Principal component regression (PCR)

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Here, I am adapting part of the lab associated with Chapter 6 of the textbook.

Data Prep

We wish to predict a baseball player's Salary on the basis of various statistics associated with performance in the previous year.

First of all, we note that the Salary variable is missing for some of the players. The is.na() function can be used to identify the missing observations. It returns a vector of the same length as the input vector, with a TRUE for any elements that are missing, and a FALSE for non-missing elements. The sum() function can then be used to count all of the missing elements.

```
library(ISLR2)
data(Hitters)
names (Hitters)
    [1] "AtBat"
                     "Hits"
                                  "HmRun"
                                               "Runs"
                                                            "RBI"
                                                                        "Walks"
##
                     "CAtBat"
                                                                        "CRBI"
    [7] "Years"
                                  "CHits"
                                               "CHmRun"
                                                            "CRuns"
## [13] "CWalks"
                     "League"
                                               "PutOuts"
                                                                        "Errors"
                                  "Division"
                                                            "Assists"
## [19] "Salary"
                     "NewLeague"
#View(Hitters)
dim(Hitters)
## [1] 322 20
sum(is.na(Hitters$Salary))
```

[1] 59

Hence we see that Salary is missing for 59 players. The na.omit() function removes all of the rows that have missing values in any variable.

```
Hitters <- na.omit(Hitters)

## [1] 263 20

sum(is.na(Hitters))

## [1] 0

All is well now, so we attach the data for ease of use.

attach(Hitters)
```

Principal Components Regression

summary(pcr.fit)

Salary

Salary

##

X

Principal components regression (PCR) can be performed using the pcr() function, which is part of the pls library. We now apply PCR to the Hitters data, in order to predict Salary.

The syntax for the pcr() function is similar to that for lm(), with a few additional options. Setting scale = TRUE has the effect of standardizing each predictor, prior to generating the principal components, so that the scale on which each variable is measured will not have an effect. Setting validation = "CV" causes pcr() to compute the ten-fold cross-validation error for each possible value of M, the number of principal components used. The resulting fit can be examined using summary().

```
## Data:
             X dimension: 263 19
    Y dimension: 263 1
## Fit method: svdpc
  Number of components considered: 19
##
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##
           (Intercept)
                        1 comps
                                  2 comps
                                            3 comps
                                                      4 comps
                                                                5 comps
                                                                          6 comps
## CV
                   452
                           352.5
                                    351.6
                                              352.3
                                                        350.7
                                                                  346.1
                                                                            345.5
                   452
                           352.1
                                    351.2
                                                        350.1
                                                                  345.5
                                                                            344.6
##
   adjCV
                                              351.8
                    8 comps
                              9 comps
                                        10 comps
                                                   11 comps
                                                             12 comps
##
          7 comps
                                                                         13 comps
                                350.4
                                                      354.5
## CV
             345.4
                      348.5
                                           353.2
                                                                 357.5
                                                                            360.3
## adjCV
             344.5
                      347.5
                                349.3
                                           351.8
                                                      353.0
                                                                 355.8
                                                                            358.5
                                                                 19 comps
##
           14 comps
                     15 comps
                                16 comps
                                           17 comps
                                                      18 comps
              352.4
                         354.3
                                    345.6
                                              346.7
                                                         346.6
                                                                    349.4
## CV
              350.2
                         352.3
                                    343.6
                                              344.5
                                                         344.3
                                                                    346.9
  adjCV
##
##
## TRAINING: % variance explained
##
            1 comps
                     2 comps
                               3 comps
                                         4 comps
                                                   5 comps
                                                            6 comps
                                                                      7 comps
                                                                                8 comps
## X
              38.31
                        60.16
                                 70.84
                                           79.03
                                                     84.29
                                                               88.63
                                                                         92.26
                                                                                  94.96
## Salary
              40.63
                        41.58
                                 42.17
                                           43.22
                                                     44.90
                                                               46.48
                                                                         46.69
                                                                                  46.75
            9 comps
                                           12 comps
                                                      13 comps
##
                     10 comps
                                11 comps
                                                                 14 comps
                                                                            15 comps
## X
              96.28
                         97.26
                                    97.98
                                              98.65
                                                         99.15
                                                                    99.47
                                                                               99.75
```

47.76

99.97

53.85

17 comps

46.86

99.89

53.01

16 comps

47.82

99.99

54.61

18 comps

The CV score is provided for each possible number of components, ranging from M=0 onwards. Note that pcr() reports the root mean squared error; in order to obtain the usual MSE, we must square this quantity.

47.85

100.00

54.61

19 comps

48.10

50.40

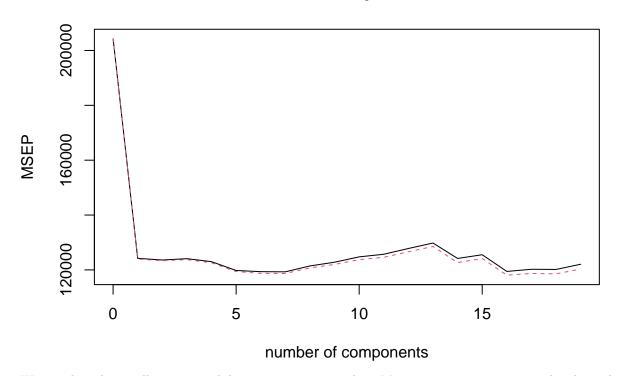
50.55

For instance, a root mean squared error of 352.8 corresponds to an MSE of $352.8^2 = 124,468$.

