

Exercise 3

Advanced Methods for Regression and Classification

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Load the necessary libraries

Load Data

```
# Load the dataset
load("building.RData")
# str(df)
```

Data Splitting

```
set.seed(12332281)

# Split the data
sample_index <- sample(1:nrow(df), size = 2/3 * nrow(df))
train_data <- df[sample_index, ]
test_data <- df[-sample_index, ]

# Display the number of samples in each set
cat("Training set size:", nrow(train_data), "\n")
```

```
## Training set size: 248
```

```
cat("Test set size:", nrow(test_data), "\n")
```

```
## Test set size: 124
```

Fit regression model on the training data

```
# Fit linear regression model
model <- lm(y ~ ., data = train_data)
# summary(model)
```

Compute RMSE (training data)

```
train_pred <- predict(model, newdata = train_data)

# Compute RMSE for training data
train_rmse <- sqrt(mean((train_data$y - train_pred)^2))
cat("Training RMSE:", train_rmse, "\n")
```

Training RMSE: 0.1928942

1. Principal Component Regression (PCR)

a) Applying PCR with Cross-Validation

```
# Fit PCR model with cross-validation and scaling
pcr_model <- pcr(y ~ ., data = train_data, scale = TRUE, validation = "CV", segments = 10)
summary(pcr_model)
```

```
## Data:      X dimension: 248 107
## Y dimension: 248 1
## Fit method: svdpc
## Number of components considered: 107
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##          (Intercept) 1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV        0.8429   0.6093   0.5938   0.5761   0.5311   0.5321   0.4648
## adjCV     0.8429   0.6091   0.5937   0.5728   0.5300   0.5328   0.4633
##          7 comps  8 comps  9 comps  10 comps 11 comps 12 comps 13 comps
## CV        0.4715   0.4126   0.3713   0.3739   0.3752   0.3725   0.3700
## adjCV     0.4724   0.4116   0.3683   0.3714   0.3705   0.3698   0.3675
##          14 comps 15 comps 16 comps 17 comps 18 comps 19 comps 20 comps
## CV        0.3702   0.3730   0.3119   0.2939   0.2923   0.2931   0.2928
## adjCV     0.3677   0.3716   0.3039   0.2895   0.2903   0.2910   0.2909
##          21 comps 22 comps 23 comps 24 comps 25 comps 26 comps 27 comps
## CV        0.2920   0.2941   0.2967   0.2983   0.3027   0.3019   0.3093
## adjCV     0.2897   0.2919   0.2944   0.2960   0.3003   0.2996   0.3065
##          28 comps 29 comps 30 comps 31 comps 32 comps 33 comps 34 comps
## CV        0.3076   0.3053   0.2968   0.2938   0.2907   0.2908   0.2802
## adjCV     0.3049   0.3019   0.2936   0.2918   0.2874   0.2880   0.2772
##          35 comps 36 comps 37 comps 38 comps 39 comps 40 comps 41 comps
## CV        0.2797   0.2764   0.2734   0.2743   0.2730   0.2703   0.2736
## adjCV     0.2753   0.2732   0.2699   0.2711   0.2697   0.2676   0.2711
##          42 comps 43 comps 44 comps 45 comps 46 comps 47 comps 48 comps
## CV        0.2750   0.2706   0.2690   0.2713   0.2713   0.2705   0.2707
## adjCV     0.2735   0.2675   0.2657   0.2681   0.2683   0.2671   0.2674
##          49 comps 50 comps 51 comps 52 comps 53 comps 54 comps 55 comps
## CV        0.2732   0.2720   0.2718   0.2728   0.2748   0.2772   0.2775
## adjCV     0.2697   0.2682   0.2682   0.2691   0.2712   0.2736   0.2733
##          56 comps 57 comps 58 comps 59 comps 60 comps 61 comps 62 comps
```

```

## CV      0.2835   0.2852   0.2890   0.2933   0.2957   0.2977   0.2968
## adjCV   0.2790   0.2806   0.2842   0.2884   0.2906   0.2924   0.2918
##       63 comps  64 comps  65 comps  66 comps  67 comps  68 comps  69 comps
## CV      0.2991   0.2983   0.2965   0.2981   0.2979   0.2971   0.3190
## adjCV   0.2946   0.2934   0.2906   0.2918   0.2914   0.2911   0.3118
##       70 comps  71 comps  72 comps  73 comps  74 comps  75 comps
## CV      2.947e+09 9.631e+10 1.727e+11 5.259e+11 4.798e+11 1.527e+12
## adjCV   2.794e+09 9.138e+10 1.638e+11 4.987e+11 4.551e+11 1.450e+12
##       76 comps  77 comps  78 comps  79 comps  80 comps  81 comps
## CV      1.626e+12 1.871e+12 1.819e+12 1.934e+12 1.829e+12 1.803e+12
## adjCV   1.544e+12 1.777e+12 1.727e+12 1.836e+12 1.737e+12 1.711e+12
##       82 comps  83 comps  84 comps  85 comps  86 comps  87 comps
## CV      1.738e+12 1.503e+12 1.724e+12 2.181e+12 2.185e+12 2.652e+12
## adjCV   1.650e+12 1.426e+12 1.635e+12 2.068e+12 2.072e+12 2.516e+12
##       88 comps  89 comps  90 comps  91 comps  92 comps  93 comps
## CV      2.815e+12 2.875e+12 3.015e+12 2.944e+12 3.059e+12 3.061e+12
## adjCV   2.671e+12 2.728e+12 2.861e+12 2.793e+12 2.903e+12 2.905e+12
##       94 comps  95 comps  96 comps  97 comps  98 comps  99 comps
## CV      3.369e+12 3.344e+12 3.433e+12 3.222e+12 3.302e+12 3.442e+12
## adjCV   3.197e+12 3.172e+12 3.257e+12 3.056e+12 3.132e+12 3.265e+12
##       100 comps 101 comps 102 comps 103 comps 104 comps 105 comps
## CV      3.291e+12 3.339e+12 3.526e+12 3.545e+12 3.603e+12 3.458e+12
## adjCV   3.121e+12 3.167e+12 3.346e+12 3.363e+12 3.419e+12 3.280e+12
##       106 comps 107 comps
## CV      3.420e+12 3.458e+12
## adjCV   3.245e+12 3.280e+12
##
## TRAINING: % variance explained
##       1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
## X      64.70    71.75   76.48   80.87   84.20   87.11   89.03   90.74
## y      48.09    51.31   58.89   63.54   63.97   72.89   72.90   79.71
##       9 comps  10 comps 11 comps 12 comps 13 comps 14 comps 15 comps
## X      92.18    93.26   94.20   95.11   95.85   96.43   96.89
## y      84.00    84.00   84.73   84.73   84.87   85.17   85.18
##       16 comps 17 comps 18 comps 19 comps 20 comps 21 comps 22 comps
## X      97.30    97.62   97.90   98.13   98.36   98.55   98.73
## y      90.17    90.33   90.39   90.43   90.47   90.59   90.61
##       23 comps 24 comps 25 comps 26 comps 27 comps 28 comps 29 comps
## X      98.88    99.02   99.14   99.24   99.33   99.40   99.46
## y      90.72    90.78   90.92   90.98   91.11   91.18   91.55
##       30 comps 31 comps 32 comps 33 comps 34 comps 35 comps 36 comps
## X      99.51    99.56   99.60   99.64   99.68   99.71   99.74
## y      91.77    91.78   92.01   92.04   92.53   92.74   92.77
##       37 comps 38 comps 39 comps 40 comps 41 comps 42 comps 43 comps
## X      99.77    99.80   99.82   99.84   99.86   99.87   99.89
## y      92.98    93.03   93.16   93.19   93.27   93.27   93.56
##       44 comps 45 comps 46 comps 47 comps 48 comps 49 comps 50 comps
## X      99.90    99.92   99.93   99.94   99.95   99.95   99.96
## y      93.66    93.67   93.69   93.77   93.79   93.91   93.97
##       51 comps 52 comps 53 comps 54 comps 55 comps 56 comps 57 comps
## X      99.97    99.97   99.97   99.98   99.98   99.99   99.99
## y      93.97    93.99   94.00   94.01   94.08   94.08   94.08
##       58 comps 59 comps 60 comps 61 comps 62 comps 63 comps 64 comps
## X      99.99    99.99   99.99   100.00  100.00  100.00  100.00

