Exercise 3

for Advanced Methods for Regression and Classification

Dzhamilia Kulikieva

06.11.2024

Let's use the data set "building.RData" from the last exercise, and make the same training/test split

load("/Users/djem/Downloads/building.RData")
head(df)

##		У	START.YEAR	START.QUART	ER COMP	LETION.	YEAR COMP	LETION.QU	ARTER Ph	nysFin1
##	1	7.696213	81		1		85		1	1
##	2	8.517193	84		1		89		4	1
##	3	7.090077	78		1		81		4	1
##	4	5.105945	72		2		73		2	1
##	5	8.612503	87		1		90		2	1
##	6	8.556414	87		1		90		1	1
##		${\tt PhysFin2}$	PhysFin3 Ph	nysFin4 Phys	Fin5 Ph	ysFin6	PhysFin7	PhysFin8	Econ1	Econ2
##	1	3150	920	598.5	190 1	.010.84	16	1200	6713.00	56.2
##	2	7600	1140	3040.0	400	963.81	23	2900	3152.00	106.0
##	3	4800	840	480.0	100	689.84	15	630	1627.00	41.0
##	4	685	202	13.7	20	459.54	4	140	2580.93	12.1
##	5	3000	800	1230.0		631.91	13	5000	6790.00	203.8
##	6	2500	640	1050.0		647.32	12		6790.00	
##		Econ3 Ec				Econ8		con10 Eco		
##				7.30 3485.8					7.3 809	
##	2			7.50 3526.1					8.4 1473	3.5
##	3		1.74 160401		34.4		6489.1		4.0 608	
##	_				13.6		154.4		3.6 211	
				3.00 10855.3					8.8 3148	
	6			3.00 10855.3					8.8 3148	3.0
##			Econ14 Econ1		Econ17	Econ1		19 Econ1.	•	
		1755.00	8003 67.8			42587.0			4986	
				52 105.32 12					2700	
			7773 45.9			39066.0			1580	
			1649 11.6		392.96				2952	
				63 169.50 10					6370	
	6	9248.40		63 169.50 10					6370	
##			•	g1 Econ4.lag		_	•		_	•
##		55				210.1	3663.5			179.63
##		103				829.2				156.60
##		40				266.8				214.35
##		11.				859.4				56.60
##		190				166.6				294.98
##	6	190.				3166.6	12930.0			294.98
##	1			ag1 Econ11.l						
##	1	9342.4	45	15 757.8	000	861.8	0 1/5	5.00	8018	

```
## 2
      13188.23
                     15
                           1424.1000
                                        1584.30
                                                   8776.71
                                                                 8799
## 3
      4866.83
                      15
                            573.7265
                                         680.29
                                                   1755.00
                                                                 6714
## 4
                                        208.60
                                                                 1582
       610.40
                      12
                            165.1000
                                                 1504.36
    52083.60
## 5
                           2595.2000
                                                   9329.64
                                                                 9396
                      11
                                        3000.00
## 6
      52083.60
                      11
                           2595.2000
                                        3000.00
                                                   9329.64
                                                                 9396
    Econ15.lag1 Econ16.lag1 Econ17.lag1 Econ18.lag1 Econ19.lag1 Econ1.lag2
       65.00 60.53
                             3538.71 31940.25 610502.7
## 2
         101.00
                   101.89
                             13571.80
                                        34474.50
                                                                 3561
                                                  1067772.0
                   36.45
                            1535.16
## 3
         43.40
                                        29299.50
                                                   466212.2
                                                                 2628
         10.86
## 4
                    9.79
                             435.10
                                        32776.00
                                                                 2649
                                                  129102.4
## 5
         148.76
                   159.00
                              9700.00
                                        37179.00 1908975.7
                                                                 5909
                              9700.00
                                        37179.00 1908975.7
                                                                 5909
## 6
        148.76
                   159.00
## Econ2.lag2 Econ3.lag2 Econ4.lag2 Econ5.lag2 Econ6.lag2 Econ7.lag2 Econ8.lag2
## 1
       54.2
               59.40
                              5.41
                                   280451.7 3755.8
                                                        58.10
                                                                  119.75
## 2
          98.2
                   98.64
                              2.76
                                    602224.7
                                                3819.0
                                                           97.20
                                                                     104.40
## 3
          39.3
                  40.21
                              1.52
                                    143737.7
                                                1284.5
                                                           33.50
                                                                     142.90
## 4
         11.4
                  6.97
                              2.25
                                    32793.7
                                                388.9
                                                          11.73
                                                                     42.45
## 5
         177.6
                  147.44
                              6.88 1451175.9
                                                8146.1
                                                          188.90
                                                                     196.65
                                                          188.90
        177.6
                  147.44
                              6.88 1451175.9
                                                8146.1
                                                                     196.65
## Econ9.lag2 Econ10.lag2 Econ11.lag2 Econ12.lag2 Econ13.lag2 Econ14.lag2
## 1
       6228.30
                  15 795.000
                                        818.50
                                                 1755.00
                                                                 8001
## 2
       8792.15
                     15
                            1298.800
                                        1389.60
                                                   8699.73
                                                                 8735
                     15
## 3
       3244.55
                            554.082
                                        663.97
                                                 1755.00
                                                                 5827
                     12
## 4
       457.80
                            167.900
                                        209.60
                                                   1450.47
                                                                 1507
      34722.40
## 5
                     11
                            2284.400
                                        2627.50
                                                 9297.06
                                                                 9347
                                                   9297.06
      34722.40
                     11
                            2284.400
                                        2627.50
    Econ15.lag2 Econ16.lag2 Econ17.lag2 Econ18.lag2 Econ19.lag2 Econ1.lag3
## 1
          63.69
                58.55
                             3347.72 21293.5 589389.6
                                                                 5728
## 2
          98.12
                     98.45
                                         22983.0
                                                   973523.7
                                                                 3157
                           13596.37
          41.79
                    34.76
                                                                 2374
                             1527.55
                                         19533.0 409677.9
                                                 123618.0
## 4
          10.17
                    9.35
                             508.64
                                         24582.0
                                                                 2312
## 5
         140.90
                    146.20
                             10149.00
                                         24786.0 1681849.3
                                                                 7045
## 6
         140.90
                  146.20 10149.00
                                         24786.0 1681849.3
                                                                 7045
## Econ2.lag3 Econ3.lag3 Econ4.lag3 Econ5.lag3 Econ6.lag3 Econ7.lag3 Econ8.lag3
       52.4 57.65 5.40 262789.00 2931.4
## 1
                                                        54.20
                                                                      59.88
## 2
          92.8
                   96.49
                              3.05 552124.40
                                                3896.7
                                                           96.90
                                                                      52.20
                                                           33.70
## 3
          38.0
                   39.43
