

# DATA24 Project 2

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## Project 2 Description

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.

## Libraries

```
library(Amelia)
library(AppliedPredictiveModeling)
library(car)
library(caret)
#library(corrgram)
library(corrplot)
library(data.table)
#library(dlookr)
library(dplyr)
library(DT)
library(e1071)
library(forecast)
library(fpp2)
#library(ggcorrplot)
library(ggplot2)
library(glmnet)
#library(glmulti)
library(gridExtra)
#library(Hmisc)
library(kableExtra)
library(knitr)
library(lubridate)
library(MASS)
library(mice)
#library(plotly)
```

```
library(pROC)
#library(pscl)
library(psych)
library(RANN)
#library(RColorBrewer)
library(readxl)
library(reshape2)
library(stringr)
library(tidyverse)
library(tseries)
library(urca)
#library(xlsx)
```

## Reading datasets.

```
# setwd("/Users/elinaazrilyan/Downloads/")
Ins_train_data <- read.csv("./StudentData.csv", stringsAsFactors = FALSE)
Ins_eval_data <- read.csv("./StudentEvaluation.csv", stringsAsFactors = FALSE)
```

## Data Exploration of StudentData.csv.

Initially, we'll do a cursory exploration of the data. After that, we'll iteratively prepare and explore the data, wherever required.

```
dim1 <- dim(Ins_train_data)
print(paste0('Dimension of training set: ', 'Number of rows: ', dim1[1], ', ', 'Number of cols: ', dim1[2]))
```

```
## [1] "Dimension of training set:   Number of rows: 2571, Number of cols: 33"
```

```
print('Head of training data set:')
```

```
## [1] "Head of training data set:"
```

```
head(Ins_train_data)
```

```
##   Brand.Code Carb.Volume Fill.Ounces PC.Volume Carb.Pressure Carb.Temp   PSC
## 1          B    5.340000    23.96667 0.2633333          68.2    141.2 0.104
## 2          A    5.426667    24.00667 0.2386667          68.4    139.6 0.124
## 3          B    5.286667    24.06000 0.2633333          70.8    144.8 0.090
## 4          A    5.440000    24.00667 0.2933333          63.0    132.6   NA
## 5          A    5.486667    24.31333 0.1113333          67.2    136.8 0.026
## 6          A    5.380000    23.92667 0.2693333          66.6    138.4 0.090
##   PSC.Fill PSC.CO2 Mnf.Flow Carb.Pressure1 Fill.Pressure Hyd.Pressure1
## 1      0.26    0.04    -100          118.8          46.0           0
## 2      0.22    0.04    -100          121.6          46.0           0
## 3      0.34    0.16    -100          120.2          46.0           0
## 4      0.42    0.04    -100          115.2          46.4           0
## 5      0.16    0.12    -100          118.4          45.8           0
## 6      0.24    0.04    -100          119.6          45.6           0
##   Hyd.Pressure2 Hyd.Pressure3 Hyd.Pressure4 Filler.Level Filler.Speed
## 1             NA             NA           118        121.2        4002
## 2             NA             NA           106        118.6        3986
## 3             NA             NA            82        120.0        4020
## 4              0              0            92        117.8        4012
## 5              0              0            92        118.6        4010
## 6              0              0           116        120.2        4014
##   Temperature Usage.cont Carb.Flow Density   MFR Balling Pressure.Vacuum   PH
## 1         66.0      16.18     2932    0.88 725.0    1.398         -4.0 8.36
## 2         67.6      19.90     3144    0.92 726.8    1.498         -4.0 8.26
## 3         67.0      17.76     2914    1.58 735.0    3.142         -3.8 8.94
## 4         65.6      17.42     3062    1.54 730.6    3.042         -4.4 8.24
## 5         65.6      17.68     3054    1.54 722.8    3.042         -4.4 8.26
## 6         66.2      23.82     2948    1.52 738.8    2.992         -4.4 8.32
##   Oxygen.Filler Bowl.Setpoint Pressure.Setpoint Air.Pressurer Alch.Rel Carb.Rel
## 1          0.022          120          46.4          142.6        6.58        5.32
## 2          0.026          120          46.8          143.0        6.56        5.30
## 3          0.024          120          46.6          142.0        7.66        5.84
## 4          0.030          120          46.0          146.2        7.14        5.42
## 5          0.030          120          46.0          146.2        7.14        5.44
## 6          0.024          120          46.0          146.6        7.16        5.44
##   Balling.Lvl
```

## 1	1.48
## 2	1.56
## 3	3.28
## 4	3.04
## 5	3.04
## 6	3.02

```
print('Structure of training data set:')
```

```
## [1] "Structure of training data set:"
```

```
str(Ins_train_data)
```

```
## 'data.frame':    2571 obs. of  33 variables:
## $ Brand.Code      : chr  "B" "A" "B" "A" ...
## $ Carb.Volume     : num  5.34 5.43 5.29 5.44 5.49 ...
## $ Fill.Ounces     : num  24 24 24.1 24 24.3 ...
## $ PC.Volume       : num  0.263 0.239 0.263 0.293 0.111 ...
## $ Carb.Pressure   : num  68.2 68.4 70.8 63 67.2 66.6 64.2 67.6 64.2 72 ...
## $ Carb.Temp       : num  141 140 145 133 137 ...
## $ PSC             : num  0.104 0.124 0.09 NA 0.026 0.09 0.128 0.154 0.132 0.014 ...
## $ PSC.Fill       : num  0.26 0.22 0.34 0.42 0.16 0.24 0.4 0.34 0.12 0.24 ...
## $ PSC.CO2        : num  0.04 0.04 0.16 0.04 0.12 0.04 0.04 0.04 0.14 0.06 ...
## $ Mnf.Flow       : num  -100 -100 -100 -100 -100 -100 -100 -100 -100 -100 ...
## $ Carb.Pressure1  : num  119 122 120 115 118 ...
## $ Fill.Pressure   : num  46 46 46 46.4 45.8 45.6 51.8 46.8 46 45.2 ...
## $ Hyd.Pressure1   : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure2   : num  NA NA NA 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure3   : num  NA NA NA 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure4   : int  118 106 82 92 92 116 124 132 90 108 ...
## $ Filler.Level    : num  121 119 120 118 119 ...
## $ Filler.Speed    : int  4002 3986 4020 4012 4010 4014 NA 1004 4014 4028 ...
## $ Temperature    : num  66 67.6 67 65.6 65.6 66.2 65.8 65.2 65.4 66.6 ...
## $ Usage.cont      : num  16.2 19.9 17.8 17.4 17.7 ...
## $ Carb.Flow       : int  2932 3144 2914 3062 3054 2948 30 684 2902 3038 ...
## $ Density         : num  0.88 0.92 1.58 1.54 1.54 1.52 0.84 0.84 0.9 0.9 ...
## $ MFR             : num  725 727 735 731 723 ...
## $ Balling         : num  1.4 1.5 3.14 3.04 3.04 ...
## $ Pressure.Vacuum : num  -4 -4 -3.8 -4.4 -4.4 -4.4 -4.4 -4.4 -4.4 -4.4 ...
## $ PH              : num  8.36 8.26 8.94 8.24 8.26 8.32 8.4 8.38 8.38 8.5 ...
## $ Oxygen.Filler   : num  0.022 0.026 0.024 0.03 0.03 0.024 0.066 0.046 0.064 0.022 ...
## $ Bowl.Setpoint   : int  120 120 120 120 120 120 120 120 120 120 ...
## $ Pressure.Setpoint: num  46.4 46.8 46.6 46 46 46 46 46 46 46 ...
## $ Air.Pressurer    : num  143 143 142 146 146 ...
## $ Alch.Rel        : num  6.58 6.56 7.66 7.14 7.14 7.16 6.54 6.52 6.52 6.54 ...
## $ Carb.Rel        : num  5.32 5.3 5.84 5.42 5.44 5.44 5.38 5.34 5.34 5.34 ...
## $ Balling.Lvl     : num  1.48 1.56 3.28 3.04 3.04 3.02 1.44 1.44 1.44 1.38 ...
```

There are few fields, which have missing values, which we'll investigate in greater details later.

## Data Preparation of StudentData.csv.

At this stage, we'll explore and prepare iteratively. Now, we'll check for NA. After that if required, we'll impute them. After that we'll show some boxplots of the numeric fields.

Checking for NA.

```
any(is.na(Ins_train_data))
```

```
## [1] TRUE
```

NA does exist. So, we'll impute with mice().

```
Ins_train_imputed <- mice(Ins_train_data, m = 1, method = "pmm", print = F) %>% mice::complete()
```

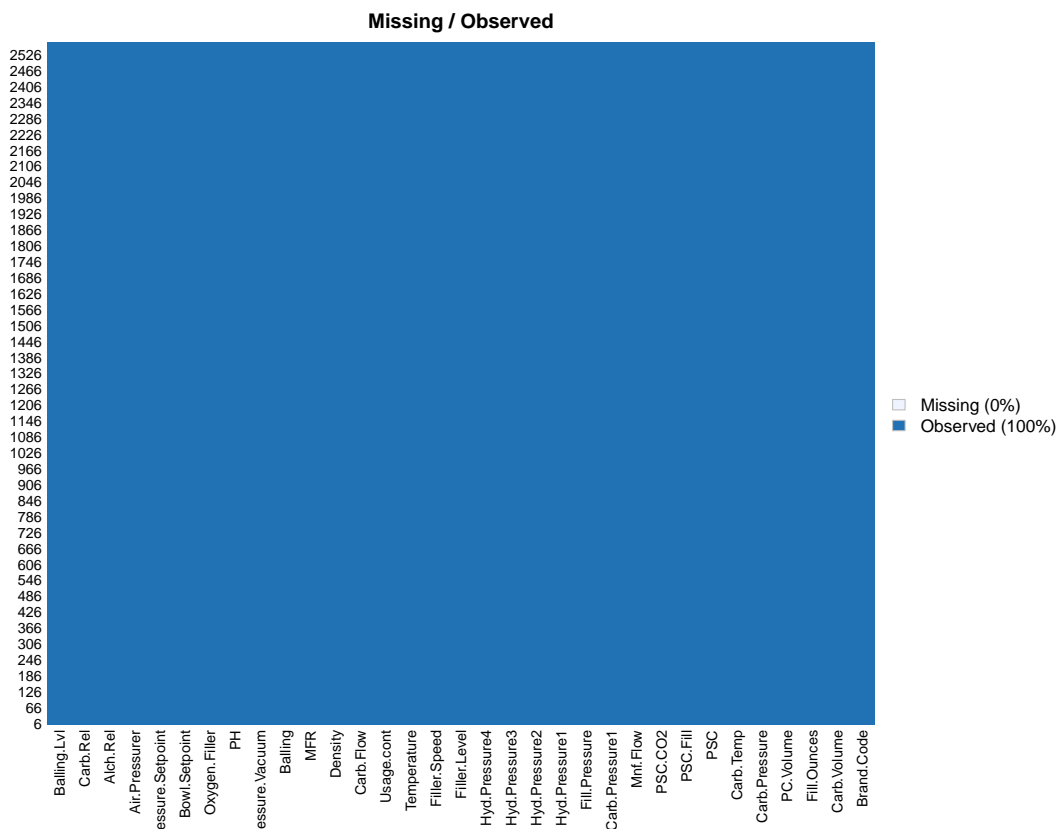
Rechecking for NA after imputation.

```
any(is.na(Ins_train_imputed))
```

```
## [1] FALSE
```

We observe that NA were removed. In the following, we'll visualize with missmap().

```
Ins_train_imputed %>% missmap(main = "Missing / Observed")
```



Both is.na() and missmap() confirm that NA were eliminated.

