2020 SISBID Dimension Reduction Lab

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7/20/2020

Quick PCA Demo Using College Data

Load in Packages

```
library(ISLR)
library(ggplot2)
```

```
## Warning: package 'ggplot2' was built under R version 3.6.2
```

```
library(GGally)
```

```
## Warning: package 'GGally' was built under R version 3.6.2
```

```
## Registered S3 method overwritten by 'GGally':
##   method from
##   +.gg   ggplot2
```

Load Digits Data

```
#code for digits - ALL
rm(list=ls())
load("UnsupL_SISBID_2020.Rdata")
```

```
data(College)
cdat = College[,2:18]
dim(cdat)
```

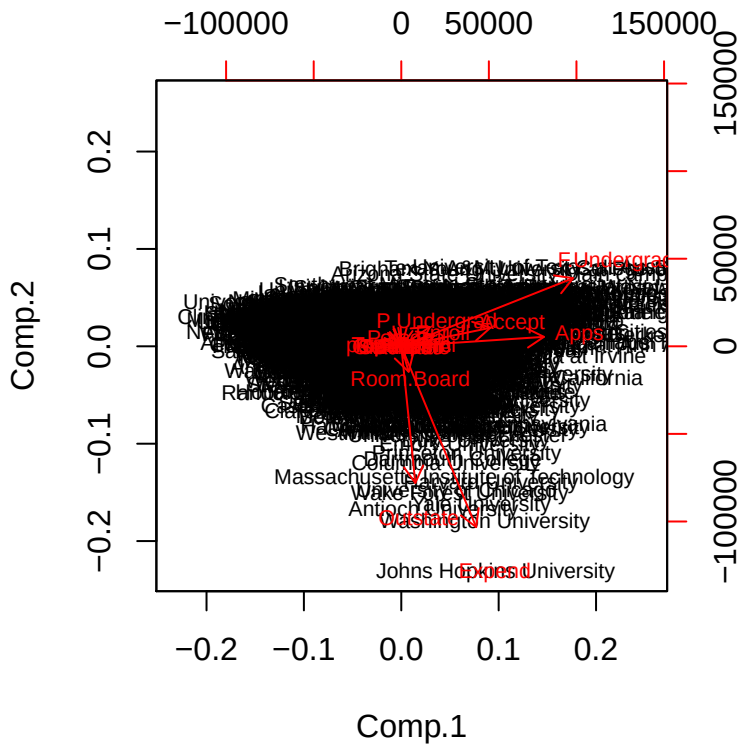
```
## [1] 777  17
```

```
names(cdat)
```

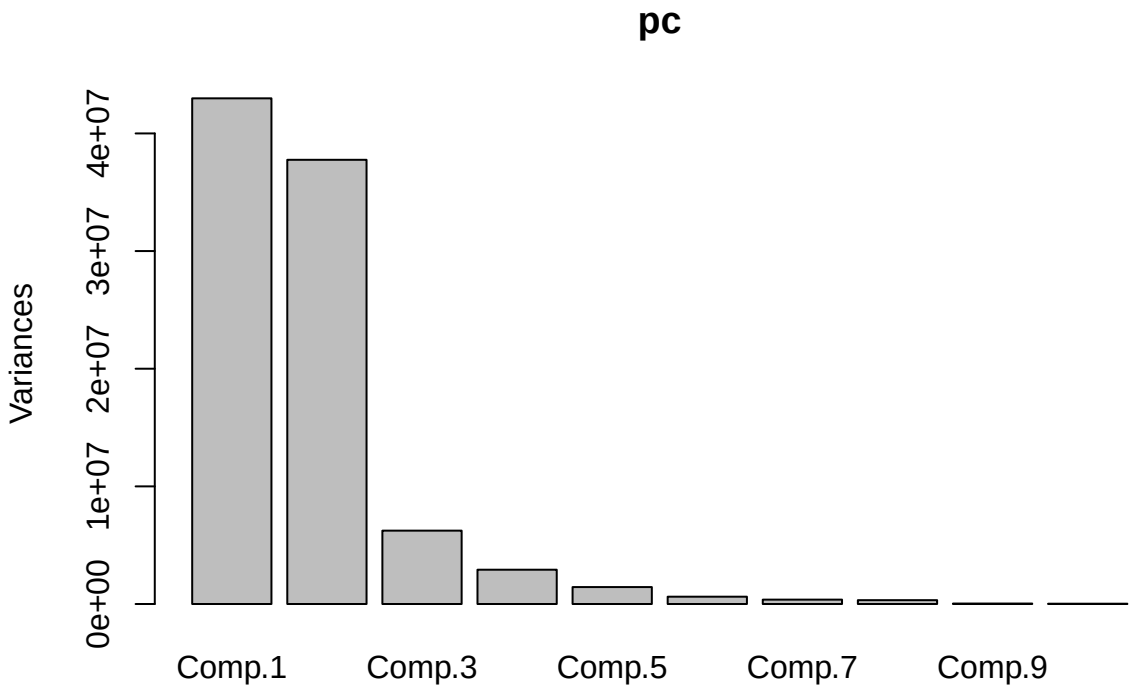
```
##  [1] "Apps"        "Accept"      "Enroll"      "Top10perc"   "Top25perc"
##  [6] "F.Undergrad" "P.Undergrad" "Outstate"    "Room.Board"  "Books"
## [11] "Personal"    "PhD"         "Terminal"    "S.F.Ratio"   "perc.alumni"
## [16] "Expend"      "Grad.Rate"
```

```
pc = princomp(cdat) #default - centers and scales

#Go back and display these plots side by side

biplot(pc,cex=.7)
```

```
## Warning in arrows(0, 0, y[, 1L] * 0.8, y[, 2L] * 0.8, col = col[2L], length =
## arrow.len): zero-length arrow is of indeterminate angle and so skipped
```



