Data reduction (PCA)

- Principal component analysis (PCA) is an *unsupervised* technique that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components (PCs).
- Mathematically, the *j*th PC can be written as

$$\text{PC}_j = (a_{j1} \times \text{Predictor } 1) + (a_{j2} \times \text{Predictor } 2) + \cdots + (a_{jP} \times \text{Predictor } P)$$

where *P* is the number of predictors.

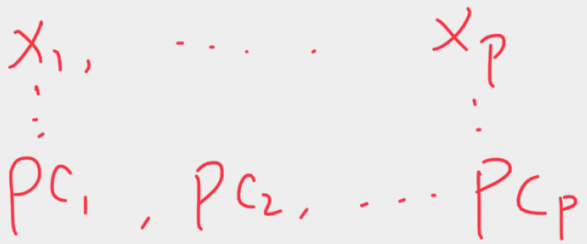
$\text{Predictor } 1 \approx X_1$, $\text{Predictor } 2 \approx X_2$, $\text{Predictor } P \approx X_P$

$\text{Cor}(PC_1, PC_2) \approx 0$

$\text{Cor}(X_1, X_2)$ is large

Remarks of PCA

- When predictors are on different scales and/or have skewed distributions, we need to
  - transform skewed data
  - center and scale data



- PCA is blind to the response (unsupervised learning)
- Use a *scree plot* to determine the number of principal components to retain. PC_s
  - The rule of thumb: the component number prior to the tapering off of variation is the maximal component that is retained.

R codes for PCA

```
library(caret)
## Use caret's preProcess function to transform for skewness
segPP <- preProcess(segTrainX, method = "BoxCox")

## Apply the transformations
segTrainTrans <- predict(segPP, segTrainX)
## R's prcomp is used to conduct PCA
pr <- prcomp(~AvgIntenCh1 + EntropyIntenCh1,
             data = segTrainTrans,  scale. = TRUE)

xyplot(AvgIntenCh1 ~ EntropyIntenCh1, data = segTrainTrans,
       groups = segTrain$Class,
       xlab = "Channel 1 Fiber Width",
       ylab = "Intensity Entropy Channel 1",
       auto.key = list(columns = 2), type = c("p", "g"),
       main = "Original Data", aspect = 1)
```

PCA:

skewness

{ centering & scaling

no response variable

Check the plot when you specify

- auto.key =FALSE
- auto.key = TRUE

R codes for PCA

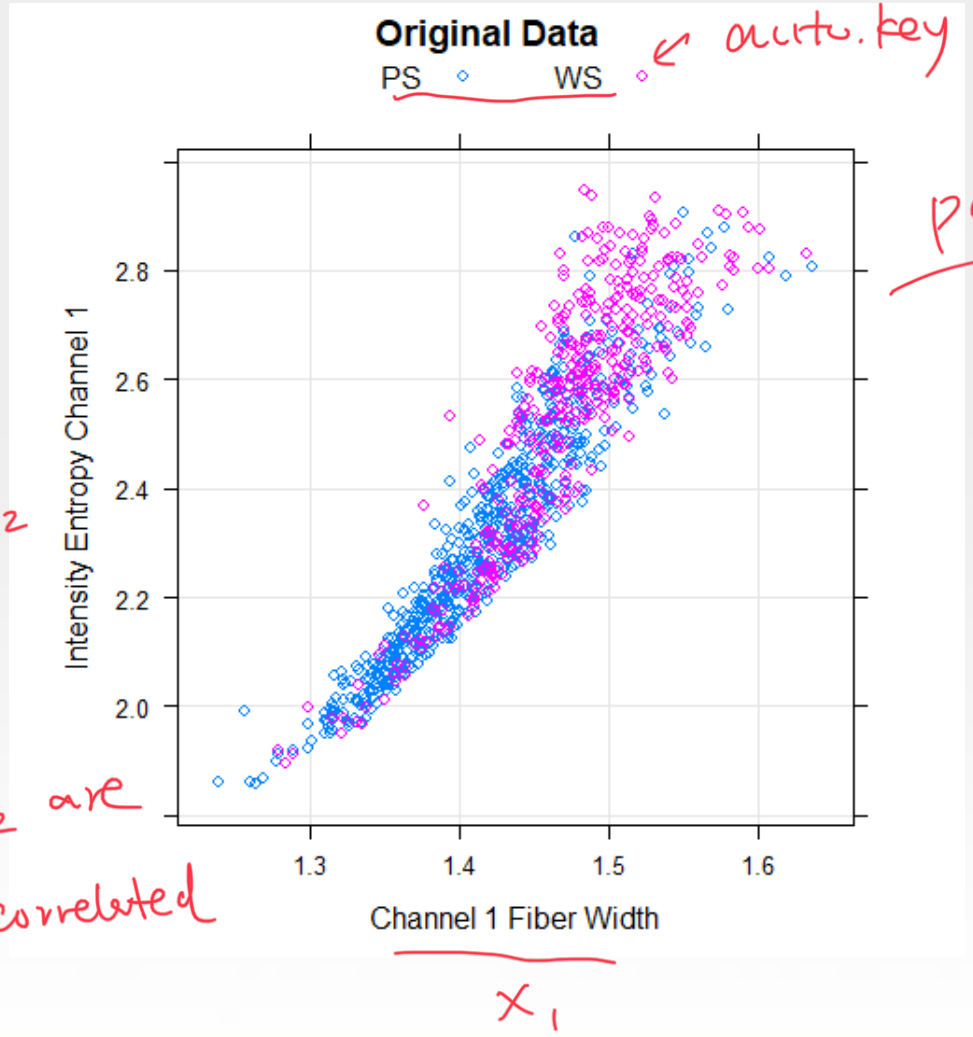
```
xyplot(PC2 ~ PC1,
      data = as.data.frame(pr$x),
      groups = segTrain$Class,
      xlab = "Principal Component #1",
      ylab = "Principal Component #2",
      main = "Transformed",
      xlim = extendrange(pr$x),
      ylim = extendrange(pr$x),
      type = c("p", "g"), aspect = 1)
```