## More Data Exploration of StudentData.csv.

Here, we'll explore the data a little further. First, we'll take a quick look at min, 1st quartile, median, mean, 2nd quartile, max etc.

```
summary(Ins_train_imputed) # %>% kable
```

```
##   Brand.Code      Carb.Volume      Fill.Ounces      PC.Volume
## Length:2571      Min.      :5.040      Min.      :23.63      Min.      :0.07933
## Class :character  1st Qu.:5.293      1st Qu.:23.92      1st Qu.:0.23933
## Mode  :character  Median :5.347      Median :23.97      Median :0.27133
##                               Mean  :5.370      Mean  :23.97      Mean  :0.27758
##                               3rd Qu.:5.453      3rd Qu.:24.03      3rd Qu.:0.31267
##                               Max.   :5.700      Max.   :24.32      Max.   :0.47800
## Carb.Pressure      Carb.Temp      PSC      PSC.Fill
## Min.      :57.00      Min.      :128.6      Min.      :0.00200      Min.      :0.000
## 1st Qu.:65.60      1st Qu.:138.4      1st Qu.:0.04900      1st Qu.:0.100
## Median :68.20      Median :140.8      Median :0.07800      Median :0.180
## Mean      :68.21      Mean      :141.1      Mean      :0.08503      Mean      :0.196
## 3rd Qu.:70.60      3rd Qu.:143.8      3rd Qu.:0.11200      3rd Qu.:0.260
## Max.      :79.40      Max.      :154.0      Max.      :0.27000      Max.      :0.620
## PSC.CO2      Mnf.Flow      Carb.Pressure1      Fill.Pressure
## Min.      :0.00000      Min.      :-100.20      Min.      :105.6      Min.      :34.60
## 1st Qu.:0.02000      1st Qu.: -100.00      1st Qu.:119.0      1st Qu.:46.00
## Median :0.04000      Median :   64.80      Median :123.2      Median :46.40
## Mean      :0.05647      Mean      :  24.47      Mean      :122.6      Mean      :47.91
## 3rd Qu.:0.08000      3rd Qu.: 140.80      3rd Qu.:125.4      3rd Qu.:50.00
## Max.      :0.24000      Max.      : 229.40      Max.      :140.2      Max.      :60.40
## Hyd.Pressure1      Hyd.Pressure2      Hyd.Pressure3      Hyd.Pressure4
## Min.      : -0.8      Min.      : 0.00      Min.      : -1.20      Min.      : 52.00
## 1st Qu.: 0.0      1st Qu.: 0.00      1st Qu.: 0.00      1st Qu.: 86.00
## Median :11.4      Median :28.60      Median :27.60      Median : 96.00
## Mean      :12.5      Mean      :20.97      Mean      :20.46      Mean      : 96.55
## 3rd Qu.:20.4      3rd Qu.:34.60      3rd Qu.:33.30      3rd Qu.:102.00
## Max.      :58.0      Max.      :59.40      Max.      :50.00      Max.      :142.00
## Filler.Level      Filler.Speed      Temperature      Usage.cont      Carb.Flow
## Min.      : 55.8      Min.      : 998      Min.      :63.60      Min.      :12.08      Min.      : 26
## 1st Qu.: 98.3      1st Qu.:3819      1st Qu.:65.20      1st Qu.:18.36      1st Qu.:1151
## Median :118.4      Median :3980      Median :65.60      Median :21.78      Median :3028
## Mean      :109.2      Mean      :3636      Mean      :65.98      Mean      :20.99      Mean      :2469
## 3rd Qu.:120.0      3rd Qu.:3996      3rd Qu.:66.40      3rd Qu.:23.75      3rd Qu.:3187
## Max.      :161.2      Max.      :4030      Max.      :76.20      Max.      :25.90      Max.      :5104
## Density      MFR      Balling      Pressure.Vacuum
## Min.      :0.240      Min.      : 31.4      Min.      : -0.170      Min.      : -6.600
## 1st Qu.:0.900      1st Qu.:695.0      1st Qu.: 1.496      1st Qu.: -5.600
## Median :0.980      Median :721.4      Median : 1.648      Median : -5.400
## Mean      :1.173      Mean      :670.2      Mean      : 2.198      Mean      : -5.216
## 3rd Qu.:1.620      3rd Qu.:730.4      3rd Qu.: 3.292      3rd Qu.: -5.000
## Max.      :1.920      Max.      :868.6      Max.      : 4.012      Max.      : -3.600
## PH      Oxygen.Filler      Bowl.Setpoint      Pressure.Setpoint
## Min.      :7.880      Min.      :0.00240      Min.      : 70.0      Min.      :44.00
## 1st Qu.:8.440      1st Qu.:0.02200      1st Qu.:100.0      1st Qu.:46.00
## Median :8.540      Median :0.03340      Median :120.0      Median :46.00
```

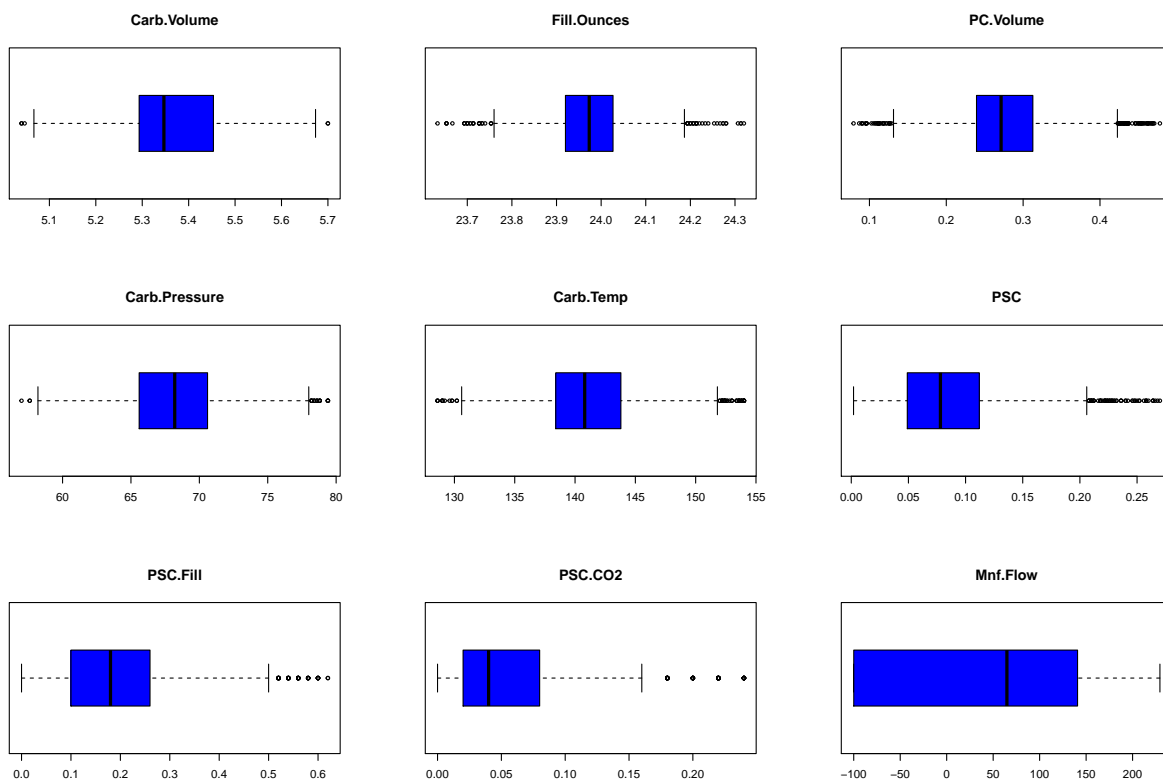
##	Mean	:8.546	Mean	:0.04713	Mean	:109.3	Mean	:47.61
##	3rd Qu.	:8.680	3rd Qu.	:0.06000	3rd Qu.	:120.0	3rd Qu.	:50.00
##	Max.	:9.360	Max.	:0.40000	Max.	:140.0	Max.	:52.00
##	Air.Pressurer		Alch.Rel		Carb.Rel		Balling.Lvl	
##	Min.	:140.8	Min.	:5.280	Min.	:4.960	Min.	:0.00
##	1st Qu.	:142.2	1st Qu.	:6.540	1st Qu.	:5.340	1st Qu.	:1.38
##	Median	:142.6	Median	:6.560	Median	:5.400	Median	:1.48
##	Mean	:142.8	Mean	:6.897	Mean	:5.436	Mean	:2.05
##	3rd Qu.	:143.0	3rd Qu.	:7.230	3rd Qu.	:5.540	3rd Qu.	:3.14
##	Max.	:148.2	Max.	:8.620	Max.	:6.060	Max.	:3.66

