Project 2: Linear Regression and Its Cousins

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Project 2 (Team) Assignment Prompt:

This is role playing. I am your new boss. I am in charge of production at ABC Beverage and you are a team of data scientists reporting to me. My leadership has told me that new regulations are requiring us to understand our manufacturing process, the predictive factors and be able to report to them our predictive model of PH.

Please use the historical data set I am providing. Build and report the factors in BOTH a technical and non-technical report. I like to use Word and Excel. Please provide your non-technical report in a business friendly readable document and your predictions in an Excel readable format. The technical report should show clearly the models you tested and how you selected your final approach.

Please submit both Rpubs links and .rmd files or other readable formats for technical and non-technical reports. Also submit the excel file showing the prediction of your models for pH.

```
library(tidyverse)
library(caret)
library(pls)
library(glmnet)
library(readxl)
library(corrplot)
library(RANN)
library(e1071)
```

Linear Regression Model

Our goal is to evaluate linear models to predict pH using the provided training data.

Explore and Preprocess

We'll explore and then pre-process the data. First, we must load the data files.

The "StudentData" file is our training data, and the "StudentEvaluation" file is our testing data.

If our data had not been provided in separate training and test files, we would subsequently perform a split of the 'main' data file into a training and a test set. In this case, since it's already been provided, we do not need to segment.

```
train_data <- read_excel("StudentData.xlsx")
test_data <- read_excel("StudentEvaluation.xlsx")
```

Since we'll be training our model on the training data, let's look at the first few rows of the data to see what we've got.

```
head(train_data)
```

```
# A tibble: 6 x 33
  `Brand Code` `Carb Volume` `Fill Ounces` `PC Volume` `Carb Pressure`
  <chr>                <dbl>         <dbl>       <dbl>           <dbl>
1 B                     5.34          24.0       0.263            68.2
2 A                     5.43          24.0       0.239            68.4
3 B                     5.29          24.1       0.263            70.8
4 A                     5.44          24.0       0.293            63
5 A                     5.49          24.3       0.111            67.2
6 A                     5.38          23.9       0.269            66.6
# i 28 more variables: `Carb Temp` <dbl>, PSC <dbl>, `PSC Fill` <dbl>,
#   `PSC CO2` <dbl>, `Mnf Flow` <dbl>, `Carb Pressure1` <dbl>,
#   `Fill Pressure` <dbl>, `Hyd Pressure1` <dbl>, `Hyd Pressure2` <dbl>,
#   `Hyd Pressure3` <dbl>, `Hyd Pressure4` <dbl>, `Filler Level` <dbl>,
#   `Filler Speed` <dbl>, Temperature <dbl>, `Usage cont` <dbl>,
#   `Carb Flow` <dbl>, Density <dbl>, MFR <dbl>, Balling <dbl>,
#   `Pressure Vacuum` <dbl>, PH <dbl>, `Oxygen Filler` <dbl>, ...
```

```
str(train_data)
```

```
tibble [2,571 x 33] (S3: tbl_df/tbl/data.frame)
 $ Brand Code       : chr [1:2571] "B" "A" "B" "A" ...
 $ Carb Volume      : num [1:2571] 5.34 5.43 5.29 5.44 5.49 ...
 $ Fill Ounces      : num [1:2571] 24 24 24.1 24 24.3 ...
 $ PC Volume        : num [1:2571] 0.263 0.239 0.263 0.293 0.111 ...
 $ Carb Pressure    : num [1:2571] 68.2 68.4 70.8 63 67.2 66.6 64.2 67.6 64.2 72 ...
 $ Carb Temp        : num [1:2571] 141 140 145 133 137 ...
 $ PSC              : num [1:2571] 0.104 0.124 0.09 NA 0.026 0.09 0.128 0.154 0.132 0.014 ...
 $ PSC Fill         : num [1:2571] 0.26 0.22 0.34 0.42 0.16 ...
 $ PSC CO2          : num [1:2571] 0.04 0.04 0.16 0.04 0.12 ...
 $ Mnf Flow         : num [1:2571] -100 -100 -100 -100 -100 -100 -100 -100 -100 -100 ...
 $ Carb Pressure1   : num [1:2571] 119 122 120 115 118 ...
 $ Fill Pressure    : num [1:2571] 46 46 46 46.4 45.8 45.6 51.8 46.8 46 45.2 ...
 $ Hyd Pressure1    : num [1:2571] 0 0 0 0 0 0 0 0 0 0 ...
 $ Hyd Pressure2    : num [1:2571] NA NA NA 0 0 0 0 0 0 0 ...
 $ Hyd Pressure3    : num [1:2571] NA NA NA 0 0 0 0 0 0 0 ...
 $ Hyd Pressure4    : num [1:2571] 118 106 82 92 92 116 124 132 90 108 ...
 $ Filler Level     : num [1:2571] 121 119 120 118 119 ...
 $ Filler Speed     : num [1:2571] 4002 3986 4020 4012 4010 ...
 $ Temperature      : num [1:2571] 66 67.6 67 65.6 65.6 66.2 65.8 65.2 65.4 66.6 ...
 $ Usage cont       : num [1:2571] 16.2 19.9 17.8 17.4 17.7 ...
 $ Carb Flow        : num [1:2571] 2932 3144 2914 3062 3054 ...
 $ Density          : num [1:2571] 0.88 0.92 1.58 1.54 1.54 1.52 0.84 0.84 0.9 0.9 ...
 $ MFR              : num [1:2571] 725 727 735 731 723 ...
 $ Balling          : num [1:2571] 1.4 1.5 3.14 3.04 3.04 ...
 $ Pressure Vacuum  : num [1:2571] -4 -4 -3.8 -4.4 -4.4 -4.4 -4.4 -4.4 -4.4 -4.4 ...
 $ PH               : num [1:2571] 8.36 8.26 8.94 8.24 8.26 8.32 8.4 8.38 8.38 8.5 ...
 $ Oxygen Filler    : num [1:2571] 0.022 0.026 0.024 0.03 0.03 0.024 0.066 0.046 0.064 0.022 ...
```

```
 $ Bowl Setpoint    : num [1:2571] 120 120 120 120 120 120 120 120 120 120 ...
 $ Pressure Setpoint: num [1:2571] 46.4 46.8 46.6 46 46 46 46 46 46 46 ...
 $ Air Pressurer    : num [1:2571] 143 143 142 146 146 ...
 $ Alch Rel         : num [1:2571] 6.58 6.56 7.66 7.14 7.14 7.16 6.54 6.52 6.52 6.54 ...
 $ Carb Rel         : num [1:2571] 5.32 5.3 5.84 5.42 5.44 5.44 5.38 5.34 5.34 5.34 ...
 $ Balling Lvl      : num [1:2571] 1.48 1.56 3.28 3.04 3.04 3.02 1.44 1.44 1.44 1.38 ...
```