One can also plot the cross-validation scores using the validationplot() function. Using val.type = "MSEP" will cause the cross-validation MSE to be plotted.

```
validationplot(pcr.fit, val.type = "MSEP")
```

Salary



We see that the smallest cross-validation error occurs when M=18 components are used. This is barely fewer than M=19, which amounts to simply performing least squares, because when all of the components are used in PCR no dimension reduction occurs. However, from the plot we also see that the cross-validation error is roughly the same when only one component is included in the model. This suggests that a model that uses just a small number of components might suffice.

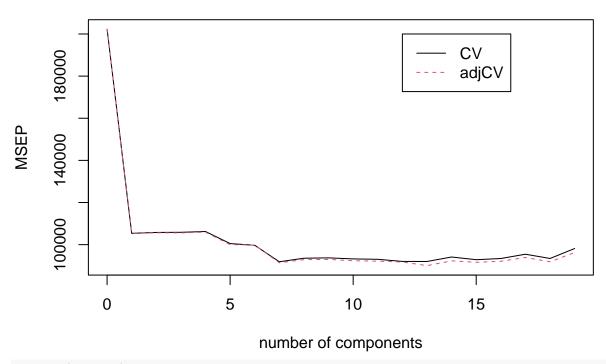
The summary() function also provides the percentage of variance explained in the predictors and in the response using different numbers of components. Briefly, we can think of this as the amount of information about the predictors or the response that is captured using M principal components. For example, setting M=1 only captures 38.31% of all the variance, or information, in the predictors. In contrast, using M=5 increases the value to 84.29%. If we were to use all M=p=19 components, this would increase to 100%.

We now perform PCR on the training data and evaluate its test set performance.

```
set.seed(1)
#splitting the data set
train <- sample(c(TRUE, FALSE), nrow(Hitters),
    replace = TRUE)
test <- (!train)

pcr.fit <- pcr(Salary ~ ., data = Hitters, subset = train,
    scale = TRUE, validation = "CV")
validationplot(pcr.fit, val.type = "MSEP", legendpos = t(c(12,200000)))</pre>
```

Salary



summary(pcr.fit)

```
X dimension: 134 19
## Data:
  Y dimension: 134 1
## Fit method: svdpc
## Number of components considered: 19
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
                       1 comps 2 comps 3 comps 4 comps 5 comps
          (Intercept)
                                                                      6 comps
## CV
                449.8
                          324.6
                                   325.3
                                            325.4
                                                      325.9
                                                               317.0
                                                                         315.8
## adjCV
                449.8
                          324.4
                                   325.0
                                            324.9
                                                      325.5
                                                               316.2
                                                                         316.0
          7 comps 8 comps 9 comps 10 comps 11 comps 12 comps 13 comps
##
            303.1
                     305.9
                               306.1
                                         305.4
                                                    305.0
                                                              303.4
## CV
                                                                         303.3
## adjCV
            302.3
                     304.8
                               304.9
                                         303.9
                                                    303.6
                                                              302.9
                                                                         300.1
##
          14 comps
                    15 comps
                               16 comps 17 comps
                                                    18 comps
                                                              19 comps
## CV
             306.8
                       304.7
                                  305.6
                                            309.0
                                                       305.7
                                                                 313.3
             303.8
                       302.7
                                  303.5
                                            306.4
                                                       303.1
                                                                 310.3
## adjCV
##
## TRAINING: % variance explained
##
           1 comps 2 comps 3 comps
                                      4 comps 5 comps
                                                          6 comps
                                                                   7 comps
                                                                             8 comps
## X
             40.68
                      61.14
                                72.31
                                         80.05
                                                   85.34
                                                                               95.54
                                                            89.31
                                                                      92.86
## Salary
             48.25
                       48.49
                                49.58
                                         50.27
                                                   53.81
                                                            54.43
           9 comps
##
                    10 comps
                                         12 comps
                                                   13 comps
                                                              14 comps
                               11 comps
                                                                        15 comps
## X
             96.96
                        97.72
                                  98.33
                                            98.75
                                                       99.11
                                                                 99.44
                                                                            99.76
                                                       63.96
## Salary
             59.87
                        61.62
                                  61.77
                                            61.84
                                                                 64.10
                                                                            64.10
##
           16 comps
                     17 comps
                               18 comps
                                          19 comps
                         99.97
                                   99.99
## X
               99.9
                                            100.00
## Salary
               64.6
                         65.43
                                   66.49
                                              66.58
```

Now we find that the lowest cross-validation error occurs when M=7 components are used. We compute the test MSE as follows.

```
x <- model.matrix(Salary ~ ., Hitters)[, -1]</pre>
y <- Hitters$Salary
y.test <- y[test]</pre>
pcr.pred <- predict(pcr.fit, x[test, ], ncomp = 7)</pre>
mean((pcr.pred - y.test)^2)
## [1] 145656
Finally, we fit PCR on the full data set, using M=7, the number of components identified by cross-validation.
pcr.fit <- pcr(y ~ x, scale = TRUE, ncomp = 7)</pre>
summary(pcr.fit)
## Data:
             X dimension: 263 19
## Y dimension: 263 1
## Fit method: svdpc
## Number of components considered: 7
## TRAINING: % variance explained
##
      1 comps 2 comps 3 comps 4 comps
                                             5 comps
                                                       6 comps
                                                                 7 comps
## X
        38.31
                  60.16
                            70.84
                                      79.03
                                                84.29
                                                         88.63
                                                                   92.26
        40.63
                  41.58
                            42.17
                                      43.22
                                                44.90
                                                         46.48
                                                                   46.69
## y
```