```
# pcr.r
# install.packages("pls")
library(pls) # needed?
library(dplyr)
library(caret)
              # createDataPartition(), train()
library(MASS)
                # Boston dataset
dim(Boston)
## [1] 506 14
# 20% test sets
set.seed(123)
training.samples <- Boston$medv %>% createDataPartition(p = 0.8, list = FALSE)
head(training.samples)
##
       Resample1
## [1,]
               1
## [2,]
## [3,]
## [4,]
               5
## [5,]
               7
## [6,]
train.data <- Boston[training.samples, ]</pre>
test.data <- Boston[-training.samples, ]</pre>
dim(train.data)
## [1] 407 14
dim(test.data)
## [1] 99 14
head(test.data)
              zn indus chas
                                                 dis rad tax ptratio black
        crim
                               nox
                                      rm
                                          age
## 3 0.02729 0.0 7.07
                          0 0.469 7.185
                                         61.1 4.9671
                                                       2 242
                                                                17.8 392.83
                           0 0.458 6.430 58.7 6.0622
## 6 0.02985 0.0 2.18
                                                       3 222
                                                                18.7 394.12
## 9 0.21124 12.5 7.87 0 0.524 5.631 100.0 6.0821 5 311
                                                                15.2 386.63
## 11 0.22489 12.5 7.87 0 0.524 6.377 94.3 6.3467 5 311 15.2 392.52
## 14 0.62976 0.0 8.14 0 0.538 5.949 61.8 4.7075 4 307
                                                                21.0 396.90
## 15 0.63796 0.0 8.14 0 0.538 6.096 84.5 4.4619 4 307
                                                                21.0 380.02
##
     1stat medv
## 3 4.03 34.7
## 6 5.21 28.7
## 9 29.93 16.5
## 11 20.45 15.0
## 14 8.26 20.4
## 15 10.26 18.2
# pcr
# fit 10 models
set.seed(1)
```

```
model <- train(medv~., data = train.data,</pre>
              method = "pcr",
              scale = TRUE,
              trControl = trainControl("cv", number = 10),
              tuneLength = 10)
str(model)
## List of 23
## $ method
                : chr "pcr"
## $ modelInfo :List of 12
##
    ..$ label
                 : chr "Principal Component Analysis"
    ..$ library : chr "pls"
##
##
    ..$ type
                 : chr "Regression"
##
     ..$ parameters:'data.frame': 1 obs. of 3 variables:
     .... $\square$ parameter: Factor w/ 1 level "ncomp": 1
    ....$ class : Factor w/ 1 level "numeric": 1
##
##
                   : Factor w/ 1 level "#Components": 1
     .. ..$ label
##
     ..$ grid
                 :function (x, y, len = NULL, search = "grid")
     ...- attr(*, "srcref")= 'srcref' int [1:8] 7 26 14 19 26 19 7 14
     ..... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
##
     ..$ loop
                  :function (grid)
     ... - attr(*, "srcref")= 'srcref' int [1:8] 15 26 20 19 26 19 15 20
##
    ..... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
##
##
                  :function (x, y, wts, param, lev, last, classProbs, ...)
##
     ... - attr(*, "srcref")= 'srcref' int [1:8] 21 25 26 19 25 19 21 26
     .... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
##
##
                 :function (modelFit, newdata, submodels = NULL)
    ..$ predict
     ... - attr(*, "srcref")= 'srcref' int [1:8] 27 29 37 19 29 19 27 37
##
##
     ..... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
##
     ..$ predictors:function (x, ...)
     ....- attr(*, "srcref")= 'srcref' int [1:8] 38 32 38 70 32 70 38 38
##
##
     ..... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
                  : chr [1:2] "Linear Regression" "Feature Extraction"
##
     ..$ tags
##
    ..$ prob
                  : NULL
##
    ..$ sort
                  :function (x)
     ....- attr(*, "srcref")= 'srcref' int [1:8] 41 26 41 53 26 53 41 41
    ..... attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x7ff6c5384a40>
##
   $ modelType : chr "Regression"
##
##
   $ results
                :'data.frame':
                                  10 obs. of 7 variables:
##
    ..$ ncomp
                 : num [1:10] 1 2 3 4 5 6 7 8 9 10
                  : num [1:10] 7.17 6.85 5.56 5.26 5.11 ...