```

```

## y      94.09      94.09      94.11      94.14      94.18      94.2       94.32
## X    65 comps   66 comps   67 comps   68 comps   69 comps   70 comps   71 comps
## y      100.00     100.00     100.00     100.00     100.00     100.00    100.0
## y      94.48      94.54      94.57      94.57      94.59      94.59      94.7
## X    72 comps   73 comps   74 comps   75 comps   76 comps   77 comps   78 comps
## y      100.00     100.00     100.00     100.00     100.00     100.00    100.0
## y      94.72      94.72      94.72      94.73      94.73      94.77      94.78
## X    79 comps   80 comps   81 comps   82 comps   83 comps   84 comps   85 comps
## y      100.00     100.00     100.00     100.00     100.00     100.00    100.0
## y      94.79      94.81      94.89      94.92      94.95      94.95      95.08
## X    86 comps   87 comps   88 comps   89 comps   90 comps   91 comps   92 comps
## X    100.0       100.0       100.0       100.0       100.0       100.0      100.0
## y      95.1       95.1       95.19      95.25      95.3       95.31      95.45
## X    93 comps   94 comps   95 comps   96 comps   97 comps   98 comps   99 comps
## X    100.00     100.00     100.00     100.00     100.00     100.00    100.0
## y      95.46      95.46      95.52      95.57      95.57      95.58      95.58
## X    100 comps  101 comps  102 comps  103 comps  104 comps  105 comps  106 comps
## X    100.00     100.00     100.00     100.00     100.00     100.00    100.0
## y      95.61      95.63      95.64      95.66      95.66      95.66      95.7
## X    107 comps
## X    100.00
## y      95.73

```

This applies Principal Component Regression (PCR) to the training data, scaling the variables and using 10-fold cross-validation to find the best number of components for accurate predictions.

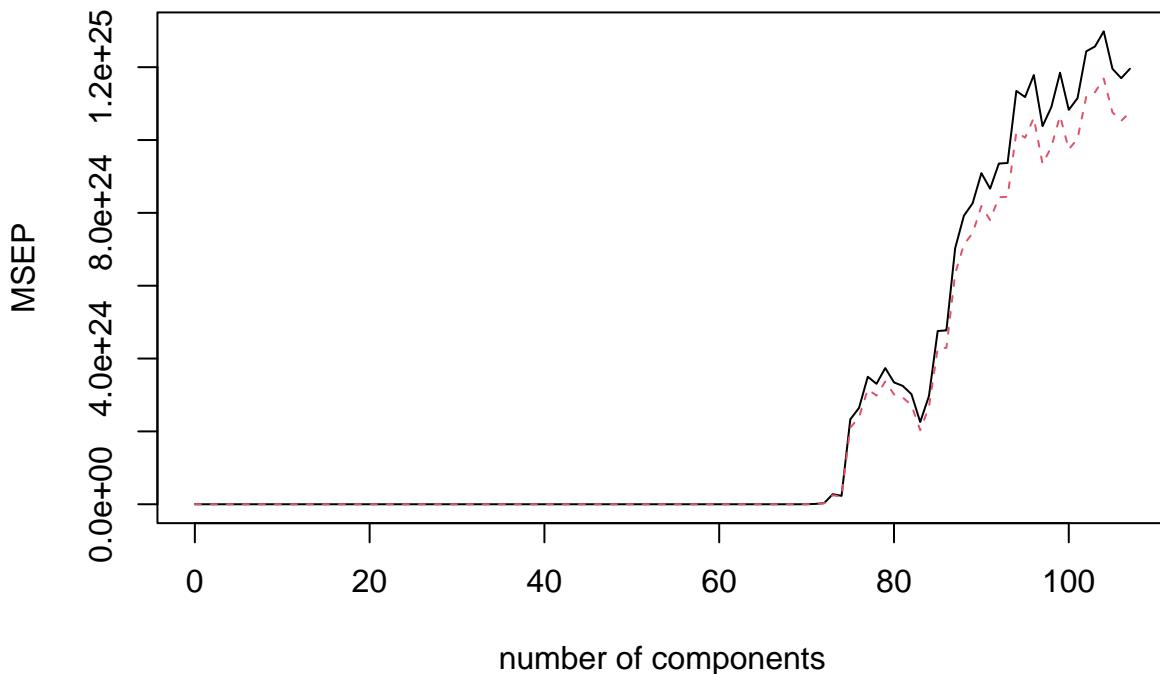
b) Cross-Validation Error Plot and Optimal Components

```

# Plot cross-validation errors for each component
validationplot(pcr_model, val.type = "MSEP", main = "PCR Cross-Validation Error Plot")

```

PCR Cross-Validation Error Plot



How many components seem to be optimal?