We can see there are 33 columns in total and 2,571 rows in total. The 33 columns includes the "PH" column which is what we will be aiming to predict – PH will be the response variable in our linear regression exploration.

We can see that we have mostly numeric values. The only character or categorical (non-numeric) is the `Brand Code`. Based on information in our team's preferred guidance on predictive modeling, to deal with non-numeric values (a.k.a. categorical values, which Brand Code is the only one) the recommendation is to either convert into dummy variables or remove if not informative or the value has too many categories.

Since the label, "Brand Code" indicates a post-manufacturing process, and our aim for this inquiry is to focus on the manufacturing process, we will choose to remove is unnecessary column entirely. We understand "Brand Code" here to be a code, not a meaningful label, so with the aim of better predicting PH for Manufacturing process improvement, it will likely enhance our ability to perform predictive modeling when we remove it from our training and test sets.

We can also see there is an assortment of null values even just in the first few rows of data, across various columns. This gives us a sense that we will need to impute missing values. This is a preferable approach to our exploratory predictive work because it enables us to keep predictors.

We can also see that there are negative values which means we won't be able to apply the BoxCox method for processing our data. Our guidance and standards state that if the data includes negatives we should use the YeoJohnson method instead.

```
colSums(is.na(train_data))
```

```
       Brand Code       Carb Volume       Fill Ounces         PC Volume 
              120                10                38                39 
   Carb Pressure         Carb Temp               PSC          PSC Fill 
               27                26                33                23 
         PSC CO2          Mnf Flow    Carb Pressure1     Fill Pressure 
               39                 2                32                22 
   Hyd Pressure1     Hyd Pressure2     Hyd Pressure3     Hyd Pressure4 
               11                15                15                30 
    Filler Level      Filler Speed       Temperature        Usage cont 
               20                57                14                 5 
       Carb Flow           Density               MFR          Balling 
                2                 1               212                 1 
  Pressure Vacuum                PH     Oxygen Filler     Bowl Setpoint 
                0                 4                12                 2 
Pressure Setpoint     Air Pressurer          Alch Rel          Carb Rel 
               12                 0                 9                10 
     Balling Lvl 
                1 
```

This is more reason to exclude brand code – there are a over 100 null values *and* it's a categorical variable which appears to be irrelevant to our manufacturing process, which is the aim of our task at hand. This is another reason to exclude it in our model training and testing.

Once we build our training and test sets, we will continue exploration and pre-processing, including by dealing with our null values and looking at the relationships among predictors, among other steps.

We also notice there are 4 missing values for PH, which will be problematic. Guidance to handle this scenario is to remove the rows where the PH is null from the training and test sets so that would include removing the rows in the predictor and response sets. We will explain more on this when we get to that step prior to training our model.

Prepare response and predictor sets

We'll prepare response and predictor sets (separating out the predictors and response variable – pH is our "response".) We'll also remove "Brand Code" from both the training and test sets.

