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,]
                               leave out 58th columns (the outcome)
M <- abs(cor(training[,-58])) Then calc correlations between all predictors.
diag(M) <- 0                   We're not interested in corr of vars with themselves.
which(M > 0.8,arr.ind=T)       Then select high correlations (>0.8)
```

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

Correlated predictors

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

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

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

-> those to Variables are extremely highly correlated.
[plot missing]

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

create 2 new variables x and y:

$$X = 0.71 \times num415 + 0.71 \times num857$$

$$Y = 0.71 \times num415 - 0.71 \times num857$$

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

[plot missing] -> most of the variability happens in x axis, almost none in y axis.

see plot on page 8.

Related problems

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

- 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

singular value decomposition

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

$$X = UDV^T$$ 3 matrices

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).

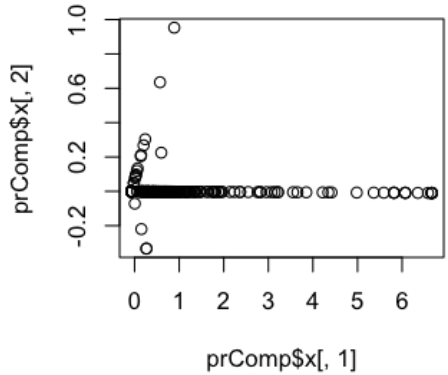
PCA

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])
```

cols 34 and 32 are those that correlate highly with each other



Principal components in R - prcomp

```
prComp$rotation
```

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

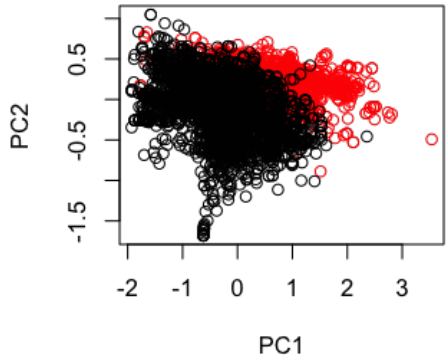
PCA on SPAM data

```
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")
```

black if not spam, red otherwise

take log to make it more gaussian

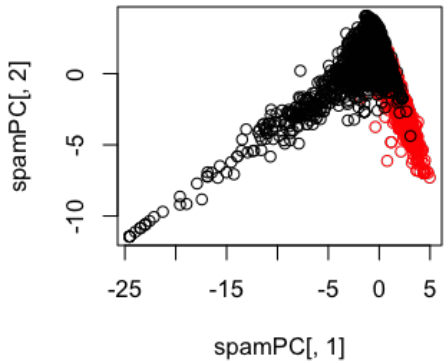
plot observations against the 2 most important principal components, coloring spam and not spam differently:



PCA with caret

tell it the number of components you want

```
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

the preProc we got from the training set!

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

but now applied on the training set

```
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
```

so: still high accuracy,
but with less components

Alternative (sets # of PCs)

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

Let caret do the pca-preprocessing automatically.
The predict function will apply the pca as well if you pass it the modelFit.

```
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
```

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