                              0.92 134548.40
                                               1191.1
                                                                     71.45
## 4
          10.6
                  5.44
                              2.58
                                   30012.46
                                                 345.3
                                                          10.79
                                                                      28.30
## 5
         160.0
                  141.34
                              4.72 1341072.80
                                                8245.0
                                                          173.80
                                                                      98.33
                                             8245.0
         160.0
                  141.34
                              4.72 1341072.80
                                                                      98.33
## 6
                                                          173.80
    Econ9.lag3 Econ10.lag3 Econ11.lag3 Econ12.lag3 Econ13.lag3 Econ14.lag3
## 1
       3114.15
                   15
                          746.8000
                                        815.50
                                                  1755.00
                                                                 8013
## 2
       4396.08
                      15
                           1294.2000
                                        1288.00
                                                   8555.54
                                                                 8585
## 3
       1622.28
                     15
                          574.6000
                                        680.50
                                                 1755.00
                                                                 5565
                            180.3715
       305.20
                     12
                                         158.45
                                                 1439.00
                                                                 1450
## 5
      17361.20
                      11
                                                                 9306
                           2451.2000
                                        2526.40
                                                   9254.28
                  11
      17361.20
                                        2526.40
                                                   9254.28
                           2451.2000
                                                                 9306
    Econ15.lag3 Econ16.lag3 Econ17.lag3 Econ18.lag3 Econ19.lag3 Econ1.lag4
## 1
          62.78
                  56.45
                              3387.72
                                        10646.75
                                                   606524.2
                                                                 7196
## 2
          95.35
                     94.34
                                                                 3678
                             12063.50
                                        11491.50
                                                   954628.6
                            1601.79
## 3
          41.03
                     33.37
                                        9766.50
                                                   403875.0
                                                                 2693
## 4
                    8.85
                             590.64
                                        16388.00 121857.2
          9.91
                                                                 1381
                138.80
138.80
## 5
         136.56
                             9291.00
                                        12393.00 1732937.5
                                                                 5606
                                        12393.00 1732937.5
## 6
        136.56
                           9291.00
                                                                 5606
```

```
Econ2.lag4 Econ3.lag4 Econ4.lag4 Econ5.lag4 Econ6.lag4 Econ7.lag4 Econ8.lag4
## 1
           51.3
                      56.13
                                   5.97
                                         249110.70
                                                        2562.3
                                                                     52.80
                                                                                217.00
                      83.21
                                   3.25
                                                        2790.6
                                                                     94.10
                                                                                334.80
## 2
           86.2
                                         526596.40
## 3
                      37.64
                                                        1529.0
                                                                     31.43
                                                                                175.70
           36.2
                                   1.55
                                         134312.50
## 4
           10.0
                       3.91
                                   3.00
                                          27231.21
                                                         316.5
                                                                      9.85
                                                                                 14.15
## 5
          149.1
                     134.80
                                   4.09 1284199.40
                                                        6622.5
                                                                    147.60
                                                                                432.40
          149.1
                     134.80
                                   4.09 1284199.40
                                                        6622.5
                                                                    147.60
                                                                                432.40
##
     Econ9.lag4 Econ10.lag4 Econ11.lag4 Econ12.lag4 Econ13.lag4 Econ14.lag4
## 1
        10445.6
                          15
                                 733.8000
                                                815.50
                                                           1755.00
                                                                           8002
        14488.6
                                1143.8000
                                                                           8393
## 2
                          15
                                               1316.30
                                                           8364.78
## 3
         3994.7
                          15
                                 589.5000
                                                765.80
                                                           1755.00
                                                                           4930
                          12
## 4
          152.6
                                 197.6796
                                                152.25
                                                           1442.31
                                                                           1456
## 5
        73143.5
                          14
                                2220.6000
                                               2244.10
                                                           9231.76
                                                                           9286
## 6
        73143.5
                          14
                                2220.6000
                                                                           9286
                                               2244.10
                                                           9231.76
     Econ15.lag4 Econ16.lag4 Econ17.lag4 Econ18.lag4 Econ19.lag4
## 1
           60.74
                        54.26
                                   2978.26
                                                  41407
                                                           601988.1
## 2
           90.95
                        89.79
                                  11379.37
                                                  44835
                                                           929027.1
## 3
           38.70
                        32.04
                                   1653.06
                                                  37933
                                                           377828.6
## 4
                         8.34
                                    686.16
                                                   8194
                                                           122031.7
            9.73
## 5
          136.60
                       140.20
                                   9821.00
                                                  48260
                                                          1734973.5
## 6
          136.60
                       140.20
                                   9821.00
                                                  48260
                                                          1734973.5
set.seed(2024)
sample_index <- sample(1:nrow(df), size = floor(2/3 * nrow(df)))</pre>
train_data <- df[sample_index, ]</pre>
test data <- df[-sample index, ]
```