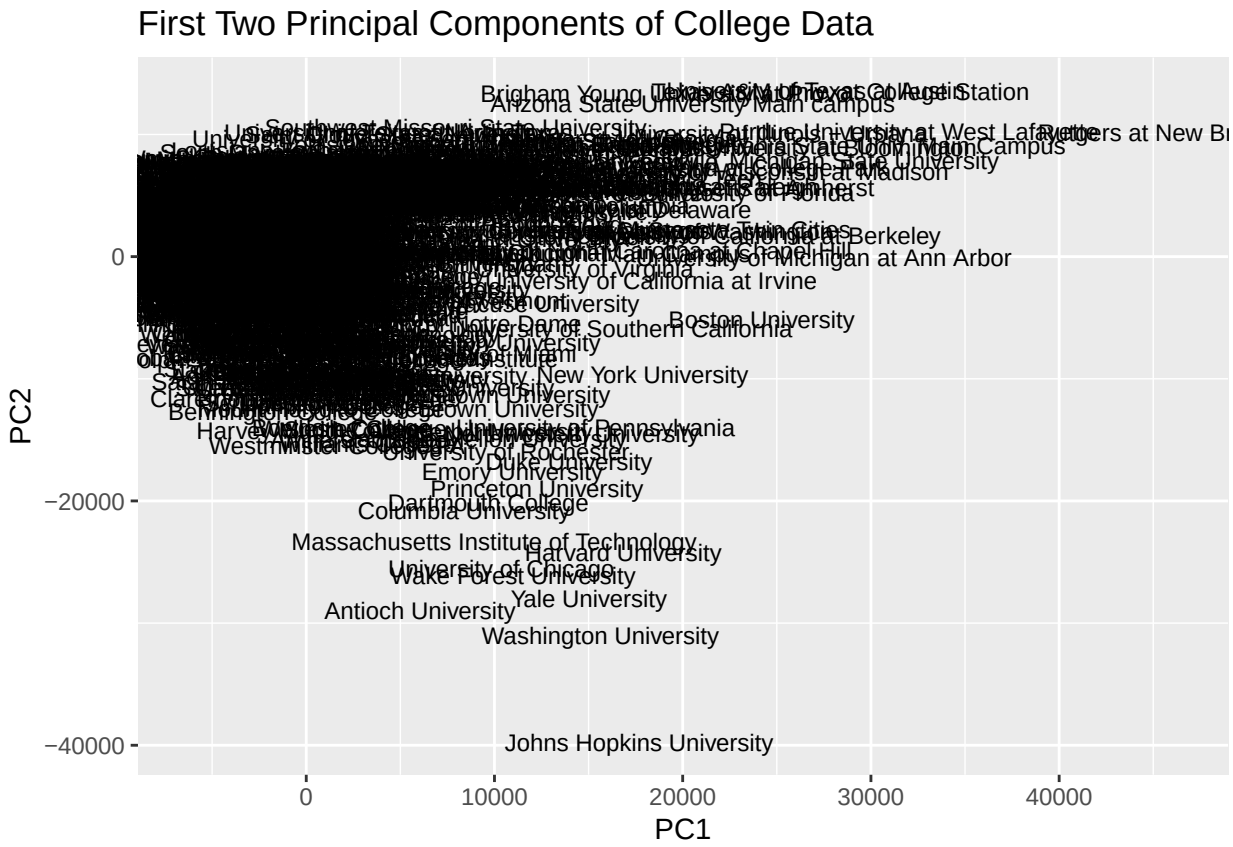

```
screeplot(pc)
```



scatter plots - patterns among observations

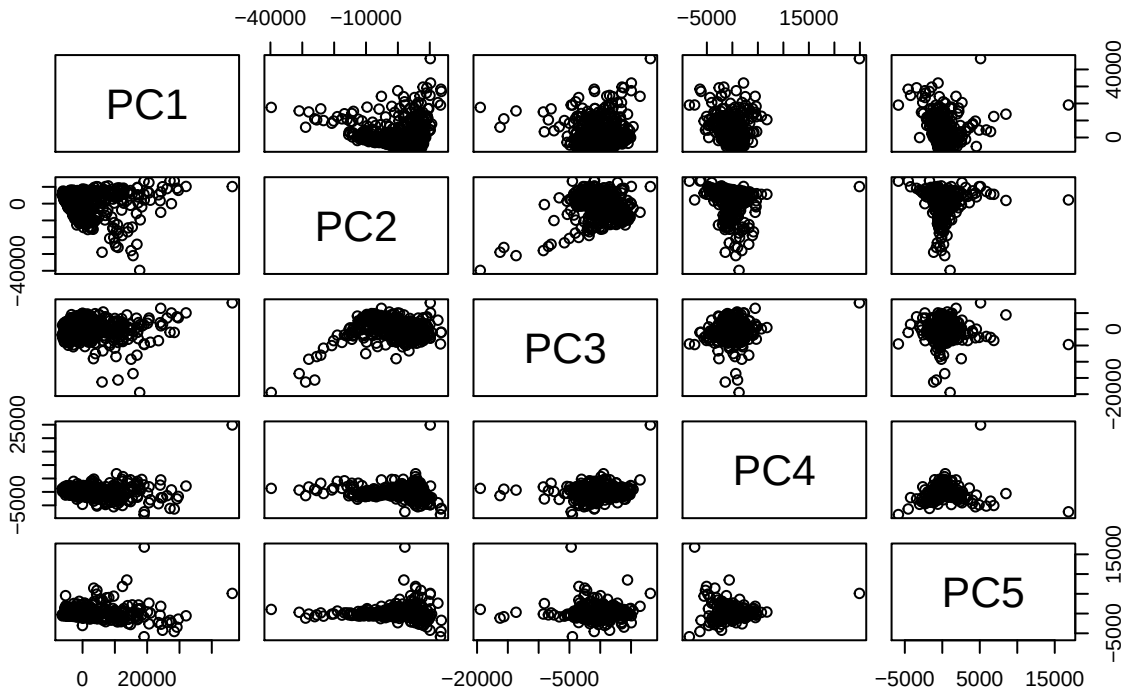
```
PC1 <- as.matrix(x=pc$scores[,1])
PC2 <- as.matrix(pc$scores[,2])

PC <- data.frame(State = row.names(cdat), PC1, PC2)
ggplot(PC, aes(PC1, PC2)) +
```

```
  geom_text(aes(label = State), size = 3) +
  xlab("PC1") +
  ylab("PC2") +
  ggtitle("First Two Principal Components of College Data")
```



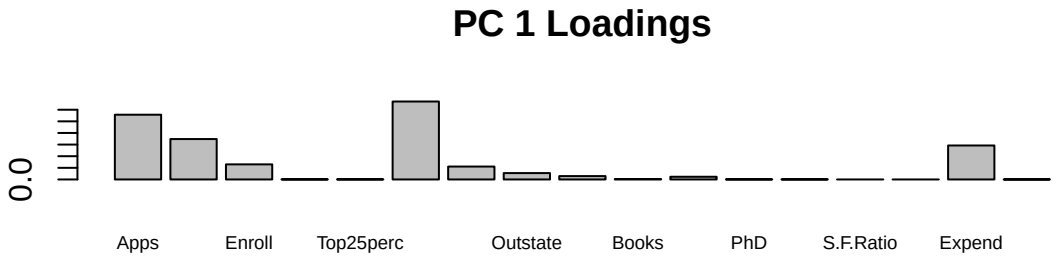
Pairs Plot

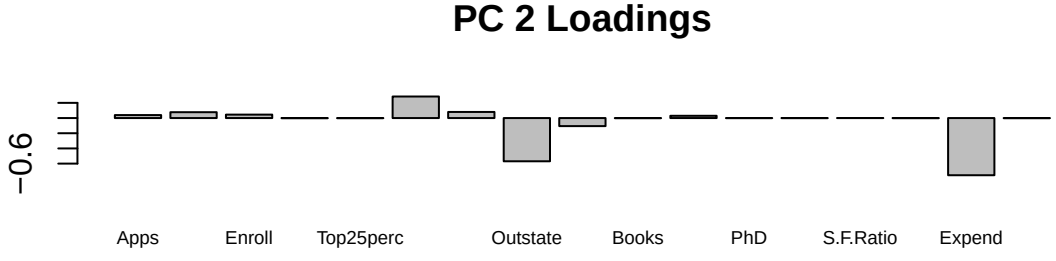
```
comp_labels<-c("PC1","PC2","PC3","PC4", "PC5")
pairs(pc$scores[,1:5], labels = comp_labels, main = "Pairs of PC's for College Data")
```



Loadings - variables that contribute to these patterns

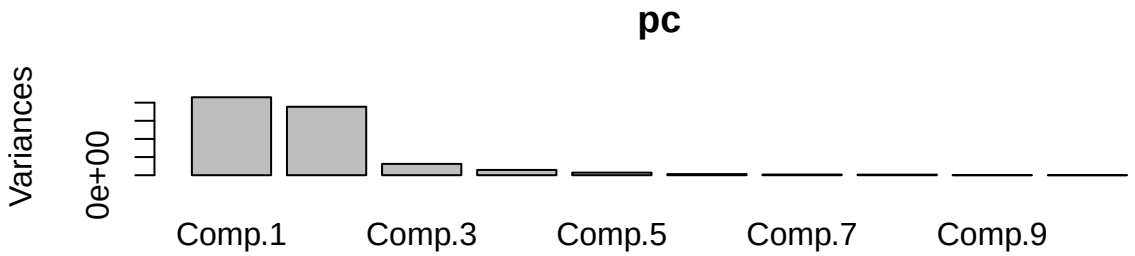
```
par(mfrow=c(2,1))
barplot(pc$loadings[,1],cex.names=.6,main="PC 1 Loadings")
barplot(pc$loadings[,2],cex.names=.6,main="PC 2 Loadings")
```