##
    ..$ RMSE
##
    ..$ Rsquared : num [1:10] 0.389 0.449 0.622 0.661 0.689 ...
                 : num [1:10] 4.99 4.98 3.84 3.54 3.42 ...
##
    ..$ MAE
                : num [1:10] 1.15 1.11 1.14 1.19 1.13 ...
##
    ..$ RMSESD
##
    ..$ RsquaredSD: num [1:10] 0.135 0.14 0.163 0.169 0.153 ...
##
                 : num [1:10] 0.59 0.602 0.489 0.448 0.449 ...
    ..$ MAESD
## $ pred
                 : NULL
                 :'data.frame': 1 obs. of 1 variable:
  $ bestTune
##
    ..$ ncomp: num 6
                 : language train.formula(form = medv ~ ., data = train.data, method = "pcr", scale = '
## $ call
## $ dots
                 :List of 1
   ..$ scale: logi TRUE
##
              : chr "RMSE"
   $ metric
```

\$ control

:List of 28

```
: chr "cv"
##
     ..$ method
##
     ..$ number
                          : num 10
##
     ..$ repeats
                          : logi NA
     ..$ search
                          : chr "grid"
##
##
     ..$ p
                          : num 0.75
##
     ..$ initialWindow
                          : NULL
##
     ..$ horizon
                          : num 1
##
     ..$ fixedWindow
                          : logi TRUE
##
     ..$ skip
                          : num O
##
     ..$ verboseIter
                         : logi FALSE
##
     ..$ returnData
                          : logi TRUE
                          : chr "final"
##
     ..$ returnResamp
     ..$ savePredictions : chr "none"
##
##
     ..$ classProbs
                          : logi FALSE
##
     ..$ summaryFunction :function (data, lev = NULL, model = NULL)
##
     ..$ selectionFunction: chr "best"
##
     ..$ preProcOptions
                          :List of 6
##
     .. ..$ thresh
                    : num 0.95
##
     ...$ ICAcomp : num 3
##
     .. ..$ k
                     : num 5
##
     ....$ freqCut : num 19
##
     .. ..$ uniqueCut: num 10
##
     .. ..$ cutoff
                    : num 0.9
##
     ..$ sampling
                          : NULL
##
     ..$ index
                          :List of 10
     ....$ Fold01: int [1:366] 1 4 5 6 7 8 9 10 11 12 ...
##
     ....$ Fold02: int [1:366] 1 2 3 4 5 6 7 8 9 10 ...
     ....$ Fold03: int [1:366] 2 3 4 5 6 8 9 10 13 14 ...
     ....$ Fold04: int [1:366] 1 2 3 5 6 7 8 9 11 12 ...
##
     ....$ Fold05: int [1:367] 1 2 3 4 6 7 9 10 11 12 ...
     ....$ Fold06: int [1:365] 1 2 3 4 5 7 8 9 10 11 ...
##
##
     ....$ Fold07: int [1:367] 1 2 3 4 5 6 7 8 10 11 ...
     ....$ Fold08: int [1:366] 1 2 3 4 5 6 7 8 9 10 ...
##
##
     ....$ Fold09: int [1:367] 1 2 3 4 5 6 7 8 9 10 ...
     ....$ Fold10: int [1:367] 1 2 3 4 5 6 7 8 9 10 ...
##
##
     ..$ indexOut
                          :List of 10
##
     ....$ Resample01: int [1:41] 2 3 22 27 39 44 57 61 72 86 ...
##
     ....$ Resample02: int [1:41] 54 64 98 110 111 131 139 145 156 167 ...
##
     ....$ Resample03: int [1:41] 1 7 11 12 36 38 45 52 85 99 ...
     ....$ Resample04: int [1:41] 4 10 31 41 42 47 51 55 68 69 ...
##
##
     ....$ Resample05: int [1:40] 5 8 16 50 63 70 71 73 77 79 ...
##
     ....$ Resample06: int [1:42] 6 13 28 37 53 65 78 83 92 93 ...
     ....$ Resample07: int [1:40] 9 19 21 24 25 30 75 81 88 101 ...