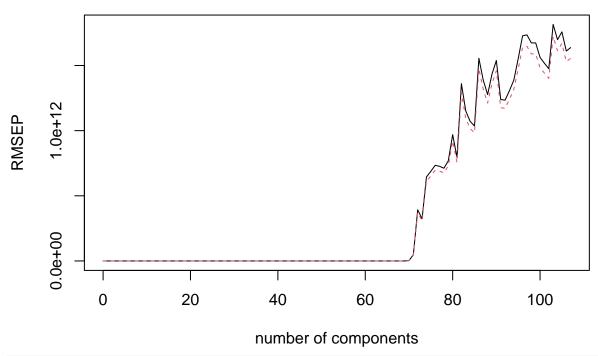
1. Principal component regression (PCR)

(1a) PCR with cross-validation into 10 segments

```
pcr_model <- pcr(y ~ ., data = train_data, scale = TRUE, validation = "CV", segments = 10)</pre>
```

(1b) Graph of cross-validation errors and selection of the optimal number of components

```
validationplot(pcr_model, val.type = "RMSEP")
```



rmsep_values <- RMSEP(pcr_model)
print(rmsep_values)</pre>

##		(Interce	pt) 1 comp	s 2 comps	3 comps	4 comps	5 comps 6	comps
##	CV	0.8	711 0.607	0.6076 0.6004		0.5309	0.5146	0.4748
##	adjCV	0.8	711 0.607	76 0.6002	0.5314	0.5307	0.5147	0.4728
##		7 comps	8 comps 9	comps 10	comps 11	l comps 12	comps 13	comps
##	CV	0.4806	0.4324	0.3828	0.3845	0.3753	0.3707	0.3502
##	adjCV	0.4790	0.4311	0.3778	0.3812	0.3699	0.3663	0.3468
##		14 comps	15 comps	16 comps	17 comps	18 comps	19 comps	20 comps
##	CV	0.3476	0.3378	0.2791	0.2793	0.2814	0.2804	0.2793
##	\mathtt{adjCV}	0.3441	0.3442	0.2762	0.2767	0.2789	0.2780	0.2773
##		21 comps	22 comps	23 comps	24 comps	25 comps	26 comps	27 comps
##	CV	0.2798	0.2837	0.2820	0.2751	0.2718	0.2758	0.2800
##	\mathtt{adjCV}	0.2781	0.2822	0.2799	0.2722	0.2694	0.2743	0.2783
##		28 comps	29 comps	30 comps	31 comps	32 comps	33 comps	34 comps
##	CV	0.2895	0.2785	0.2819	0.2726	0.2648	0.2609	0.2570
##	adjCV	0.2873	0.2757	0.2783	0.2691	0.2608	0.2582	0.2546
##		35 comps	36 comps	37 comps	38 comps	39 comps	40 comps	41 comps
##	CV	0.2581	0.2581	0.2582	0.2600	0.2611	0.2635	0.2653
##	adjCV	0.2554	0.2554	0.2557	0.2583	0.2583	0.2605	0.2622
##		42 comps	43 comps	44 comps	45 comps	46 comps	47 comps	48 comps
##	CV	0.2683	0.2702	0.2688	0.2714	0.2723	0.2739	0.2757
##	adjCV	0.2651	0.2669	0.2654	0.2678	0.2687	0.2702	0.2720
##		49 comps	50 comps	51 comps	52 comps	53 comps	54 comps	55 comps
##	CV	0.2719	0.2695	0.2662	0.2689	0.2686	0.2706	0.2727
##	adjCV	0.2672	0.2651	0.2624	0.2654	0.2645	0.2664	0.2685
##		56 comps	57 comps	58 comps	59 comps	60 comps	61 comps	62 comps
##	CV	0.2753	0.2729	0.2752	0.2753	0.2747	0.2793	0.2808
##	adjCV	0.2709	0.2690	0.2719	0.2707	0.2696	0.2743	0.2754

```
##
          63 comps
                     64 comps
                                65 comps
                                          66 comps
                                                     67 comps
                                                                68 comps
                                                                           69 comps
            0.2826
                       0.2900
                                  0.2908
                                             0.3048
                                                       0.3239
                                                                  0.3459
                                                                             0.3433
## CV
                                                       0.3159
                                                                  0.3368
##
   adjCV
            0.2778
                       0.2848
                                  0.2864
                                             0.2981
                                                                             0.3341
##
                                                         74 comps
                                                                     75 comps
          70 comps
                      71 comps
                                  72 comps
                                              73 comps
##
          2.90e+09
                     4.757e+10
                                 3.924e+11
                                             3.241e+11
                                                        6.445e+11
                                                                    6.879e+11
  adjCV
                                 3.722e+11
                                                        6.112e+11
                                                                    6.526e+11
          2.75e+09
                     4.511e+10
                                             3.074e+11
##
##
           76 comps
                       77 comps
                                   78 comps
                                               79 comps
                                                           80 comps
                                                                      81 comps
                                                                     7.950e+11
## CV
          7.341e+11
                      7.262e+11
                                  7.117e+11
                                             7.685e+11
                                                         9.688e+11
## adjCV
          6.963e+11
