PRINCIPAL COMPONENTS AND PARTIAL LEAST SQUARES

1. Eigenvalues and eigenvectors. Spectral decomposition.

```
> attach(Auto);
> library(ISLR2); attach(Auto);
> X = model.matrix( mpg ~ weight + horsepower + cylinders - 1, data=Auto )
> A = cor(X)
> A
              weight horsepower cylinders
weight     1.0000000  0.8645377 0.8975273
horsepower 0.8645377  1.0000000 0.8429834
cylinders  0.8975273  0.8429834 1.0000000
>
> eigen(A)          # This produces eigenvalues and eigenvectors
eigen() decomposition
$values
[1] 2.73689293 0.16323918 0.09986789

$vectors
           [,1]       [,2]       [,3]
[1,] -0.5829268  0.2531535  0.7720813
[2,] -0.5708026 -0.8038435 -0.1673921
[3,] -0.5782566  0.5382834 -0.6130826

> lambda = eigen(A)$values
> Q = eigen(A)$vectors
>
> # Check QQ' = Q'Q = I and the spectral decomposition
>
> Q %*% t(Q)
             [,1]         [,2]         [,3]
[1,] 1.000000e+00 5.551115e-17 2.220446e-16
[2,] 5.551115e-17 1.000000e+00 8.326673e-17
[3,] 2.220446e-16 8.326673e-17 1.000000e+00
> t(Q) %*% Q
              [,1]          [,2]          [,3]
[1,]  1.000000e+00 -5.551115e-17 -1.110223e-16
[2,] -5.551115e-17  1.000000e+00  1.665335e-16
[3,] -1.110223e-16  1.665335e-16  1.000000e+00
>
> # These are identity matrices, all off-diagonal elements are practically 0
>
> LAMBDA = diag(lambda)         # Diagonal matrix with eigenvalues on the diagonal
> lambda
```

```
[1] 2.73689293 0.16323918 0.09986789
> LAMBDA
         [,1]      [,2]       [,3]
[1,] 2.736893 0.0000000 0.00000000
[2,] 0.000000 0.1632392 0.00000000
[3,] 0.000000 0.0000000 0.09986789
> Q %*% LAMBDA %*% t(Q)        # Spectral decomposition of matrix A
          [,1]      [,2]      [,3]
[1,] 1.0000000 0.8645377 0.8975273
[2,] 0.8645377 1.0000000 0.8429834
[3,] 0.8975273 0.8429834 1.0000000
> A
             weight horsepower cylinders
weight     1.0000000  0.8645377 0.8975273
horsepower 0.8645377  1.0000000 0.8429834
cylinders  0.8975273  0.8429834 1.0000000
>
> # This is the same matrix: Q %*% LAMBDA %*% t(Q) = A.
```

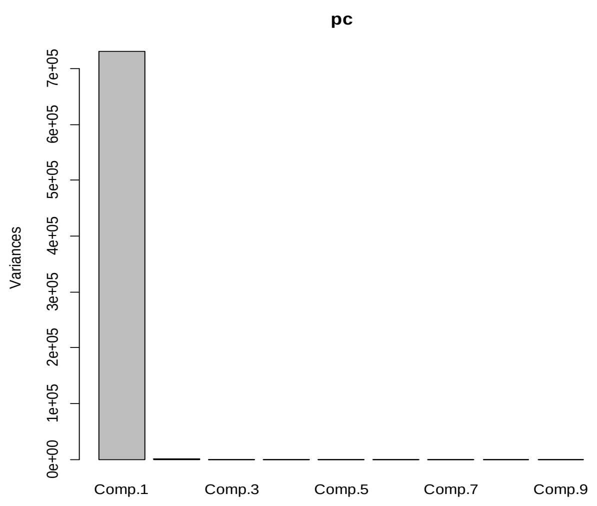
2. Principal Components

# Let's investigate the principal components, and how much variance they explain.

```
> X = model.matrix( mpg ~ .-name-origin+as.factor(origin), data=Auto )
> pc = princomp(X)
> summary(pc)
Importance of components:
                            Comp.1       Comp.2       Comp.3       Comp.4       Comp.5
Standard deviation     854.5664182 38.860050688 1.614144e+01 3.309297e+00 1.694518e+00
Proportion of Variance   0.9975617  0.002062789 3.559039e-04 1.495959e-05 3.922297e-06
Cumulative Proportion    0.9975617  0.999624521 9.999804e-01 9.999954e-01 9.999993e-01
                             Comp.6       Comp.7       Comp.8       Comp.9
Standard deviation     5.242357e-01 4.162175e-01 2.443204e-01 1.110223e-16
Proportion of Variance 3.754062e-07 2.366403e-07 8.153944e-08 1.683715e-38
Cumulative Proportion  9.999997e-01 9.999999e-01 1.000000e+00 1.000000e+00
```