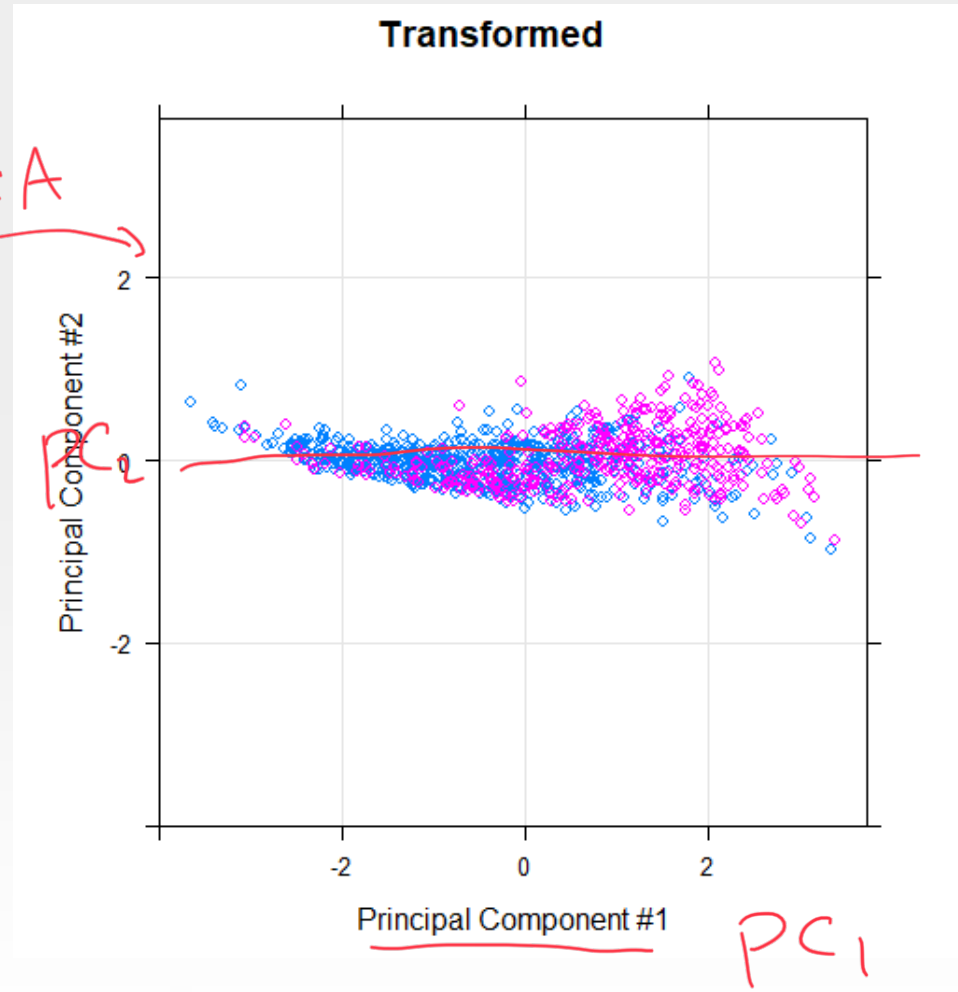
"p" → point; "g" → grid of the plot

For xyplot's type, you may refer to https://stat.ethz.ch/R-manual/R-devel/library/lattice/html/panel.xyplot.html