                      6.892e+11
                                  6.756e+11
                                             7.294e+11
                                                         9.194e+11
                                                                     7.547e+11
##
           82 comps
                       83 comps
                                   84 comps
                                               85 comps
                                                           86 comps
                                                                      87 comps
## CV
          1.360e+12
                      1.151e+12
                                  1.071e+12
                                             1.036e+12
                                                         1.555e+12
                                                                     1.387e+12
          1.291e+12
                      1.092e+12
                                                         1.476e+12
##
   adjCV
                                  1.017e+12
                                             9.834e+11
                                                                     1.316e+12
                                                          92 comps
##
           88 comps
                                   90 comps
                       89 comps
                                               91 comps
                                                                      93 comps
## CV
          1.277e+12
                      1.434e+12
                                  1.538e+12
                                              1.239e+12
                                                         1.234e+12
                                                                     1.307e+12
## adjCV
                                                         1.172e+12
                                                                     1.241e+12
          1.212e+12
                      1.361e+12
                                  1.460e+12
                                              1.176e+12
##
           94 comps
                       95 comps
                                   96 comps
                                               97 comps
                                                           98 comps
                                                                      99 comps
                                  1.728e+12
## CV
          1.388e+12
                      1.553e+12
                                              1.735e+12
                                                         1.674e+12
                                                                     1.673e+12
          1.317e+12
                      1.474e+12
                                  1.640e+12
                                              1.647e+12
                                                         1.589e+12
                                                                     1.589e+12
  adiCV
##
          100 comps
                      101 comps
                                  102 comps
                                             103 comps
                                                         104 comps
                                                                     105 comps
## CV
          1.562e+12
                      1.517e+12
                                  1.475e+12
                                              1.815e+12
                                                         1.698e+12
                                                                     1.758e+12
##
  adjCV
          1.483e+12
                      1.441e+12
                                  1.401e+12
                                             1.723e+12
                                                         1.613e+12
                                                                     1.669e+12
##
          106 comps
                      107 comps
## CV
          1.611e+12
                      1.638e+12
## adjCV
         1.530e+12
                      1.555e+12
```

The optimal number of components may be that at which the RMSEP(CV and adjCV) is at a minimum level and remains relatively stable before it starts a sharp increase.

In our case, the RMSEP values continue to decrease until around 34 components, after which the error starts to stabilize and even increase slightly in some places. At around 34 components, the RMSEP reaches a relatively low and stable value before starting to increase significantly after 70 components. Therefore, 34 components seems to be an optimal choice, as adding more components does not significantly reduce the RMSEP and could lead to overfitting.