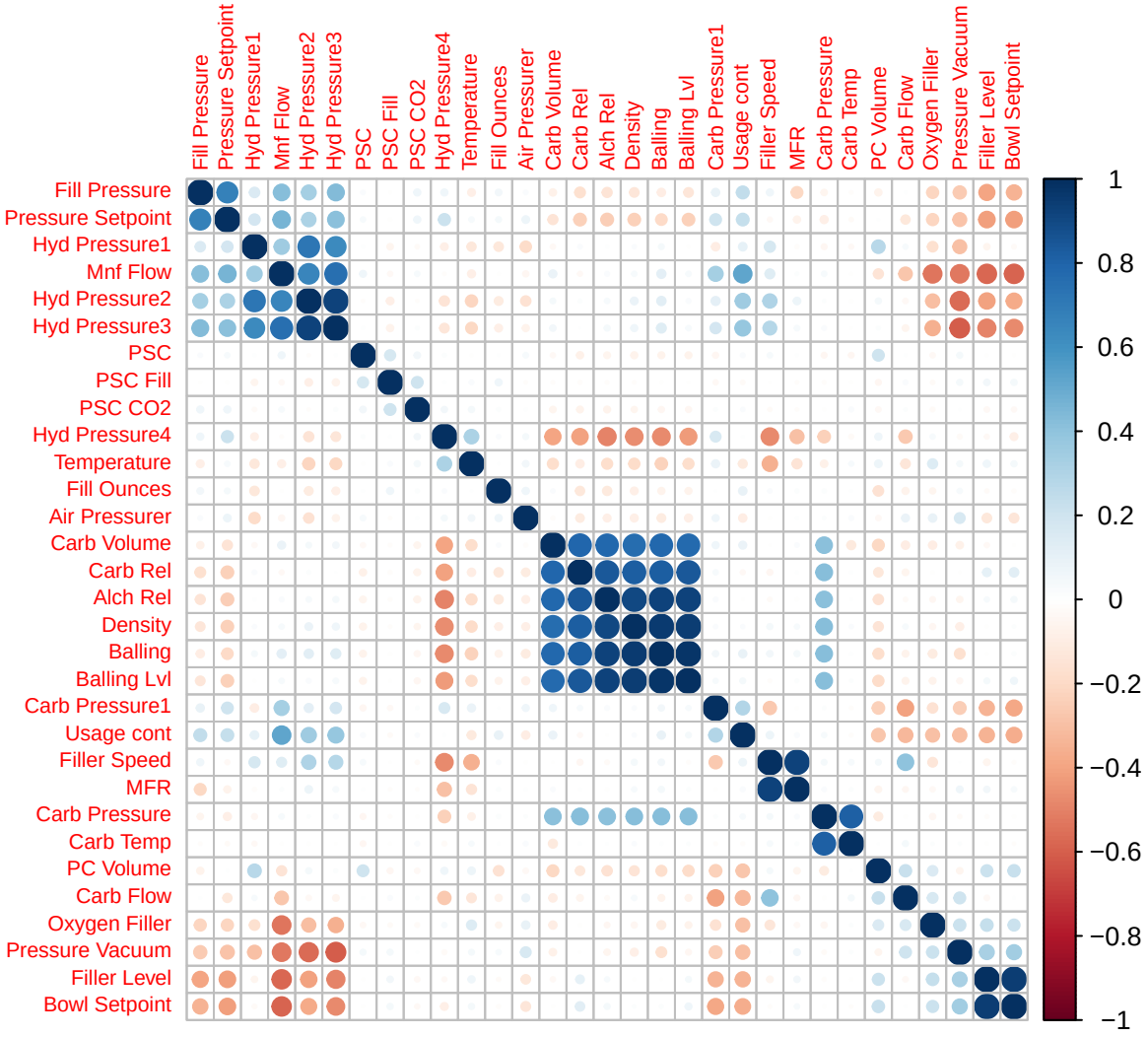
```
train_y <- train_data$PH
train_x <- train_data |> select(-PH, -"Brand Code")
```

```
test_y <- test_data$PH
test_x <- test_data |> select(-PH, -"Brand Code")
```

Correlation matrix

A correlation matrix is used to understand the relationships among predictor variables.

```
cor_matrix <- cor(train_x, use = "pairwise.complete.obs")
corrplot(cor_matrix, order = "hclust", tl.cex = 0.7)
```



We will choose to only remove extremely correlated predictors using a threshold of 0.95. While the "starting point" for removing highly collinear predictors is 0.75, this would be too aggressive in our situation. There are a few reasons for this, including that PLS (Partial Least Squares) handles collinearity well (it extracts components and is designed to deal with collinearity) and 0.95 is sufficient for traditional linear regression (OLS). As recommended by our preferred guidance source – the gold standard here – we will seek a less aggressive approach and instead retain more features.

```
high_corr <- findCorrelation(cor_matrix, cutoff = 0.95)
train_x <- train_x[, -high_corr]
test_x <- test_x[, -high_corr]
```

We removed only near-duplicate predictors with a correlation threshold of 0.95 to preserve interpretability for linear models while retaining useful variance for PLS.