# So, Z_1, the first PC, contains 99.76% of the total variation of X variables. The first two PCs together contain 99.96%. Here is a plot of these percents called a *screeplot*.

```
> screeplot(pc)
```



# The actual coefficients can be obtained by prcomp().

```
> prcomp(X)
                              PC1           PC2          PC3          PC4           PC5
(Intercept)          0.0000000000  0.0000000000  0.000000000  0.000000000  0.000000e+00
cylinders           -0.0017926225  0.0133245279 -0.007294275  0.001414710  1.719368e-02
displacement        -0.1143412856  0.9457785881 -0.303312504 -0.009143349 -1.059355e-02
horsepower          -0.0389670412  0.2982553337  0.948761071 -0.043076559 -8.646402e-02
weight              -0.9926735354 -0.1207516411 -0.002454212  0.001480458  3.152970e-03
acceleration         0.0013528348 -0.0348264293 -0.077006895  0.059516278 -9.944974e-01
year                 0.0013368415 -0.0238516081 -0.042819254 -0.996935229 -5.549653e-02
as.factor(origin)2   0.0001308250 -0.0024889942  0.002857670  0.022100094 -9.052576e-05
as.factor(origin)3   0.0002103564 -0.0003765828  0.004796684 -0.012089823 -1.150938e-03
                              PC6           PC7           PC8 PC9
(Intercept)          0.0000000000  0.0000000000  0.000000e+00   1
cylinders            0.9911554803  0.1211162208 -4.909265e-02   0
displacement        -0.0146594359 -0.0006512752  4.394368e-03   0
horsepower           0.0038232742  0.0034425206 -4.435100e-03   0
weight              -0.0002093216 -0.0003053766  5.729471e-06   0
acceleration         0.0168319859  0.0012233398 -1.799780e-03   0
year                -0.0001647840  0.0240346554  7.643176e-03   0
as.factor(origin)2  -0.0483462982  0.6888706846  7.229226e-01   0
as.factor(origin)3   0.1214929883 -0.7142804151  6.891098e-01   0
```

<u>**Standardized scale**</u>

So, we see that the 1st principal component contains a huge portion of the total variation of X variables, and it is dominated by variable "weight". Of course! Looking at the data, we see that weight simply has the largest values.

```
> head(Auto)
  mpg cylinders displacement horsepower weight acceleration year origin
1  18         8          307        130   3504         12.0   70      1
2  15         8          350        165   3693         11.5   70      1
3  18         8          318        150   3436         11.0   70      1
4  16         8          304        150   3433         12.0   70      1
5  17         8          302        140   3449         10.5   70      1
6  15         8          429        198   4341         10.0   70      1
```

