Preprocessing with Principal Components Analysis (PCA)

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Correlated predictors

```
library(caret); library(kernlab); data(spam)
```

```
## Loading required package: lattice

## Loading required package: ggplot2

##
## Attaching package: 'kernlab'

## The following object is masked from 'package:ggplot2':
##
##     alpha
```

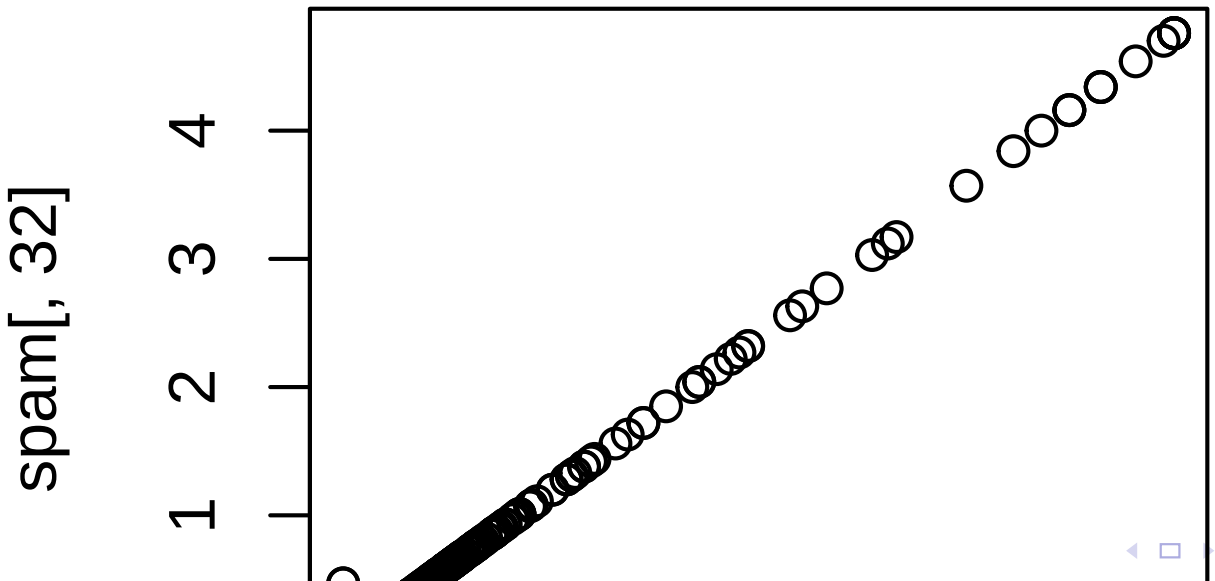
```
inTrain <- createDataPartition(y=spam$type,
                               p=0.75, list=FALSE)
training <- spam[inTrain,]
testing <- spam[-inTrain,]

M <- abs(cor(training[,-58]))
```

Correlated predictors

```
names(spam)[c(34,32)]
```

```
## [1] "num415" "num857"
```

```
plot(spam[,34],spam[,32])
```



Basic PCA idea

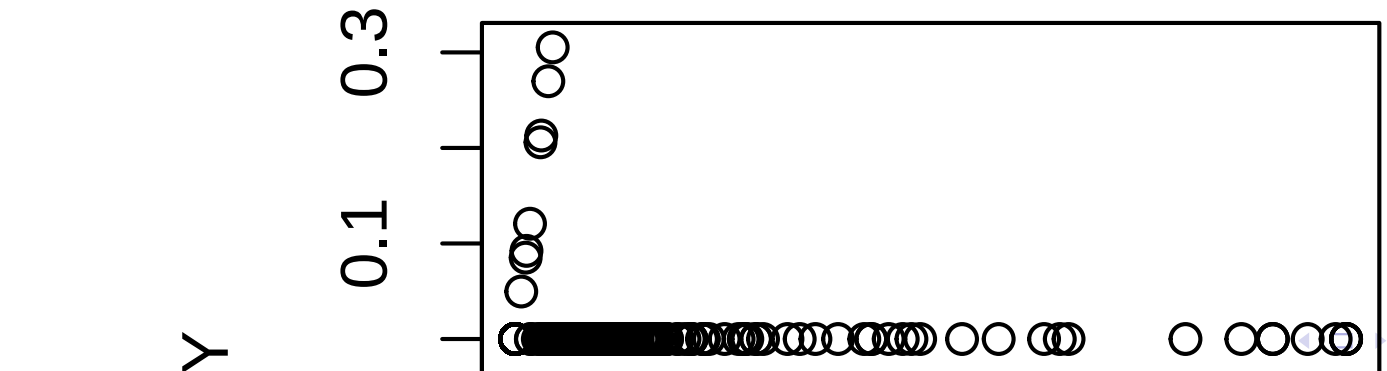
- We might not need every predictor
- A weighted combination of predictors might be better
- We should pick this combination to capture the "most information" possible
- Benefits
- Reduced number of predictors
- Reduced noise (due to averaging)