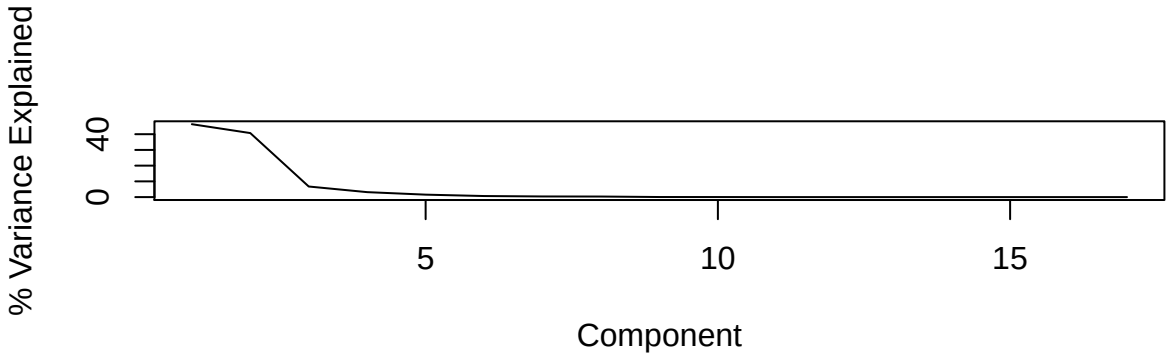




Variance explained

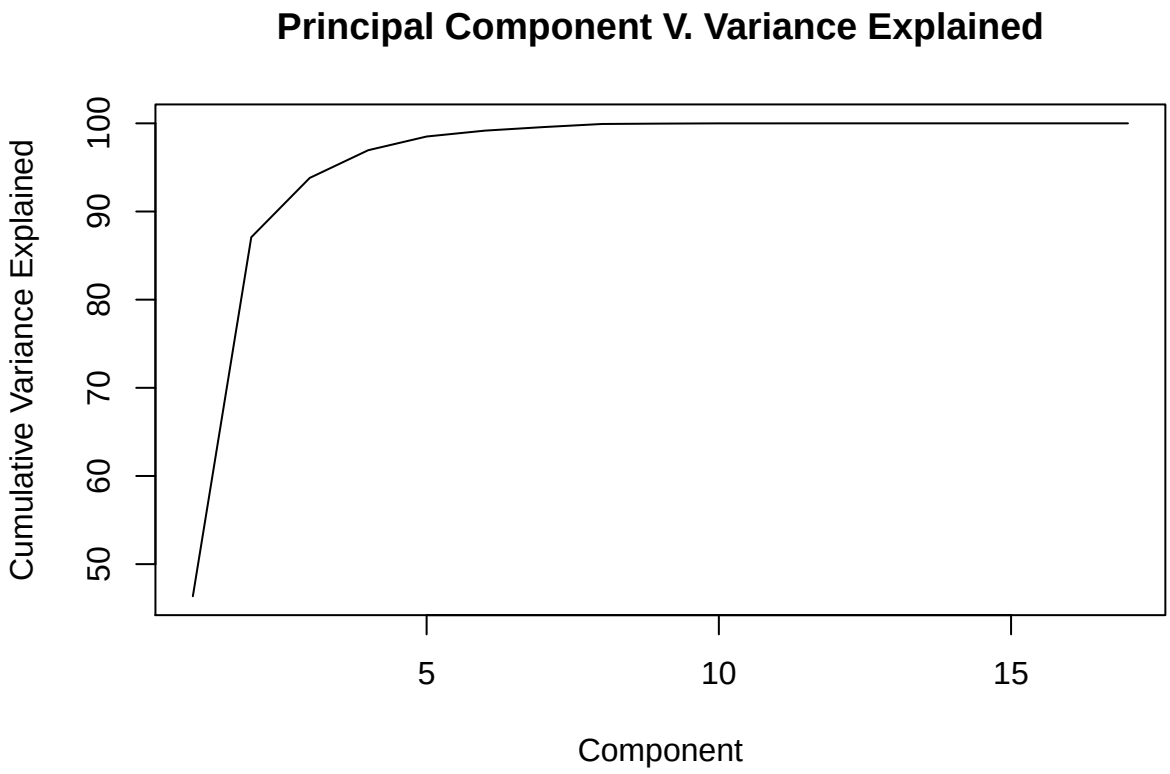
```r
varex = 100*pc$sdev^2/sum(pc$sdev^2)
par(mfrow=c(2,1))
screeplot(pc)
plot(varex,type="l",ylab="% Variance Explained",xlab="Component")
```





Cumulative variance explained

```r
#cumulative variance explained
cvarex = NULL
for(i in 1:ncol(cdat)){
  cvarex[i] = sum(varex[1:i])
}
plot(cvarex,type="l",ylab="Cumulative Variance Explained",xlab="Component", main = "Principal Component
```



Sparse PCA

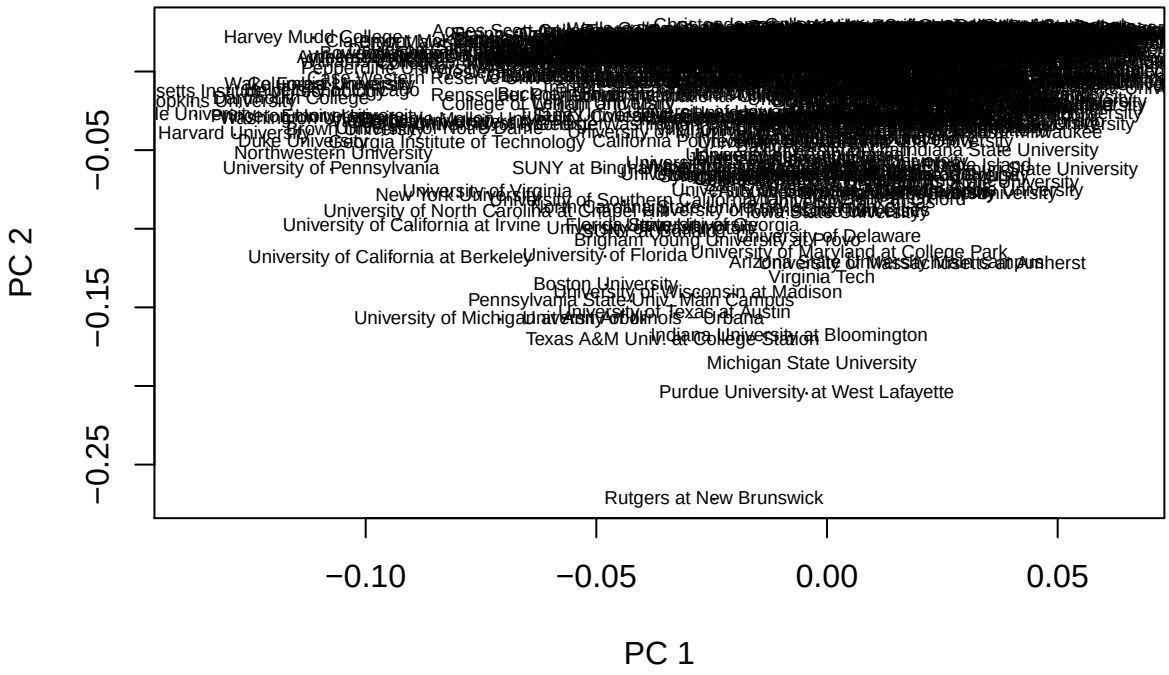
```
library(PMA)

spc = SPC(scale(cdat),sumabsv=2,K=3)
```

```
## 1234567891011121314151617181920
## 1234567891011
## 1234567891011121314151617181920
```

```
spcL = spc$v
rownames(spcL) = names(cdat)
```

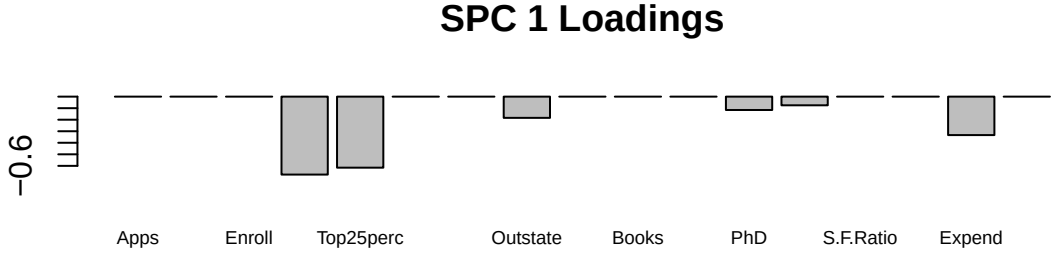
Scatterplots of Sparse PCs

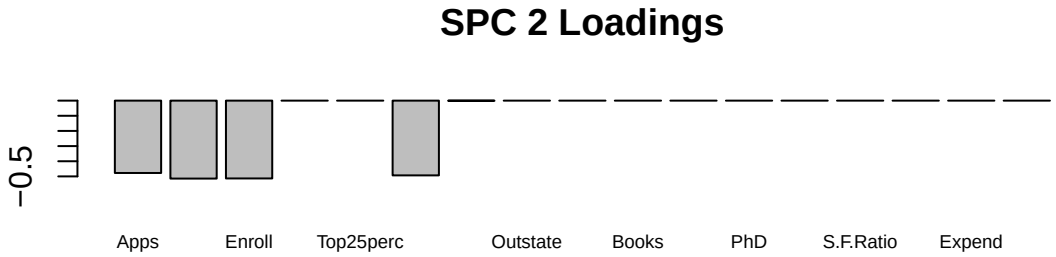
```
i = 1; j = 2;
plot(spc$u[,i],spc$u[,j],pch=16,cex=.2, xlab = "PC 1", ylab = "PC 2", main = "Scatterplot of Sparse PC'
text(spc$u[,i],spc$u[,j],rownames(cdat),cex=.6)
```