Let's check the conclusion above by extracting the RMSEP value for the optimal number of components:

```
optimal_rmsep <- min(rmsep_values$val)
optimal_rmsep</pre>
```

[1] 0.2546155

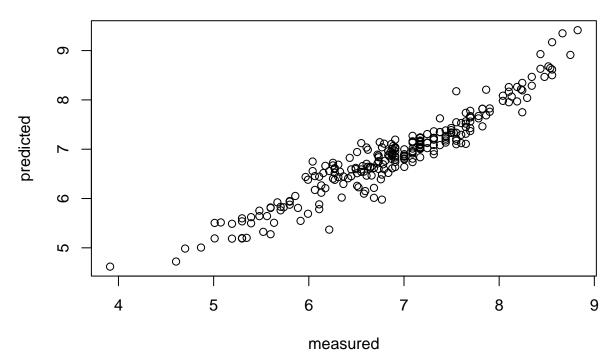
At 34 components, the RMSEP values are approximately: CV (RMSEP): 0.2570 adjCV (Adjusted RMSEP): 0.2546

This value represents a low and stable point in the RMSEP, suggesting that 34 components could be considered an optimal choice. While the RMSEP values remain relatively low until around 40 components, choosing 34 components might balance complexity and accuracy effectively, as adding more components beyond this point provides diminishing returns.

(1c) A graph of predicted(cross-validated) values vs observed values with optimal model

```
predplot(pcr_model, ncomp = 34, main = "Cross-validated predictions vs Measured values")
```

Cross-validated predictions vs Measured values



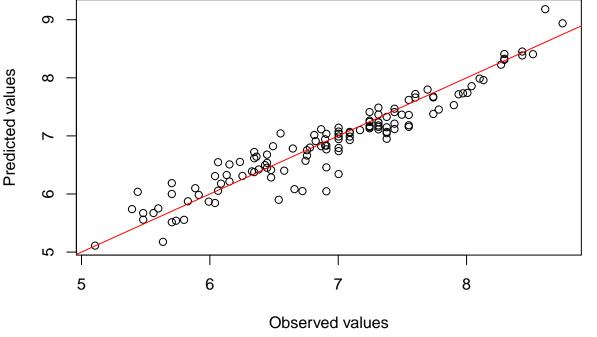
In an ideal model, the predicted values would be close to the actual values, and the points would be aligned along a 45° diagonal line (where predicted = measured).

Here, while there is a general diagonal trend, there is still some scatter, which indicates minor prediction errors. This is expected even in a well-fitted model due to natural variability. In summary, the plot indicates that the model with 34 components is making reasonably accurate predictions on the cross-validated data, with most points following a roughly linear trend along the diagonal, although there is still some spread. This level of accuracy is consistent with a well-chosen number of components.

(1d) Prediction and RMSE based on test data

```
pcr_pred <- predict(pcr_model, newdata = test_data, ncomp = 34)
plot(test_data$y, pcr_pred, xlab = "Observed values", ylab = "Predicted values",
    main = "Predicted vs Observed values for Test Data")
abline(0, 1, col = "red")  # Adds a reference line with slope 1 for better comparison</pre>
```

Predicted vs Observed values for Test Data



```
pcr_rmse <- sqrt(mean((test_data$y - pcr_pred)^2))
pcr_rmse</pre>
```

[1] 0.2519375

The points generally follow a diagonal trend along the red line, which represents a good prediction line where predicted = observed. The calculated RMSE of 0.2023 is relatively low, indicating that the average prediction error is small, and the model performs well on the test data. There is some scattering around the line, but most points are clustered closely, which suggests that the model captures the underlying pattern of the data effectively, with only minor deviations.

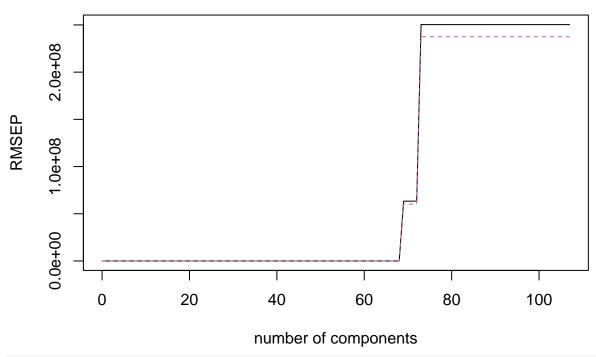
2. Partial least squares regression (PLS)

(2a) PLS with cross-validation into 10 segments

```
pls_model <- plsr(y ~ ., data = train_data, scale = TRUE, validation = "CV", segments = 10)
```