We could rotate the plot

$$X = 0.71 \times \text{num415} + 0.71 \times \text{num857}$$

$$Y = 0.71 \times \text{num415} - 0.71 \times \text{num857}$$

```
X <- 0.71*training$num415 + 0.71*training$num857
Y <- 0.71*training$num415 - 0.71*training$num857
plot(X,Y)
```



Related problems

You have multivariate variables $X_1, \ldots, X_n$ so $X_1 = (X_{11}, \ldots, X_{1m})$

- Find a new set of multivariate variables that are uncorrelated and explain as much variance as possible.
- If you put all the variables together in one matrix, find the best matrix created with fewer variables (lower rank) that explains the original data.

The first goal is statistical and the second goal is data compression.

Related solutions - PCA/SVD

SVD

If X is a matrix with each variable in a column and each observation in a row then the SVD is a "matrix decomposition"

$$X = UDV^T$$

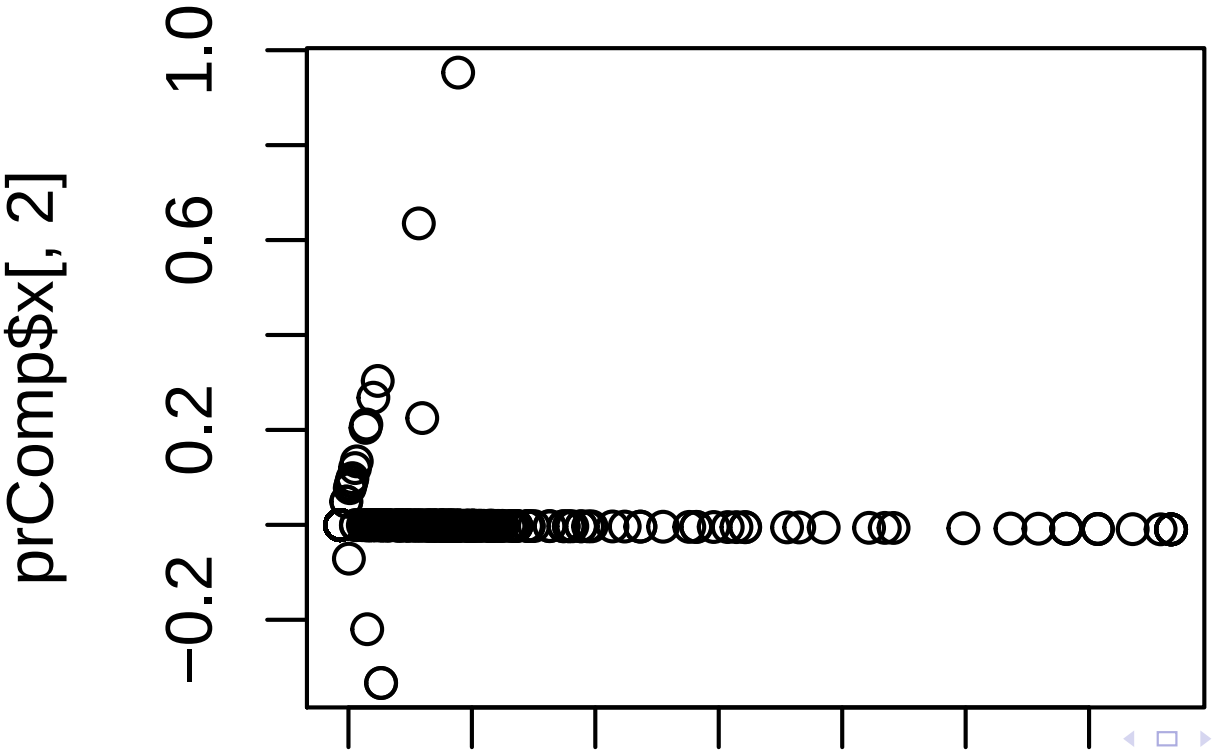
where the columns of U are orthogonal (left singular vectors), the columns of V are orthogonal (right singluar vectors) and D is a diagonal matrix (singular values).