Extendrange: Extends a numerical range by a small percentage

PC transformation for the cell segmentation data

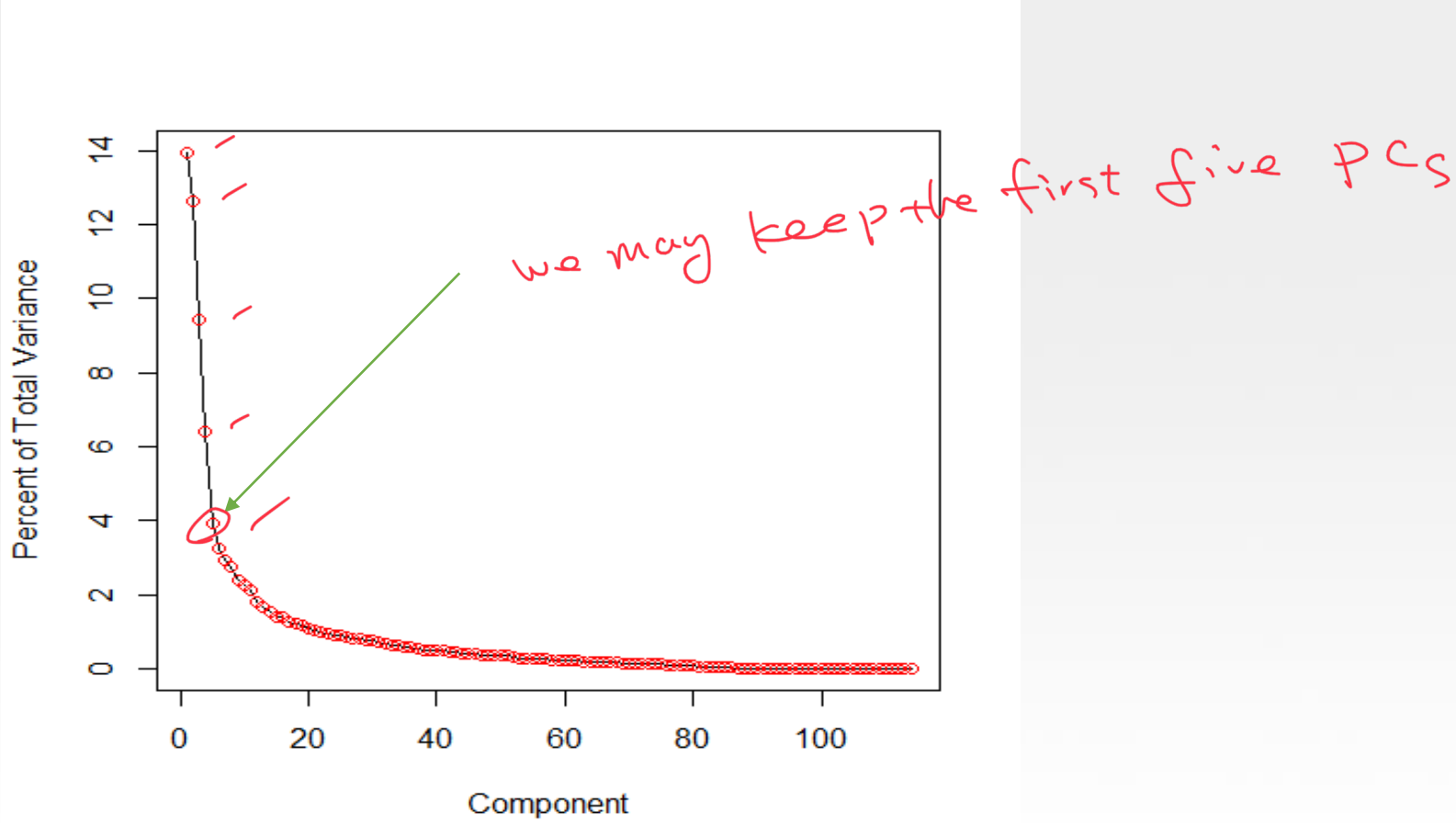




Fit PCA to entire set of segmentation data

```
## There are a few predictors with only a single value, so we remove these first
## (since PCA uses variances, which would be zero)

isZV <- apply(segTrainX, 2, function(x) length(unique(x)) == 1)  #identify the predictor with a single value
segTrainX <- segTrainX[, !isZV]

segPP <- preProcess(segTrainX, c("BoxCox", "center", "scale"))
segTrainTrans <- predict(segPP, segTrainX)

segPCA <- prcomp(segTrainTrans, center = TRUE, scale. = TRUE)

#Scree plot
PTotalVariance = (segPCA$sdev^2)/sum(segPCA$sdev^2)*100