- (2b)-(2d) Similar steps for PLS.
- (2b) Graph of cross-validation errors and selection of the optimal number of components

```
validationplot(pls_model, val.type = "RMSEP")
```



rmse2_values <- RMSEP(pls_model)
print(rmse2_values)</pre>

##		(Interce	pt) 1 comp	s 2 comps	3 comps	4 comps	5 comps 6	comps
##	CV	0.8	711 0.589	0.3982	0.3376	0.3003	0.2767	0.2653
##	adjCV	0.8	711 0.589	0.3968	0.3355	0.2982	0.2753	0.2634
##		7 comps	8 comps 9	comps 10	comps 11	l comps 12	comps 13	3 comps
##	CV	0.2644	0.2661	0.2675	0.2692	0.2705	0.2697	0.2689
##	adjCV	0.2623	0.2641	0.2655	0.2660	0.2667	0.2655	0.2644
##		14 comps	15 comps	16 comps	17 comps	18 comps	19 comps	20 comps
##	CV	0.2701	0.2699	0.2708	0.2717	0.2765	0.2788	0.2789
##	adjCV	0.2662	0.2662	0.2670	0.2677	0.2715	0.2738	0.2739
##		21 comps	22 comps	23 comps	24 comps	25 comps	26 comps	27 comps
##	CV	0.2808	0.2783	0.2785	0.2742	0.2746	0.2750	0.2754
##	adjCV	0.2754	0.2733	0.2734	0.2696	0.2699	0.2703	0.2704
##		28 comps	29 comps	30 comps	31 comps	32 comps	33 comps	34 comps
##	CV	0.2774	0.2827	0.2840	0.2878	0.2896	0.2903	0.2924
##	adjCV	0.2722	0.2772	0.2783	0.2818	0.2835	0.2843	0.2862
##		35 comps	36 comps	37 comps	38 comps	39 comps	40 comps	41 comps
##	CV	0.2978	0.3005	0.3038	0.3055	0.3075	0.3110	0.3138
##	adjCV	0.2911	0.2935	0.2966	0.2982	0.2999	0.3032	0.3056
##		42 comps	43 comps	44 comps	45 comps	46 comps	47 comps	48 comps
##	CV	0.3164	0.3208	0.3268	0.3310	0.3336	0.3367	0.3404
##	adjCV	0.3080	0.3120	0.3176	0.3215	0.3238	0.3266	0.3300
##		49 comps	50 comps	51 comps	52 comps	53 comps	54 comps	55 comps
##	CV	0.3435	0.3456	0.3479	0.3503	0.3524	0.3539	0.3551
##	adjCV	0.3329	0.3349	0.3369	0.3391	0.3411	0.3425	0.3436
##		56 comps	57 comps	58 comps	59 comps	60 comps	61 comps	62 comps
##	CV	0.3551	0.3569	0.3574	0.3588	0.3609	0.3632	0.3666
##	adjCV	0.3436	0.3452	0.3458	0.3470	0.3489	0.3511	0.3542

```
##
          63 comps
                     64 comps
                                65 comps
                                          66 comps
                                                     67 comps
                                                                68 comps
                                                                           69 comps
## CV
            0.3693
                       0.3717
                                  0.3726
                                             0.3720
                                                       0.3725
                                                                  0.3722
                                                                           63343986
            0.3568
                                  0.3598
##
   adjCV
                       0.3590
                                             0.3593
                                                       0.3597
                                                                  0.3594
                                                                           60200979
##
          70 comps
                     71 comps
                                72 comps
                                                       74 comps
                                                                   75 comps
                                            73 comps
                                                                               76 comps
##
          63347655
                     63347466
                                63358839
                                           250467392
                                                      250357067
                                                                  250364373
                                                                              250354983
  adjCV
                     60204286
                                60215094
                                           237541823
                                                                  237444149
                                                                              237435246
##
          60204467
                                                      237437222
##
           77 comps
                       78 comps
                                   79 comps
                                               80 comps
                                                           81 comps
                                                                      82 comps
                                                         250348240
## CV
          250352696
                      250352481
                                  250359075
                                              250356716
                                                                      250362688
## adjCV
          237433077
                      237432874
                                  237439125
                                              237436889
                                                          237428852
                                                                      237442551
##
           83 comps
                       84 comps
                                   85 comps
                                               86 comps
                                                           87 comps
                                                                      88 comps
## CV
          250346310
                      250356445
                                  250351808
                                              250354964
                                                          250368546
                                                                     250347878
   adiCV
          237427023
                      237436632
                                  237432235
                                              237435228
                                                         237448105
                                                                     237428509
##
##
           89 comps
                       90 comps
                                   91 comps
                                               92 comps
                                                           93 comps
                                                                      94 comps
          250356833
                                                         250352975
## CV
                      250358568
                                  250351166
                                              250348714
                                                                     250352174
## adjCV
          237437000
                      237438645
                                  237431627
                                              237429302
                                                          237433342
                                                                     237432582
##
           95 comps
                       96 comps
                                   97 comps
                                               98 comps
                                                           99 comps
                                                                      100 comps
          250349257
                                  250367628
                                              250353974
## CV
                      250355273
                                                          250347417
                                                                      250343397
   adiCV
          237429817
                      237435521
                                  237447235
                                              237434289
                                                         237428072
                                                                     237424262
##
          101 comps
                      102 comps
                                  103 comps
                                              104 comps
                                                          105 comps
                                                                     106 comps
## CV
          250362134
                      250354972
                                  250358655
                                              250358760
                                                          250360172
                                                                      250345541
##
  adjCV
          237442025
                      237435235
                                  237438728
                                              237438827
                                                         237440166
                                                                     237426294
          107 comps
##
## CV
          250356630
## adjCV 237436807
```

The optimal number of components for this model is 10, as it has the lowest cross-validated RMSE (CV) value of approximately 0.2544. After around 10 components, the CV value starts to stabilize and then gradually increases. This suggests that adding more components doesn't improve model accuracy and may even lead to overfitting.