Optimal number of components is around 68. The curve shows how the prediction error changes as more components are added. Initially, the error decreases, indicating an improvement in the model's accuracy as components are included. However, after a certain number of components, the error increases, suggesting that adding more components leads to overfitting, where the model becomes too complex and loses its generalizability.

```
rmsep_results <- RMSEP(pcr_model)
rmsep_values <- rmsep_results$val

# Now you can find the optimal RMSE
optimal_components <- 68
optimal_rmse <- rmsep_values[optimal_components]
cat("Resulting RMSE at optimal components:", optimal_rmse, "\n")

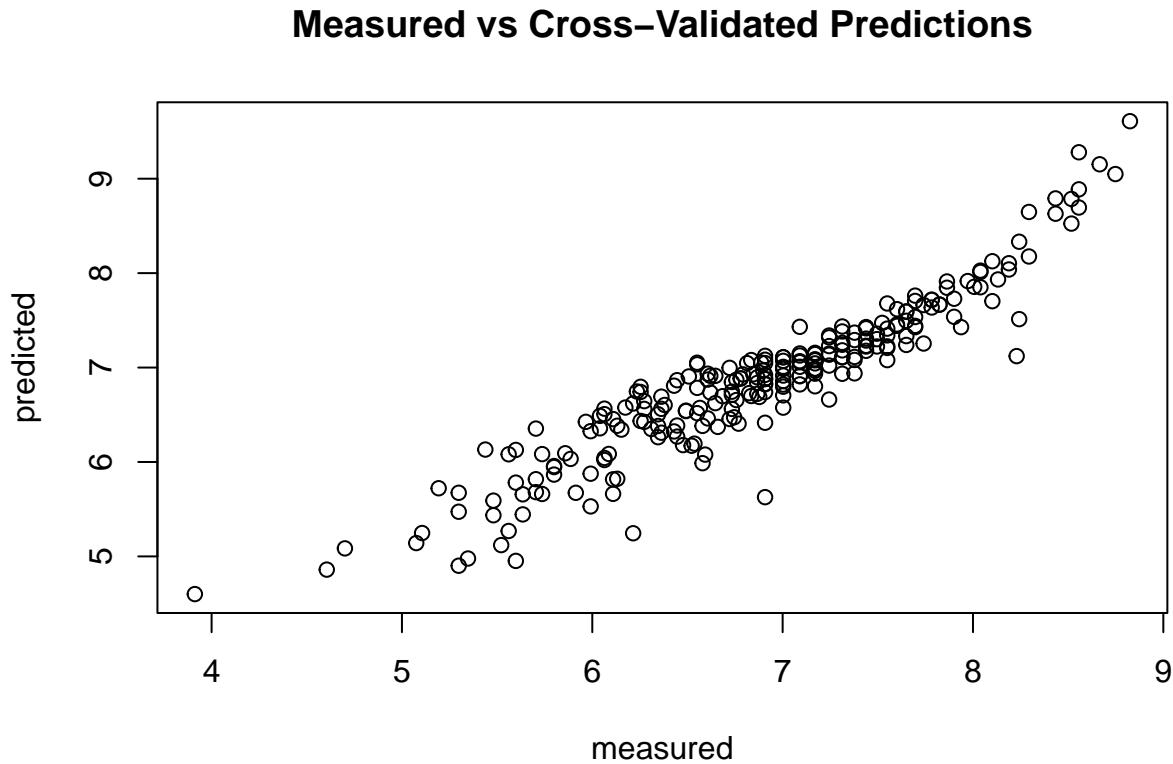
## Resulting RMSE at optimal components: 0.2880382
```

The RMSE increased when moving from a simple training RMSE to a cross-validated RMSE in PCR, because:

- Overfitting on Training Data: The initial RMSE of 0.1929 was calculated directly on the training data, which means the model was fitted to the same data used to evaluate it.
- Cross-Validation for Generalization: When you switch to using cross-validation in PCR, the model is repeatedly trained on different subsets of the data and tested on other subsets. The cross-validated RMSE, better reflects how well the model generalizes to unseen data.

c) Plotting Measured vs. Cross-Validated Predictions

```
# Plot measured vs cross-validated predictions
predplot(pcr_model, ncomp = optimal_components, main = "Measured vs Cross-Validated Predictions")
```



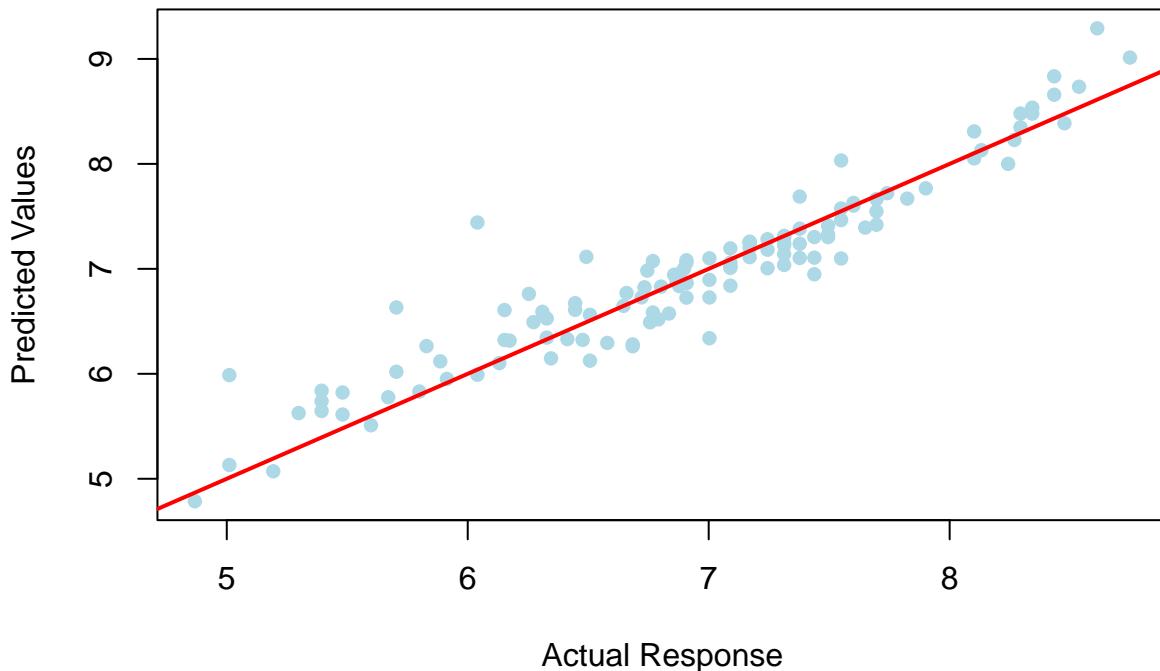
This plot visualizes the relationship between the actual measured values of the response variable (y) and the cross-validated predictions generated by the PCR model using 68 components. The plot shows that the cross-validated predictions closely align with the actual values along the diagonal, indicating the model's generally accurate fit, with some minor variance at the edges.