Impute, transform, center and scale

To accommodate both traditional linear regression and PLS models, we will apply a preprocessing pipeline that includes transformations, centering, scaling, and imputation. Again based on our expert guidance from Applied Predictive Modeling, we will use the training set to fit preprocessing, and apply it to both training and test sets. We're setting the "seed" here to ensure reproducibility of results.

We will be imputing values using "knnImpute" to handle our NULL (missing) values; we will be using "YeoJohnson" for handling skewness and negative values (which we observed in our dataset – hence BoxCox method would not be appropriate), and we will center and scale the values, which is important for applied predictive modeling.

```
train_x <- as.data.frame(train_x)
test_x <- as.data.frame(test_x)
```

We coerced the entire dataset to a dataframe to ensure that our preprocessing steps will work.

However, before we move on we remember there are missing values in our outcome variable.

```
sum(is.na(train_y))
```

```
[1] 4
```

```
sum(is.na(test_y))
```

```
[1] 267
```

All 267 rows of the test set are missing values for PH because that is what we are trying to predict. This means that we can't remove all the corresponding predictor variables in the test set because that would literally remove all the values in our test set.

We'll remove rows from the training set where the outcome is missing. Modeling cannot proceed with missing values in the outcome.

```
complete_rows <- complete.cases(train_y)
train_y <- train_y[complete_rows]
train_x <- train_x[complete_rows, ]
```

To ensure that KNN imputation of missing values will work, we'll coerce the entire dataset to avoid hidden issues and then preprocess.

```
set.seed(5889)
preProc <- preProcess(train_x, method = c("knnImpute", "YeoJohnson", "center", "scale"))
train_x_proc <- predict(preProc, train_x)
test_x_proc <- predict(preProc, test_x)
```

These preprocessing steps are essential to ensure that both OLS and PLS models can operate effectively and fairly. Missing values were imputed using K-nearest neighbors (knnImpute), which leverages the similarity between observations to fill gaps in the data. Since our dataset includes both negative values and skewed distributions, we used the YeoJohnson transformation, which is suitable for normalizing such data (unlike BoxCox, which only works on positive values). Centering and scaling ensure that all predictors contribute equally to model training and are especially important for distance-based algorithms like PLS and KNN.

Now we are ready to train with linear regression using the processed data. This ensures fair comparison of model performance across the different algorithms.

Preprocessing continued

We'll now set up trainControl setup for model training.

```
ctrl <- trainControl(method = "repeatedcv", number = 10, repeats = 5)
```

Train Partial Least Squares (PLS) model

```
set.seed(5889)
pls_model <- train(
  x = train_x_proc,
  y = train_y,
  method = "pls",
  tuneLength = 20,
  trControl = ctrl
)
```

Train Ordinary Least Squares (OLS) Model

Ordinary Least Squares (OLS) is a benchmark linear modeling method. We've already preprocessed the data in a way which suits both PLS and OLS. We'll determine which of these two models is best among linear regression - to do that let's fit an OLS model.

```
set.seed(5889)
ols_model <- train(
  x = train_x_proc,
  y = train_y,
  method = "lm",
  trControl = ctrl
)
```

Since test_y is missing, we evaluate the different linear models using cross-validation results, since our test set doesn't contain any PH values.

OLS is interpretable and useful as a baseline. It assumes linear relationships and independence. It may not perform as well as more complex models if predictors are collinear or relationships are nonlinear.

Train Lasso Regression model

To further assess whether regularization improves performance, models like Lasso could be explored. These approaches can reduce overfitting and handle correlated predictors more effectively than OLS. In future work or production deployment, it would be advisable to test these variants and compare their performance using the same repeated cross-validation framework.

```
set.seed(5889)

lasso_model <- train(
  x = train_x_proc,
  y = train_y,
```

```
  method = "lasso",
  tuneLength = 20,
  trControl = ctrl,
  preProcess = NULL
)
```