PCA

The principal components are equal to the right singular values if you first scale (subtract the mean, divide by the standard deviation) the variables.

Principal components in R - prcomp

```
smallSpam <- spam[,c(34,32)]
prComp <- prcomp(smallSpam)
plot(prComp$x[,1],prComp$x[,2])
```



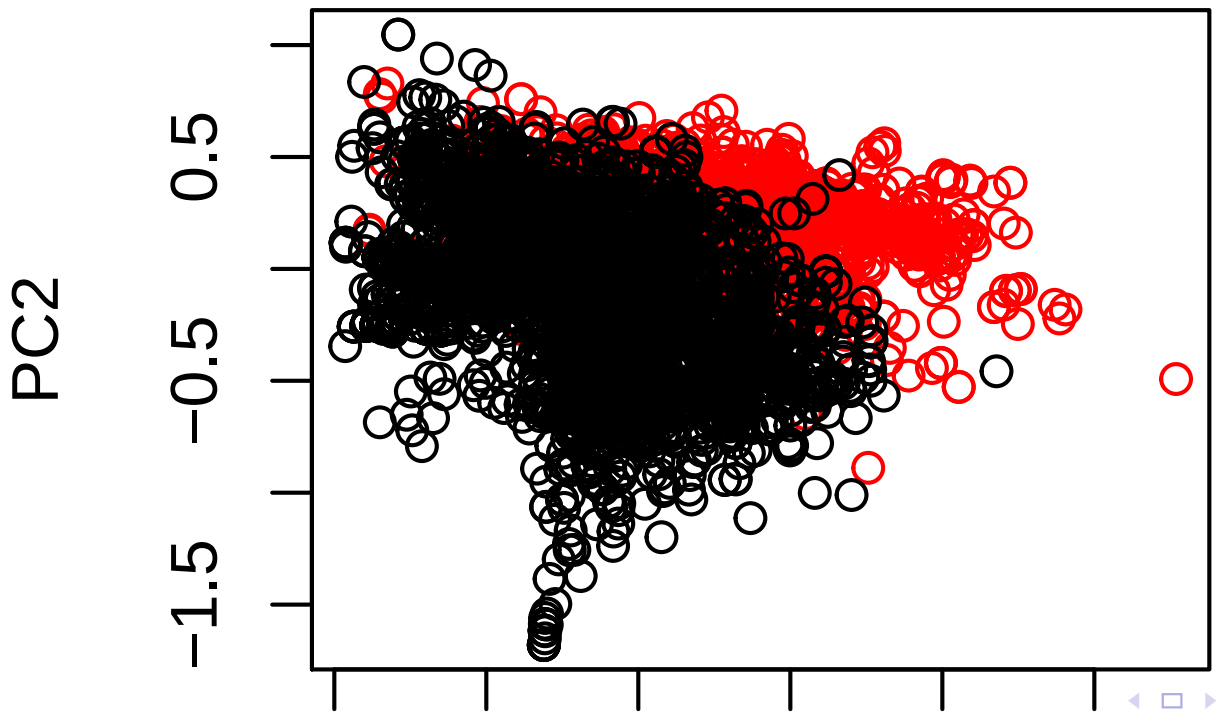
Principal components in R - prcomp

```
prComp$rotation
```

```
##                PC1         PC2
## num415 0.7080625  0.7061498
## num857 0.7061498 -0.7080625
```

