HW-10-PCA_Wes_Wilson

Packages

```
library(tidyverse)
library(ISLR2)
library(pls)
library(MASS)
library(leaps)
library(glmnet)
```

Data and Functions

```
data("Boston")
data("College")
split_train_and_test_data <- function(split_pct, data, seed){
    set.seed(seed)
    z <- sample(nrow(data), split_pct * nrow(data))
    train <- data[z,]
    test <- data[-z,]

    return(list(train = train, test = test))
}

calc_mse <- function(y_actual, y_predicted) {
    if (!is.vector(y_actual) || !is.vector(y_predicted)) {
        warning("Both y_actual and y_predicted should be vectors.")
        return(NULL) # Return NULL to indicate an issue
    }
    mse <- mean((y_actual - y_predicted)^2)

return(mse)</pre>
```

College Applications Continued

This continues the College data problem from the previous h/w. (Chap. 6, # 9 cd, p.286-287)

Predict the number of applications received based on the other variables in the College data set.

• This data set is from our textbook. Access it with library(ISLR2).

Now fit models using two additional regularization methods using the validation set based on 50% split where appropriate and set.seed(123) where appropriate:

(a) PCR model, with M, the number of principal components, chosen by cross-validation

```
pcr_reg <- pcr(Apps ~ ., data = model_data$train, validation = "CV")
summary(pcr_reg)</pre>
```

Data: X dimension: 388 17

Y dimension: 388 1

Fit method: svdpc

Number of components considered: 17

VALIDATION: RMSEP

Cross-validated using 10 random segments.

	(Interce	pt) 1	comp	s 2 co	mps	3 com	ps	4 comps	5	comps	6	comps
CV	32	258	3258	3 1	482	14	63	1342	2	1235		1076
${\tt adjCV}$	32	258	3258	3 1	481	14	62	1339)	1234		1073
	7 comps	8 comp	os 9	comps	10	comps	11	comps	12	comps	13	comps
CV	1075	108	32	1083		1065		1050		1053		1047
${\tt adjCV}$	1073	108	30	1080		1062		1047		1049		1044
	14 comps	15 c	omps	16 com	ps	17 com	ps					
CV	1042	-	1039	10	42	10	23					
\mathtt{adjCV}	1038	-	1035	10	38	10	18					

```
TRAINING: % variance explained
```

```
1 comps
              2 comps 3 comps
                                4 comps 5 comps 6 comps
                                                            7 comps 8 comps
Х
       53.738
                 87.86
                          95.79
                                   97.67
                                             98.77
                                                      99.40
                                                               99.91
                                                                        99.96
Apps
        1.547
                 79.79
                          80.49
                                   83.71
                                             86.45
                                                      89.88
                                                               89.91
                                                                        89.91
                                                                  15 comps
      9 comps
              10 comps
                         11 comps
                                  12 comps 13 comps 14 comps
Х
       100.00
                 100.00
                           100.00
                                      100.00
                                                100.00
                                                          100.00
                                                                    100.00
                            90.65
                                      90.69
                                                 90.85
                                                           91.05
                                                                     91.19
Apps
        89.92
                  90.36
      16 comps
               17 comps
Х
         100.0
                  100.00
          91.2
                   91.58
Apps
```

(b) PLS model, with M, the number of principal components, chosen by cross-validation.

```
pls_reg <- plsr(Apps ~ ., data = model_data$train, validation = "CV")
summary(pls_reg)</pre>
```

Data: X dimension: 388 17

Y dimension: 388 1 Fit method: kernelpls

Number of components considered: 17

VALIDATION: RMSEP

Cross-validated using 10 random segments.

		_			_							
	(Interce	pt) 1	compa	2 co	mps	3 com	.ps	4 comps	5	comps	6	comps
CV	3:	258	1472	2 1	430	12	56	1123	L	1070		1066
${\tt adjCV}$	3:	258	1466	5 1	446	12	56	1120)	1068		1065
	7 comps	8 com	ps 9	comps	10	comps	11	comps	12	comps	13	comps
CV	1072	10	75	1056		1041		1034		1030		1028
${\tt adjCV}$	1070	10	73	1059		1038		1031		1026		1025
	14 comps	15 c	omps	16 com	ps	17 com	ps					
CV	1029		1029	10	26	10	14					
${\tt adjCV}$	1025		1026	10	23	10	10					