Compare model performance via resampling

We combine cross-validation results and show summary statistics (RMSE, R-squared, MAE)

```
model_results <- resamples(list(PLS = pls_model, OLS = ols_model, Lasso = lasso_model))
summary(model_results)
```

```
Call:
summary.resamples(object = model_results)

Models: PLS, OLS, Lasso
Number of resamples: 50

MAE
            Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
PLS   0.09906755 0.1043541 0.1073073 0.1078058 0.1111548 0.1202731    0
OLS   0.09910651 0.1043522 0.1072920 0.1078006 0.1111750 0.1202642    0
Lasso 0.09906564 0.1042513 0.1073125 0.1078211 0.1111845 0.1200218    0

RMSE
           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
PLS   0.1295312 0.1346997 0.1397781 0.1395524 0.1428140 0.1554479    0
OLS   0.1295745 0.1347359 0.1397813 0.1395543 0.1428206 0.1554490    0
Lasso 0.1295466 0.1350859 0.1397972 0.1395239 0.1429452 0.1553670    0

Rsquared
           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
PLS   0.2602509 0.3233976 0.3462202 0.3472244 0.3756546 0.4318679    0
OLS   0.2605439 0.3232182 0.3463302 0.3472042 0.3758451 0.4311958    0
Lasso 0.2599246 0.3238391 0.3465396 0.3472994 0.3745320 0.4281998    0
```

Comparison of OLS, PLS, and Lasso

We evaluated three linear modeling approaches—Ordinary Least Squares (OLS), Partial Least Squares (PLS), and Lasso Regression—using repeated 10-fold cross-validation. The models were compared using three key performance metrics: RMSE (Root Mean Squared Error), R-squared, and MAE (Mean Absolute Error).

The results showed extremely small differences in average performance across the three models:

```
model_summary <- summary(model_results)$statistics

model_summary$RMSE[,"Mean"]
```

```
      PLS       OLS     Lasso
0.1395524 0.1395543 0.1395239
```

```
model_summary$Rsquared[,"Mean"]
```

```
      PLS       OLS     Lasso
0.3472244 0.3472042 0.3472994
```

```
model_summary$MAE[,"Mean"]
```

```
      PLS       OLS     Lasso
0.1078058 0.1078006 0.1078211
```

Key Takeaways:

Lasso Regression slightly outperformed both PLS and OLS on RMSE and R^2, making it the top performer in this comparison. Its use of L1 regularization likely helped by reducing variance and handling minor predictor redundancy.

PLS was the next-best performer. It achieved marginally better RMSE and R-squared than OLS, indicating that dimensionality reduction via latent components helped modestly, likely due to mild multicollinearity present in the predictor space.

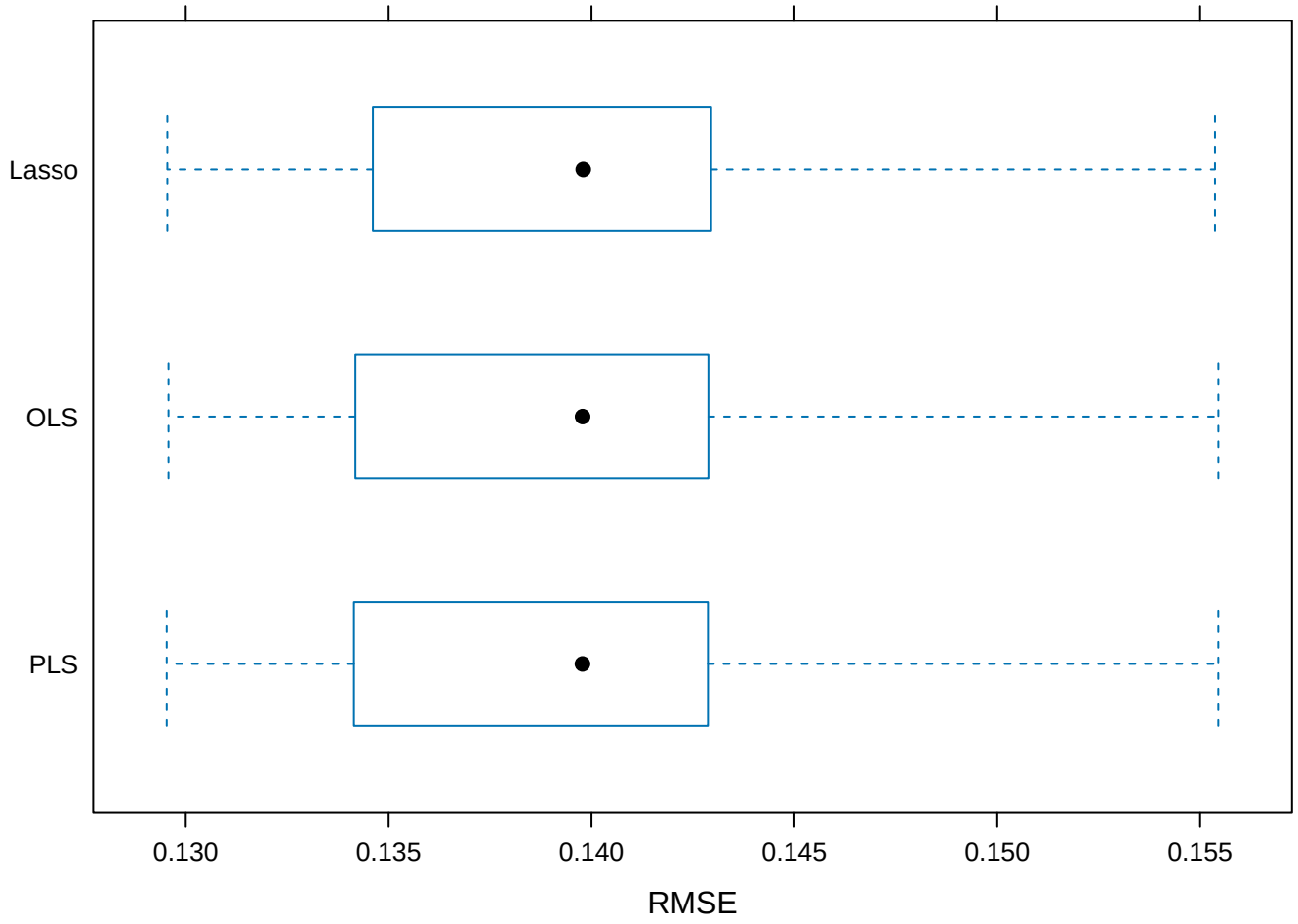
OLS was the weakest of the three, although its performance was still extremely close to the others—especially in terms of MAE.