d) Plotting Predicted vs Observed Values for Test Data and Computing RMSE

```
test_pred <- predict(pcr_model, newdata = test_data, ncomp = 68)

# Plot Predicted vs Observed values for Test Data
plot(test_data$y, test_pred, main = "Predicted vs Actual Response (Test Data)", xlab = "Actual Response",
     ylab = "Predicted Values", pch = 16, col = "lightblue")
abline(0, 1, col = "red", lwd = 2)
```

Predicted vs Actual Response (Test Data)



```
# Calculate RMSE for Test Data
test_rmse <- sqrt(mean((test_data$y - test_pred)^2))
cat("Test RMSE:", test_rmse, "\n")
```

```
## Test RMSE: 0.2872396
```

The plot shows a strong alignment of the predicted values with the actual values for the test data. The relatively low Test RMSE of 0.2872, indicates minimal error in predictions.

2. Partial least squares regression (PLS)

a) Applying PLS with Cross-Validation

```
# Apply PLS on the training data with cross-validation and scaling
pls_model <- plsr(y ~ ., data = train_data, scale = TRUE, validation = "CV", segments = 10)
summary(pls_model)

## Data:      X dimension: 248 107
##   Y dimension: 248 1
## Fit method: kernelpls
## Number of components considered: 107
##
## VALIDATION: RMSEP
```

```

## Cross-validated using 10 random segments.
##          (Intercept) 1 comps 2 comps 3 comps 4 comps 5 comps 6 comps
## CV          0.8429  0.5874  0.4073  0.3518  0.3192  0.2944  0.2823
## adjCV       0.8429  0.5873  0.4052  0.3498  0.3171  0.2929  0.2804
##          7 comps 8 comps 9 comps 10 comps 11 comps 12 comps 13 comps
## CV          0.2829  0.2863  0.2891  0.2932  0.2944  0.2898  0.2815
## adjCV       0.2810  0.2836  0.2859  0.2884  0.2892  0.2841  0.2764
##          14 comps 15 comps 16 comps 17 comps 18 comps 19 comps 20 comps
## CV          0.2744  0.2725  0.2725  0.2735  0.2762  0.2766  0.2787
## adjCV       0.2707  0.2690  0.2688  0.2696  0.2722  0.2724  0.2745
##          21 comps 22 comps 23 comps 24 comps 25 comps 26 comps 27 comps
## CV          0.2801  0.2811  0.2827  0.2866  0.2865  0.2899  0.2945
## adjCV       0.2758  0.2767  0.2782  0.2819  0.2818  0.2849  0.2891
##          28 comps 29 comps 30 comps 31 comps 32 comps 33 comps 34 comps
## CV          0.2973  0.3028  0.3030  0.3059  0.3081  0.3076  0.3105
## adjCV       0.2917  0.2967  0.2968  0.2994  0.3013  0.3008  0.3034
##          35 comps 36 comps 37 comps 38 comps 39 comps 40 comps 41 comps
## CV          0.3122  0.3115  0.3128  0.3123  0.3150  0.3184  0.3197
## adjCV       0.3049  0.3042  0.3053  0.3049  0.3074  0.3106  0.3118
##          42 comps 43 comps 44 comps 45 comps 46 comps 47 comps 48 comps
## CV          0.3230  0.3265  0.3315  0.3372  0.3445  0.3503  0.3539
## adjCV       0.3148  0.3181  0.3226  0.3279  0.3346  0.3400  0.3434
##          49 comps 50 comps 51 comps 52 comps 53 comps 54 comps 55 comps
## CV          0.3574  0.3611  0.3629  0.3648  0.3667  0.3674  0.3682
## adjCV       0.3466  0.3501  0.3516  0.3534  0.3552  0.3558  0.3566
##          56 comps 57 comps 58 comps 59 comps 60 comps 61 comps 62 comps
## CV          0.3686  0.3684  0.3683  0.3687  0.3697  0.3700  0.3700
## adjCV       0.3570  0.3568  0.3567  0.3570  0.3579  0.3582  0.3582
##          63 comps 64 comps 65 comps 66 comps 67 comps 68 comps 69 comps
## CV          0.3703  0.3705  0.3705  0.3705  0.3704  6060898 24816893
## adjCV       0.3585  0.3587  0.3587  0.3587  0.3586  5747296 23532821
##          70 comps 71 comps 72 comps 73 comps 74 comps 75 comps
## CV          24817022 48213846 216233529 216229331 216230956 216230322
## adjCV       23532944 45719190 205045213 205041233 205042773 205042172
##          76 comps 77 comps 78 comps 79 comps 80 comps 81 comps
## CV          216229731 216230773 216230118 216231031 216230406 216231416
## adjCV       205041612 205042600 205041979 205042844 205042252 205043209
##          82 comps 83 comps 84 comps 85 comps 86 comps 87 comps
## CV          216231316 216231089 216230179 216231494 216229654 216231161
## adjCV       205043115 205042899 205042036 205043283 205041539 205042968
##          88 comps 89 comps 90 comps 91 comps 92 comps 93 comps
## CV          216230331 216230826 216229842 216231296 216232423 216231344
## adjCV       205042181 205042650 205041717 205043096 205044164 205043141
##          94 comps 95 comps 96 comps 97 comps 98 comps 99 comps
## CV          216232113 216230959 216230749 216231978 216230177 216232575
## adjCV       205043870 205042777 205042577 205043743 205042034 205044308
##          100 comps 101 comps 102 comps 103 comps 104 comps 105 comps
## CV          216230956 216231194 216231562 216232052 216232291 216232238
## adjCV       205042773 205042999 205043348 205043812 205044039 205043989
##          106 comps 107 comps
## CV          216231325 216231550
## adjCV       205043123 205043336
##
## TRAINING: % variance explained