ts.plot(PTotalVariance, xlab='Component', ylab='Percent of Total Variance')
points(PTotalVariance, col=2)
```

A "scree plot" where the percentage of the total variance explained by each component



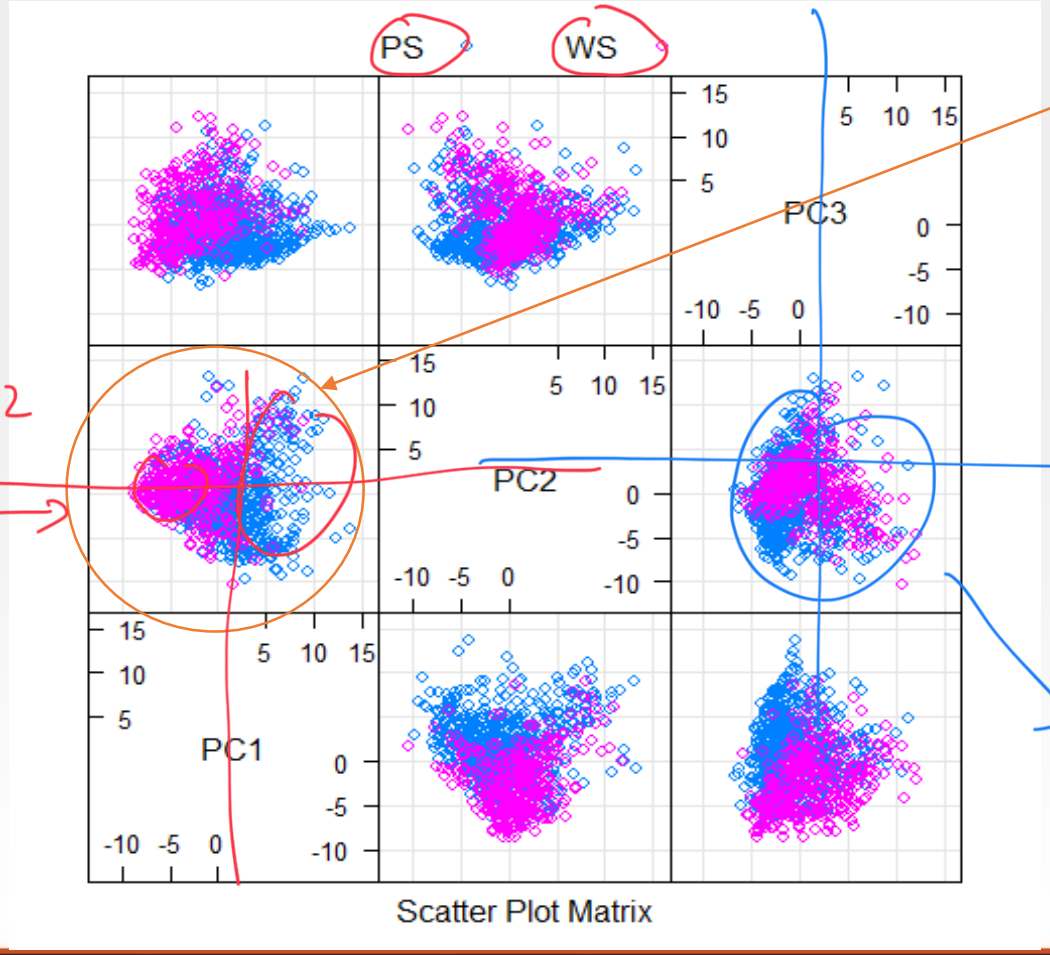
Plot a scatterplot matrix of the first three components

```
panelRange <- extendrange(segPCA$x[, 1:3])
splom(as.data.frame(segPCA$x[, 1:3]), #a data matrix consisting of three PCs
      groups = segTrainClass,
      type = c("p", "g"),
      auto.key = list(columns = 2),
      prepanel.limits = function(x) panelRange)
```

first three PCs

- *splom*: draw conditional scatter plot matrices and parallel coordinate plots.
- You may refer to http://127.0.0.1:29519/library/lattice/html/splom.html