##
     \dots $\ Resample08: int [1:41] 14 17 18 20 23 29 32 35 46 58 \dots
     ....$ Resample09: int [1:40] 15 33 49 76 82 84 90 95 102 120 ...
##
     ....$ Resample10: int [1:40] 26 34 40 43 48 56 59 60 62 66 ...
##
     ..$ indexFinal
                          : NULL
##
     ..$ timingSamps
                          : num 0
##
     ...$ predictionBounds : logi [1:2] FALSE FALSE
##
     ..$ seeds
                          :List of 11
##
     ....$ : int 452737
##
     ....$ : int 124413
##
     ....$ : int 436523
     ....$ : int 856018
##
```

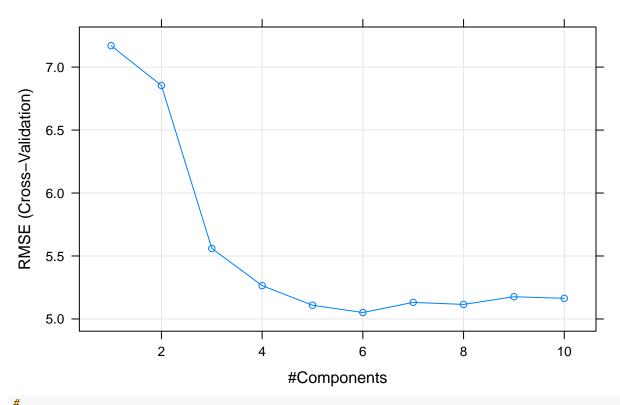
```
##
    .. ..$ : int 666931
##
    ....$ : int 25173
    ....$ : int 294762
##
##
    ....$ : int 392686
##
    ....$ : int 640775
##
    ....$ : int 538191
    ....$ : int 270373
##
     ..$ adaptive
                         :List of 4
##
    ....$ min : num 5
##
    ....$ alpha : num 0.05
     .... $ method : chr "gls"
##
     ....$ complete: logi TRUE
    ..$ trim
##
                  : logi FALSE
    ..$ allowParallel : logi TRUE
##
##
    ..$ yLimits
                       : num [1:2] 2.75 52.25
   $ finalModel :List of 23
##
    ..$ coefficients : num [1:13, 1, 1:6] -0.5735 0.567 -0.7786 0.0146 -0.7678 ...
##
    ...- attr(*, "dimnames")=List of 3
     .....$ : chr [1:13] "crim" "zn" "indus" "chas" ...
##
    .. ...$ : chr ".outcome"
##
##
    .....$ : chr [1:6] "1 comps" "2 comps" "3 comps" "4 comps" ...
                : 'scores' num [1:407, 1:6] -2.13 -1.47 -2.63 -2.47 -1.39 ...
     ... - attr(*, "dimnames")=List of 2
##
    ....$ : chr [1:407] "X1" "X2" "X4" "X5" ...
    .....$ : chr [1:6] "Comp 1" "Comp 2" "Comp 3" "Comp 4" ...
##
    ..$ loadings : 'loadings' num [1:13, 1:6] 0.25424 -0.25133 0.34515 -0.00649 0.34034 ...
     ....- attr(*, "dimnames")=List of 2
##
    .....$ : chr [1:13] "crim" "zn" "indus" "chas" ...
    ....$ : chr [1:6] "Comp 1" "Comp 2" "Comp 3" "Comp 4" ...
     ..$ Yloadings : 'loadings' num [1, 1:6] -2.26 1.89 3.65 2.11 -1.21 ...
     ... - attr(*, "dimnames")=List of 2
##
    .. ... ..$ : chr ".outcome"
##
     ....$ : chr [1:6] "Comp 1" "Comp 2" "Comp 3" "Comp 4" ...
##
     ..$ projection : num [1:13, 1:6] 0.25424 -0.25133 0.34515 -0.00649 0.34034 ...
##
     ... - attr(*, "dimnames")=List of 2
##
    .....$ : chr [1:13] "crim" "zn" "indus" "chas" ...
##
    .....$ : chr [1:6] "Comp 1" "Comp 2" "Comp 3" "Comp 4" ...