TRAINING: % variance explained

	1 comps	2 comps	3 comps 4	comps 5	comps 6	comps 7 c	omps 8 comps
X	35.02	86.48	93.11	97.29	98.47	99.40 9	9.77 99.96
Apps	80.22	81.34	85.77	88.84	89.82	89.91 8	9.93 89.95
	9 comps	10 comps	11 comps	12 comps	13 comps	14 comps	15 comps
X	99.99	100.00	100	100.00	100.00	100.0	100.0
Apps	90.24	90.75	91	91.16	91.19	91.2	91.2
	16 comps	17 comps	1				
Х	100.00	100.00	1				

Apps 91.22 91.58

- (c) Evaluate performance of each method in terms of **prediction MSE** and add the results into the summary table.
- (d) Comment on the results obtained.

With the PCR model, around 6 components appears to be the optimal number. Once we move beyond 10 or so components, the changes in the variance explained by the x values and the rmse is nominal.

With the plsr model, around 9 components looks to be an optimal number; though I suppose that is arguable depending on who you ask. I am going create new models that have the optimal number of components and use that to predict and evaluate performance.

[1] 1068315

[1] 1030691

Do on the test data now.

• How accurately can we predict the number of college applications?

```
tibble(method = c("step_lse", "step_k_fold", "ridge", "lasso_1se", "lasso_min", "pcr"
    results = c(sqrt(1327026), sqrt(1264962), sqrt(2092402),
    sqrt(1528732), sqrt(1391186), pcr_rmse, plsr_rmse))
```

```
# A tibble: 7 x 2
 method
              results
  <chr>
                 <dbl>
1 step_lse
                1152.
2 step_k_fold
                1125.
3 ridge
                1447.
4 lasso_1se
                1236.
5 lasso_min
                1179.
6 pcr
                 1286.
7 pls
                1258.
```

- Is there much difference among the test errors resulting from these five approaches?
- Which method appears most accurate?

There does not appear to be a drastic difference in the model accuracy between our approaches. We are able to predict the number of applications with rmse of between 1,150 and 1,300. It looks like the stepwise approach was the most accurate with 12 predictors.

• Look at help for: pls::validationplot(), pls::R2(), pls::MSEP()

	(Intercept)	1 comps	2 comps	3 comps	4 comps	5 comps	6 comps
train	3249	3224	1461	1435	1311	1196	1034
CV	3258	3258	1482	1463	1342	1235	1076
${\tt adjCV}$	3258	3258	1481	1462	1339	1234	1073
test	4401	4404	2155	2096	1973	1742	1286
	7 comps 8 c	omps 9 c	omps 10	comps 11	comps 12	comps	13 comps

train	1032	1032	1032	1009	993.4	991.5	982.7
CV	1075	1082	1083	1065	1049.9	1052.6	1047.2
\mathtt{adjCV}	1073	1080	1080	1062	1046.8	1049.4	1043.8
test	1276	1270	1270	1221	1193.3	1192.3	1205.9
	14 comps	15 comps	16 comps	17 comps	1		
train	971.9	964.4	963.9	943	}		
CV	1041.8	1038.5	1042.4	1023	}		
\mathtt{adjCV}	1037.7	1034.5	1038.1	1018	}		
test	1181.6	1163.5	1161.0	1172	}		

this appears to do the same thing that I did earlier manually, but faster. I can pass no

Comparison of Dimension Reduction Methods

We will now try to predict per capita crime rate in the Boston data set in the {MASS} package (library(MASS)).

- Leave rad as an integer.
- Use set.seed(1234) and 50% validation where appropriate.

a. Try out at least four of the dimension reduction methods that we explored over the last two weeks, such as the best subset selection, lasso, ridge regression, PCR, and PLS. Discuss results.

Principal Component Analysis Model

```
pcr_model <- pcr(crim ~ ., data = model_data$train, validation = "CV")
summary(pcr_model)

Data: X dimension: 253 13</pre>
```

Fit method: svdpc

Y dimension: 253 1

Number of components considered: 13

VALIDATION: RMSEP

Cross-validated using 10 random segments.