```

```

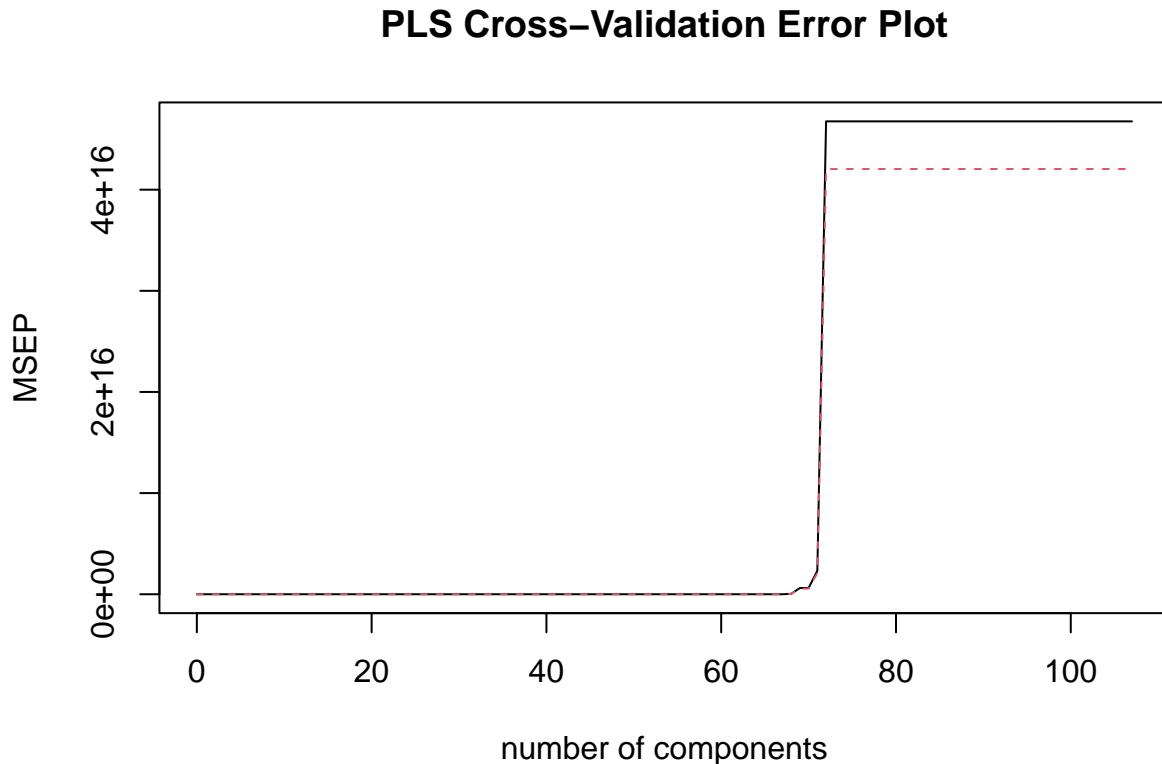
##   1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
## X 64.55    69.53    74.23    77.93    80.34    82.10    85.65    87.14
## y 51.98    79.47    85.64    88.38    90.00    91.28    91.57    91.91
##   9 comps  10 comps 11 comps 12 comps 13 comps 14 comps 15 comps
## X 89.40    90.79    91.64    92.16    93.07    94.37    94.86
## y 92.26    92.82    93.21    93.47    93.63    93.71    93.80
## 16 comps 17 comps 18 comps 19 comps 20 comps 21 comps 22 comps
## X 95.24    95.73    96.47    96.67    97.26    97.73    98.05
## y 93.89    93.95    93.99    94.06    94.08    94.11    94.14
## 23 comps 24 comps 25 comps 26 comps 27 comps 28 comps 29 comps
## X 98.26    98.44    98.58    98.70    98.81    98.94    99.07
## y 94.17    94.20    94.24    94.27    94.31    94.34    94.37
## 30 comps 31 comps 32 comps 33 comps 34 comps 35 comps 36 comps
## X 99.17    99.26    99.35    99.45    99.50    99.57    99.6
## y 94.41    94.46    94.49    94.52    94.55    94.57    94.6
## 37 comps 38 comps 39 comps 40 comps 41 comps 42 comps 43 comps
## X 99.63    99.66    99.68    99.70    99.73    99.75    99.77
## y 94.61    94.62    94.63    94.64    94.65    94.65    94.66
## 44 comps 45 comps 46 comps 47 comps 48 comps 49 comps 50 comps
## X 99.79    99.81    99.84    99.85    99.87    99.89    99.9
## y 94.67    94.67    94.68    94.68    94.69    94.69    94.7
## 51 comps 52 comps 53 comps 54 comps 55 comps 56 comps 57 comps
## X 99.92    99.93    99.93    99.94    99.95    99.96    99.97
## y 94.70    94.71    94.71    94.71    94.71    94.71    94.71
## 58 comps 59 comps 60 comps 61 comps 62 comps 63 comps 64 comps
## X 99.97    99.98    99.98    99.98    99.99    99.99    99.99
## y 94.71    94.72    94.72    94.72    94.72    94.72    94.72
## 65 comps 66 comps 67 comps 68 comps 69 comps 70 comps 71 comps
## X 99.99    100.00   100.00   100.00   100.00   100.00   100.00
## y 94.72    94.72    94.72    94.72    94.72    94.72    94.72
## 72 comps 73 comps 74 comps 75 comps 76 comps 77 comps 78 comps
## X 100.00   100.00   100.01   100.01   100.01   100.02   100.02
## y 94.72    94.69    94.69    94.69    94.69    94.69    94.69
## 79 comps 80 comps 81 comps 82 comps 83 comps 84 comps 85 comps
## X 100.02   100.03   100.03   100.03   100.04   100.04   100.04
## y 94.69    94.69    94.69    94.69    94.69    94.69    94.69
## 86 comps 87 comps 88 comps 89 comps 90 comps 91 comps 92 comps
## X 100.04   100.05   100.05   100.06   100.06   100.06   100.07
## y 94.69    94.69    94.69    94.69    94.69    94.69    94.69
## 93 comps 94 comps 95 comps 96 comps 97 comps 98 comps 99 comps
## X 100.07   100.07   100.08   100.08   100.08   100.09   100.09
## y 94.69    94.69    94.69    94.69    94.69    94.69    94.69
## 100 comps 101 comps 102 comps 103 comps 104 comps 105 comps 106 comps
## X 100.09   100.10   100.10   100.10   100.11   100.11   100.11
## y 94.69    94.69    94.69    94.69    94.69    94.69    94.69
## 107 comps
## X 100.12
## y 94.69

```

This code fits a PLS model to the train_data dataset, using scaling and 10-fold cross-validation to assess model performance.

b) Cross-Validation Error Plot and Optimal Components

```
# Plot cross-validation errors for each component
validationplot(pls_model, val.type = "MSEP", main = "PLS Cross-Validation Error Plot")
```



How many components seem to be optimal? In the PLS Cross-Validation Error Plot, the optimal number of components appears to be where the Mean Squared Error of Prediction (MSEP) is at its lowest before any significant increase. From the plot, this seems to occur at around 65 components. After this point, the MSEP value increases sharply, indicating that adding more components does not improve the model's performance and may lead to overfitting.