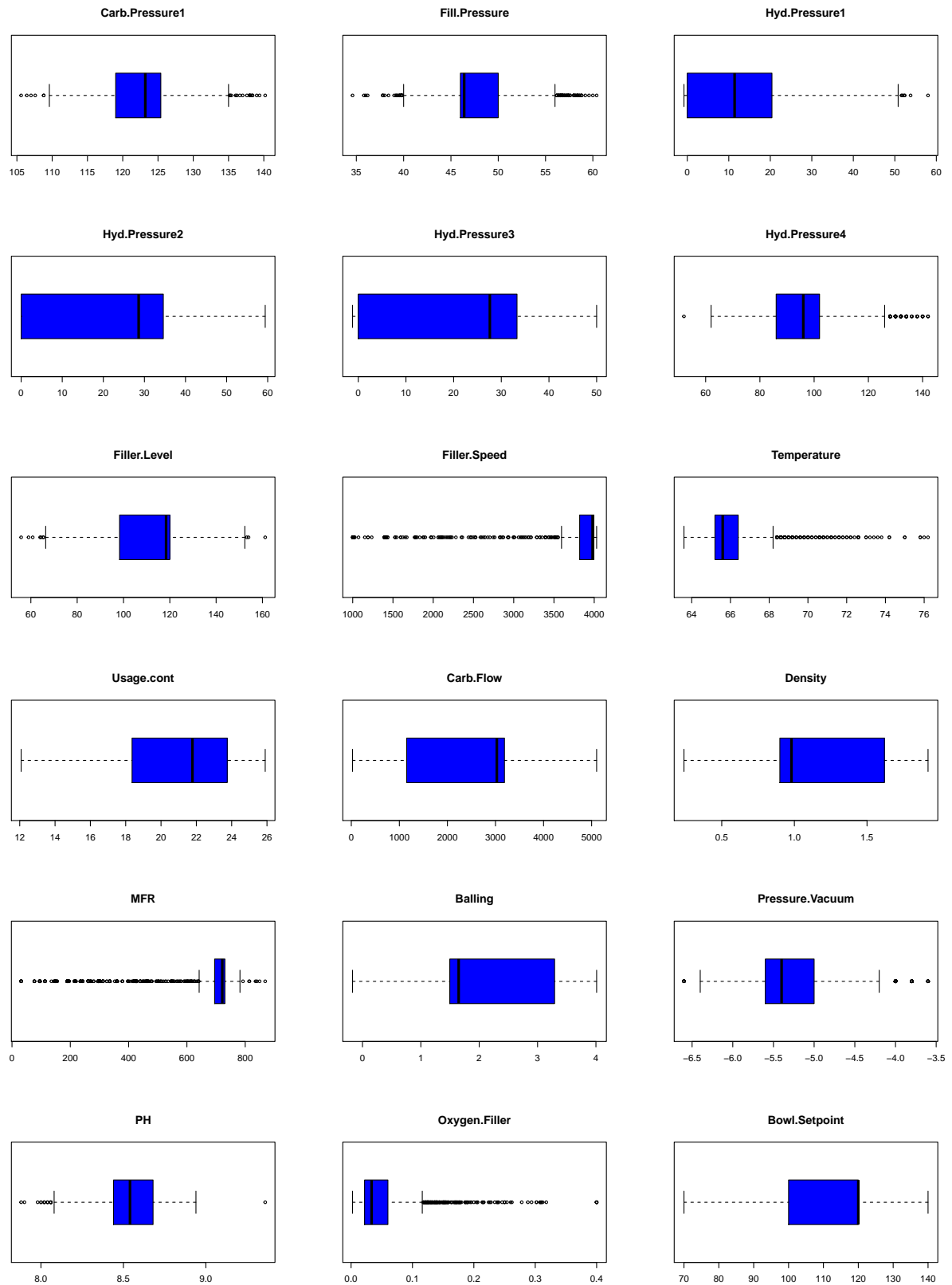


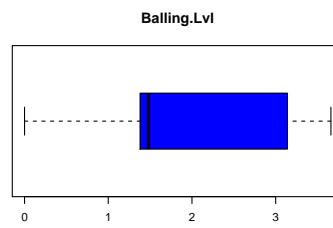
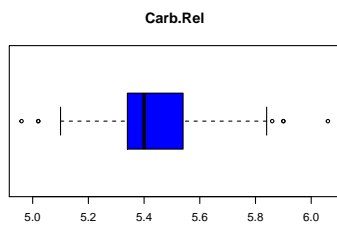
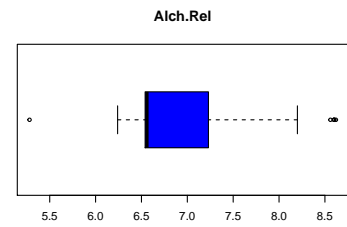
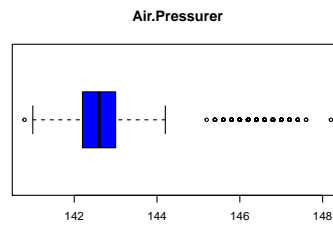
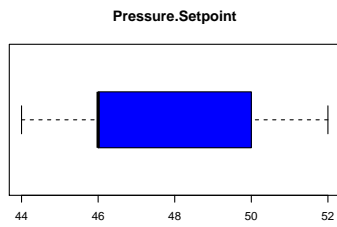
## Boxplots

First look at the boxplots.

```
par(mfrow = c(3, 3))
for(i in 2:33) {
  if (is.numeric(Ins_train_imputed[,i])) {
    boxplot(Ins_train_imputed[,i], main = names(Ins_train_imputed[i]), col = 4, horizontal = TRUE)
  }
}
```







The boxplots show that some of the variables have outliers in them. So, we'll cap them.

```

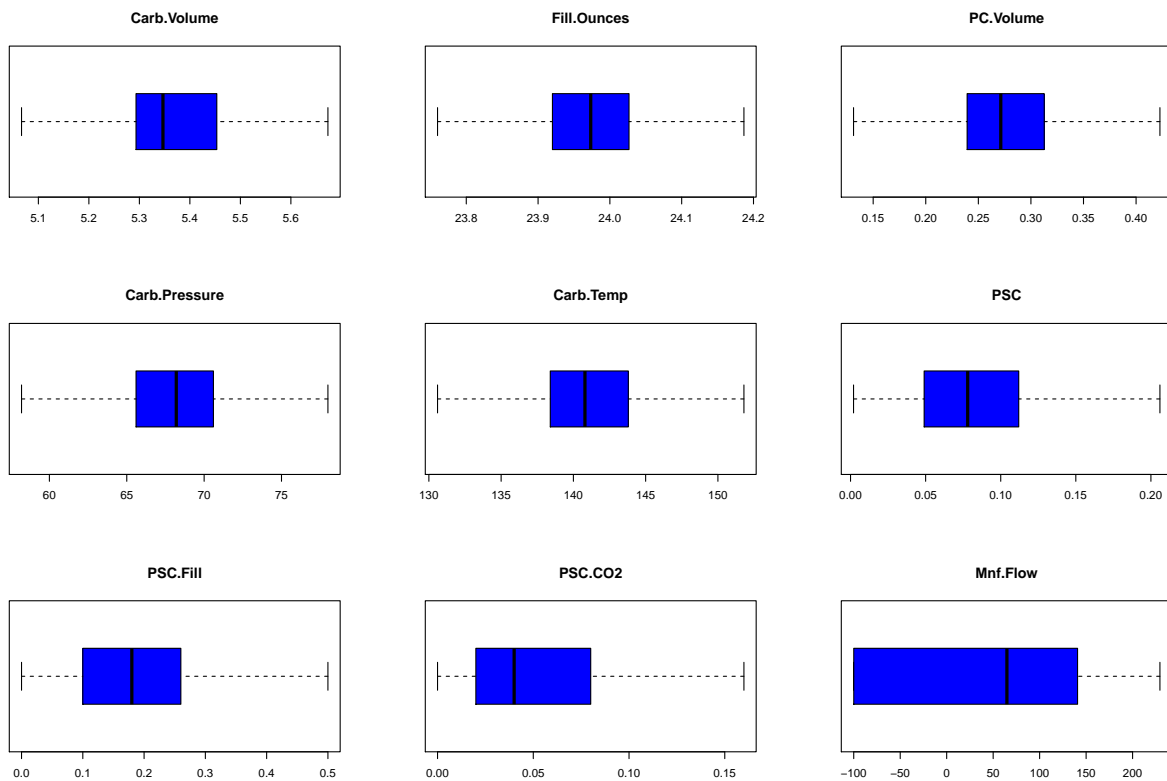
Ins_train_cap <- Ins_train_imputed

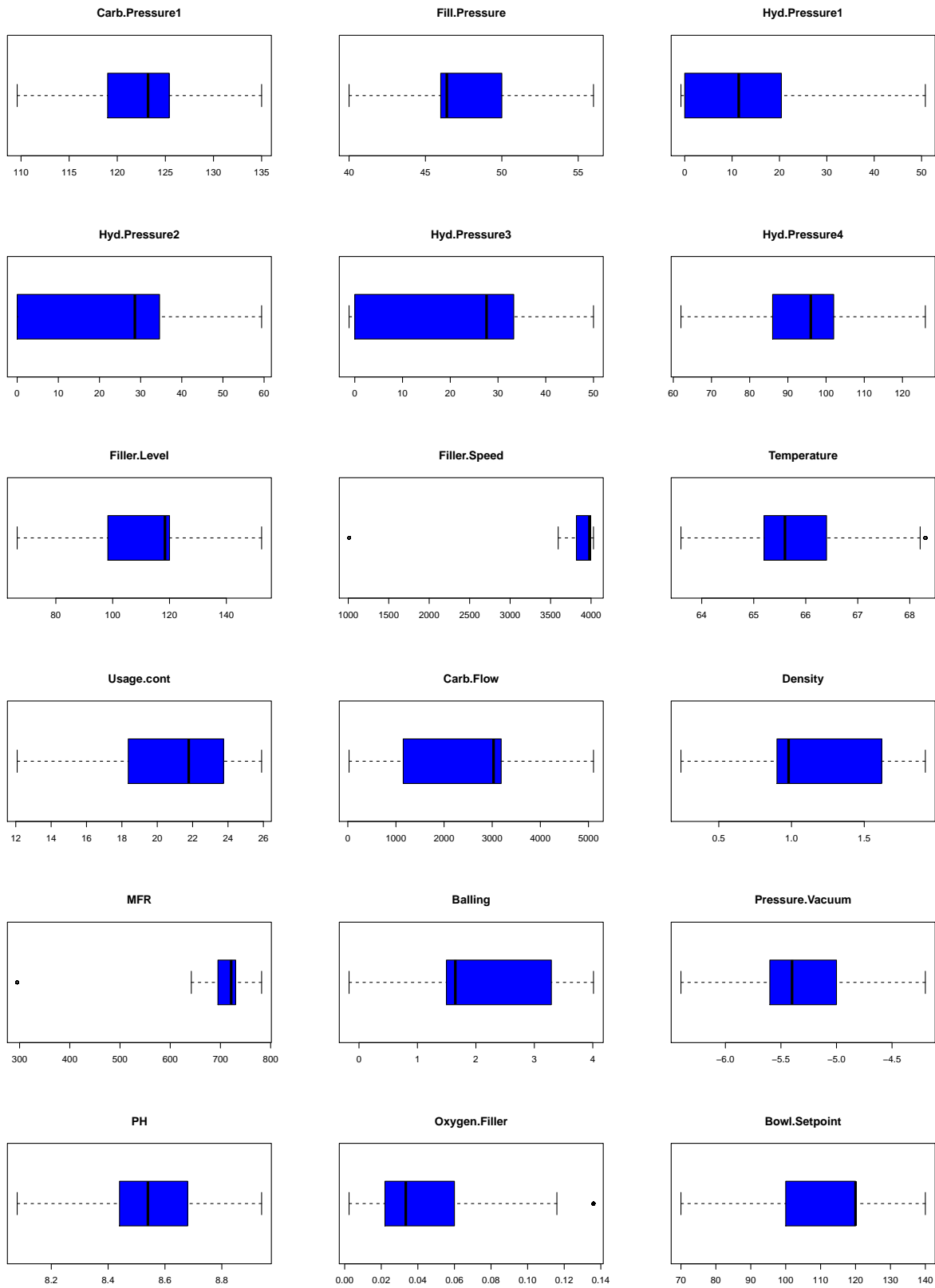
for (i in 2:33) {
  qnt1 <- quantile(Ins_train_cap[,i], probs = c(0.25, 0.75), na.rm = T)
  cap_amt <- quantile(Ins_train_cap[,i], probs = c(0.05, 0.95), na.rm = T)
  High <- 1.5 * IQR(Ins_train_cap[,i], na.rm = T)

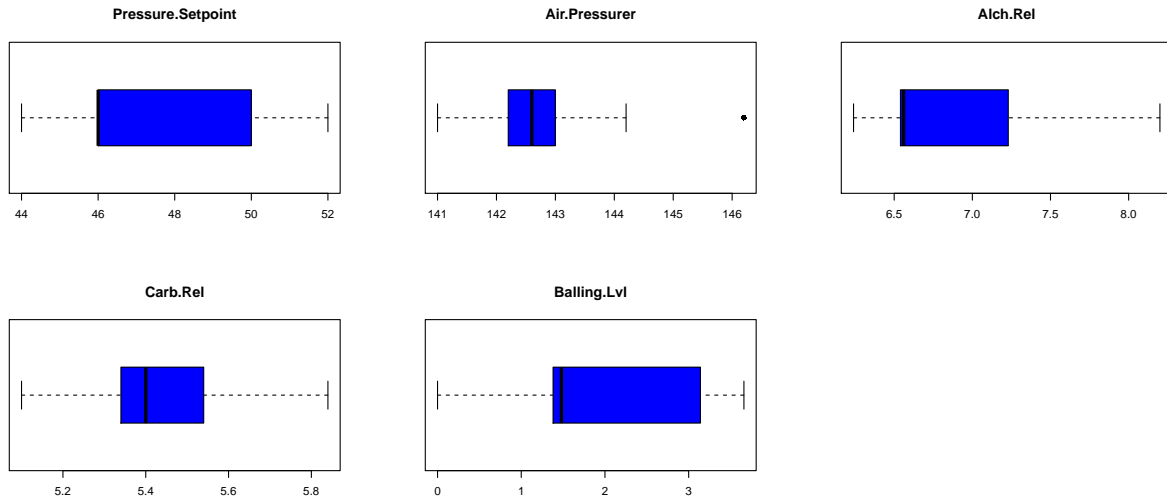
  Ins_train_cap[,i][Ins_train_cap[,i] < (qnt1[1] - High)] <- cap_amt[1]
  Ins_train_cap[,i][Ins_train_cap[,i] > (qnt1[2] + High)] <- cap_amt[2]
}

par(mfrow = c(3, 3))
for(i in 2:33) {
  if (is.numeric(Ins_train_cap[,i])) {
    boxplot(Ins_train_cap[,i], main = names(Ins_train_cap[i]), col = 4, horizontal = TRUE)
  }
}