	(Interce	pt) 1	comps	2 co	mps	3 com	ıps	4 comp	S	5 comps	6	comps
CV	10	.32	8.701	8.	735	8.7	34	8.72	2	8.660		8.345
${\tt adjCV}$	10	.32	8.696	8.	726	8.7	24	8.71	2	8.647		8.331
	7 comps	8 comp	s 9	comps	10	comps	11	comps	12	comps	13	comps
CV	8.304	8.24	<u> 1</u> 7	8.233		8.203		8.246		8.248		8.227
adjCV	8.289	8.23	31	8.217		8.185		8.224		8.225		8.203

TRAINING: % variance explained

	1 comps	2 comps	3 comps 4	comps 5	comps 6 comp	s 7 comps	8 comps
X	82.53	96.85	98.99	99.68	99.86 99.9	99.96	99.99
crim	29.95	30.74	30.81	31.12	32.91 38.2	4 39.15	40.17
	9 comps	10 comps	11 comps	12 comps	13 comps		
X	100.00	100.00	100.00	100.0	100.0		
crim	40.55	41.36	42.07	42.2	42.7		

It appears that 7 components is the optimal number. After that, the increases are extremely marginal. Still, the model is only accounting for $\sim 42\%$ of the variance and the RMSE is pretty high.

 $RMSE = \sim 8.7$

Partial Least Squares Model

```
plsr_model <- plsr(crim ~ ., data = model_data$train, validation = "CV")
summary(plsr_model)</pre>
```

Data: X dimension: 253 13

Y dimension: 253 1 Fit method: kernelpls

Number of components considered: 13

VALIDATION: RMSEP

Cross-validated using 10 random segments.

	(Intercep	pt) 1 d	comps	2 co	nps	3 com	ps	4 comp	s .	5 comps	6	comps
CV	10.	.32	3.749	8.	763	8.6	75	8.52	9	8.362		8.234
${\tt adjCV}$	10.	.32	3.741	8.	752	8.6	62	8.51	5	8.348		8.220
	7 comps	8 comps	9	comps	10	comps	11	comps	12	comps	13	comps
CV	8.226	8.236	3	8.217		8.237		8.303		8.318		8.300
adjCV	8.210	8.219)	8.200		8.218		8.278		8.291		8.273

TRAINING: % variance explained 6 comps 1 comps 2 comps 3 comps 4 comps 5 comps 7 comps Х 82.48 96.79 98.18 99.36 99.81 99.92 99.95 99.97 crim 30.22 30.92 33.16 35.68 38.24 40.24 40.79 41.18 9 comps 10 comps 11 comps 12 comps 13 comps Х 99.99 100.00 100.00 100.00 100.0 crim 41.49 41.71 42.18 42.29 42.7

The pls model performs quite similarly and its pretty hard to tell what the optimal number of components should be. After one component, the changes in variance and RMSE is pretty small.

 $RMSE = \sim 8.7$

Stepwise Regression

```
y_train <- model_data$train$crim</pre>
  full_regression <- lm(crim ~ ., data = model_data$train)</pre>
  step_output <- step(object = full_regression, method = "backward")</pre>
Start: AIC=1066.32
crim ~ zn + indus + chas + nox + rm + age + dis + rad + tax +
    ptratio + black + lstat + medv
          Df Sum of Sq
                          RSS
                                  AIC
- age
           1
                   0.00 15328 1064.3
- chas
           1
                  22.82 15350 1064.7
- indus
           1
                  23.96 15352 1064.7
                  29.55 15357 1064.8
- tax
           1
                  62.15 15390 1065.3
- black
           1
- ptratio
                 85.09 15413 1065.7
<none>
                        15328 1066.3
                 135.92 15464 1066.5
- nox
           1
           1
                 164.66 15492 1067.0
- rm
- zn
           1
                170.49 15498 1067.1
                223.60 15551 1068.0
- lstat
           1
- dis
           1
                331.43 15659 1069.7
- medv
                622.51 15950 1074.4
           1
               1320.70 16648 1085.2
- rad
```