Loadings

```
par(mfrow=c(2,1))
barplot(spc$v[,1],names=names(cdat),cex.names=.6,main="SPC 1 Loadings")
barplot(spc$v[,2],names=names(cdat),cex.names=.6,main="SPC 2 Loadings")
```





Try Princomp Function for Digits 3 and 8

```
dat38 = rbind(digits[which(rownames(digits)==3),],digits[which(rownames(digits)==8),])
```

```
pc = princomp(dat38) #default - centers and scales
```

Pairs plot Using ggpairs

```
PC1 <- as.matrix(x=pc$scores[,1])
PC2 <- as.matrix(pc$scores[,2])
PC3 <- as.matrix(pc$scores[,3])
PC4 <- as.matrix(pc$scores[,4])
PC5<-as.matrix(pc$scores[,5])

pc.df.digits <- data.frame(digit_name = row.names(dat38), PC1, PC2,PC3, PC4, PC5)

ggpairs(pc.df.digits, mapping = aes(color = digit_name))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
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```
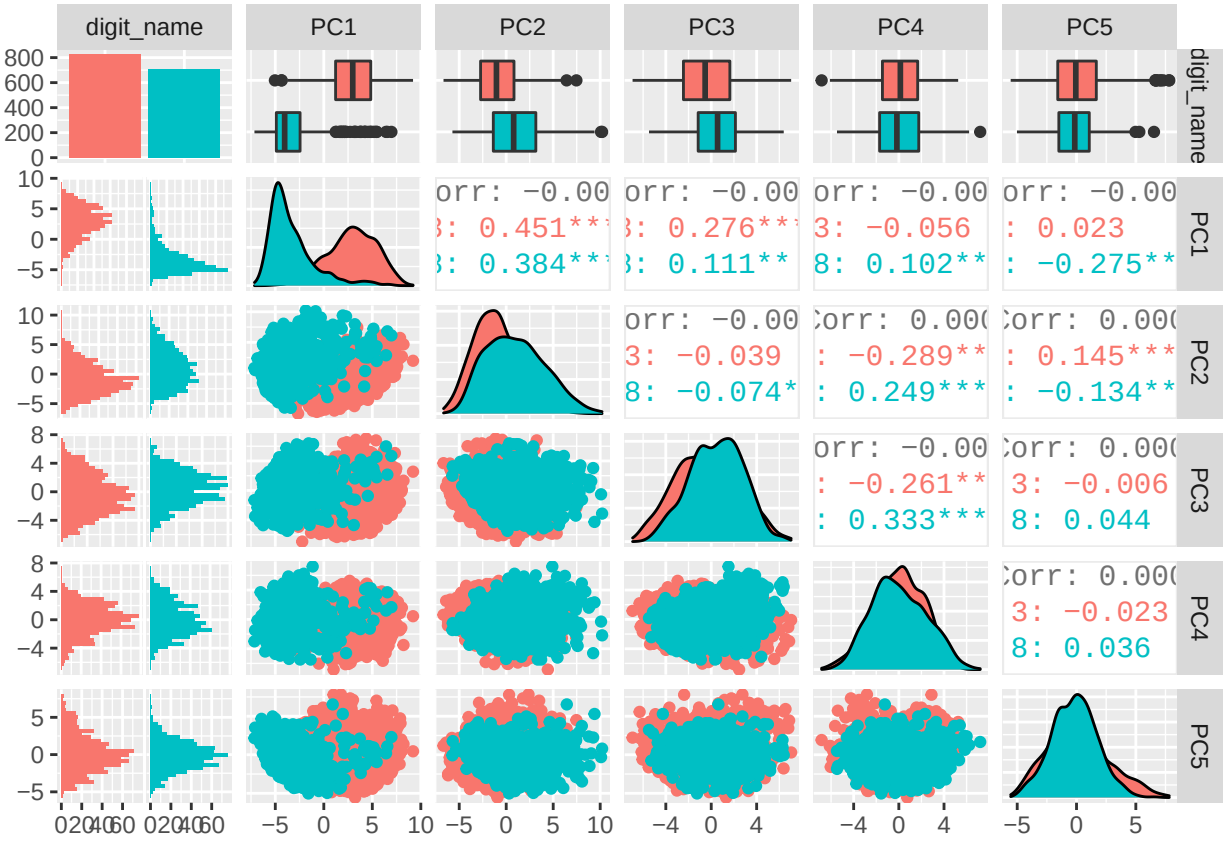
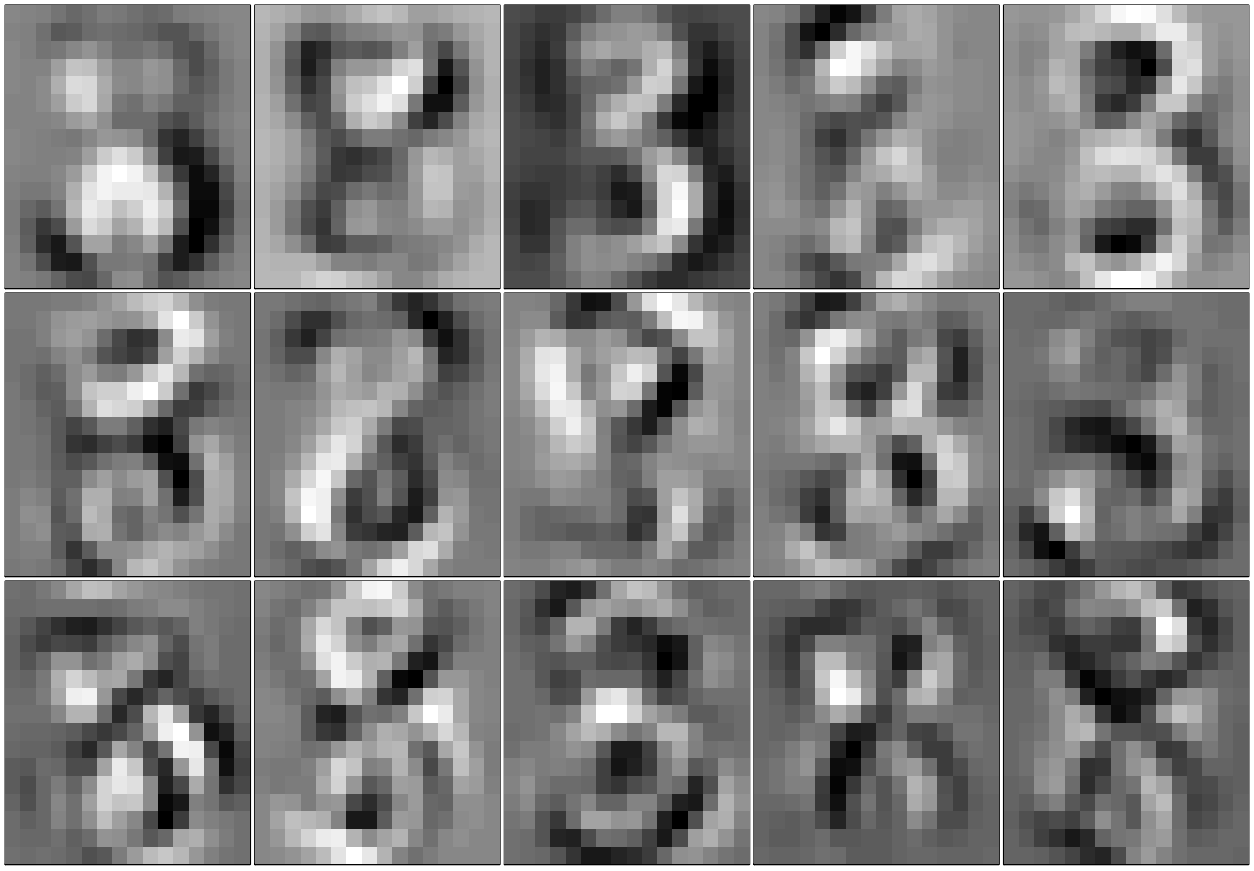



PC Loadings