##
                    : Named num [1:13] 0.435 0.488 1.623 0.282 4.806 ...
     ..$ Xmeans
     ....- attr(*, "names")= chr [1:13] "crim" "zn" "indus" "chas" ...
##
                   : Named num 22.5
##
     ..$ Ymeans
    ....- attr(*, "names")= chr ".outcome"
     ..$ fitted.values: num [1:407, 1, 1:6] 27.3 25.8 28.4 28.1 25.7 ...
##
    ...- attr(*, "dimnames")=List of 3
##
    .. .. ..$ : chr [1:407] "X1" "X2" "X4" "X5" ...
##
     .. ...$ : chr ".outcome"
     .....$ : chr [1:6] "1 comps" "2 comps" "3 comps" "4 comps" ...
##
    ..$ residuals : num [1:407, 1, 1:6] -3.31 -4.24 4.96 8.11 -2.75 ...
##
##
    ....- attr(*, "dimnames")=List of 3
     .....$ : chr [1:407] "X1" "X2" "X4" "X5" ...
##
    .. .. ..$ : chr ".outcome"
##
    .....$ : chr [1:6] "1 comps" "2 comps" "3 comps" "4 comps" ...
##
                   : Named num [1:6] 2535 570 483 360 331 ...
##
##
     ... - attr(*, "names")= chr [1:6] "Comp 1" "Comp 2" "Comp 3" "Comp 4" ...
##
    ..$ Xtotvar : num 5278
```

```
##
                   : Named num 0.001
    ..$ fit.time
    .. ..- attr(*, "names")= chr "elapsed"
##
##
    ..$ ncomp
                    : num 6
                     : chr "svdpc"
##
    ..$ method
                    : Named num [1:13] 8.264 22.715 6.809 0.262 0.116 ...
##
    ..$ scale
    ....- attr(*, "names")= chr [1:13] "crim" "zn" "indus" "chas" ...
##
                    : language pcr(formula = .outcome ~ ., ncomp = ncomp, data = dat, scale = TRUE)
    ..$ call
                     :Classes 'terms', 'formula' language .outcome ~ crim + zn + indus + chas + nox +
##
    ..$ terms
##
    ..... attr(*, "variables")= language list(.outcome, crim, zn, indus, chas, nox, rm, age, dis,
    ..... attr(*, "factors")= int [1:14, 1:13] 0 1 0 0 0 0 0 0 0 ...
##
    ..... attr(*, "dimnames")=List of 2
    .....$ : chr [1:14] ".outcome" "crim" "zn" "indus" ...
##
    ..... s: chr [1:13] "crim" "zn" "indus" "chas" ...
    ..... attr(*, "term.labels")= chr [1:13] "crim" "zn" "indus" "chas" ...
##
     ..... attr(*, "order")= int [1:13] 1 1 1 1 1 1 1 1 1 1 ...
    .. .. ..- attr(*, "intercept")= int 1
##
    .. .. ..- attr(*, "response")= int 1
##
    ..... attr(*, ".Environment")=<environment: 0x7ff6b0a1b440>
     .... - attr(*, "predvars")= language list(.outcome, crim, zn, indus, chas, nox, rm, age, dis, r
##
    .... attr(*, "dataClasses")= Named chr [1:14] "numeric" "numeric" "numeric" "numeric" ...
##
##
    ..... attr(*, "names")= chr [1:14] ".outcome" "crim" "zn" "indus" ...
                     :'data.frame':
                                    407 obs. of 14 variables:
     ....$ .outcome: num [1:407] 24 21.6 33.4 36.2 22.9 27.1 18.9 18.9 21.7 19.9 ...
##
                : num [1:407] 0.00632 0.02731 0.03237 0.06905 0.08829 ...
##
    .. ..$ crim
                   : num [1:407] 18 0 0 0 12.5 12.5 12.5 12.5 12.5 0 ...
##
    .. ..$ zn
    ....$ indus : num [1:407] 2.31 7.07 2.18 2.18 7.87 7.87 7.87 7.87 7.87 8.14 ...
                  : num [1:407] 0 0 0 0 0 0 0 0 0 0 ...
##
     .. ..$ chas
                  : num [1:407] 0.538 0.469 0.458 0.458 0.524 0.524 0.524 0.524 0.524 0.538 ...