A plot of the first three principal components for the cell segmentation data, colored by cell type



PC1 and PC2

Some separation between the class when plotting the first and second components

PC2 vs. PC3

Implement a series of transformations to multiple data

- The *caret* class *preProcess* has the ability to transform, center, scale, or impute values, as well as apply the spatial sign transformation and feature extraction.
- The *preProcess* function can be integrated into the *train* function for constructing predictive models.
- For example, to Box–Cox transform, center, and scale the data, then execute PCA for signal extraction.

R code

```
#Implement a series of transformations to multiple data
trans <- preProcess(segTrainX, method = c("BoxCox", "center", "scale", "pca"))
trans

# Apply the transformations:
transformed <- predict(trans, segTrainX)
# These values are different than the previous PCA components since
# they were transformed prior to PCA
head(transformed[, 1:6])
```

predict matrix

Implement a series of transformations to multiple data

```
> #Implement a series of transformations to multiple data
> trans <- preProcess(segTrainX, method = c("BoxCox", "center", "scale", "pca"))
> trans
Created from 1009 samples and 114 variables

Pre-processing:
  - Box-Cox transformation (47)
  - centered (114)
  - ignored (0)
  - principal component signal extraction (114)
  - scaled (114)

Lambda estimates for Box-Cox transformation:
    Min.  1st Qu.   Median     Mean  3rd Qu.     Max.
-2.00000 -0.50000 -0.10000  0.05106  0.30000  2.00000

PCA needed 55 components to capture 95 percent of the variance
```

114 predictors → 100% of variance

55 Pc → 95% of the variance

dimension reduction

Implement a series of transformations to multiple data

```
> # Apply the transformations:
> transformed <- predict(trans, segTrainX)
> # These values are different than the previous PCA components since
> # they were transformed prior to PCA
> head(transformed[, 1:6])
          PC1        PC2        PC3        PC4        PC5        PC6
2   4.3560119 10.1198090  0.2870062 -0.8592671 -5.2499525  0.7331065
3  -0.5444723  1.6283869 -1.6533073 -3.8354232 -1.2555453  1.2558205
4   3.5512811 -0.5033273 -1.4852323 -1.0083940 -1.1571055 -3.2644940
12 -0.4318782 -1.7221518  0.9324858 -4.1005766 -2.4346531 -1.3982350
15  0.4826446 -0.6522716 -1.4394427 -4.6004477 -1.6368873 -0.7714049
16 -0.7522627  0.5447819 -0.3864860 -3.3520698 -0.1278511  1.7248114
```

Dealing with missing values

- In many cases, some predictors have no values for a given sample.
- Rubin (1976) classified missing data into three mechanisms, namely,
  - Missing completely at random (MCAR), where the missing process is completely independent from observed and missing quantities;
  - Missing at random (MAR), where the missing process depends on observed quantities, but not on missing quantities;
  - Nonignorable missing or not missing at random (NMAR), where the missing process may depend on both observed and missing quantities.
- The missing data mechanism could be ignored if the missingness is either MCAR or MAR. However, if the data are NMAR then the mechanism is not ignorable.

Dealing with missing values

- Understand *why* the values are missing
- Some methods
  - Remove the missing data (not applicable for NMAR!)
  - Some predictive models, such as tree-based techniques, can account for missing data
  - Imputing the missing data (Use MICE package in R)
  - Please refer to https://www.r-bloggers.com/imputing-missing-data-with-r-mice-package/

Removing predictors

- Few predictors means decreased computational time and complexity.
- Removing highly correlated predictors could promise the performance of the model and might lead to a more parsimonious and interpretable model.
- Removing predictors with degenerate distributions (e.g., near-zero variance predictor) could be a significant improvement in model performance and/or stability without the problematic variables.