```
par(mfrow=c(3,5),mar=c(.1,.1,.1,.1))
for(i in 1:15){
  imagedigit(pc$loadings[,i])
```

```
}
```



PCA LAB Using Digits Data

Data set - Digits Data. Either use all digits or choose 2-3 digits if computational speed is a problem. Looking at 3's, 8's and 5's are interesting.

Problem 1 - PCA

Problem 1a - Apply PCA to this data.

Problem 1b - Do the first several PCs well separate different digits? Why or why not?

Problem 1c - Use the first several PCs and PC loadings to evaluate the major patterns in the digits data. Can you come up with a description of the pattern found by each of the first five PCs?

Problem 1d - How many PCs are needed to explain 95% of the variance? You must decide how many PCs to retain. Which do you pick and why?

Problem 2 - MDS

Problem 2a - Apply MDS (classical or non-metric) to this data. Try out several distance metrics and different numbers of MDS components.

Problem 2b - Which distance metric is best for this data? Which one reveals the most separation of the digits?

Problem 2c - Compare and contrast the MDS component maps to the dimension reduction of PCA. Which is preferable?

Problem 3 - ICA.

Problem 3a - Apply ICA to this data set.

Problem 3b - Which value of K did you use? Why? What happens when you slightly change your chosen K?

Problem 3c - Interpret the independent image signals found. Do any other them accurately reflect the different digits? Which ones?

Problem 4 - UMAP

Problem 5a - Apply UMAP on this data set.

Problem 5 - tSNE

Problem 5a - Apply tSNE on this data set

Problem 6 - Comparisons.

Problem 6a - Compare and contrast PCA, MDS and ICA, TSNE, and UMAP on this data set. Which one best separates the different digits? Which one reveals the most interesting patterns?

Problem 6b - Overall, which method do you recommend for this data set and why?

Additional Data set - NCI Microarray data

(If you have time - take a further look at this data set using various methods for dimension reduction. Also you may be interested in trying MDS to visualize this data.)

##R scripts to help out with the Dimension Reduction Lab #Don't peek at this if you want to practice coding on your own!!

```
library(ISLR)
library(ggplot2)
library(tidyr)
```

```
## Warning: package 'tidyr' was built under R version 3.6.2
```

Load in data and visualize

```
#code for digits - ALL
rm(list=ls())
load("UnsupL_SISBID_2020.Rdata")

#visulaize
pdf("temp.pdf")
par(mfrow=c(4,8), mar=c(.1,.1,.1,.1))
for(i in 1:32){
  imagedigit(digits[i,])
}
dev.off()
```

```
## pdf
##   2
```

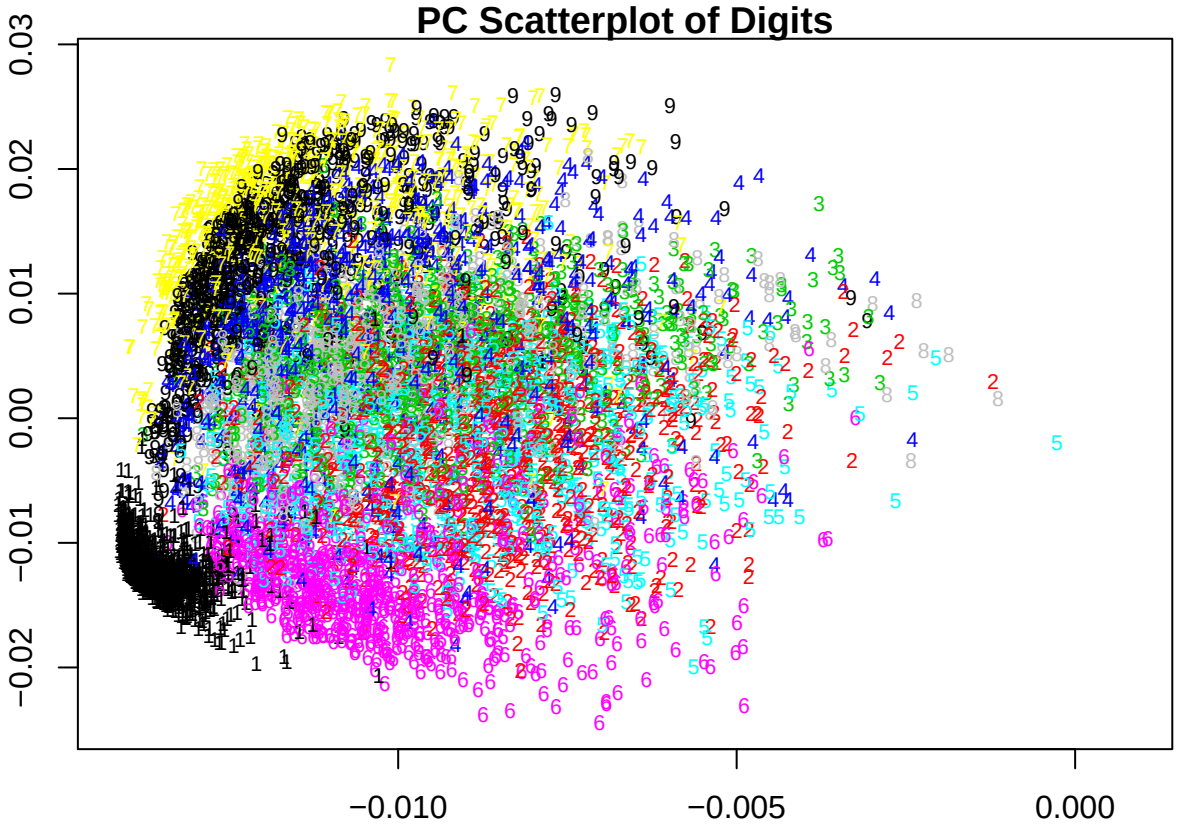
##Problem 1 - PCA

PCA - take SVD to get solution don't center and scale to retain interpretation as images