```





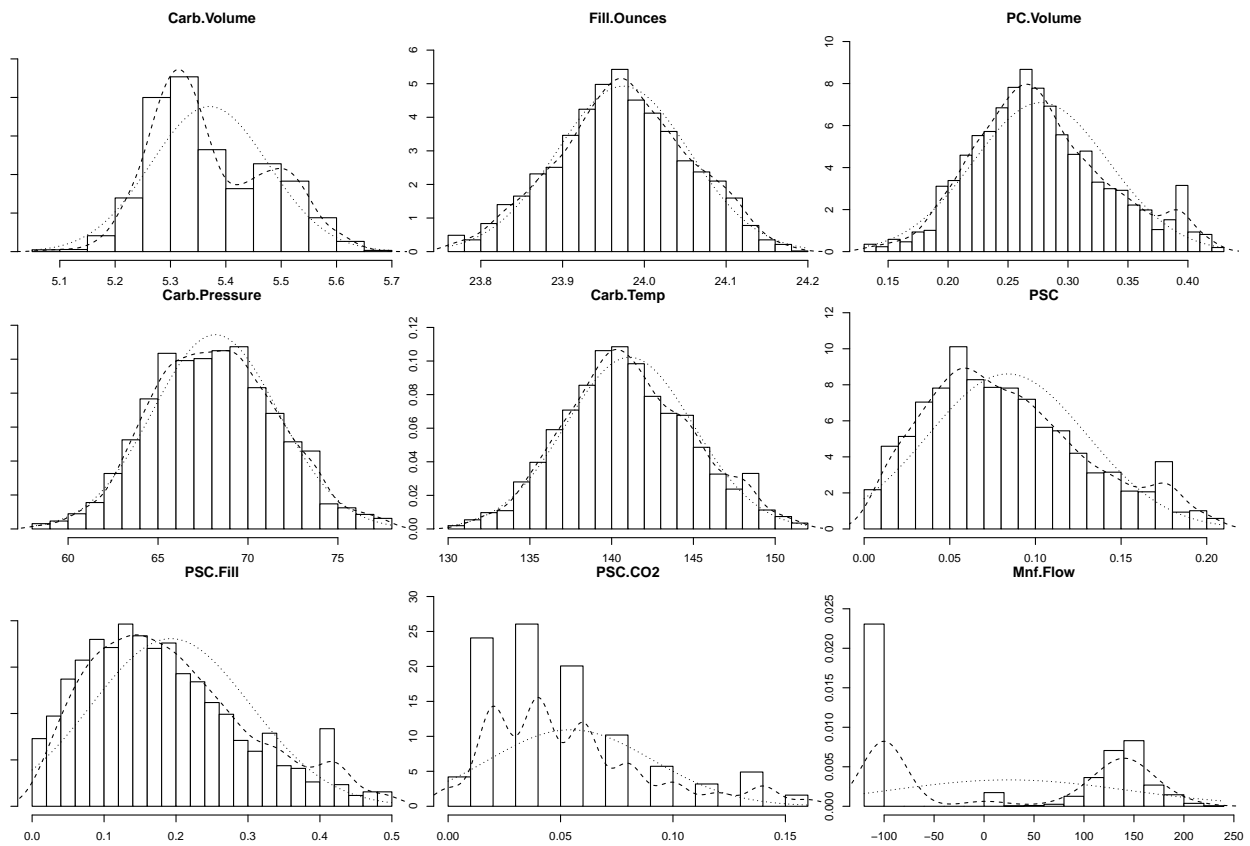


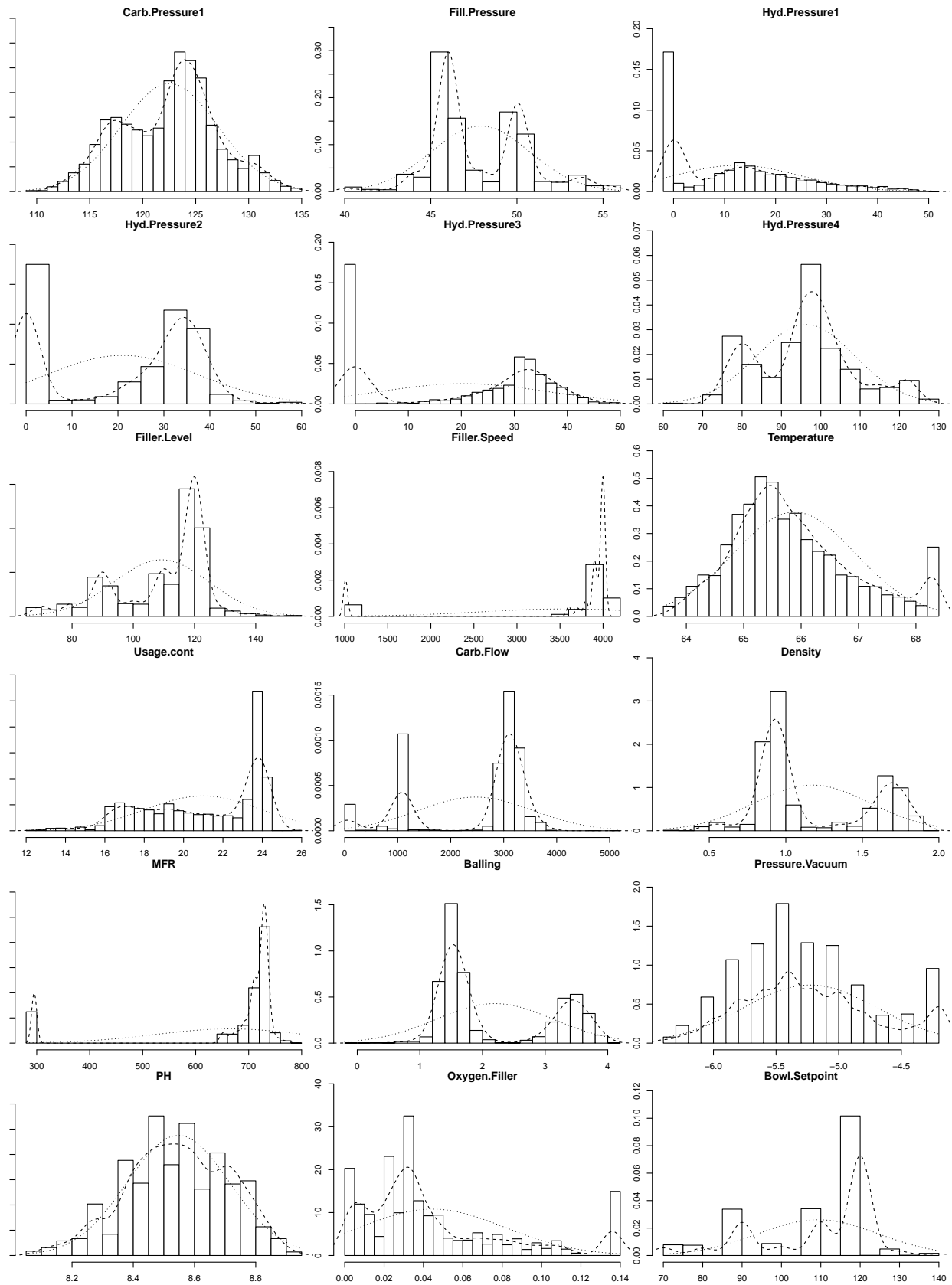
The outliers were capped and now we see that several fields PSC.FILL, PSC.C02, Mnf.Flow, Hyd.Pressure1, Hyd.Pressure2, Hyd.Pressure3, Usage.cont, Carb.Flow, Density, Balling, Oxygen.Filler, Bowl.Setpoint, Pressure.Setpoint, Alch.Rel, Balling.Lvl have high variance.