Step: AIC=1064.32

```
black + lstat + medv
         Df Sum of Sq
                       RSS
                             AIC
               22.86 15350 1062.7
- chas
- indus
               23.96 15352 1062.7
- tax
              29.55 15357 1062.8
              62.21 15390 1063.3
- black
          1
- ptratio 1
              85.37 15413 1063.7
<none>
                     15328 1064.3
            146.70 15474 1064.7
- nox
          1
- rm
          1 174.32 15502 1065.2
          1 177.64 15505 1065.2
- zn
- lstat
         1 240.94 15568 1066.3
          1 357.01 15685 1068.1
- dis
         1 625.62 15953 1072.4
- medv
- rad
          1 1328.81 16656 1083.3
Step: AIC=1062.69
crim ~ zn + indus + nox + rm + dis + rad + tax + ptratio + black +
   lstat + medv
         Df Sum of Sq
                       RSS
               25.43 15376 1061.1
- tax
- indus
         1
               27.71 15378 1061.2
- black
               65.67 15416 1061.8
       1
- ptratio 1
              84.66 15435 1062.1
<none>
                     15350 1062.7
            164.37 15515 1063.4
- nox
- zn
          1 177.55 15528 1063.6
          1 178.03 15528 1063.6
- rm
- lstat
         1 241.90 15592 1064.7
         1 362.41 15713 1066.6
- dis
- medv
          1 663.50 16014 1071.4
- rad
          1 1312.14 16662 1081.4
Step: AIC=1061.11
crim ~ zn + indus + nox + rm + dis + rad + ptratio + black +
   lstat + medv
         Df Sum of Sq RSS
                             AIC
- black
         1
               64.59 15440 1060.2
- indus
        1 91.95 15468 1060.6
```

crim ~ zn + indus + chas + nox + rm + dis + rad + tax + ptratio +

```
- ptratio 1
            93.80 15470 1060.7
<none>
                     15376 1061.1
               156.90 15533 1061.7
- zn
          1
- nox
          1 169.01 15545 1061.9
          1 171.53 15547 1061.9
- rm
            244.71 15620 1063.1
- lstat
- dis
          1 363.02 15739 1065.0
          1 639.24 16015 1069.4
- medv
          1 2698.70 18074 1100.0
- rad
Step: AIC=1060.17
crim ~ zn + indus + nox + rm + dis + rad + ptratio + lstat +
   medv
         Df Sum of Sq
                       RSS
- indus
          1
                87.57 15528 1059.6
- ptratio 1
               110.00 15550 1060.0
                     15440 1060.2
<none>
- zn
            162.05 15602 1060.8
          1
          1 179.36 15620 1061.1
- nox
          1 219.95 15660 1061.8
- rm
          1 282.44 15723 1062.8
- lstat
          1 379.04 15820 1064.3
- dis
              741.43 16182 1070.0
- medv
          1
- rad
          1
              2984.79 18425 1102.9
Step: AIC=1059.6
crim ~ zn + nox + rm + dis + rad + ptratio + lstat + medv
         Df Sum of Sq
                       RSS
                              AIC
<none>
                     15528 1059.6
- ptratio 1
               132.06 15660 1059.8
            176.56 15705 1060.5
- zn
          1
- rm
          1
            251.19 15779 1061.7
          1 273.81 15802 1062.0
- lstat
          1 274.82 15803 1062.0
- nox
- dis
          1 308.96 15837 1062.6
- medv
              695.31 16223 1068.7
          1
```

1 2916.19 18444 1101.2

- rad

[1] 7.834251

Stepwise regression selection selected 7 variables from the original 12 and resulted with rmse of 7.83.

