluster)) {
 for (j in 1:length(thickness[,i])) {
    if (thickness[j,i] != 0 ) {
       thickness[j,i] \leftarrow adjust(thickness[j,i] * abs(mydata.dist.sym[j,i]))
      thickness[j,i] <- thickness[j,i] * abs(mydata.dist.sym[j,i])</pre>
    } else { thickness[j,i] <- 0}</pre>
 }
diag(thickness) <- 0</pre>
```

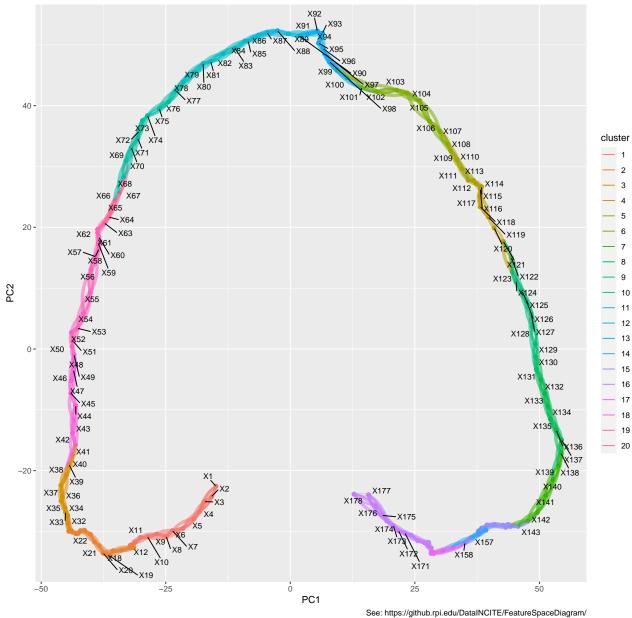
```
# Switching to networks
# Create igraph structure
network <- graph from adjacency matrix(selector, weighted = TRUE)</pre>
network.t <- graph_from_adjacency_matrix(thickness, weighted = TRUE)</pre>
# Gets us our edges!
mydata.edges <- get.data.frame(network) %>% # this is where "weight" is introduced
  dplyr::rename(Cluster = weight)
mydata.edges.t <- get.data.frame(network.t) %>% # this is where "weight" is introduced
  dplyr::rename(thickness = weight) %>%
# mutate(thickness = as.integer(thickness))
 mutate(thickness = thickness)
# replace `from` with X1 and Y1, and `to` with X2 and Y2
# These will be our line segments!
mydata.segments <- mydata.edges %>%
 left_join(mydata.dist.sym.pca.plot, by=c("from"="name")) %>%
  dplyr::select(-cluster) %>%
  mutate(X1=PC1, Y1=PC2) %>%
  dplyr::select(-PC1, -PC2)
mydata.segments <- mydata.segments %>%
  left_join(mydata.dist.sym.pca.plot, by=c("to"="name")) %>%
  dplyr::select(-cluster) %>%
  mutate(X2=PC1, Y2=PC2) %>%
  dplyr::select(-PC1, -PC2)
mydata.segments <- mydata.segments %>%
  dplyr::rename(cluster = Cluster)
mydata.dist.sym.pca.plot$cluster <- as.factor(mydata.dist.sym.pca.plot$cluster)</pre>
# NEW: cluster used for coloring
mydata.segments$cluster <- as.factor(mydata.segments$cluster)</pre>
#mydata.segments$thickness <- as.integer(mydata.edges.t$thickness)</pre>
mydata.segments$thickness <- mydata.edges.t$thickness</pre>
```

### Building the Plot

```
# Adding line segments to PCA plot
p <- ggplot(mydata.dist.sym.pca.plot, aes(x=PC1, y=PC2)) +
    geom_point(aes(color=cluster, size=6), show.legend = FALSE) +
    geom_curve(aes(x=X1, y=Y1, xend=X2, yend=Y2, color=cluster, size=thickness, alpha=0.4), curvature=0.2
    guides(alpha = FALSE) +
    scale_size(range = c(0.1, 2), guide = guide_none()) +
    geom_text_repel(aes(label=name),hjust=1, vjust=0, size=3) +
    labs(title="Feature Space Diagram for the Boston Housing data set") +
    labs(title="Feature Space Diagram for the Wisconsin Breast Cancer data set") +
    labs(title="Feature Space Diagram for the Epileptic Seizure Recognition Dataset") +
    labs(title="Feature Space Diagram for the classic `mtcars` data set") +
    labs(caption = "See: https://github.rpi.edu/DataINCITE/FeatureSpaceDiagram/")</pre>
```

p





ggsave(filename="fsd\_esr.png", plot = p)

## Saving 10 x 10 in image

## Sanity check: Biplot on the original dataset

Usually we review the feature space using a PCA biplot. Let's see how it compares!