Preprocessing with Principal Components Analysis (PCA)

Jeffrey Leek
Johns Hopkins Bloomberg School of Public Health

Correlated predictors

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

M <- abs(cor(training[,-58]))
diag(M) <- 0
which(M > 0.8,arr.ind=T)
```

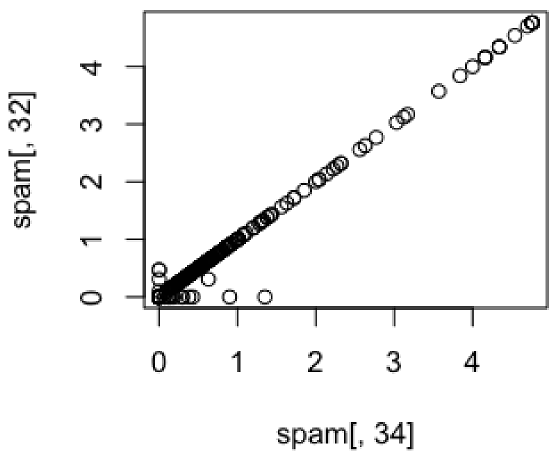
```
       row col
num415  34  32
num857  32  34
```

Correlated predictors

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

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

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



Basic PCA idea

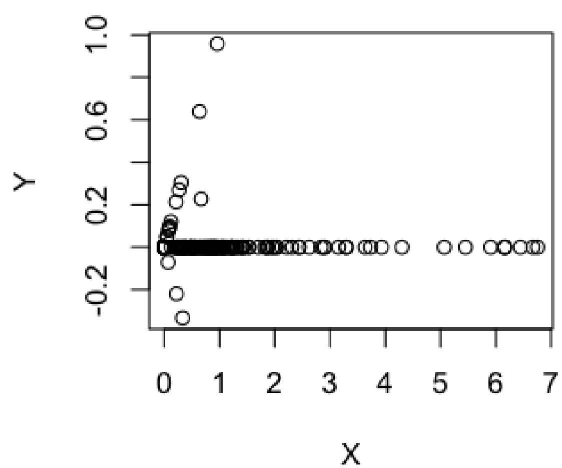
- We might not need every predictor
- A weighted combination of predictors might be better
- We should pick this combination to capture the "most information" possible
- Benefits
    - Reduced number of predictors
    - Reduced noise (due to averaging)

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"

$$X = UDV^T$$

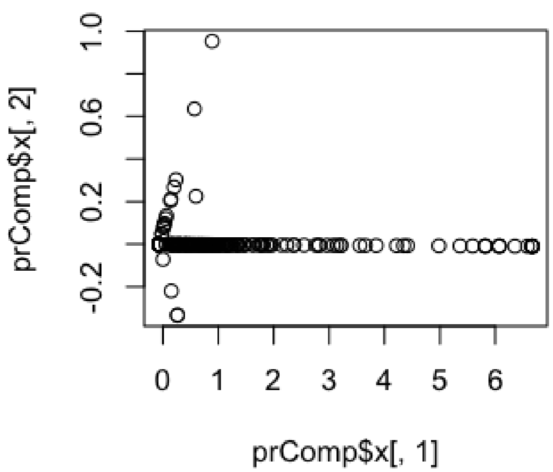
where the columns of U are orthogonal (left singular vectors), the columns of V are orthogonal (right singluar vectors) and D is a diagonal matrix (singular values).

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])
```



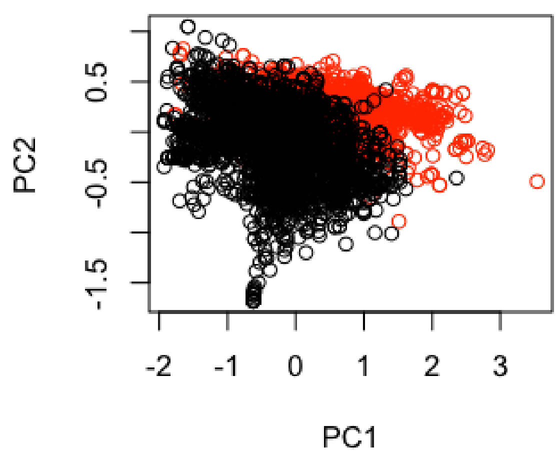
Principal components in R - prcomp

```
prComp$rotation
```

```
          PC1     PC2
num415 0.7081  0.7061
num857 0.7061 -0.7081
```

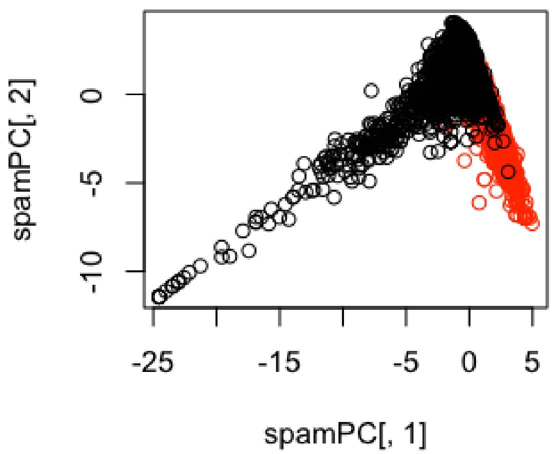
PCA on SPAM data

```
typeColor <- ((spam$type=="spam")*1 + 1)
prComp <- prcomp(log10(spam[,-58]+1))
plot(prComp$x[,1],prComp$x[,2],col=typeColor,xlab="PC1",ylab="PC2")
```



PCA with caret

```
preProc <- preProcess(log10(spam[,-58]+1),method="pca",pcaComp=2)
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",pcaComp=2)
trainPC <- predict(preProc,log10(training[,-58]+1))
modelFit <- train(training$type ~ .,method="glm",data=trainPC)
```

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     646   51
   spam         64  389

               Accuracy : 0.9
                 95% CI : (0.881, 0.917)
    No Information Rate : 0.617
    P-Value [Acc > NIR] : <2e-16

                  Kappa : 0.79
 Mcnemar's Test P-Value : 0.263

            Sensitivity : 0.910
            Specificity : 0.884
         Pos Pred Value : 0.927
         Neg Pred Value : 0.859
             Prevalence : 0.617
```

Alternative (sets # of PCs)

```
modelFit <- train(training$type ~ .,method="glm",preProcess="pca",data=training)
confusionMatrix(testing$type,predict(modelFit,testing))
```

```
Confusion Matrix and Statistics

          Reference
Prediction nonspam spam
   nonspam     660   37
   spam         54  399

               Accuracy : 0.921
                 95% CI : (0.904, 0.936)
    No Information Rate : 0.621
    P-Value [Acc > NIR] : <2e-16

                  Kappa : 0.833
 Mcnemar's Test P-Value : 0.0935

            Sensitivity : 0.924
            Specificity : 0.915
         Pos Pred Value : 0.947
         Neg Pred Value : 0.881
             Prevalence : 0.621
```

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