```
########Problem 1 - PCA
#PCA - take SVD to get solution
#don't center and scale to retain interpretation as images
svdd = svd(digits)
U = svdd$u
V = svdd$v #PC loadings
D = svdd$d
Z = digits%*%V #PCs
```

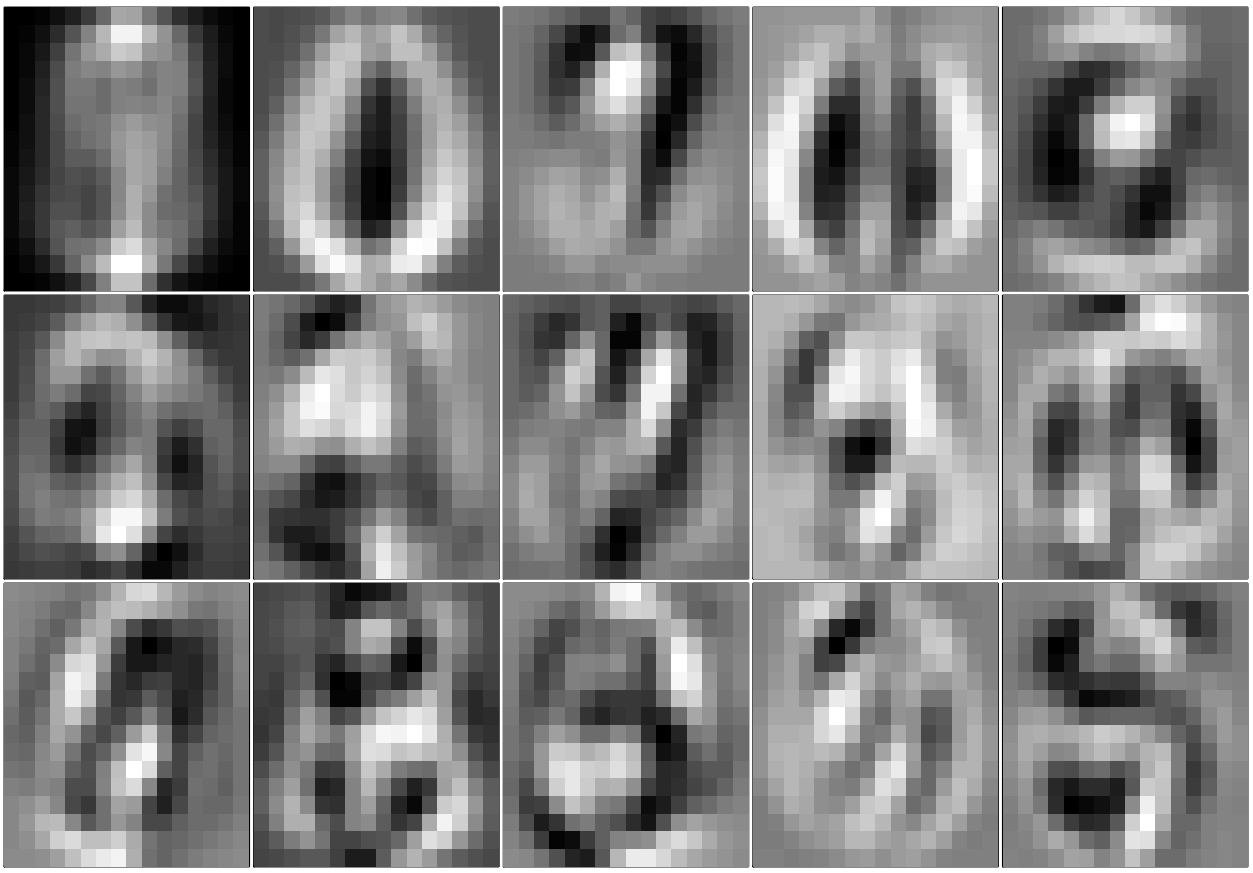
PC scatterplot

```
i = 1; j = 3;
par(mfrow=c(1,1), mar=c(3,3,1,1))
plot(U[,i],U[,j],type="n", xlab = "PC1", ylab = "PC2", main = "PC Scatterplot of Digits")
text(U[,i],U[,j],rownames(digits),col=rownames(digits),cex=.7)
```



PC loadings

```
#PC loadings
par(mfrow=c(3,5),mar=c(.1,.1,.1,.1))
for(i in 1:15){
  imagedigit(V[,i])
}
```

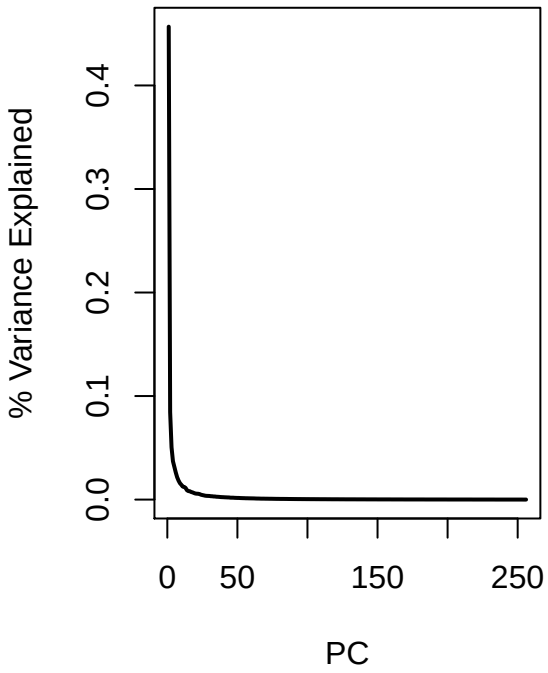


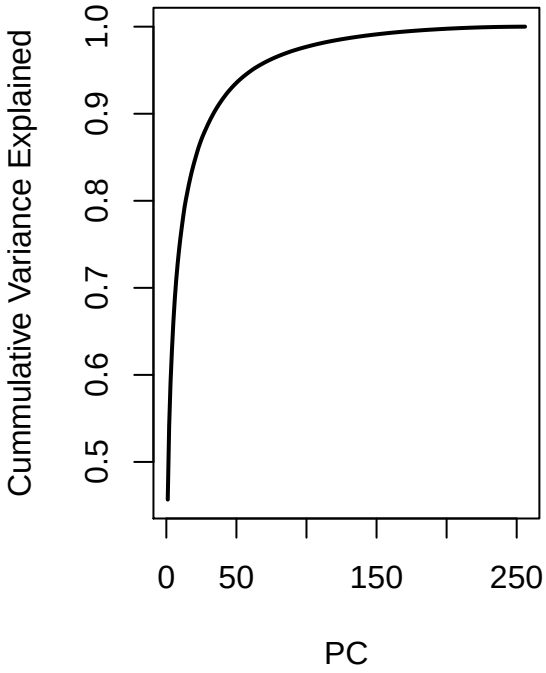
Variance Explained

```
#Variance Explained
varex = 0
cumvar = 0
denom = sum(D^2)
for(i in 1:256){
  varex[i] = D[i]^2/denom
  cumvar[i] = sum(D[1:i]^2)/denom
}
```

Screeplot

```
par(mfrow=c(1,2))
plot(1:256,varex,type="l",lwd=2,xlab="PC",ylab="% Variance Explained")
plot(1:256,cumvar,type="l",lwd=2,xlab="PC",ylab="Cummulative Variance Explained")
```

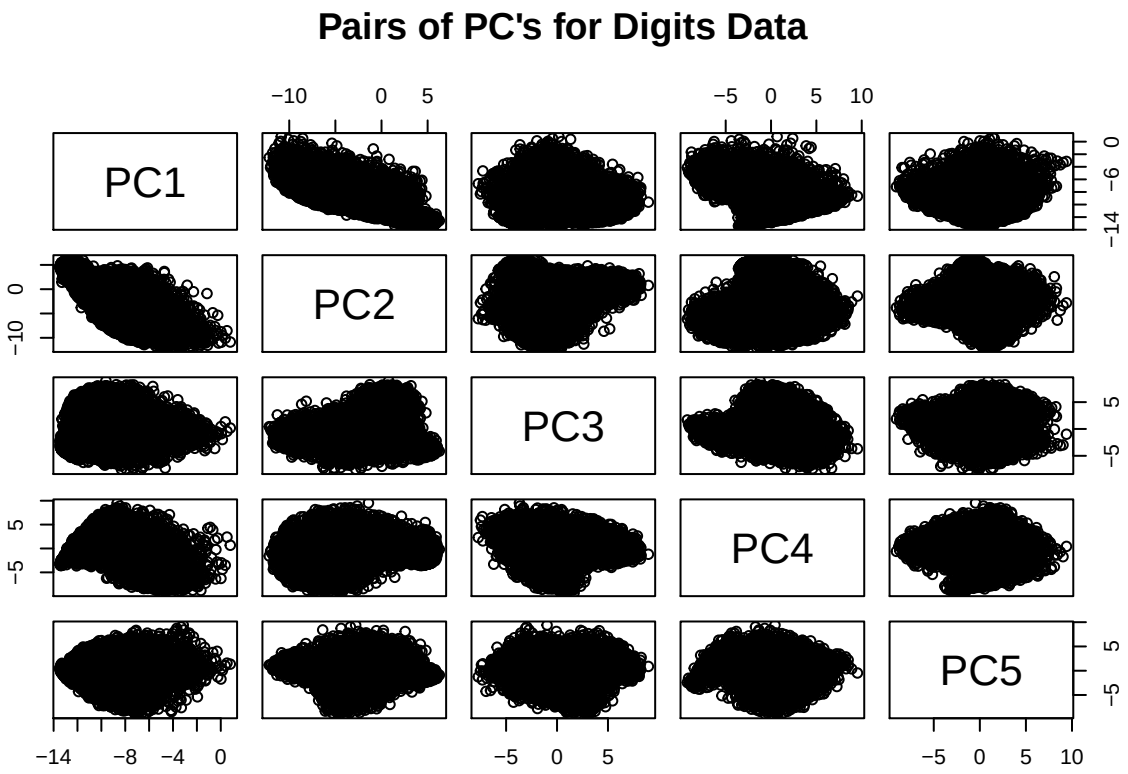




Pairs Plot