##
    .. ..$ nox
##
                 : num [1:407] 6.58 6.42 7 7.15 6.01 ...
                  : num [1:407] 65.2 78.9 45.8 54.2 66.6 96.1 85.9 82.9 39 56.5 ...
     .. ..$ age
##
    .. ..$ dis
                  : num [1:407] 4.09 4.97 6.06 6.06 5.56 ...
##
    .. ..$ rad
                  : num [1:407] 1 2 3 3 5 5 5 5 5 4 ...
##
                  : num [1:407] 296 242 222 222 311 311 311 311 311 307 ...
    ....$ ptratio: num [1:407] 15.3 17.8 18.7 18.7 15.2 15.2 15.2 15.2 15.2 21 ...
##
    ....$ black : num [1:407] 397 397 395 397 396 ...
    ....$ lstat : num [1:407] 4.98 9.14 2.94 5.33 12.43 ...
##
    ...- attr(*, "terms")=Classes 'terms', 'formula' language .outcome ~ crim + zn + indus + chas +
    ..... attr(*, "variables")= language list(.outcome, crim, zn, indus, chas, nox, rm, age, di
##
    ..... attr(*, "factors")= int [1:14, 1:13] 0 1 0 0 0 0 0 0 0 0 ...
##
    ..... attr(*, "dimnames")=List of 2
##
    ..... s: chr [1:14] ".outcome" "crim" "zn" "indus" ...
    .....$ : chr [1:13] "crim" "zn" "indus" "chas" ...
##
    ..... attr(*, "term.labels")= chr [1:13] "crim" "zn" "indus" "chas" ...
    ..... attr(*, "order")= int [1:13] 1 1 1 1 1 1 1 1 1 1 ...
##
    .. .. .. - attr(*, "intercept")= int 1
    .. .. .. - attr(*, "response")= int 1
##
##
    ..... attr(*, ".Environment")=<environment: 0x7ff6b0a1b440>
    ..... attr(*, "predvars")= language list(.outcome, crim, zn, indus, chas, nox, rm, age, dis
    ..... attr(*, "dataClasses")= Named chr [1:14] "numeric" "numeric" "numeric" "numeric" ...
##
    ..... attr(*, "names")= chr [1:14] ".outcome" "crim" "zn" "indus" ...
##
                    : chr [1:13] "crim" "zn" "indus" "chas" ...
##
##
    ..$ problemType : chr "Regression"
##
    ..$ tuneValue :'data.frame': 1 obs. of 1 variable:
##
    .. ..$ ncomp: num 6
```

```
##
     ..$ obsLevels
                     : logi NA
##
     ..$ param
                     :List of 1
##
     ....$ scale: logi TRUE
     ..- attr(*, "class")= chr "mvr"
##
   $ preProcess : NULL
##
   $ trainingData:'data.frame':
                                   407 obs. of 14 variables:
##
     ..$ .outcome: num [1:407] 24 21.6 33.4 36.2 22.9 27.1 18.9 18.9 21.7 19.9 ...
##
                : num [1:407] 0.00632 0.02731 0.03237 0.06905 0.08829 ...
##
     ..$ zn
                 : num [1:407] 18 0 0 0 12.5 12.5 12.5 12.5 12.5 0 ...
##
     ..$ indus : num [1:407] 2.31 7.07 2.18 2.18 7.87 7.87 7.87 7.87 7.87 8.14 ...
                : int [1:407] 0 0 0 0 0 0 0 0 0 0 ...
##
                : num [1:407] 0.538 0.469 0.458 0.458 0.524 0.524 0.524 0.524 0.524 0.538 ...
     ..$ nox
##
     ..$ rm
                : num [1:407] 6.58 6.42 7 7.15 6.01 ...
##
                : num [1:407] 65.2 78.9 45.8 54.2 66.6 96.1 85.9 82.9 39 56.5 ...
##
                : num [1:407] 4.09 4.97 6.06 6.06 5.56 ...
     ..$ dis
##
     ..$ rad
                : int [1:407] 1 2 3 3 5 5 5 5 5 4 ...