These differences are numerically small and fall within overlapping confidence intervals, so none of the models is dramatically better. However, when forced to rank them:

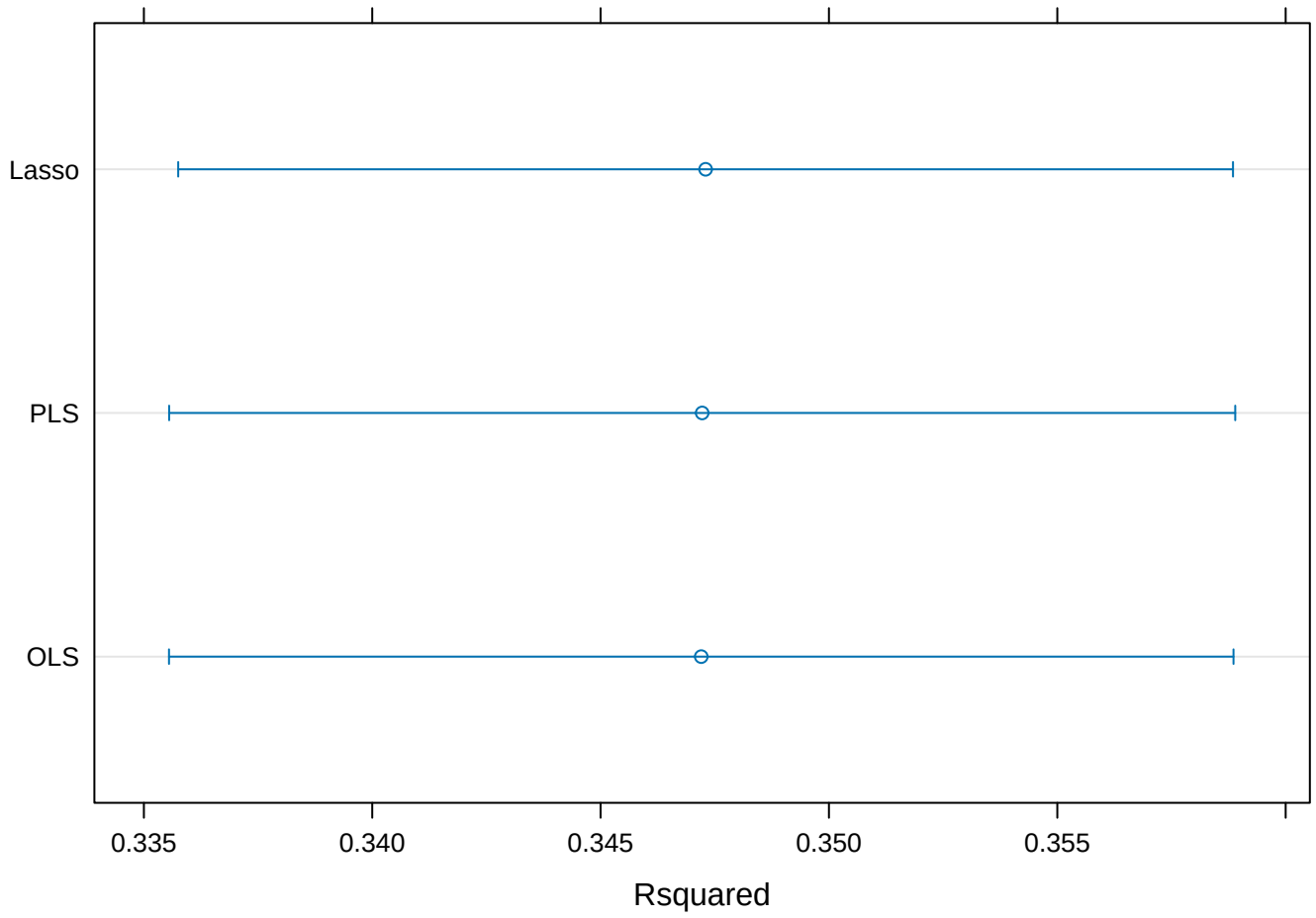
- Lasso is recommended as the best linear model for predicting pH
- PLS is a strong second-best, particularly valuable when predictors are correlated, since it builds new variables (called components) that summarize the most important patterns in the data
- OLS performed well, but slightly lagged behind the others in explaining variance and minimizing error