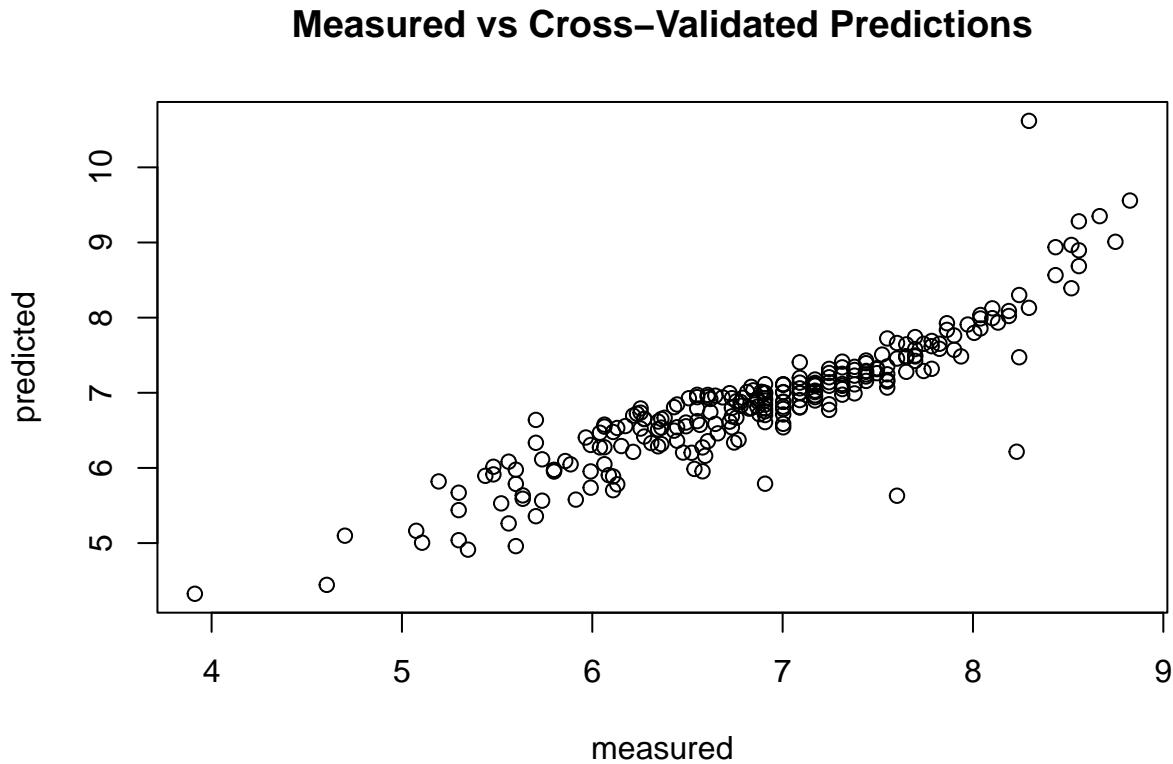
```
rmsep_results2 <- RMSEP(pls_model)
rmsep_values2 <- rmsep_results2$val

# Now you can find the optimal RMSE
optimal_components <- 65
optimal_rmse <- rmsep_values2[optimal_components]
cat("Resulting RMSE at optimal components:", optimal_rmse, "\n")

## Resulting RMSE at optimal components: 0.3080849
```

c) Plotting Measured vs. Cross-Validated Predictions

```
# Plot measured vs cross-validated predictions
predplot(pls_model, ncomp = optimal_components, main = "Measured vs Cross-Validated Predictions")
```



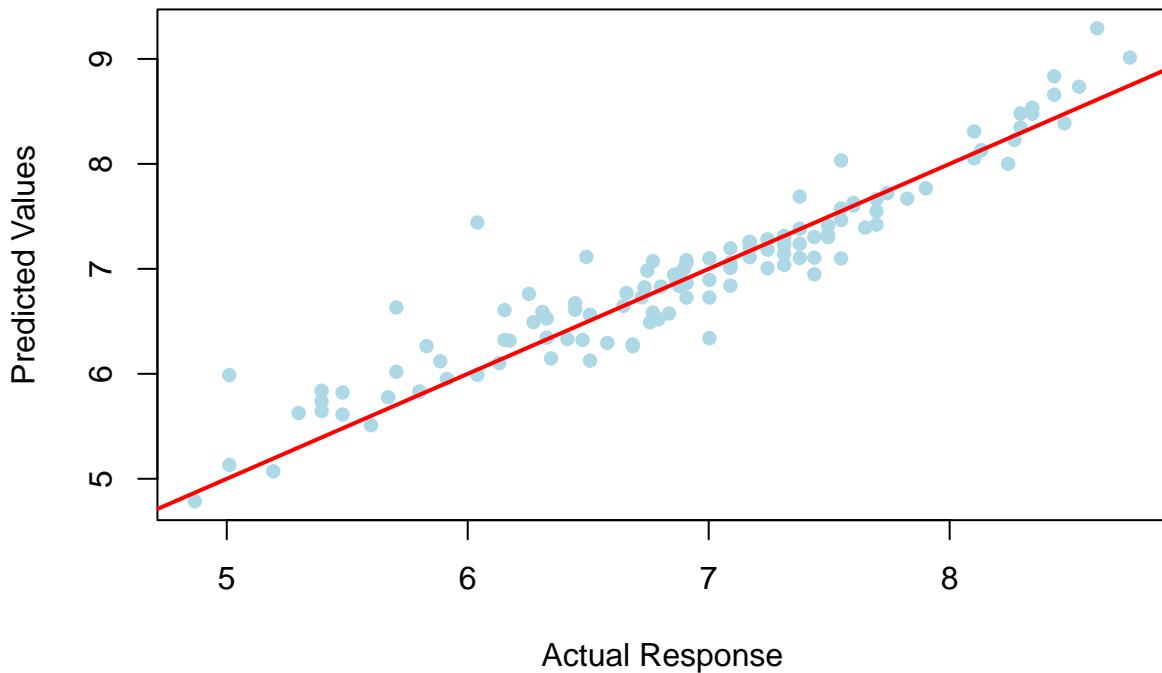
This plot visualizes the relationship between the actual measured values of the response variable (y) and the cross-validated predictions generated by the PLS model using 65 components. The plot shows that the cross-validated predictions closely align with the actual values along the diagonal, indicating the model's generally accurate fit, with some minor variance at the edges.