##
                : num [1:407] 296 242 222 222 311 311 311 311 311 307 ...
     ..$ tax
##
     ..$ ptratio : num [1:407] 15.3 17.8 18.7 18.7 15.2 15.2 15.2 15.2 15.2 21 ...
     ..$ black : num [1:407] 397 397 395 397 396 ...
##
               : num [1:407] 4.98 9.14 2.94 5.33 12.43 ...
##
     ..$ lstat
##
   $ resample
               :'data.frame':
                                   10 obs. of 4 variables:
               : num [1:10] 4.17 4.36 4.8 5.15 6.01 ...
     ..$ RMSE
##
     ..$ Rsquared: num [1:10] 0.807 0.698 0.79 0.662 0.58 ...
                : num [1:10] 3.25 2.86 3.23 3.51 3.65 ...
     ..$ Resample: chr [1:10] "Fold03" "Fold08" "Fold02" "Fold06" ...
##
   $ resampledCM : NULL
   $ perfNames
                : chr [1:3] "RMSE" "Rsquared" "MAE"
##
   $ maximize
                 : logi FALSE
## $ yLimits
                 : num [1:2] 2.75 52.25
   $ times
                 :List of 3
##
     ..$ everything: 'proc_time' Named num [1:5] 1.218 0.045 1.273 0 0
##
     ... - attr(*, "names")= chr [1:5] "user.self" "sys.self" "elapsed" "user.child" ...
##
                  : 'proc_time' Named num [1:5] 0.006 0.001 0.006 0 0
     ... - attr(*, "names")= chr [1:5] "user.self" "sys.self" "elapsed" "user.child" ...
##
##
     ..$ prediction: logi [1:3] NA NA NA
##
   $ levels
                 : logi NA
                  :Classes 'terms', 'formula' language medv ~ crim + zn + indus + chas + nox + rm + ag
##
     ... - attr(*, "variables") = language list(medv, crim, zn, indus, chas, nox, rm, age, dis, rad, ta
     ....- attr(*, "factors")= int [1:14, 1:13] 0 1 0 0 0 0 0 0 0 ...
##
##
     .. .. - attr(*, "dimnames")=List of 2
     .....$ : chr [1:14] "medv" "crim" "zn" "indus" ...
     .....$ : chr [1:13] "crim" "zn" "indus" "chas" ...
##
     ... - attr(*, "term.labels")= chr [1:13] "crim" "zn" "indus" "chas" ...
##
     ... - attr(*, "order")= int [1:13] 1 1 1 1 1 1 1 1 1 ...
##
     .. ..- attr(*, "intercept")= int 1
     .. ..- attr(*, "response")= int 1
##
     ....- attr(*, ".Environment")=<environment: R_GlobalEnv>
##
     ... - attr(*, "predvars")= language list(medv, crim, zn, indus, chas, nox, rm, age, dis, rad, tax
##
     ... - attr(*, "dataClasses")= Named chr [1:14] "numeric" "numeric" "numeric" "numeric" ...
     ..... attr(*, "names")= chr [1:14] "medv" "crim" "zn" "indus" ...