Visualize performance comparison

```
bwplot(model_results, metric = "RMSE")
```




```
dotplot(model_results, metric = "Rsquared")
```



This shows the models performed nearly the same.

To predict on each test set, for reference:

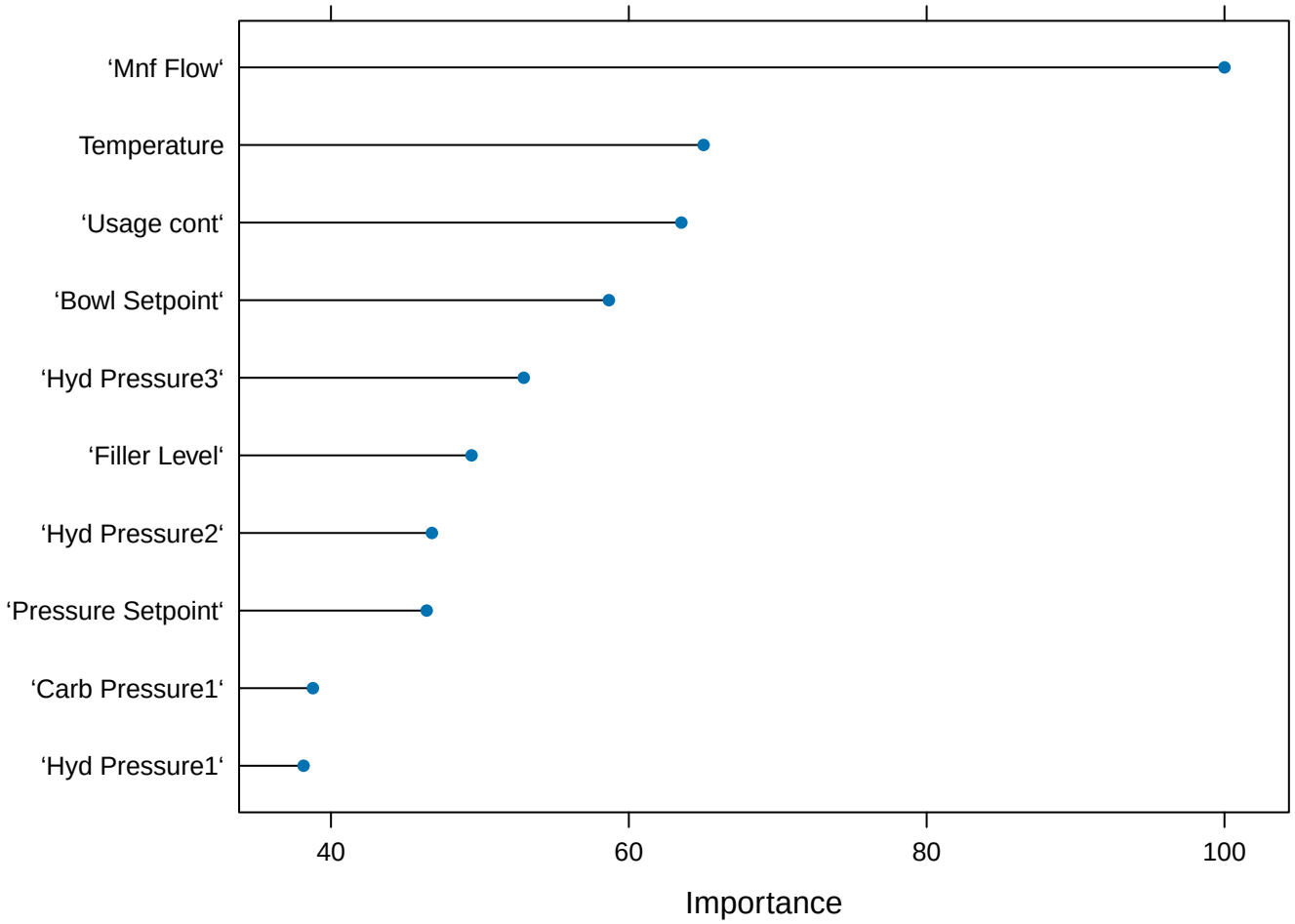
```
pls_pred <- predict(pls_model, newdata = test_x_proc)
ols_pred <- predict(ols_model, newdata = test_x_proc)
lasso_pred <- predict(lasso_model, newdata = test_x_proc)
```