d) Plotting Predicted vs Observed Values for Test Data and Computing RMSE

```
pls_test_pred <- predict(pls_model, newdata = test_data, ncomp = 65)

# Plot Predicted vs Observed values for Test Data
plot(test_data$y, test_pred, main = "Predicted vs Actual Response (Test Data)", xlab = "Actual Response",
     ylab = "Predicted Values", pch = 16, col = "lightblue")
abline(0, 1, col = "red", lwd = 2)
```

Predicted vs Actual Response (Test Data)



```
# Calculate RMSE for test data predictions
pls_test_rmse <- sqrt(mean((test_data$y - pls_test_pred)^2))
cat("Test RMSE for PLS:", pls_test_rmse, "\n")
```

Test RMSE for PLS: 0.2988856

The plot shows a strong alignment of the predicted values with the actual values for the test data. The relatively low Test RMSE of 0.2992037, indicates minimal error in predictions.

e)) Compare the regression coefficients from PCR and PLS

```
# Extract coefficients for the optimal number of components in PCR and PLS
pcr_coefs <- coef(pcr_model, ncomp = optimal_components)
pls_coefs <- coef(pls_model, ncomp = optimal_components)

# Convert to data frame for easy plotting
coef_data <- data.frame(Predictor = rownames(pcr_coefs), PCR = as.vector(pcr_coefs),
PLS = as.vector(pls_coefs))

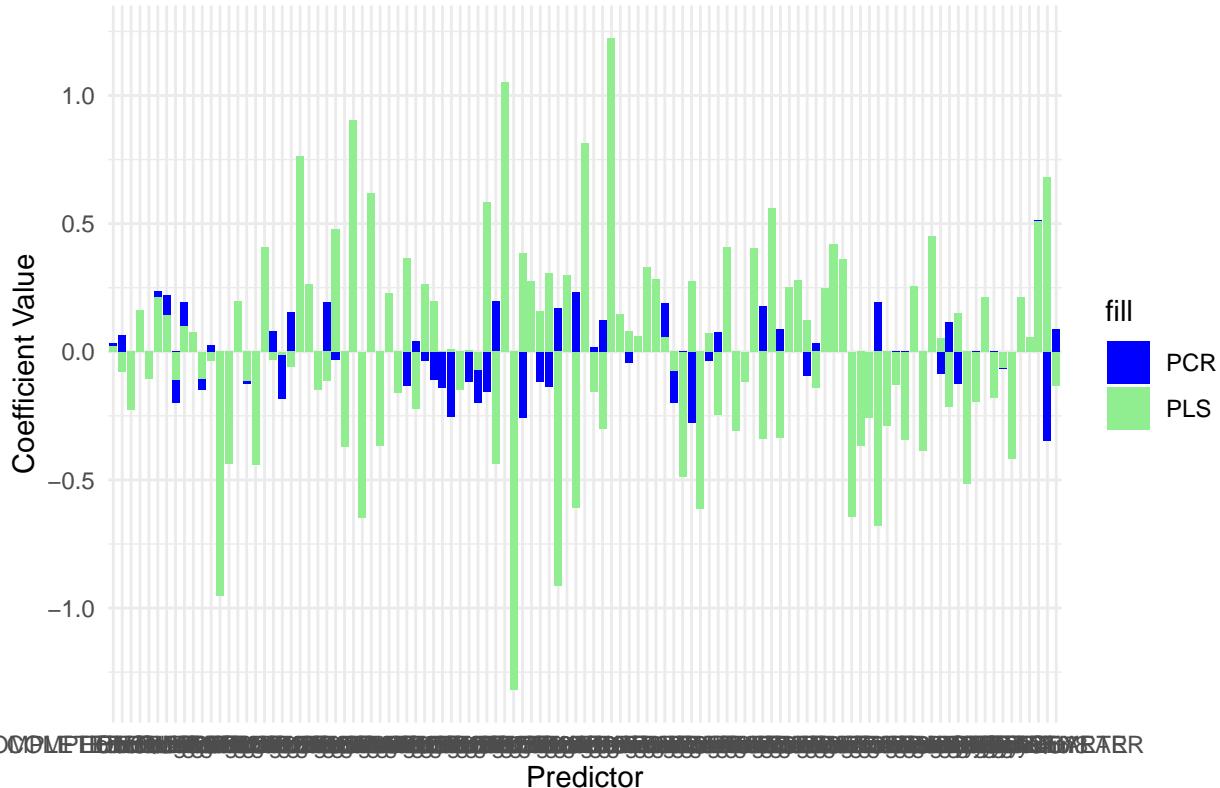
# Plot the coefficients for PCR and PLS
library(ggplot2)
ggplot(coef_data, aes(x = Predictor)) + geom_bar(aes(y = PCR, fill = "PCR"), stat = "identity",
position = "dodge") + geom_bar(aes(y = PLS, fill = "PLS"), stat = "identity",
```

```

position = "dodge") + labs(title = "Comparison of Regression Coefficients for PCR and PLS",
y = "Coefficient Value") + scale_fill_manual(values = c(PCR = "blue", PLS = "lightgreen")) +
theme(axis.text.x = element_text(angle = 90, hjust = 1)) + theme_minimal()

```

Comparison of Regression Coefficients for PCR and PLS



From this comparison plot of regression coefficients for PCR (blue) and PLS (green), we can observe:

- Coefficient Magnitudes:** PLS generally shows larger coefficients than PCR across several predictors, suggesting that PLS places more emphasis on certain variables than PCR. This is because PLS aims to maximize the covariance between predictors and the response variable, while PCR focuses on capturing the variance of predictors.
- Direction of Coefficients:** In some predictors, the direction of the coefficients differs between PCR and PLS, indicating that each method might be capturing slightly different relationships between predictors and the response.
- Stability and Selection:** PCR seems to yield smaller coefficients, particularly around zero for several predictors, which could indicate that only the most influential predictors have noticeable effects.