## $ coefnames : chr [1:13] "crim" "zn" "indus" "chas" ...
                 : Named list()
## - attr(*, "class")= chr [1:2] "train" "train.formula"
```

```
model$results
##
      ncomp
               RMSE Rsquared
                                    MAE
                                           RMSESD RsquaredSD
                                                                 MAESD
## 1
          1 7.170043 0.3889250 4.987823 1.1458409 0.1352420 0.5901698
## 2
          2 6.853749 0.4488643 4.984816 1.1099369 0.1401927 0.6023489
## 3
         3 5.560047 0.6219351 3.837986 1.1413884 0.1632687 0.4889031
## 4
         4 5.264562 0.6612251 3.536613 1.1938471 0.1686282 0.4484231
## 5
         5 5.108941 0.6885868 3.415854 1.1334370 0.1534321 0.4491089
         6 5.051134 0.6963419 3.366435 1.1530716 0.1531997 0.4614229
## 7
         7 5.131647 0.6891018 3.399233 1.1319485 0.1548154 0.4460782
         8 5.115450 0.6908804 3.404935 1.0950841 0.1491827 0.4304041
## 8
## 9
         9 5.176459 0.6827258 3.448911 1.0937752 0.1521372 0.4133588
         10 5.163884 0.6845580 3.512858 0.9806345 0.1350371 0.3864128
# plot train RMSE vs number of components
plot(model,main="Principal Components Regression")
```

Principal Components Regression



```
# best tuning parameter ncomp that minimize the cross-validation error, RMSE
model$bestTune

## ncomp
## 6 6
#
# variance per model
summary(model$finalModel)
```

```
## Data:
           X dimension: 407 13
## Y dimension: 407 1
## Fit method: svdpc
## Number of components considered: 6
## TRAINING: % variance explained
##
            1 comps 2 comps 3 comps 4 comps 5 comps 6 comps
                                 67.97
              48.02
                        58.82
                                          74.78
                                                   81.04
                                                            86.16
## X
                                                   68.66
              37.80
                        43.76
                                          67.24
                                                            69.30
## .outcome
                                 62.57
# variance explained in predictors (1st row) and in the response (2nd row)
#
# test performance
predictions = model %>% predict(test.data)
RMSE = caret::RMSE(predictions, test.data$medv)
Rsquare = caret::R2(predictions, test.data$medv)
d1 = data.frame(RMSE, Rsquare)
rownames(d1) = c('pcr')
##
           RMSE
                 Rsquare
## pcr 4.847172 0.7488739
#
# pls
set.seed(1)
model <- train(medv~., data = train.data,</pre>
              method = "pls",
              scale = TRUE,
               trControl = trainControl("cv", number = 10),
               tuneLength = 10)
model$results
               RMSE Rsquared
                                    MAE
                                           RMSESD RsquaredSD
     ncomp
         1 6.494611 0.4955165 4.447078 1.1137875 0.1443515 0.5343725
## 1
         2 5.015789 0.6980533 3.392457 1.1443205 0.1531122 0.4772334
## 2
## 3
         3 4.995150 0.7025177 3.368314 1.0116818 0.1375136 0.3761320
         4 4.989396 0.7059699 3.430505 0.9674060 0.1306264 0.4482073
## 5
         5 4.955958 0.7070120 3.453991 0.8937295 0.1227171 0.4176809
## 6
         6 4.888249 0.7145149 3.423969 0.9125166 0.1201442 0.4126241
         7 4.865945 0.7167157 3.402248 0.9238277 0.1212114 0.4289319
## 7
## 8
        8 4.868566 0.7165412 3.409289 0.9209121 0.1208916 0.4320559
         9 4.869615 0.7164567 3.411307 0.9196800 0.1208792 0.4312978
## 9
## 10
        10 4.871954 0.7161181 3.415144 0.9176257 0.1206587 0.4296808
#
# plot train RMSE vs number of components
plot(model,main="Partial least Squares Regression")
```

Partial least Squares Regression

```
6.5 (Conponents)

6.5 (Components)

6.5 (Components)
```

```
# best tuning parameter ncomp that minimize the cross-validation error, RMSE
model$bestTune
##
     ncomp
## 7
#
# variance per model
summary(model$finalModel)
            X dimension: 407 13
## Data:
  Y dimension: 407 1
## Fit method: oscorespls
## Number of components considered: 7
## TRAINING: % variance explained
##
             1 comps 2 comps 3 comps
                                        4 comps 5 comps
                                                           6 comps
## X
               46.91
                        57.21
                                 64.47
                                          69.89
                                                    75.76
                                                             79.59
                                                                      83.17
               49.21
## .outcome
                        70.10
                                 71.68
                                          72.72
                                                    73.13
                                                             73.28
                                                                      73.38
# variance explained in predictors (1st row) and in the response (2nd row)
#
# test performance
predictions = model %>% predict(test.data)
RMSE = caret::RMSE(predictions, test.data$medv)
Rsquare = caret::R2(predictions, test.data$medv)
d2 = data.frame(RMSE,Rsquare)
rownames(d2) = c('pls')
```

```
#
# compare models
d3 = rbind(d1,d2)
d3
```

```
## RMSE Rsquare
## pcr 4.847172 0.7488739
## pls 4.581767 0.7620960
```