Lasso

Algorithm for removing highly correlated predictors

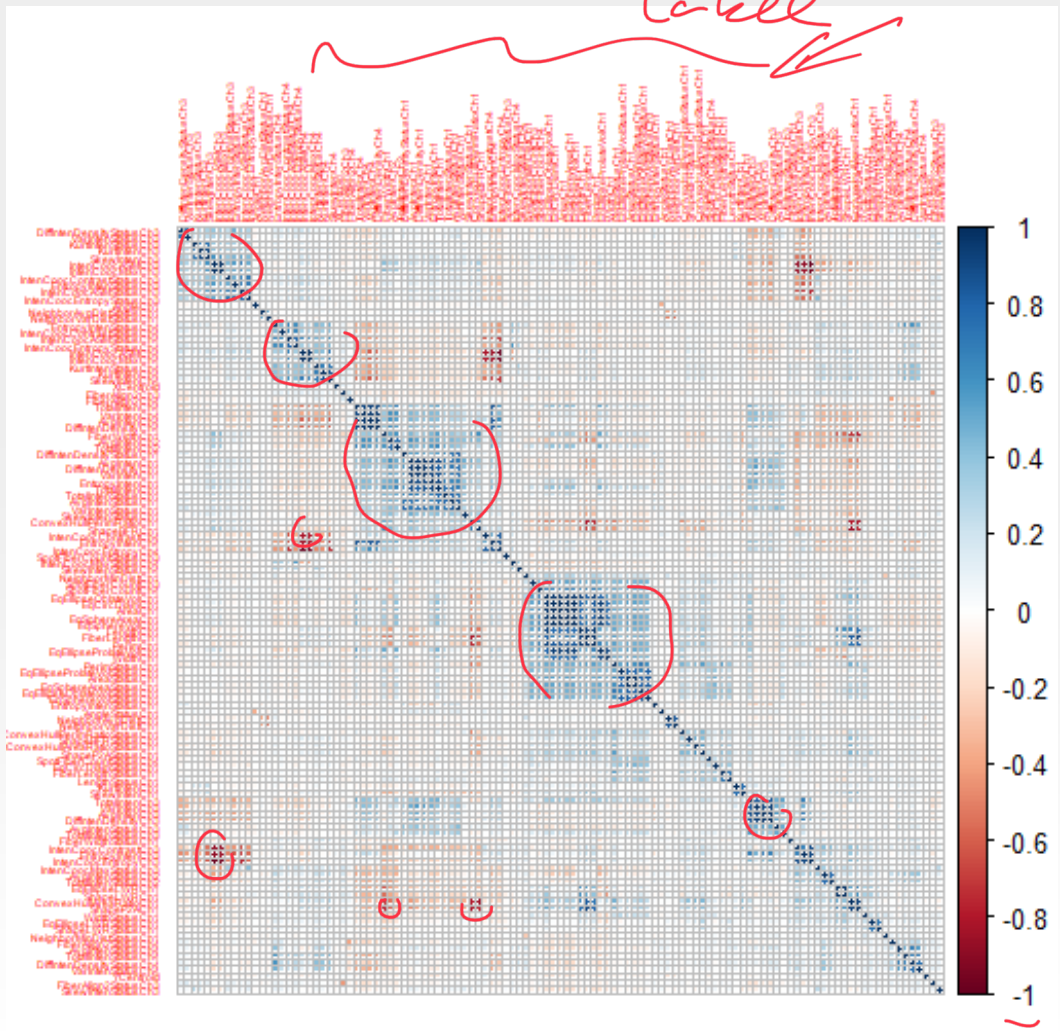
1. Calculate the correlation matrix of the predictors.
2. Determine the two predictors associated with the largest absolute pairwise correlation (call them predictors A and B).
3. Determine the average correlation between A and the other variables. Do the same for predictor B.
4. If A has a larger average correlation, remove it; otherwise, remove predictor B.
5. Repeat Steps 2–4 until no absolute correlations are above the threshold.

0.7 or 0.8 for correlation

R-codes for removing predictors

```
#Near zero variance predictor
nearZeroVar(segTrainTrans)
#Remove the near zero variance predictor
segTrainTrans1 = segTrainTrans[, -nearZeroVar(segTrainTrans)]
nearZeroVar(segTrainTrans1)

## To filter on correlations, we first get the correlation matrix for the
## predictor set
segCorr <- cor(segTrainTrans1)

library(corrplot)
corrplot(segCorr, order = "hclust", tl.cex = .35)
#tl.cexfor the size of text label (variable names).
## caret's findCorrelation function is used to identify columns to remove.
highCorr <- findCorrelation(segCorr, .75)
highCorr
```