```
library(GGally)
```

```
Z_sub = Z[,1:5]
comp_labels<-c("PC1","PC2","PC3","PC4", "PC5")
pairs(Z_sub, labels = comp_labels, main = "Pairs of PC's for Digits Data")
```



Problem 2 - MDS

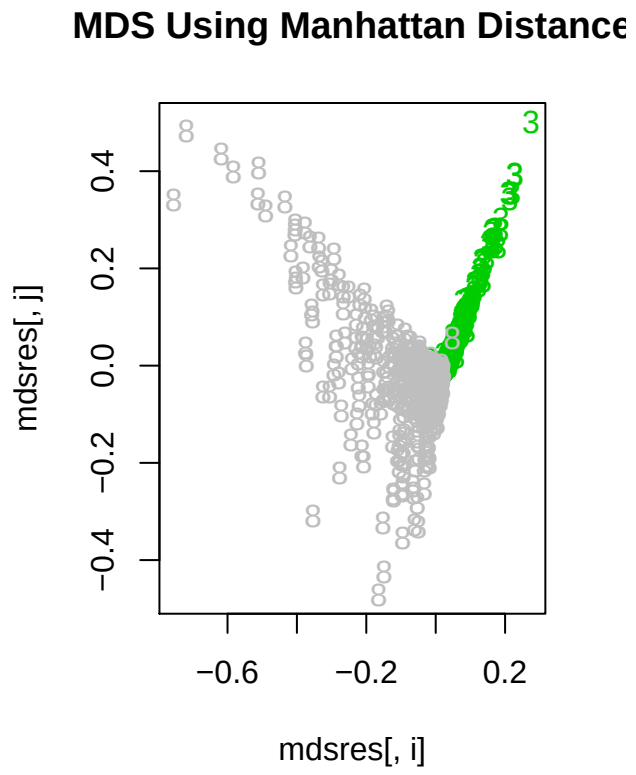
classical MDS (Note, this may take some time - try only on 3's and 8's)

```
dat38 = rbind(digits[which(rownames(digits)==3),],digits[which(rownames(digits)==8),])
dim(dat38)
```

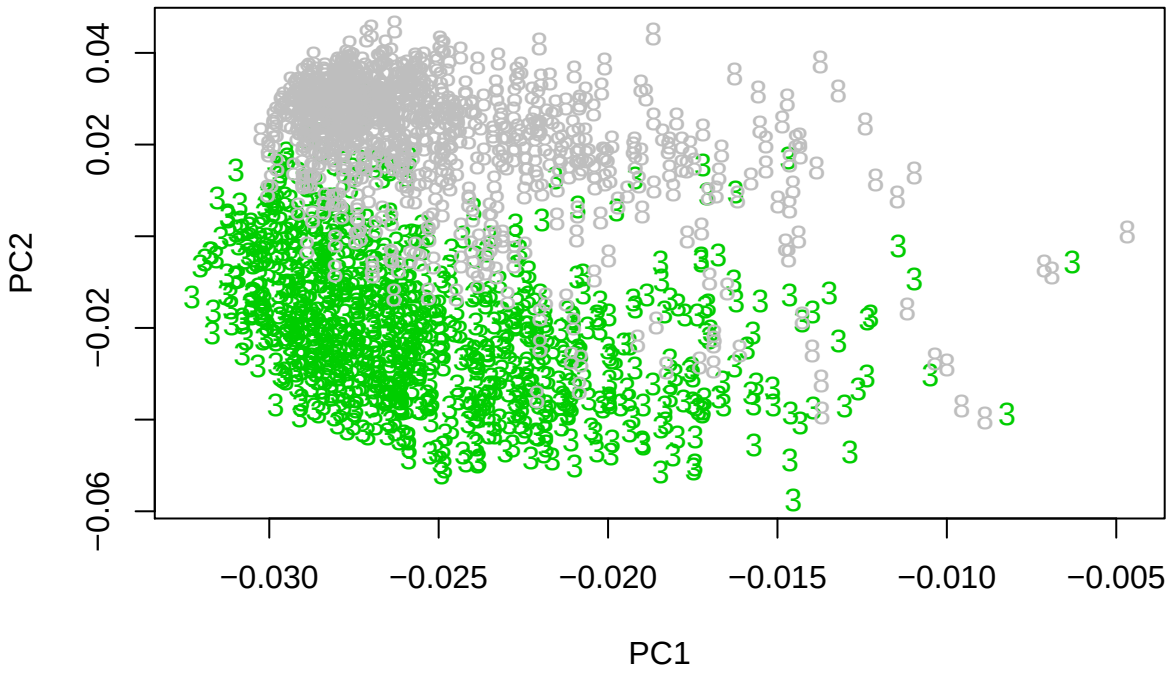
```
## [1] 1532  256
```

```
#PCA for comparison
svdd = svd(dat38)
U = svdd$u
V = svdd$v #PC loadings
D = svdd$d
Z = digits%*%V #PCs
```

```
#MDS
Dmat = dist(dat38,method="maximum") #Manhattan (L1) Distance
mdsres = cmdscale(Dmat,k=10)

i = 1; j = 2;
par(mfrow=c(1,2))
plot(mdsres[,i],mdsres[,j],type="n", main = "MDS Using Manhattan Distance")
text(mdsres[,i],mdsres[,j],rownames(dat38),col=rownames(dat38))
```

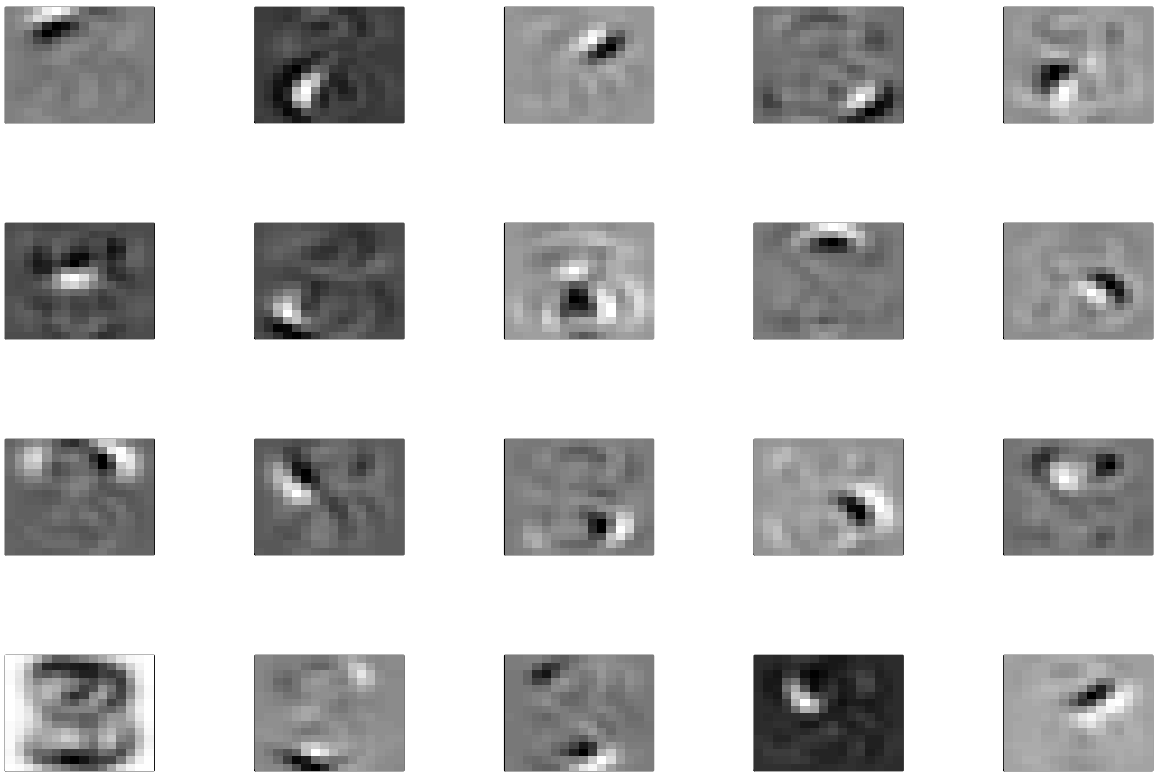