## Histograms

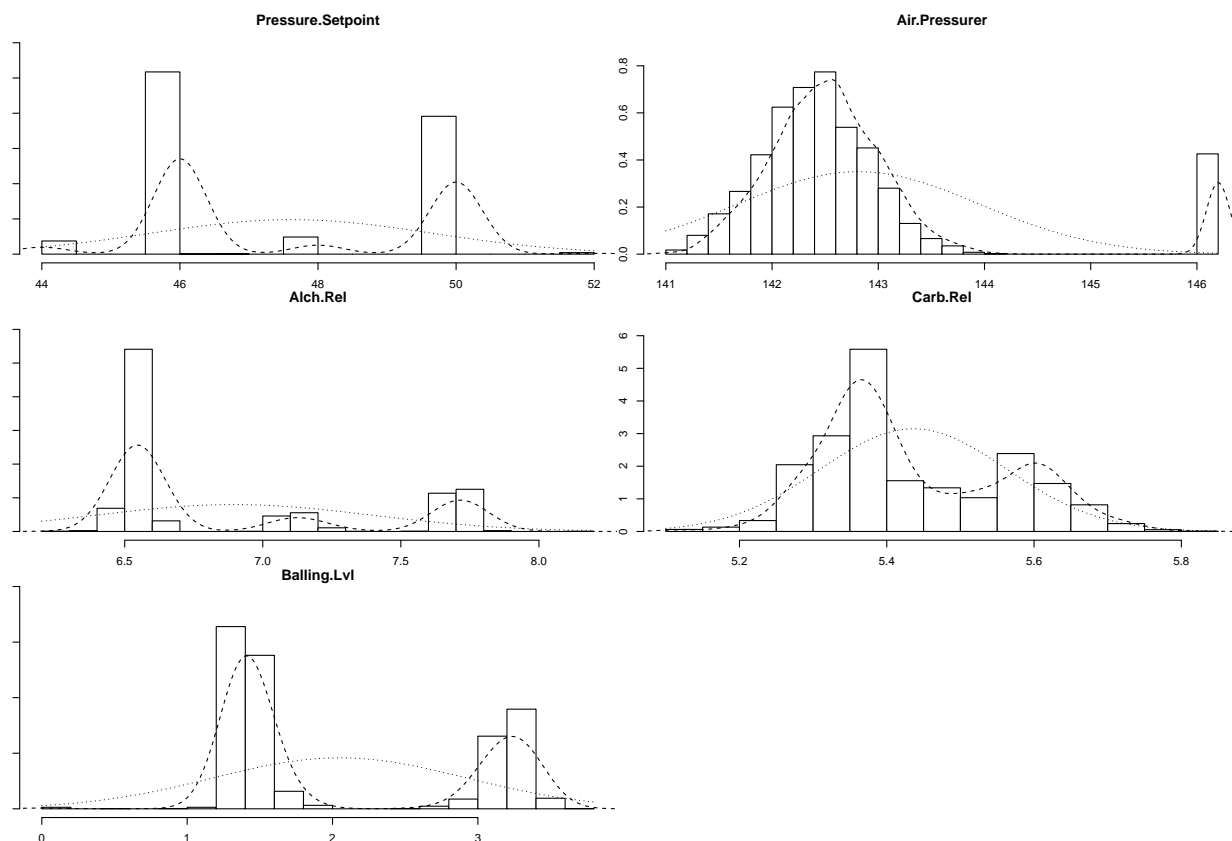
Histograms tell us how the data is distributed in the dataset (numeric fields).

```
for(i in seq(from = 2, to = length(Ins_train_cap), by = 9)) {  
  if(i <= 27) {  
    multi.hist(Ins_train_cap[i:(i + 8)])  
  } else {  
    multi.hist(Ins_train_cap[i:(i + 4)])  
  }  
}
```









Observing the above histograms, I decided the critical skewness, needing BoxCox transformation, to be 0.75 or higher. Based on this critical value, I am creating a vector `transform_cols`, which'll contain the column names of skewed columns.

The columns, whose skewness exceed the critical value of 0.75, are printed below.

```
transform_cols <- c()

for(i in seq(from = 2, to = length(Ins_train_cap), by = 1)) {
  if(abs(skewness(Ins_train_cap[, i])) >= 1) {
    transform_cols <- append(transform_cols, names(Ins_train_cap[i]))
    print(paste0(names(Ins_train_cap[i]), ": ", skewness(Ins_train_cap[, i])))
  }
}
```

```
## [1] "Filler.Speed: -2.19541624072288"
## [1] "MFR: -2.18086384109116"
## [1] "Oxygen.Filler: 1.18562238421133"
## [1] "Air.Pressurer: 2.07962689734424"
```

Many of these histograms are skewed. So, following the recommendations of “Applied Statistical Learning” (page 105, 2nd para), I’ll apply Box-Cox transformation to remove the skewness.

```
lambda <- NULL
data_imputed_2 <- Ins_train_cap

for (i in 1:length(transform_cols)) {
  lambda[transform_cols[i]] <- BoxCox.lambda(abs(Ins_train_cap[, transform_cols[i]]))

  data_imputed_2[c(transform_cols[i])] <- BoxCox(Ins_train_cap[transform_cols[i]], lambda[transform_cols[i]])
}
```

Now, we don’t need to observe the histograms all over again. It will suffice to see the skewness.

We observe that skewness of most or all of the columns reduced and some even reduced to less than 1.

```
for(i in seq(from = 2, to = length(data_imputed_2), by = 1)) {
  if(abs(skewness(data_imputed_2[, i])) >= 1) {
    print(paste0(names(data_imputed_2[i]), ": ", skewness(data_imputed_2[, i])))
  }
}
```

```
## [1] "Filler.Speed: -2.14118664976147"
## [1] "MFR: -2.10088378864193"
## [1] "Air.Pressurer: 2.04308315860091"
```

## Categorical variables

Now, we'll explore the Categorical variables.

```
cat('Brand.Code:')
```

```
## Brand.Code:
```

```
table(data_imputed_2$Brand.Code)
```

```
##  
##      A      B      C      D  
## 120  293 1239  304  615
```

Observation: In Brand.Code column, 120 rows are empty. So, we'll impute them with "X".

```
Ins_train_cap_imputed <- data_imputed_2 %>% mutate(Brand.Code = ifelse((Brand.Code == ""), "X", Brand.C  
cat("Brand.Code: ")
```

```
## Brand.Code:
```

```
table(Ins_train_cap_imputed$Brand.Code)
```

```
##  
##      A      B      C      D      X  
## 293 1239  304  615  120
```

## Correlations

At this point the data is prepared. So, we'll explore the top correlated variables.

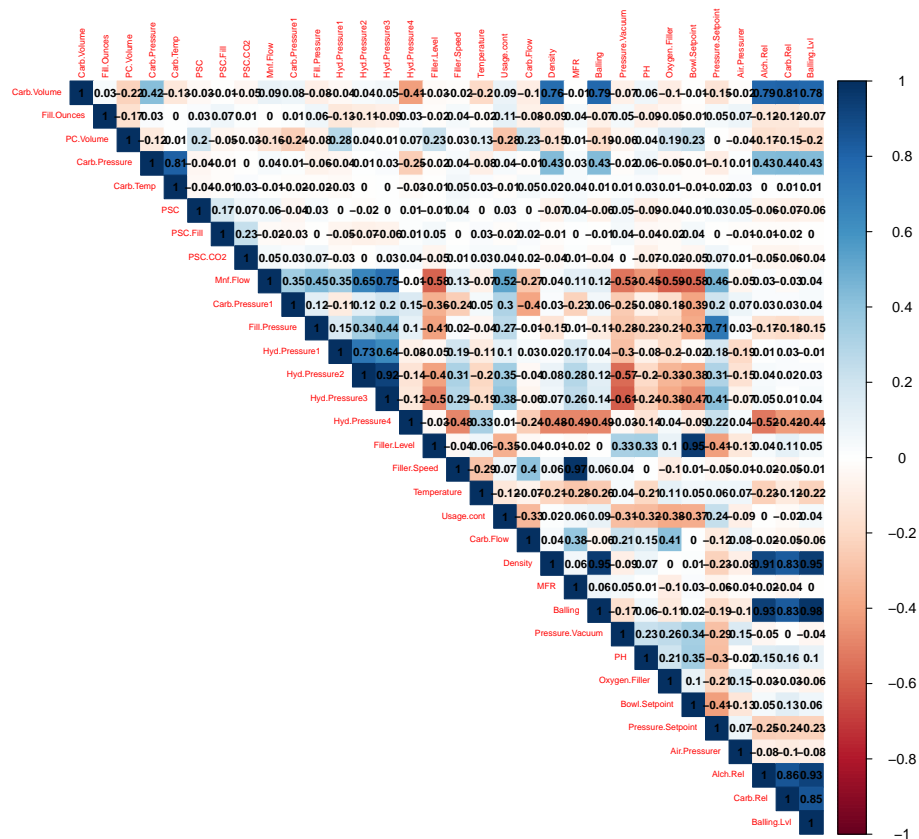
For the purpose of correlation, we'll remove the only non-numeric field Brand.Code, out of the correlation.

Now, we'll look at the correlation matrix of the variables.

```
Ins_train_corr <- Ins_train_cap_imputed[-1]

cor_mx = cor(Ins_train_corr, use = "pairwise.complete.obs", method = "pearson")

corrplot(cor_mx, method = "color", type = "upper", order = "original", number.cex = .7, addCoef.col = "t",
          tl.srt = 90, # Text label color and rotation
          diag = TRUE, # hide correlation coefficient on the principal diagonal
          tl.cex = 0.5)
```



At this point exploration, preparation and pair-wise correlations of **StudentData.csv** are done. So, I'll begin the same exercise for **StudentEvaluation.csv**.