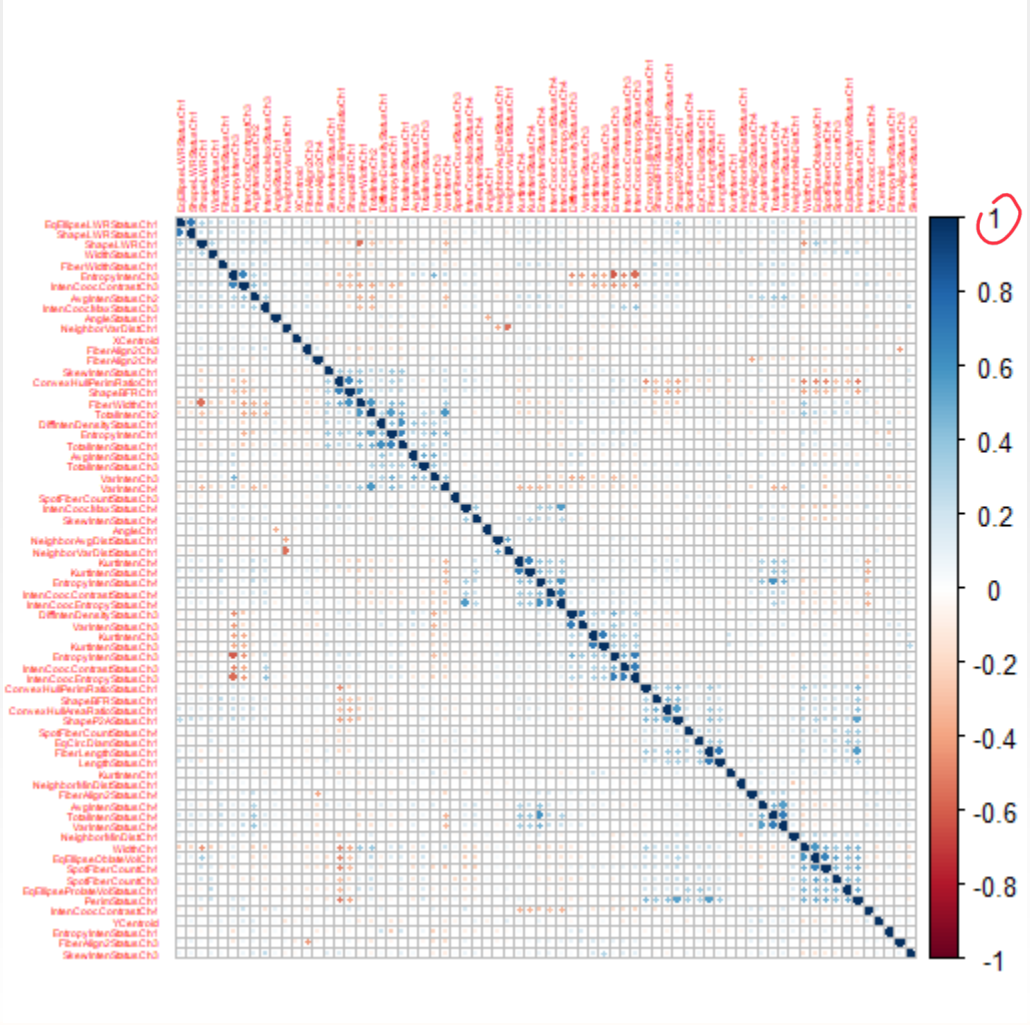
A visualization of the cell segmentation correlation matrix



R-codes for removing highly correlated predictors

```
## caret's findCorrelation function is used to identify columns to remove.
highCorr <- findCorrelation(segCorr, .75)
highCorr

#Removing highly correlated predictors
segCorr1 <- cor(segTrainTrans1[,-highCorr])
corrplot(segCorr1, order = "hclust", tl.cex = .35)
```

A visualization of the cell segmentation correlation matrix



Creating dummy variables

- When a predictor is categorical, such as gender, car type, it is common to decompose the predictor into a set of more specific variables.
- The categories are re-encoded into smaller bits of information called "dummy variables."
- Usually, each category get its own *dummy variable* that is a *zero/one indicator* for that group.