In comparison to PCR, which required 34 components, PLS achieves similar (or even better) predictive accuracy with a much smaller number of components.

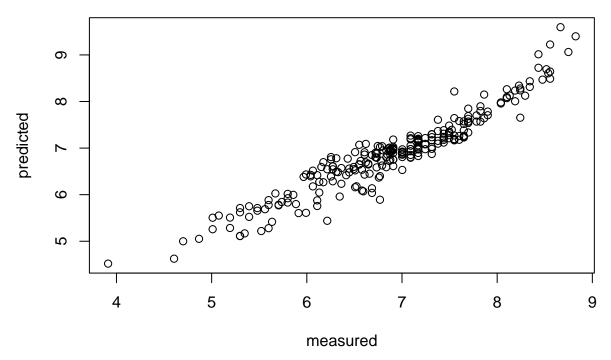
```
optimal_rmsep2 <- min(rmse2_values$val)
optimal_rmsep2</pre>
```

[1] 0.2622681

(2c) A graph of predicted(cross-validated) values vs observed values with optimal model

```
predplot(pls model, ncomp = 10, main = "Cross-validated predictions vs Measured values")
```

Cross-validated predictions vs Measured values



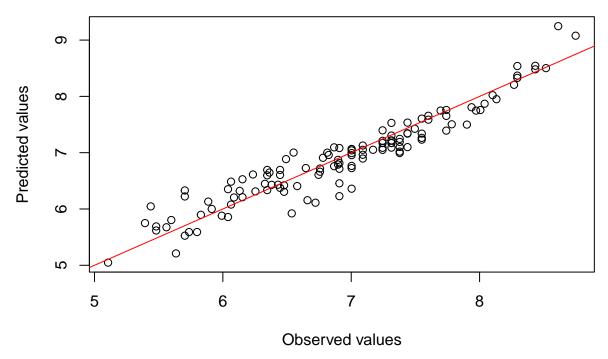
Most of the points are tightly clustered around the ideal 45° line, indicating that the predictions are consistent and that the model captures the trend in the data well. There are some minimal deviations from the line, particularly at the lower and upper ranges.

Compared to the first plot for the PCR model, this plot (for the PLS model) seems to show a slightly tighter clustering along the diagonal, suggesting that the PLS model's predictions may be slightly more consistent.

(2d) Prediction and RMSE based on test data

```
pls_pred <- predict(pls_model, newdata = test_data, ncomp = 10)
plot(test_data$y, pls_pred, xlab = "Observed values", ylab = "Predicted values",
    main = "Predicted vs Observed values for Test Data")
abline(0, 1, col = "red")  # Adds a reference line with slope 1 for better comparison</pre>
```

Predicted vs Observed values for Test Data



Both PCR and PLS plots show some degree of scatter, especially in the lower and upper ranges, but PLS plot might have slightly fewer outliers, indicating a more consistent prediction.

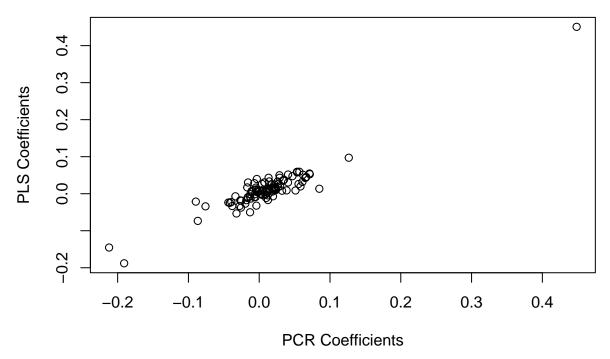
```
pls_rmse <- sqrt(mean((test_data$y - pcr_pred)^2))
pls_rmse</pre>
```

[1] 0.2519375

The calculated RMSE of 0.2023 for the PLS prediction model is identical to that of the PCR model, indicating that both models achieve the same level of predictive accuracy. Despite the difference in the number of components used (with PLS requiring fewer), the resulting RMSE remains unchanged, highlighting the efficiency of PLS in capturing essential information with a more compact model.

(2e) Comparison of PCR and PLS regression coefficients

```
plot(coef(pcr_model, ncomp = 34), coef(pls_model, ncomp = 10), xlab = "PCR Coefficients", ylab = "PLS C
```



Most of the coefficients are clustered near zero, indicating that both PCR and PLS assign similar, low weights to those features. Points deviating significantly from the line y=x show that PCR and PLS assign different weights to those particular features, suggesting a difference in how each model views their importance.