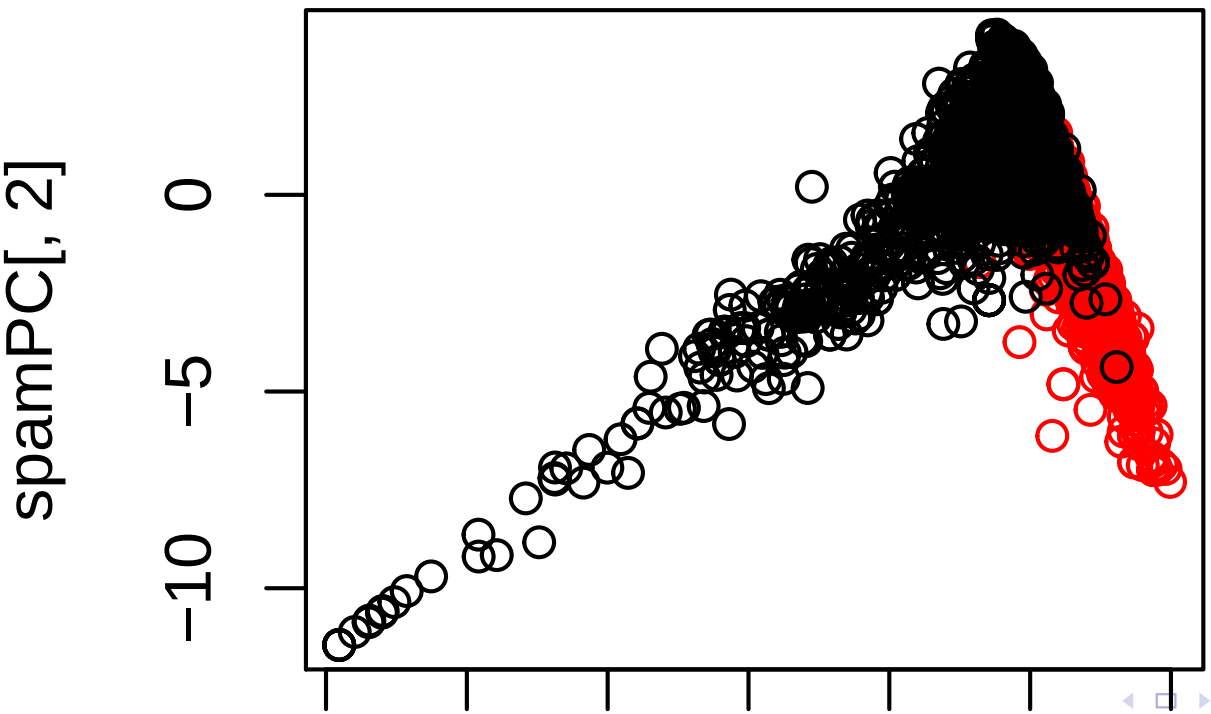
PCA on SPAM data

```
typeColor <- ((spam$type=="spam")*1 + 1)
prComp <- prcomp(log10(spam[,-58]+1))
plot(prComp$x[,1],prComp$x[,2],col=typeColor,xlab="PC1",yla
```



PCA with caret

```
preProc <- preProcess(log10(spam[,-58]+1),method="pca",pca(
spamPC <- predict(preProc,log10(spam[,-58]+1))
plot(spamPC[,1],spamPC[,2],col=typeColor)
```



Preprocessing with PCA

```
preProc <- preProcess(log10(training[,-58]+1),method="pca"
trainPC <- predict(preProc,log10(training[,-58]+1))
modelFit <- train(training$type ~ .,method="glm",data=train
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or

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```

Preprocessing with PCA

```
testPC <- predict(preProc,log10(testing[,-58]+1))
confusionMatrix(testing$type,predict(modelFit,testPC))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction nonspam spam
##    nonspam     648   49
##    spam         66  387
##
##                Accuracy : 0.9
##                  95% CI : (0.8812, 0.9167)
##     No Information Rate : 0.6209
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.7892
##  Mcnemar's Test P-Value : 0.1357
##
```

Alternative (sets # of PCs)

```
modelFit <- train(training$type ~ .,method="glm",preProcess
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or
```

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Final thoughts on PCs

- Most useful for linear-type models
- Can make it harder to interpret predictors
- Watch out for outliers!
- Transform first (with logs/Box Cox)
- Plot predictors to identify problems
- For more info see
- Exploratory Data Analysis
- Elements of Statistical Learning