## Data Exploration of StudentEvaluation.csv.

Initially, we'll do a cursory exploration of the data. After that, we'll iteratively prepare and explore the data, wherever required.

```
dim2 <- dim(Ins_eval_data)
print(paste0('Dimension of training set: ', 'Number of rows: ', dim2[1], ', ', 'Number of cols: ', dim2[2]))
```

```
## [1] "Dimension of training set:   Number of rows: 267, Number of cols: 33"
```

```
print('Head of training data set:')
```

```
## [1] "Head of training data set:"
```

```
head(Ins_eval_data)
```

```
##   Brand.Code Carb.Volume Fill.Ounces PC.Volume Carb.Pressure Carb.Temp   PSC
## 1          D    5.480000    24.03333 0.2700000         65.4    134.6 0.236
## 2          A    5.393333    23.95333 0.2266667         63.2    135.0 0.042
## 3          B    5.293333    23.92000 0.3033333         66.4    140.4 0.068
## 4          B    5.266667    23.94000 0.1860000         64.8    139.0 0.004
## 5          B    5.406667    24.20000 0.1600000         69.4    142.2 0.040
## 6          B    5.286667    24.10667 0.2120000         73.4    147.2 0.078
##   PSC.Fill PSC.CO2 Mnf.Flow Carb.Pressure1 Fill.Pressure Hyd.Pressure1
## 1    0.40    0.04   -100         116.6         46.0           0
## 2    0.22    0.08   -100         118.8         46.2           0
## 3    0.10    0.02   -100         120.2         45.8           0
## 4    0.20    0.02   -100         124.8         40.0           0
## 5    0.30    0.06   -100         115.0         51.4           0
## 6    0.22     NA   -100         118.6         46.4           0
##   Hyd.Pressure2 Hyd.Pressure3 Hyd.Pressure4 Filler.Level Filler.Speed
## 1           NA           NA           96      129.4      3986
## 2           0           0           112      120.0      4012
## 3           0           0           98      119.4      4010
## 4           0           0          132      120.2         NA
## 5           0           0           94      116.0      4018
## 6           0           0           94      120.4      4010
##   Temperature Usage.cont Carb.Flow Density   MFR Balling Pressure.Vacuum PH
## 1        66.0     21.66     2950    0.88 727.6    1.398        -3.8 NA
## 2        65.6     17.60     2916    1.50 735.8    2.942        -4.4 NA
## 3        65.6     24.18     3056    0.90 734.8    1.448        -4.2 NA
## 4        74.4     18.12        28    0.74   NA    1.056        -4.0 NA
## 5        66.4     21.32     3214    0.88 752.0    1.398        -4.0 NA
## 6        66.6     18.00     3064    0.84 732.0    1.298        -3.8 NA
##   Oxygen.Filler Bowl.Setpoint Pressure.Setpoint Air.Pressurer Alch.Rel Carb.Rel
## 1         0.022         130         45.2         142.6      6.56      5.34
## 2         0.030         120         46.0         147.2      7.14      5.58
## 3         0.046         120         46.0         146.6      6.52      5.34
## 4          NA         120         46.0         146.4      6.48      5.50
## 5         0.082         120         50.0         145.8      6.50      5.38
## 6         0.064         120         46.0         146.0      6.50      5.42
##   Balling.Lvl
```

## 1	1.48
## 2	3.04
## 3	1.46
## 4	1.48
## 5	1.46
## 6	1.44

```
print('Structure of training data set:')
```

```
## [1] "Structure of training data set:"
```

```
str(Ins_eval_data)
```

```
## 'data.frame':    267 obs. of  33 variables:
## $ Brand.Code      : chr  "D" "A" "B" "B" ...
## $ Carb.Volume     : num  5.48 5.39 5.29 5.27 5.41 ...
## $ Fill.Ounces     : num  24 24 23.9 23.9 24.2 ...
## $ PC.Volume       : num  0.27 0.227 0.303 0.186 0.16 ...
## $ Carb.Pressure   : num  65.4 63.2 66.4 64.8 69.4 73.4 65.2 67.4 66.8 72.6 ...
## $ Carb.Temp       : num  135 135 140 139 142 ...
## $ PSC             : num  0.236 0.042 0.068 0.004 0.04 0.078 0.088 0.076 0.246 0.146 ...
## $ PSC.Fill       : num  0.4 0.22 0.1 0.2 0.3 0.22 0.14 0.1 0.48 0.1 ...
## $ PSC.CO2        : num  0.04 0.08 0.02 0.02 0.06 NA 0 0.04 0.04 0.02 ...
## $ Mnf.Flow        : num  -100 -100 -100 -100 -100 -100 -100 -100 -100 -100 ...
## $ Carb.Pressure1  : num  117 119 120 125 115 ...
## $ Fill.Pressure   : num  46 46.2 45.8 40 51.4 46.4 46.2 40 43.8 40.8 ...
## $ Hyd.Pressure1   : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure2   : num  NA 0 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure3   : num  NA 0 0 0 0 0 0 0 0 ...
## $ Hyd.Pressure4   : int   96 112 98 132 94 94 108 108 110 106 ...
## $ Filler.Level    : num  129 120 119 120 116 ...
## $ Filler.Speed    : int   3986 4012 4010 NA 4018 4010 4010 NA 4010 1006 ...
## $ Temperature     : num  66 65.6 65.6 74.4 66.4 66.6 66.8 NA 65.8 66 ...
## $ Usage.cont      : num  21.7 17.6 24.2 18.1 21.3 ...
## $ Carb.Flow       : int   2950 2916 3056 28 3214 3064 3042 1972 2502 28 ...
## $ Density         : num  0.88 1.5 0.9 0.74 0.88 0.84 1.48 1.6 1.52 1.48 ...
## $ MFR             : num  728 736 735 NA 752 ...
## $ Balling         : num  1.4 2.94 1.45 1.06 1.4 ...
## $ Pressure.Vacuum : num  -3.8 -4.4 -4.2 -4 -4 -3.8 -4.2 -4.4 -4.4 -4.2 ...
## $ PH              : logi  NA NA NA NA NA NA ...
## $ Oxygen.Filler   : num  0.022 0.03 0.046 NA 0.082 0.064 0.042 0.096 0.046 0.096 ...
## $ Bowl.Setpoint   : int   130 120 120 120 120 120 120 120 120 120 ...
## $ Pressure.Setpoint: num  45.2 46 46 46 50 46 46 46 46 46 ...
## $ Air.Pressurer   : num  143 147 147 146 146 ...
## $ Alch.Rel        : num  6.56 7.14 6.52 6.48 6.5 6.5 7.18 7.16 7.14 7.78 ...
## $ Carb.Rel        : num  5.34 5.58 5.34 5.5 5.38 5.42 5.46 5.42 5.44 5.52 ...
## $ Balling.Lvl     : num  1.48 3.04 1.46 1.48 1.46 1.44 3.02 3 3.1 3.12 ...
```

There are few fields, which have missing values, which we'll investigate in greater details later.

## Data Preparation of StudentEvaluation.csv.

At this stage, we'll explore and prepare iteratively. Now, we'll check for NA. After that if required, we'll impute them.

After that we'll show some boxplots of the numeric fields.

Checking for NA.

```
any(is.na(Ins_eval_data))
```

```
## [1] TRUE
```

NA does exist. So, we'll impute with mice().

```
Ins_eval_imputed <- mice(Ins_eval_data, m = 1, method = "pmm", print = F) %>% mice::complete()
```

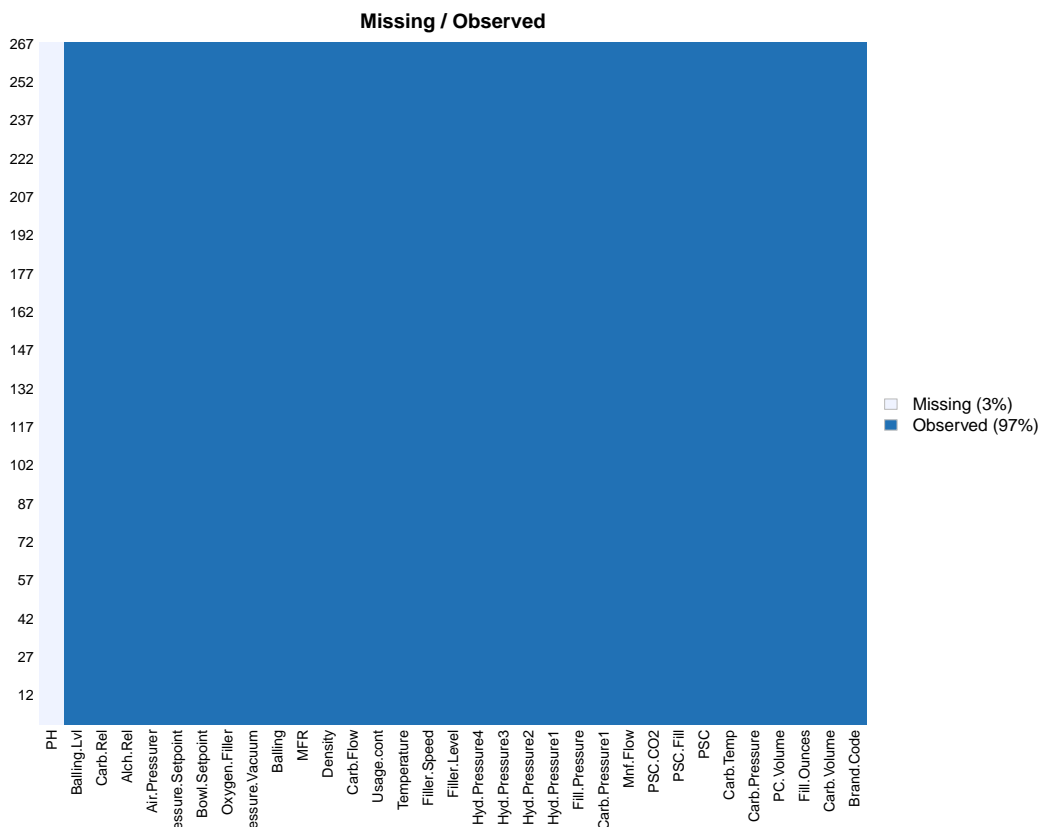
Rechecking for NA after imputation.

```
any(is.na(subset(Ins_eval_imputed, select = -c(PH))))
```

```
## [1] FALSE
```

We observe that NA were removed in all columns except TARGET\_FLAG and TARGET\_AMT, which is what we want. In the following, we'll visualize with missmap().

```
Ins_eval_imputed %>% missmap(main = "Missing / Observed")
```



Both is.na() and missmap() confirm that NA were eliminated.