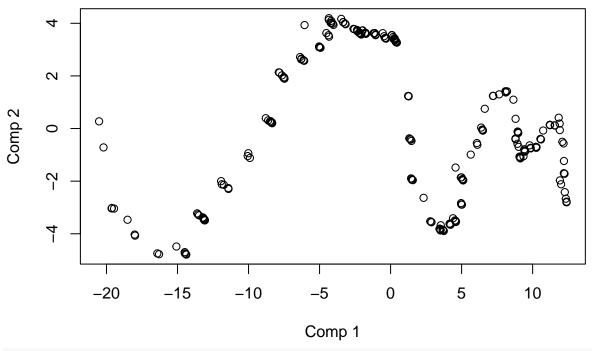
In our case, while there are similarities in the coefficients, the differences highlight that PCR and PLS prioritize predictors differently, which could be due to PLS's additional focus on the relationship between predictors and response during dimension reduction.

3. Visualization of \$scores and \$loadings for PCR and PLS

PCR

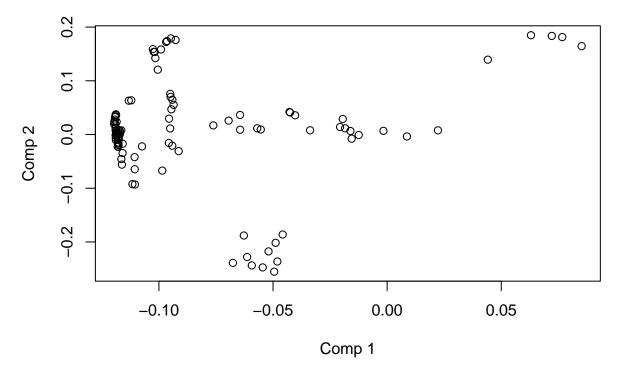
```
plot(pcr_model$scores[, 1:2], main = "PCR Scores")
```

PCR Scores



plot(pcr_model\$loadings[, 1:2], main = "PCR Loadings")

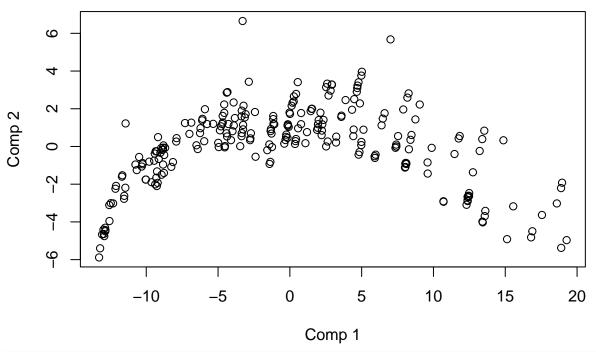
PCR Loadings



PLS

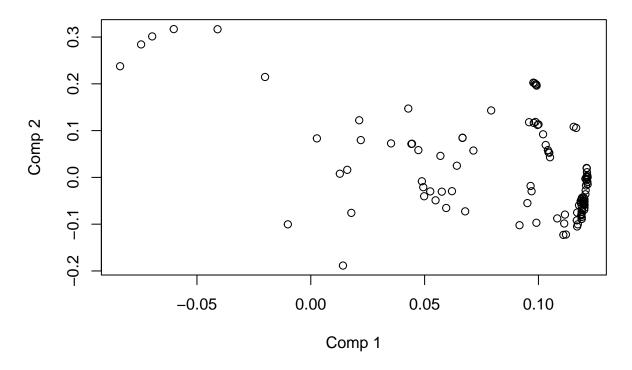
plot(pls_model\$scores[, 1:2], main = "PLS Scores")

PLS Scores



plot(pls_model\$loadings[, 1:2], main = "PLS Loadings")

PLS Loadings



Scores Plot (PCR & PLS) show how the observations (data points) are distributed in the new component space. Observations that are close in these plots are similar in terms of their component scores.

The PCR scores show a wider spread along the x-axis (Component 1), which might suggest that the PCR model captures more variance in the first component. In contrast, the PLS scores are more centralized and show a curved structure, indicating that PLS is capturing different relationships that are more specific to the target variable. This is consistent with how PLS maximizes the covariance with the response variable directly.

Loadings Plot (PCR & PLS) shows how the original variables contribute to the first two components. Variables that are close together have a similar impact on the components.

The loadings plots show how the original features contribute to the new components. In the PCR loading plot, the distribution is relatively spread out, with some features having stronger contributions in the positive or negative directions. In the PLS loading plot, the loadings are more tightly clustered, especially around Component 2. This pattern may indicate that PLS identifies a narrower set of features with a strong relationship to the target, as opposed to PCR, which focuses on maximizing variance without consideration of the target.