3. Score vectors and loadings vectors

```

library(ggplot2)
library(gridExtra)

# Extract scores and loadings for PCR

```

```

pcr_scores <- pcr_model$scores[, 1:2] # First two score vectors (Z1 and Z2)
pcr_loadings <- pcr_model$loadings[, 1:2] # First two loading vectors (V1 and V2)

# Extract scores and loadings for PLS
pls_scores <- pls_model$scores[, 1:2] # First two score vectors (T1 and T2)
pls_loadings <- pls_model$loadings[, 1:2] # First two loading vectors (W1 and W2)

# Convert to data frames for ggplot
pcr_scores_df <- as.data.frame(pcr_scores)
pcr_loadings_df <- as.data.frame(pcr_loadings)
pls_scores_df <- as.data.frame(pls_scores)
pls_loadings_df <- as.data.frame(pls_loadings)

# Plot PCR scores
p1 <- ggplot(pcr_scores_df, aes(x = `Comp 1`, y = `Comp 2`)) + geom_point(color = "blue") +
  labs(title = "PCR Scores (Z1 vs Z2)", x = "Z1", y = "Z2")

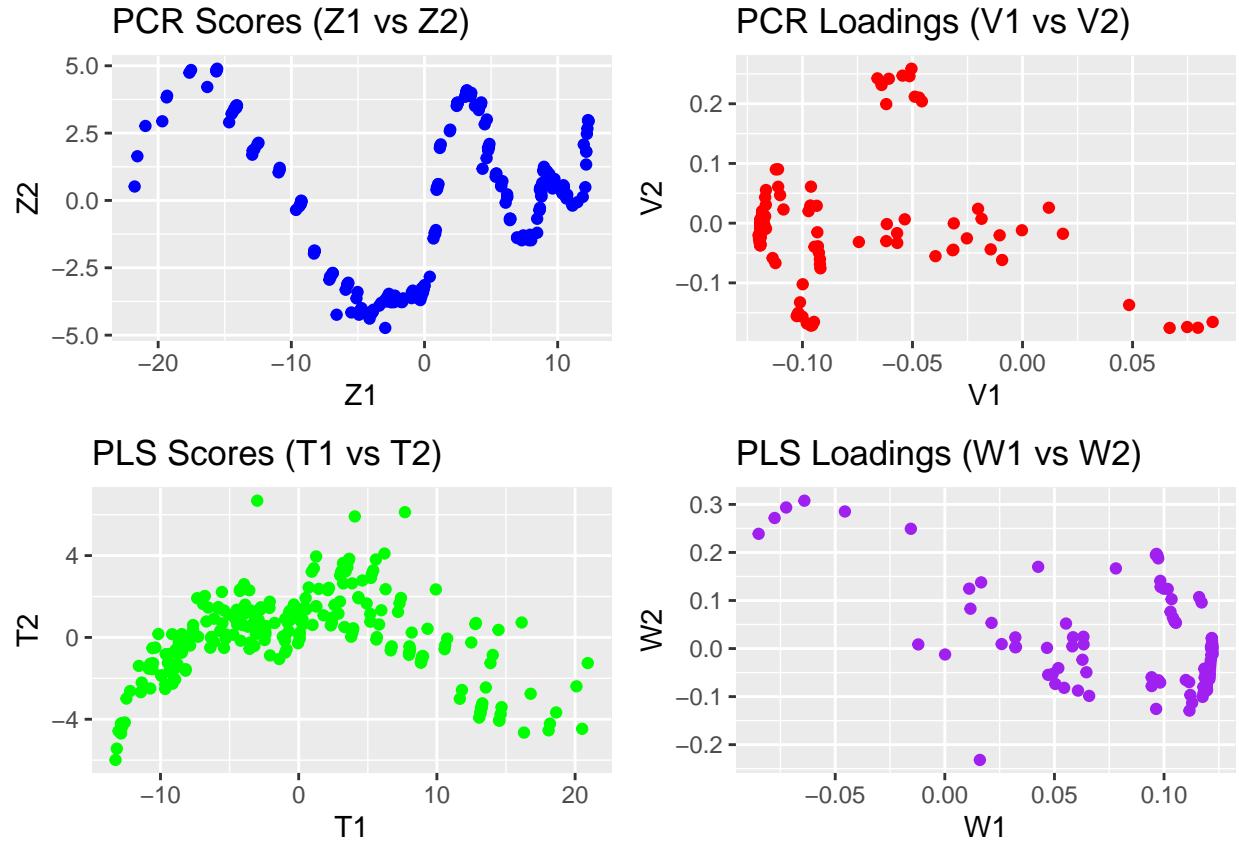
# Plot PCR loadings
p2 <- ggplot(pcr_loadings_df, aes(x = `Comp 1`, y = `Comp 2`)) + geom_point(color = "red") +
  labs(title = "PCR Loadings (V1 vs V2)", x = "V1", y = "V2")

# Plot PLS scores
p3 <- ggplot(pls_scores_df, aes(x = `Comp 1`, y = `Comp 2`)) + geom_point(color = "green") +
  labs(title = "PLS Scores (T1 vs T2)", x = "T1", y = "T2")

# Plot PLS loadings
p4 <- ggplot(pls_loadings_df, aes(x = `Comp 1`, y = `Comp 2`)) + geom_point(color = "purple") +
  labs(title = "PLS Loadings (W1 vs W2)", x = "W1", y = "W2")

# Arrange the plots in a 2x2 grid
grid.arrange(p1, p2, p3, p4, ncol = 2)

```



- PCR Scores (Z1 vs Z2):** The plot of the first two principal component scores (Z1 and Z2) shows a clear pattern, indicating that the first two components capture a meaningful structure in the data. There seems to be a trend within the points, suggesting a relationship between the variables that these components represent.
- PCR Loadings (V1 vs V2):** This plot of the loadings (V1 and V2) shows how the original predictors contribute to the first two principal components. The spread of points here implies that certain variables are more heavily weighted on either V1 or V2, helping shape the data's primary directions.
- PLS Scores (T1 vs T2):** The PLS scores (T1 and T2) also show a pattern, with points spread across a curve. This indicates that PLS, like PCR, captures a trend in the data. However, PLS components focus on maximizing the correlation with the response variable, so these patterns are influenced by that goal.
- PLS Loadings (W1 vs W2):** The loadings for PLS (W1 vs W2) indicate how the original variables contribute to the first two PLS components. The distribution of points suggests some variables contribute more to these components, capturing relationships specifically targeted to predict the response.