## More Data exploration of StudentEvaluation.csv.

Now, we'll explore the data a little further. First, we'll take a quick look at min, 1st quartile, median, mean, 2nd quartile, max etc.

```
summary(Ins_eval_imputed) # %>% kable
```

```
##   Brand.Code      Carb.Volume      Fill.Ounces      PC.Volume
## Length:267      Min.      :5.147      Min.      :23.75      Min.      :0.09867
## Class :character 1st Qu.:5.283      1st Qu.:23.92      1st Qu.:0.23333
## Mode  :character Median :5.340      Median :23.97      Median :0.27600
##                               Mean  :5.368      Mean  :23.97      Mean  :0.27845
##                               3rd Qu.:5.463      3rd Qu.:24.01      3rd Qu.:0.32267
##                               Max.   :5.667      Max.   :24.20      Max.   :0.46400
## Carb.Pressure     Carb.Temp      PSC              PSC.Fill
## Min.      :60.20      Min.      :130.0      Min.      :0.00400      Min.      :0.0200
## 1st Qu.:65.30      1st Qu.:138.4      1st Qu.:0.04600      1st Qu.:0.1100
## Median :68.00      Median :140.8      Median :0.07600      Median :0.1800
## Mean  :68.25      Mean  :141.3      Mean  :0.08617      Mean  :0.1915
## 3rd Qu.:70.60      3rd Qu.:143.9      3rd Qu.:0.11200      3rd Qu.:0.2600
## Max.   :77.60      Max.   :154.0      Max.   :0.24600      Max.   :0.6200
## PSC.CO2           Mnf.Flow      Carb.Pressure1      Fill.Pressure
## Min.      :0.00000      Min.      :-100.20      Min.      :113.0      Min.      :37.80
## 1st Qu.:0.02000      1st Qu.: -100.00      1st Qu.:120.1      1st Qu.:46.00
## Median :0.04000      Median :    0.20      Median :123.4      Median :47.80
## Mean  :0.05086      Mean  :   21.03      Mean  :123.0      Mean  :48.14
## 3rd Qu.:0.06000      3rd Qu.: 141.30      3rd Qu.:125.5      3rd Qu.:50.20
## Max.   :0.24000      Max.   : 220.40      Max.   :136.0      Max.   :60.20
## Hyd.Pressure1      Hyd.Pressure2      Hyd.Pressure3      Hyd.Pressure4
## Min.      :-50.00      Min.      :-50.00      Min.      :-50.00      Min.      : 68.00
## 1st Qu.:  0.00      1st Qu.:  0.00      1st Qu.:  0.00      1st Qu.: 90.00
## Median : 10.40      Median : 26.80      Median : 27.60      Median : 98.00
## Mean  : 12.01      Mean  : 20.04      Mean  : 19.54      Mean  : 98.33
## 3rd Qu.: 20.40      3rd Qu.: 34.80      3rd Qu.: 33.00      3rd Qu.:104.00
## Max.   : 50.00      Max.   : 61.40      Max.   : 49.20      Max.   :140.00
## Filler.Level      Filler.Speed      Temperature      Usage.cont      Carb.Flow
## Min.      : 69.2      Min.      :1006      Min.      :63.80      Min.      :12.90      Min.      :  0
## 1st Qu.:100.6      1st Qu.:3795      1st Qu.:65.40      1st Qu.:18.10      1st Qu.:1083
## Median :118.6      Median :3918      Median :65.80      Median :21.40      Median :3038
## Mean  :110.3      Mean  :3507      Mean  :66.25      Mean  :20.88      Mean  :2409
## 3rd Qu.:120.2      3rd Qu.:3996      3rd Qu.:66.60      3rd Qu.:23.74      3rd Qu.:3215
## Max.   :153.2      Max.   :4020      Max.   :75.40      Max.   :24.60      Max.   :3858
## Density           MFR              Balling      Pressure.Vacuum
## Min.      :0.060      Min.      : 15.6      Min.      :0.902      Min.      : -6.400
## 1st Qu.:0.910      1st Qu.:688.1      1st Qu.:1.497      1st Qu.: -5.600
## Median :0.980      Median :720.4      Median :1.648      Median : -5.200
## Mean  :1.175      Mean  :652.1      Mean  :2.199      Mean  : -5.176
## 3rd Qu.:1.600      3rd Qu.:730.7      3rd Qu.:3.242      3rd Qu.: -4.800
## Max.   :1.840      Max.   :784.8      Max.   :3.788      Max.   : -3.600
## PH              Oxygen.Filler      Bowl.Setpoint      Pressure.Setpoint
## Mode:logical      Min.      :0.00240      Min.      : 70.0      Min.      :44.00
## NA's:267          1st Qu.:0.02070      1st Qu.:100.0      1st Qu.:46.00
##                               Median :0.03380      Median :120.0      Median :46.00
```

```
##           Mean    :0.04768   Mean    :109.6   Mean    :47.73
##           3rd Qu.:0.05630   3rd Qu.:120.0   3rd Qu.:50.00
##           Max.    :0.39800   Max.    :130.0   Max.    :52.00
## Air.Pressurer   Alch.Rel      Carb.Rel      Balling.Lvl
## Min.      :141.2   Min.      :6.400   Min.      :5.18   Min.      :0.000
## 1st Qu.   :142.2   1st Qu.   :6.540   1st Qu.   :5.34   1st Qu.   :1.380
## Median    :142.6   Median    :6.580   Median    :5.40   Median    :1.480
## Mean      :142.8   Mean      :6.903   Mean      :5.44   Mean      :2.051
## 3rd Qu.   :142.8   3rd Qu.   :7.180   3rd Qu.   :5.56   3rd Qu.   :3.080
## Max.      :147.2   Max.      :7.820   Max.      :5.74   Max.      :3.420
```

## Zeroing PH column

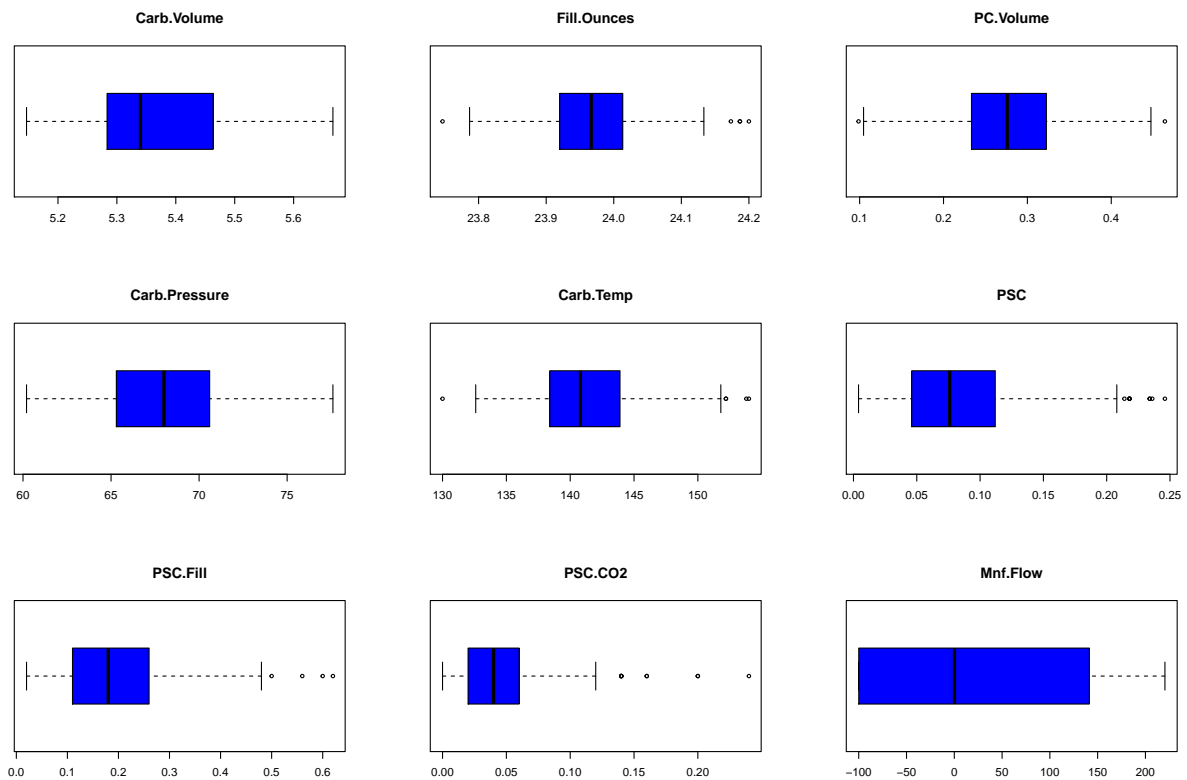
Currently, PH has NA. We'll insert zero into column PH, for convenience of analysis.

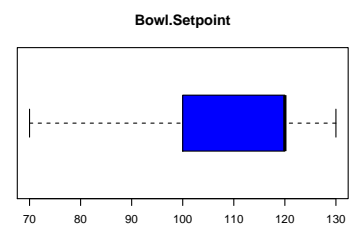
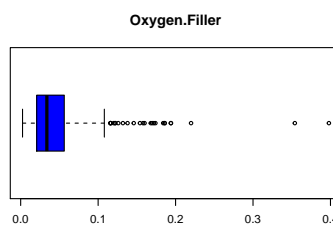
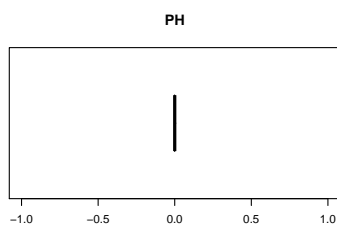
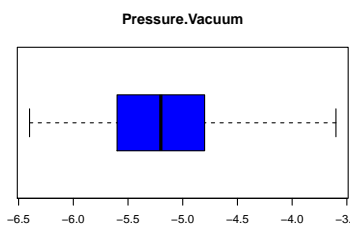
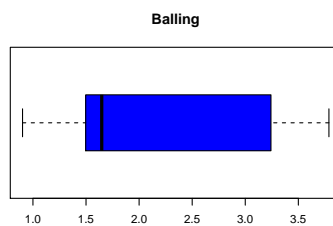
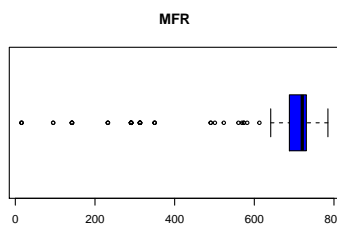
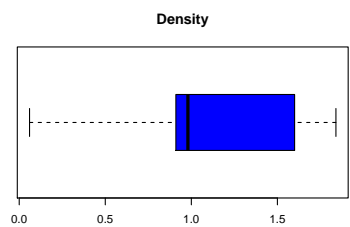
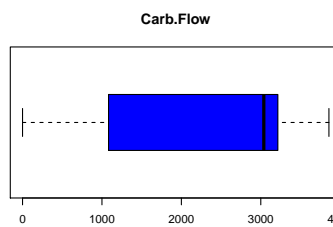
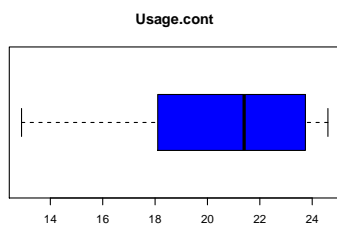
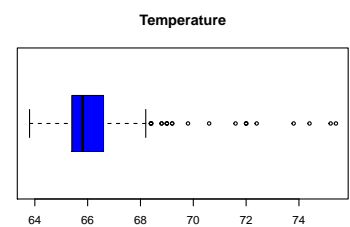
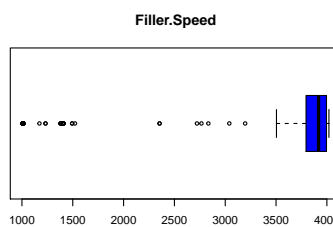
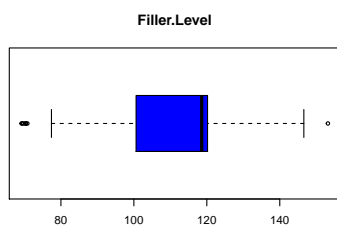
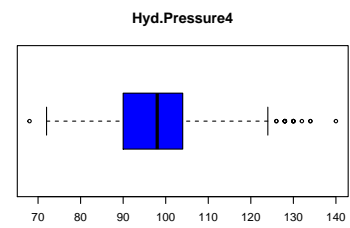
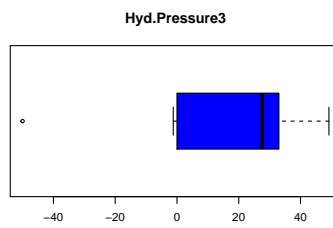
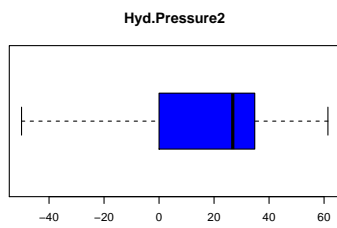
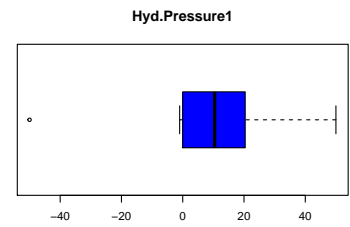
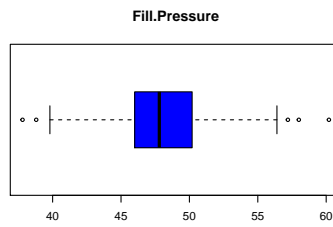
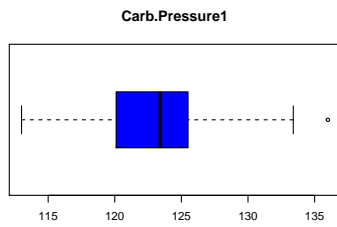
```
Ins_eval_imputed$PH[is.na(Ins_eval_imputed$PH)] <- 0
```