Ridge Regression

```
x train <- model.matrix(lm(formula = crim ~ .,</pre>
                            data = model_data$train))[,-1]
 r_train <- cv.glmnet(x = x_train, y = y_train, alpha = 0)
 ridge_predictions <- predict(r_train, newx = x_train) %>% as.vector()
 ridge_predictions
[1] 1.612530 3.283893 5.885659 3.807628 5.172257 3.927413 5.889116 4.456629
[9] 5.632322 5.989434 6.057029 2.824525 4.544568 3.335639 3.103409 3.144530
[17] 3.692734 5.331243 4.800348 3.385360 5.617881 3.174858 3.730548 2.699924
[25] 4.010553 5.075539 2.573706 4.032486 5.753436 2.423660 3.429051 4.158854
[33] 6.069259 2.625611 3.561721 6.143913 5.654299 5.469102 2.753608 4.151851
[41] 4.543778 3.312781 2.392795 4.080233 3.428088 3.501909 6.448969 3.504647
[49] 2.626781 2.826792 3.998475 5.539902 3.121006 2.862221 5.223336 4.928210
[57] 3.051871 5.728671 5.458974 3.536729 3.493848 4.034943 3.916215 4.669889
[65] 2.569136 5.181098 4.284687 3.397671 2.940994 3.161263 3.972334 2.660683
[73] 3.135902 3.808443 5.172708 2.478554 2.470502 3.634692 3.725109 3.406174
[81] 4.822377 4.662451 5.857774 3.022307 3.563799 5.873913 3.601747 3.941436
[89] 5.717717 2.811296 4.250093 3.124699 3.517978 2.687095 6.255103 5.794497
[97] 4.661772 5.583352 5.222162 3.335123 3.675303 6.200523 3.925205 4.731010
```

```
[105] 4.173565 3.684115 3.660640 4.307700 5.754074 3.737641 4.875767 3.720710
[113] 5.535622 3.187702 4.251081 4.390558 3.860719 3.492540 5.702490 3.083529
[121] 4.814622 2.952592 3.483246 3.872219 2.761304 3.268598 5.165511 2.738989
[129] 5.569939 4.644664 3.256783 5.739562 3.204553 6.102026 5.185986 3.921102
[137] 6.382558 3.524596 3.140672 3.311948 5.906258 5.415257 6.005334 3.236285
[145] 3.113515 5.289821 5.127521 6.737446 2.946142 2.879296 4.256979 4.756471
[153] 6.294249 4.227496 3.868277 2.988178 3.484438 5.770035 5.274886 2.875234
[161] 1.960236 3.150972 5.415163 2.926357 4.849388 2.467219 5.475836 5.037559
[169] 3.841829 6.034724 5.470242 6.039459 3.611647 3.144789 5.133556 3.540403
[177] 2.704194 5.344277 3.003421 5.455231 4.288729 2.710407 5.364268 4.305857
[185] 3.012002 4.361344 2.930048 2.885458 4.669527 2.895473 3.405247 4.448731
[193] 3.414483 5.575409 3.432226 3.397185 5.961657 2.255470 6.081084 3.062482
[201] 3.775953 4.205282 3.607564 3.255160 5.554167 3.115011 5.847252 3.205094
[209] 3.087763 5.146055 2.501293 2.083660 3.182924 3.149880 2.568591 3.522708
[217] 2.410190 3.457947 2.017172 2.265563 3.633992 3.547817 1.954263 4.116003
[225] 4.037627 4.104865 5.003165 5.566102 3.277276 5.152197 3.324057 5.541940
[233] 3.673378 6.057449 3.874799 2.350740 3.632658 3.390823 2.656352 5.252871
[241] 4.129647 2.326829 3.166769 3.328426 5.568014 5.473942 3.477075 5.519424
[249] 4.106352 3.355919 4.239522 2.832617 3.198019
  sqrt(calc_mse(y_actual = y_train, y_predicted = ridge_predictions))
```

[1] 9.683361

The ridge regression doesn't remove any variables and the rmse is 9.46.

Overall, there was not a huge difference in performance. The stepwise selected model performed the best, with an rmse of \sim 7.9. The PCR and PLSR model perform similarly and the ridge regression did the worst.

Create Plots

- a. For all possible values of K, compare
- regression models that are based on the best subset of -variables.

```
n_predictors <- ncol(model_data$train) - 1

# empty data frame to store the results.
results <- data.frame(matrix(NA, ncol = 3, nrow = n_predictors))
colnames(results) <- c("Variables", "adjusted_r2", "rmse")</pre>
```

```
for(k in 1:n_predictors) {
    #browser()
    predictor_combinations <- regsubsets(crim ~ .,</pre>
                                           data = model_data$train,
                                           nvmax = k, intercept = FALSE)
    # Fit models for each combination and obtain adjusted R-squared and MSE
    models <- summary(predictor_combinations)</pre>
    adj_r_squared_values <- models$rsq</pre>
    # Find the index of the model with the highest adjusted R-squared
    best_model_index <- which.max(adj_r_squared_values)</pre>
    # Extract the names of selected predictors
    selected_predictors <- names(coef(predictor_combinations, id = best_model_index))</pre>
    # Fit a linear model using the selected predictors
    lm_model <- lm(crim ~ .,</pre>
                    data = model_data$train[,c("crim", selected_predictors)])
    # Calculate MSE
    y_predicted <- predict(lm_model, newdata = model_data$train)</pre>
    rmse_value <- sqrt(mean((model_data$train$crim - y_predicted)^2))</pre>
    # Store results for the current k
  results[k, 1] <- length(names(coef(predictor_combinations, id = best_model_index)))</pre>
  results[k, 2] <- adj_r_squared_values[best_model_index]</pre>
  results[k, 3] <- rmse_value
  step_results <- results</pre>
  step_results
   Variables adjusted_r2
                              rmse
           1 0.4090749 8.318242
1
2
           2 0.4545558 8.121705
           3 0.4709485 8.044823
3
4
           4 0.4744398 8.018398
           5 0.4811558 7.956229
```