To export predictions to CSV, for reference:

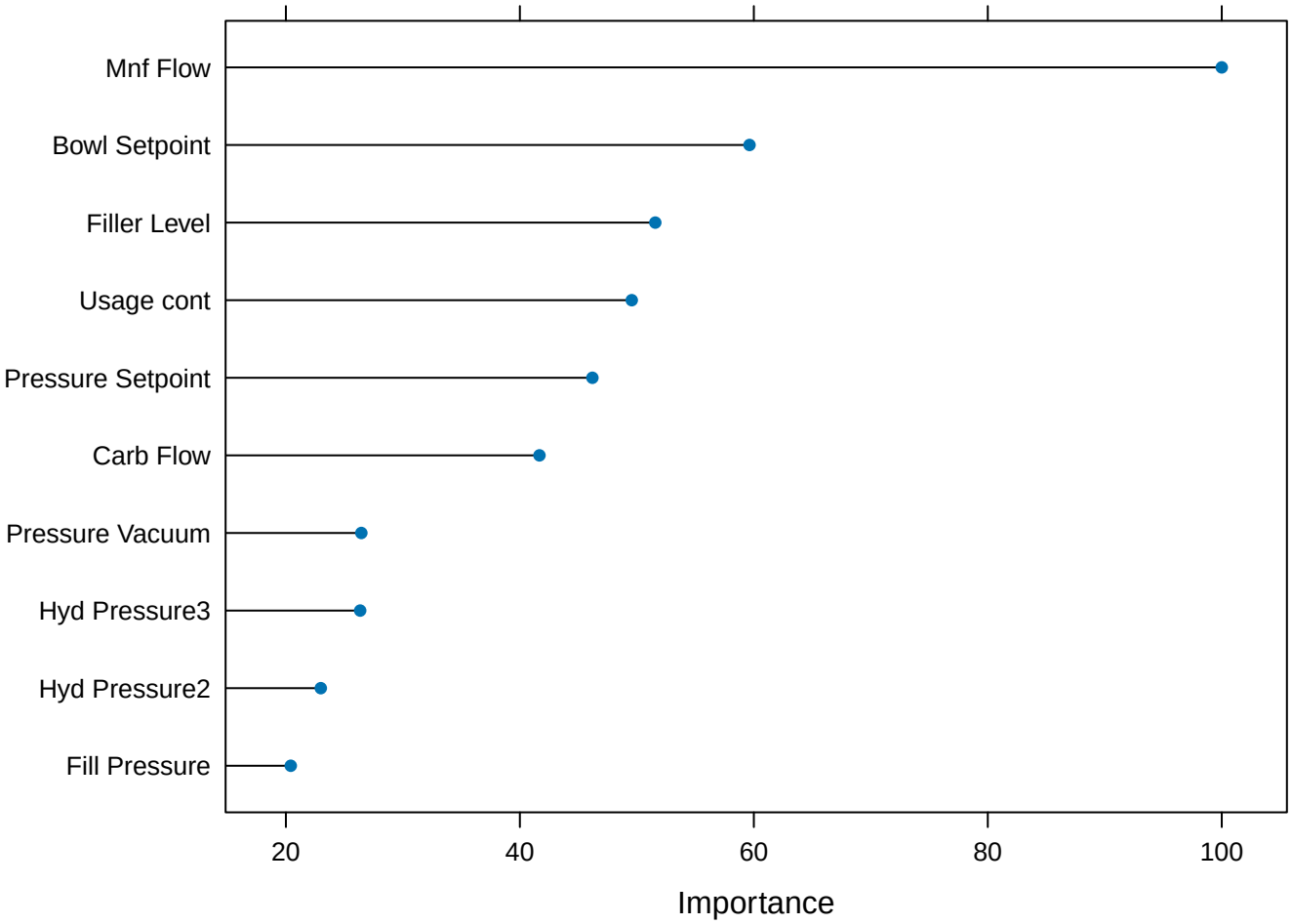
```
write.csv(data.frame(SampleID = 1:nrow(test_x_proc), Predicted_pH = pls_pred), "ph_predictions_pls.cs
write.csv(data.frame(SampleID = 1:nrow(test_x_proc), Predicted_pH = ols_pred), "ph_predictions_ols.cs
write.csv(data.frame(SampleID = 1:nrow(test_x_proc), Predicted_pH = lasso_pred), "ph_predictions_lass
```

Variable importance plot for PLS

```
vip <- varImp(pls_model)
plot(vip, top = 10)
```




```r
vip2 <- varImp(lasso_model)
plot(vip2, top = 10)
```


Mnf Flow
Bowl Setpoint
Filler Level
Usage cont
Pressure Setpoint
Carb Flow
Pressure Vacuum
Hyd Pressure3
Hyd Pressure2
Fill Pressure
20
40
60
80
100
Importance