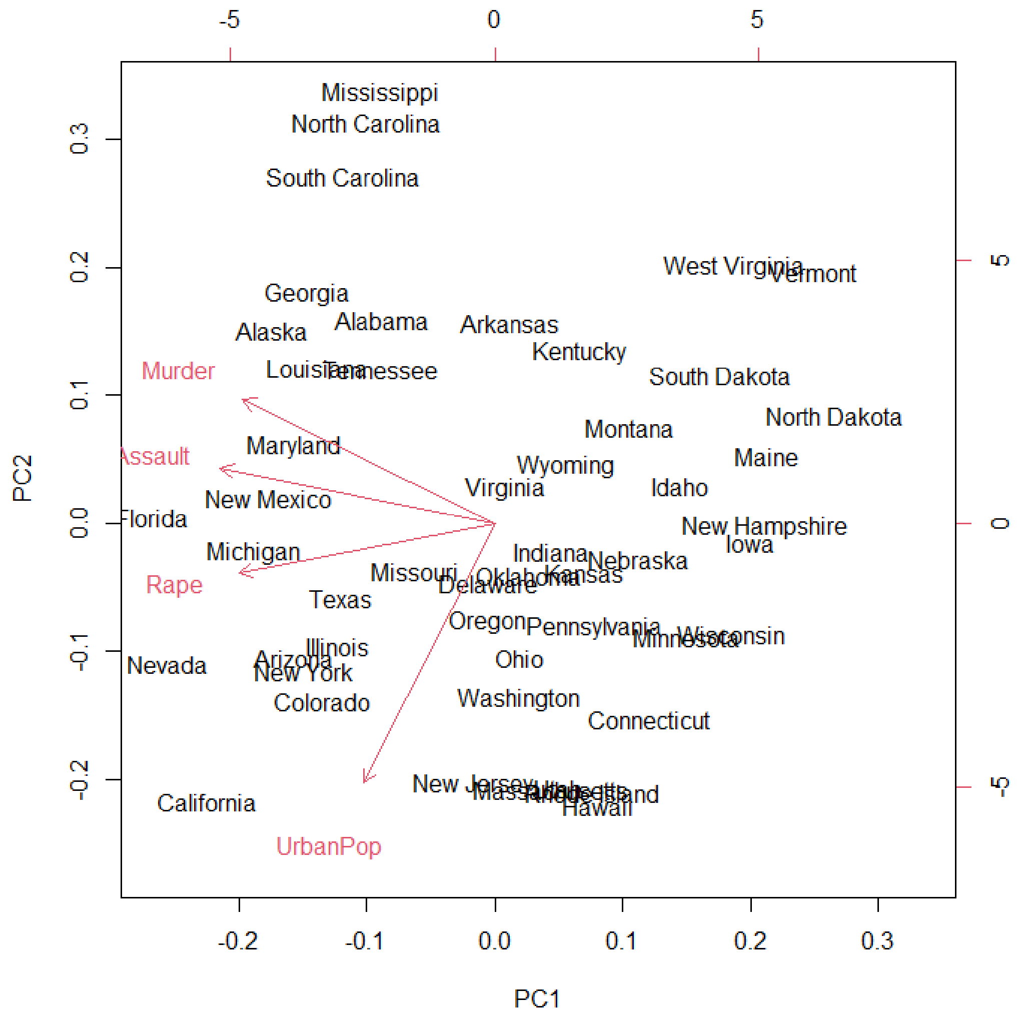
# For this reason, usually, X variables are standardized first (subtract each X-variable's mean and divide by the standard deviation).

> pcr.fit = pcr(mpg ~ .-name-origin+as.factor(origin), data=Auto, scale=TRUE)
> summary(pcr.fit)

```
TRAINING: % variance explained
     1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X       56.9    73.02    84.29    92.38    97.29    98.86    99.59   100.00
mpg     71.8    73.64    73.96    79.25    79.25    80.22    81.55    82.42
```

Visualization

```
> names(USArrests)
[1] "Murder"   "Assault"  "UrbanPop" "Rape"
> pc = prcomp(USArrests, scale=TRUE)
> biplot(pc)
```



3. Principal Components Regression

```
> library(pls)
> pcr.fit = pcr( mpg ~ . ╥ name ╥ origin + as.factor(origin),  data=Auto )
# Using all variables except name

> summary(pcr.fit)


TRAINING: % variance explained
     1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X      99.76    99.96   100.00   100.00   100.00   100.00   100.00   100.00
mpg    69.35    70.09    70.75    80.79    80.88    80.91    80.93    82.42
```

# The “X” row shows % of X variation contained in the given number of PCs.
# The “mpg” row shows R^2 (% of Y variation explained) from the PC regression. The usual linear regression on all 8 variables has the same R^2 as PCR that uses all 8 principal components.

```
> reg = lm( mpg ~ .-name-origin+as.factor(origin), data=Auto )
> summary(reg)
Multiple R-squared:  0.8242
```