```
plot(U[,i],U[,j],type="n",xlab="PC1",ylab="PC2")
text(U[,i],U[,j],rownames(dat38),col=rownames(dat38))
```



Problem 3 - ICA

```
library(fastICA)
require("fastICA")

K = 20
icafit = fastICA(t(dat38),n.comp=K)

#plot independent source signals
options(width = 60)
par(mfrow=c(4,5),mar = c(2, 2, 2, 2))
for(i in 1:K){
  imagedigit(icafit$S[,i])
}
```



Problem 4 - UMAP

Install Packages

```
#install.packages('umap')
#install.packages('Rtsne')
library(umap)
```

```
## Warning: package 'umap' was built under R version 3.6.2
```

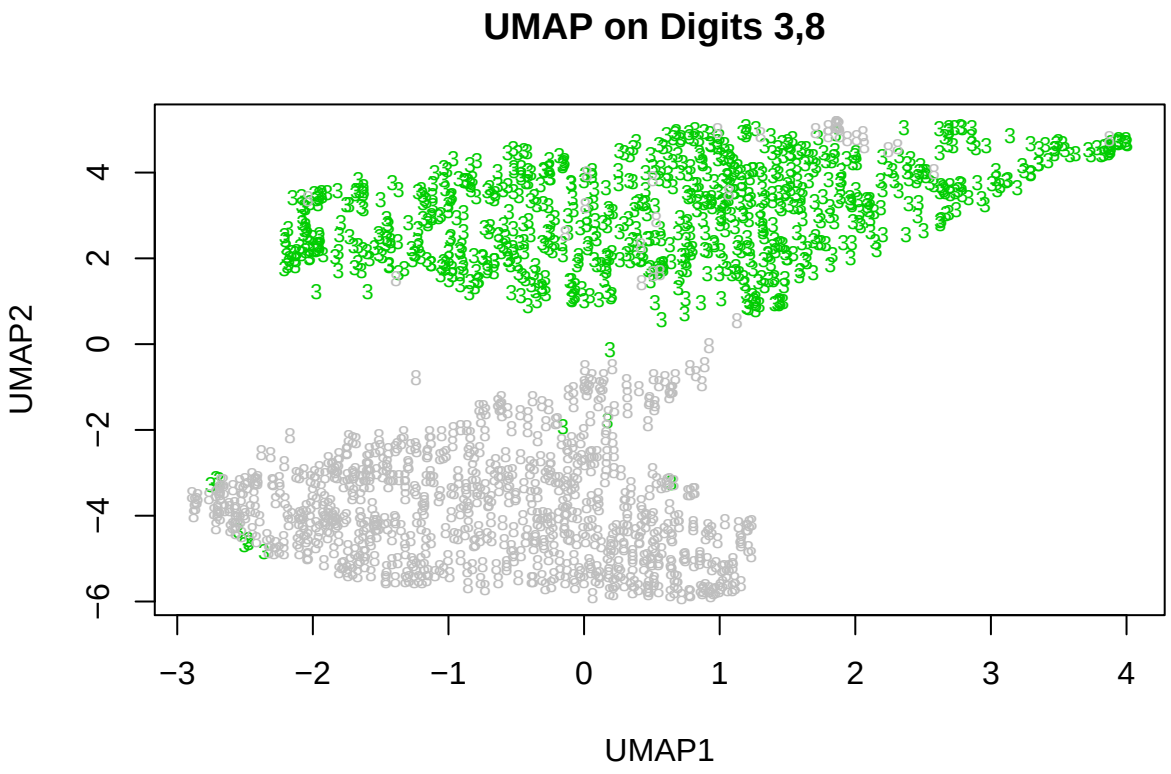
```
library(Rtsne)
```

Run UMAP

```
digits.umap = umap(dat38)
```

Plot UMAP

```
plot(digits.umap$layout[,1],y=digits.umap$layout[,2], type ='n', main = "UMAP on Digits 3,8 ", xlab = "U
text(digits.umap$layout[,1],y=digits.umap$layout[,2],rownames(dat38),col=rownames(dat38),cex=.7)
```

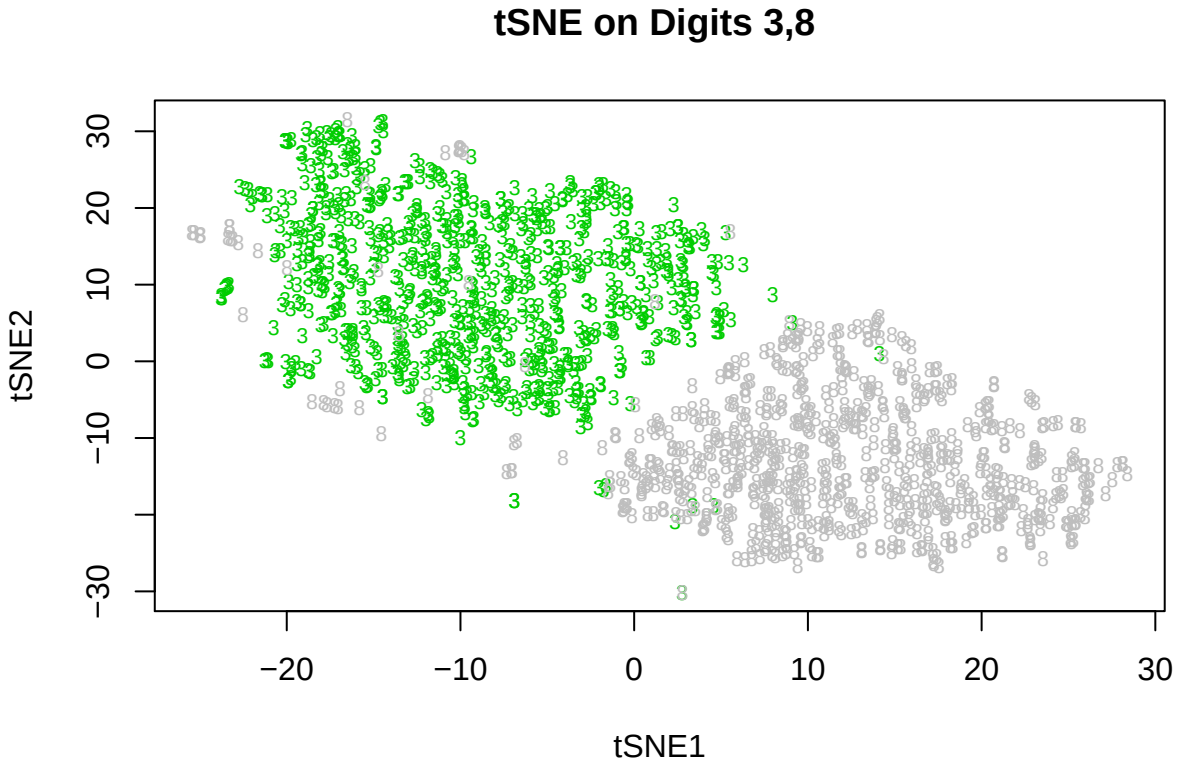


Problem 5 - tSNE

Run tSNE

```
tsne_digit <- Rtsne(as.matrix(dat38))
```

```
plot(tsne_digit$Y[,1],y=tsne_digit$Y[,2], type ='n', main = "tSNE on Digits 3,8 ", xlab = "tSNE1", ylab
text(tsne_digit$Y[,1],y=tsne_digit$Y[,2],rownames(dat38),col=rownames(dat38),cex=.7)
```


tSNE on Digits 3,8
tSNE2
30
20
10
0
−10
−30
−20
−10
0
10
20
30
tSNE1