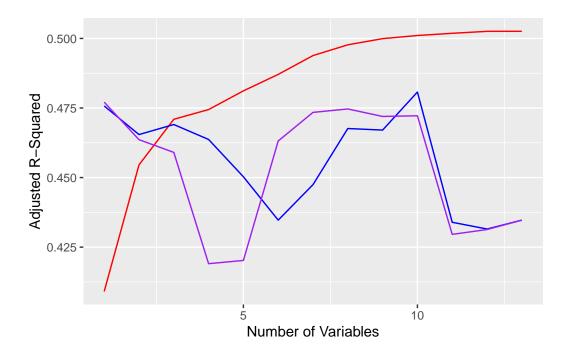
```
6
               0.4870767 7.921192
7
               0.4938450 7.867494
           7
8
               0.4977103 7.838929
9
           9
               0.4999329 7.819515
              0.5010587 7.795773
10
          10
               0.5018515 7.789602
11
          11
12
          12
               0.5025528 7.783521
13
          13
               0.5025659 7.783521
```

- PCR based on first principal components;
- The pls::R2() and pls::MSEP() functions calculate this automatically, so I will just extract those values as a vector.

```
pcr_model <- pcr(crim ~ . -1, data = model_data$train,</pre>
                  validation = "CV", scaled = TRUE)
pcr_r_squared <- pls::R2(pcr_model, estimate = "test",</pre>
                          newdata = model_data$test)$val %>%
data.frame() %>%
  pivot_longer(cols = everything(),
               names_to = "component",
                values_to = "r_squared") %>%
  slice(-1)
pcr_rmse <- pls::RMSEP(pcr_model, estimate = "test",</pre>
                        newdata = model data$test)$val %>%
data.frame() %>%
  pivot_longer(cols = everything(),
                names_to = "component",
                values_to = "rmse") %>%
  slice(-1) %>%
  dplyr::select(rmse)
pcr_results <- bind_cols(pcr_r_squared, pcr_rmse)</pre>
• PLS based on first PLS components.
plsr_model <- plsr(crim ~ ., data = model_data$train,</pre>
                    validation = "CV", scaled = TRUE)
```

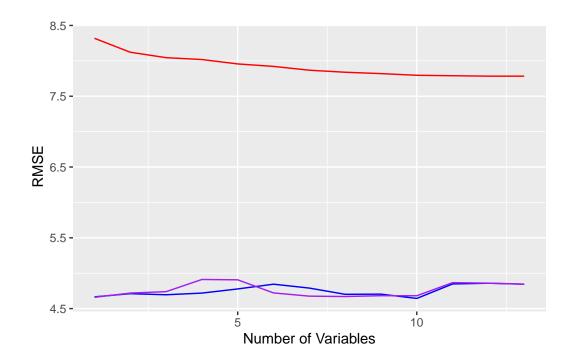
For each , compare these methods in terms of the **explained proportion of the total** variation of crime rate per capita (adjusted) and in terms of the prediction mean-squared error.

- Hint: Look at the regsubsets output object list elements. The \$adjR2 will be useful. You may find it helpful to use the \$which matrix in a for-loop to get the cross-validated MSEP.
- c. Create one plot comparing adjusted- 2 for different values of for subset regression, PCR, and PLS and interpret the plot.



Based on the r-squared values, the stepwise model selection performed best with a max adjusted r-squared value of roughly 50% when it used all of the variables. Interestingly, the partial least squared model was outperforming the PCR model until the number of dimensions exceeded 8 or so. I am guessing this is an issue with scaling the variables.

c. Create one plot comparing Prediction MSE for different values of for subset regression, PCR, and PLS and interpret the plot.



- e. Propose a model (or set of models) that seem to perform well on this data set, and justify your answer. Make sure you are evaluating model performance on basis of cross-validation, as opposed to using training error.
- f. Does your chosen model involve all of the features in the data set? Why or why not?

I am not entirely sure that I set this up correctly. I don't fully understand estimate argument in the PCR/PLS function. I have changed it several times and get widely different results. It decided to make the estimate "test" which given that the model was created with the training makes sense to me.

I would select the PCR models with somewhere between 2-3 components. As we can see from the plot, the RMSE is pretty stable for with 2 components vs 10; therefore, its not worth the degrees-of-freedom price we pay to get an extra .001 in precision in the rmse.