R-codes for creating dummy variables

```
data(cars)
type <- c("convertible", "coupe", "hatchback", "sedan", "wagon")
cars$Type <- factor(apply(cars[, 14:18], 1, function(x) type[which(x == 1)]))

carSubset <- cars[sample(1:nrow(cars), 20), c(1, 2, 19)]

head(carSubset)
levels(carSubset$Type)

simpleMod <- dummyVars(~Mileage + Type,
                       data = carSubset,
                       ## Remove the variable name from the
                       ## column name
                       levelsOnly = TRUE)
simpleMod
```

now

subset of data

20 obs

choose 3 columns: 1, 2, 19

dummyVars: https://www.rdocumentation.org/packages/caret/versions/6.0-92/topics/dummyVars

R-codes for creating dummy variables with interaction

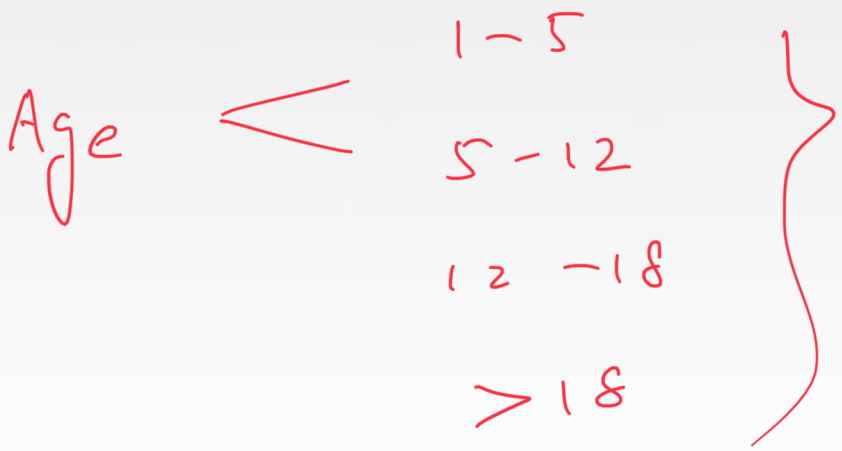
```
withInteraction <- dummyVars(~Mileage + Type + Mileage:Type,
                             data = carSubset,
                             levelsOnly = TRUE)
withInteraction
predict(withInteraction, head(carSubset))
```

Creating dummy variables

```
> predict(withInteraction, head(carSubset))
    Mileage convertible coupe hatchback sedan wagon Mileage:Typeconvertible
107   24318           0     1         0     0     0                       0
181   21132           0     0         0     1     0                       0
30    21545           0     0         0     0     1                       0
75    30502           1     0         0     0     0                   30502
326   22152           0     1         0     0     0                       0
71     5239           1     0         0     0     0                    5239
    Mileage:Typecoupe Mileage:Typehatchback Mileage:Typesedan Mileage:Typewagon
107             24318                     0                 0                 0
181                 0                     0             21132                 0
30                  0                     0                 0             21545
75                  0                     0                 0                 0
326             22152                     0                 0                 0
71                  0                     0                 0                 0
```

Should we bin predictors?

- While there are recommended techniques for pre-processing data, there are also methods to avoid.
- One common approach to simplifying a data set is to take a numeric predictor and pre-categorize or “bin” it into two or more groups prior to data analysis.



SIRS

- Bone et al. (1992) define a set of clinical symptoms to diagnose Systemic Inflammatory Response Syndrome (SIRS). SIRS can occur after a person is subjected to some sort of physical trauma (e.g., car crash). A simplified version of the clinical criteria for SIRS are:
  - Temperature less than 36 ° C or greater than 38°C.
  - Heart rate greater than 90 beats per minute.
  - Respiratory rate greater than 20 breaths per minute.
  - White blood cell count less than 4,000 cells/mm^3 or greater than 12,000 cells/mm3.
- A person who shows two or more of these criteria would be diagnosed as having SIRS.

SIRS

The perceived *advantages* to this approach are:

- The ability to make seemingly simple statements, either for sake of having a simple decision rule (as in the SIRS example) or the belief that there will be a simple interpretation of the model.
- The modeler does not have to know the exact relationship between the predictors and the outcome.
- A higher response rate for survey questions where the choices are binned. For example, asking the date of a person's last tetanus shot is likely to have fewer responses than asking for a range (e.g., in the last 2 years, in the last 4 years).

SIRS

The perceived issues to this approach are:

- There can be a significant loss of performance in the model
- There is a loss of precision in the predictions when the predictors are categorized.
- The research has shown (Austin and Brunner 2004) that categorizing predictors can lead to a high rate of false positives (i.e., noise predictors determined to be informative).

Remark: The predictive models that are most powerful are usually the least interpretable.

R demonstration 3(2)

- R demonstration 3(2): PCA, creating dummy variables, removing and binning predictors.

Exercise 2