### Cross-validation

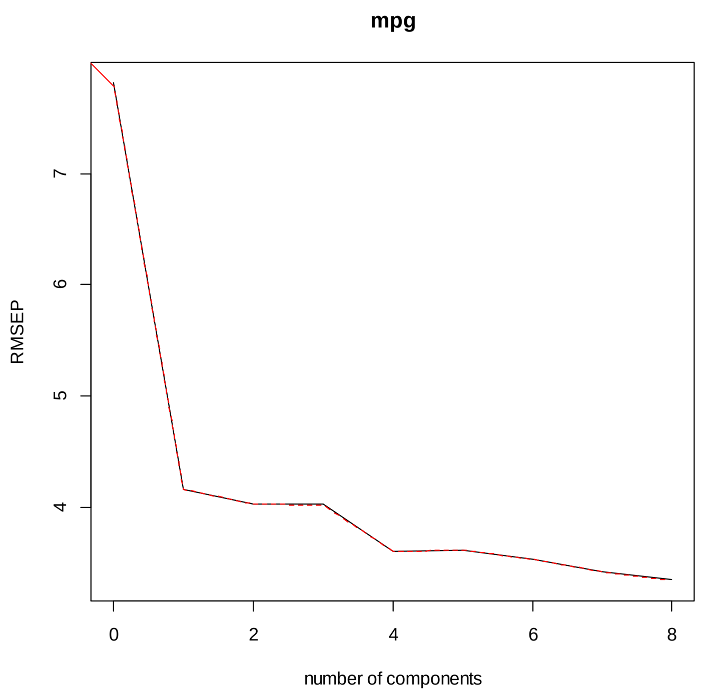
# Cross-validation. Option `validation="CV"` does a K-fold cross-validation with K=10, for LOOCV, use `validation="LOO"`.

```
> pcr.fit = pcr( mpg ~ .-name-origin+as.factor(origin), data=Auto, scale=TRUE, validation="CV" )
> summary(pcr.fit)

VALIDATION: RMSEP
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
CV           7.815    4.162    4.036    4.028    3.611    3.616    3.537    3.427    3.350
adjCV        7.815    4.161    4.034    4.026    3.607    3.613    3.533    3.422    3.346
```

# The predicted error (by cross-validation) is minimized by using all M=8 principal components.
# We can see the graph of *root mean-squared error of prediction* (or specify val.type)

```
> validationplot(pcr.fit)
```



3. Partial Least Squares

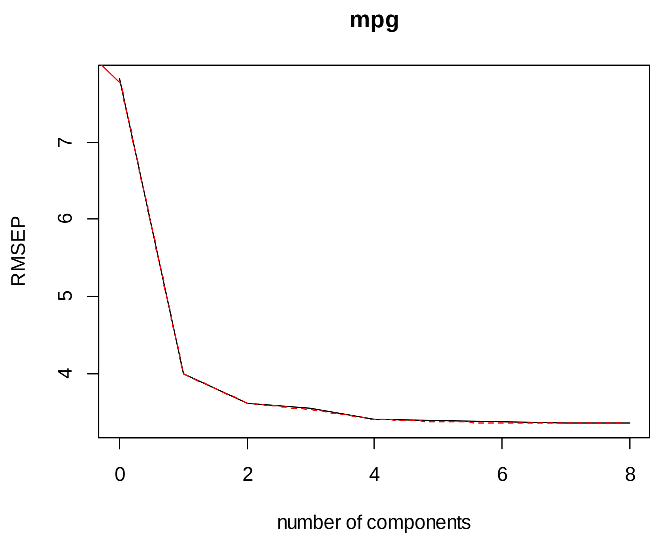
# Similar commands, just replace "pcr" with "plsr". M=6 components gives the lowest prediction MSE.

```
> pls = plsr( mpg ~ .-name-origin+as.factor(origin), data=Auto, scale=TRUE, validation="CV" )
> summary(pls)
```

```
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
CV           7.815    3.994    3.616    3.540    3.395    3.379    3.351    3.364    3.362
adjCV        7.815    3.992    3.612    3.535    3.390    3.376    3.345    3.359    3.357

TRAINING: % variance explained
     1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X      56.73    68.84    80.75    84.08    93.48    94.88    99.33   100.00
mpg    74.32    79.37    80.29    81.71    82.00    82.35    82.38    82.42
```

```
> validationplot(pls)
```



# Next, we can fit a model with the desired number of principal components, obtain predicted values, and calculate the prediction mean-squared error. For example:

```
> n = length(mpg);
> Z = sample(n,n/2);
> PLS = plsr( mpg ~ .-name-origin+as.factor(origin), data=Auto[Z,], scale=TRUE, ncomp=6 );
> Yhat = predict( PLS, newdata=Auto[-Z,], ncomp=6 )
> MSE = mean((Yhat - mpg[-Z])^2)
> MSE
[1] 9.619134
> RMSE = sqrt(MSE)
> RMSE
[1] 3.101473
```