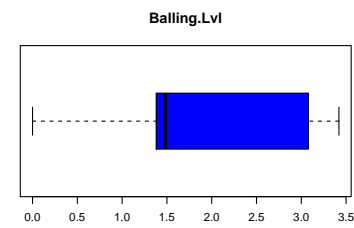
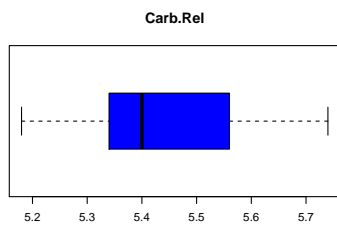
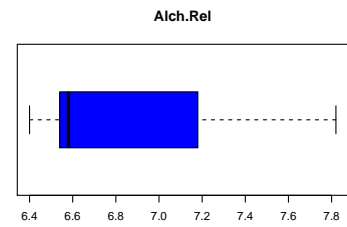
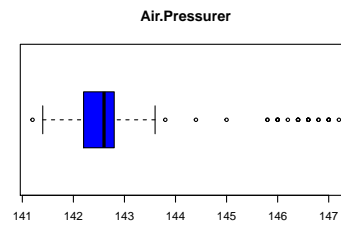
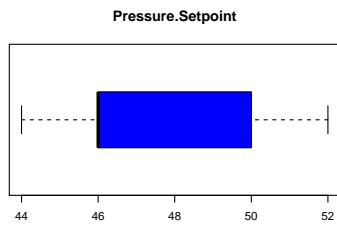
## Boxplots

Let's take a first look at the boxplots

```
par(mfrow = c(3, 3))
for(i in 2:33) {
  if (is.numeric(Ins_eval_imputed[,i])) {
    boxplot(Ins_eval_imputed[,i], main = names(Ins_eval_imputed[i]), col = 4, horizontal = TRUE)
  }
}
```







The boxplots show that some of the variables have outliers in them. So, we'll cap them.

```

Ins_eval_cap <- Ins_eval_imputed

for (i in 2:33) {
  if(i == 26) next # skipping the PH column, which is a 26th column position.

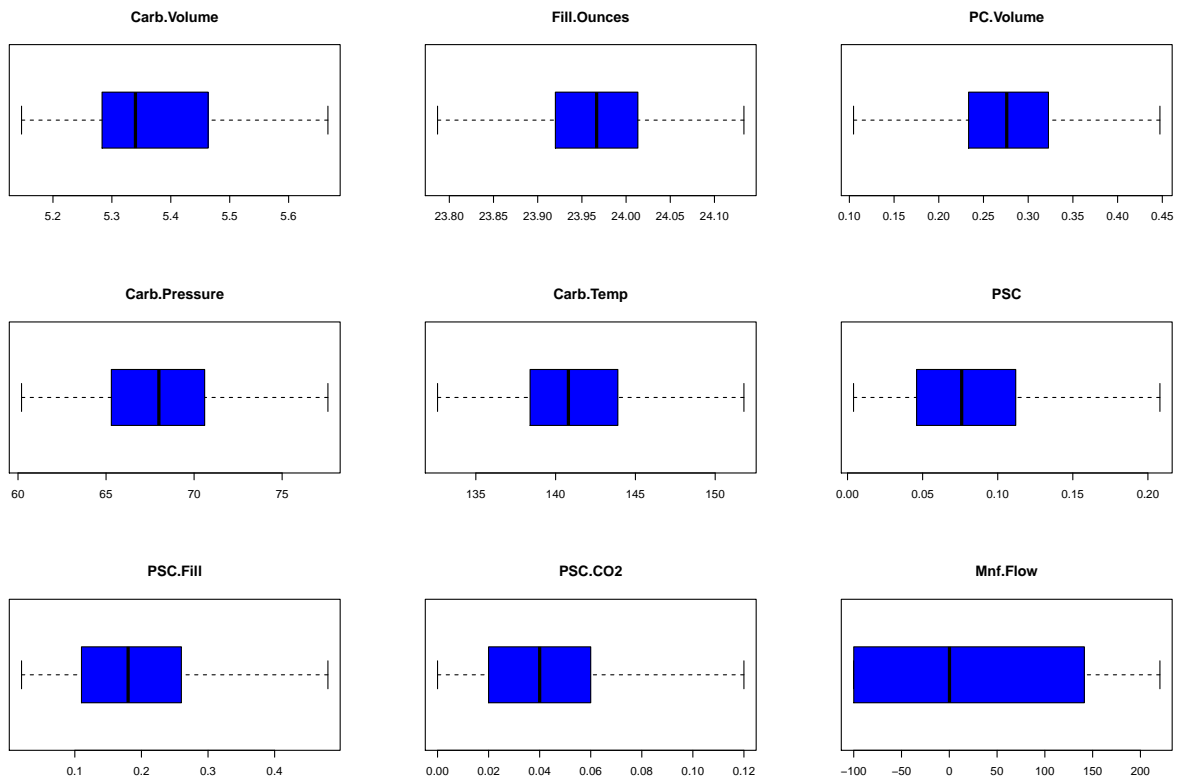
  qnt1 <- quantile(Ins_eval_cap[,i], probs = c(0.25, 0.75), na.rm = T)
  cap_amt <- quantile(Ins_eval_cap[,i], probs = c(0.05, 0.95), na.rm = T)
  High <- 1.5 * IQR(Ins_eval_cap[,i], na.rm = T)

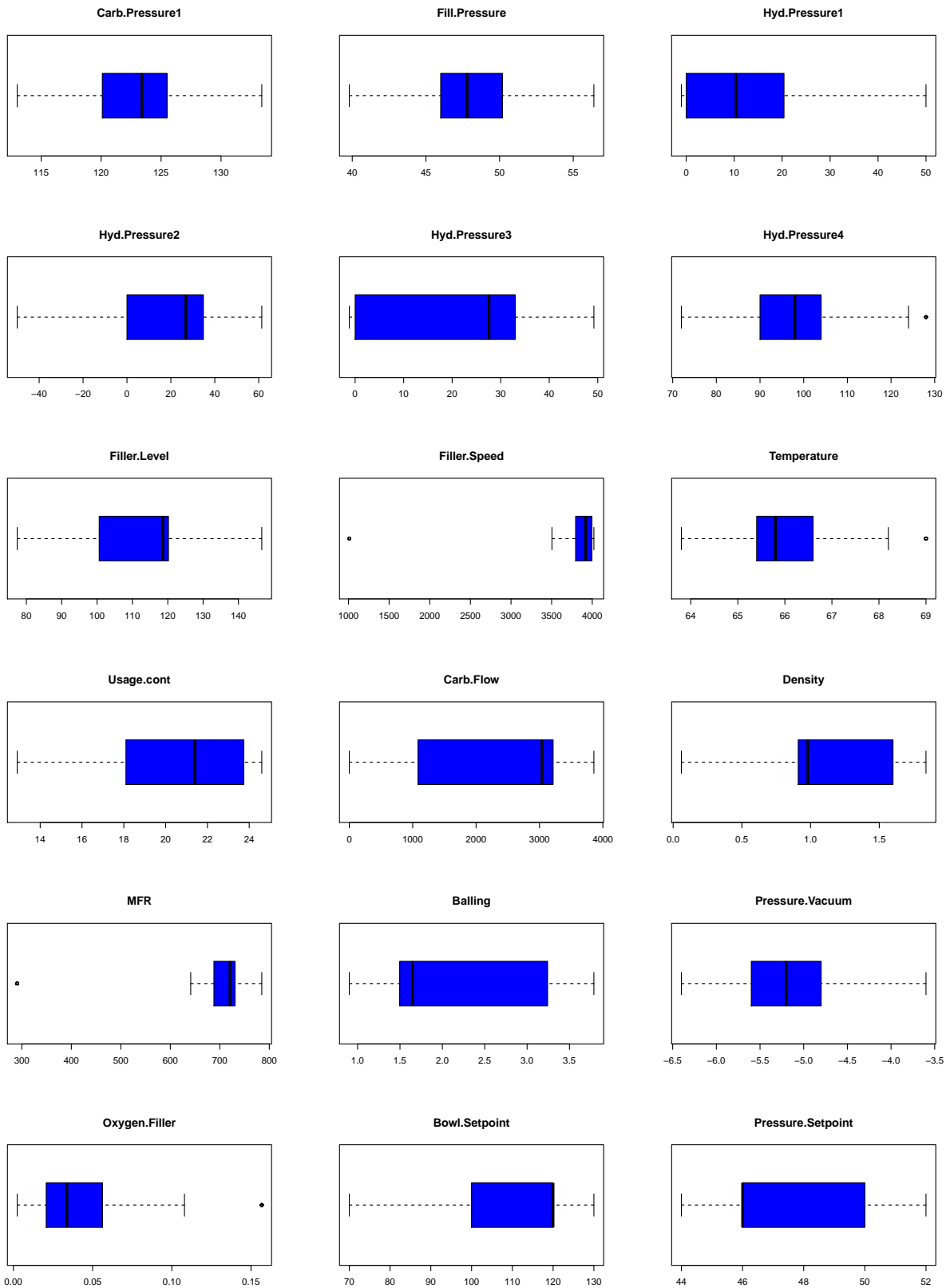
  Ins_eval_cap[,i][Ins_eval_cap[,i] < (qnt1[1] - High)] <- cap_amt[1]
  Ins_eval_cap[,i][Ins_eval_cap[,i] > (qnt1[2] + High)] <- cap_amt[2]
}

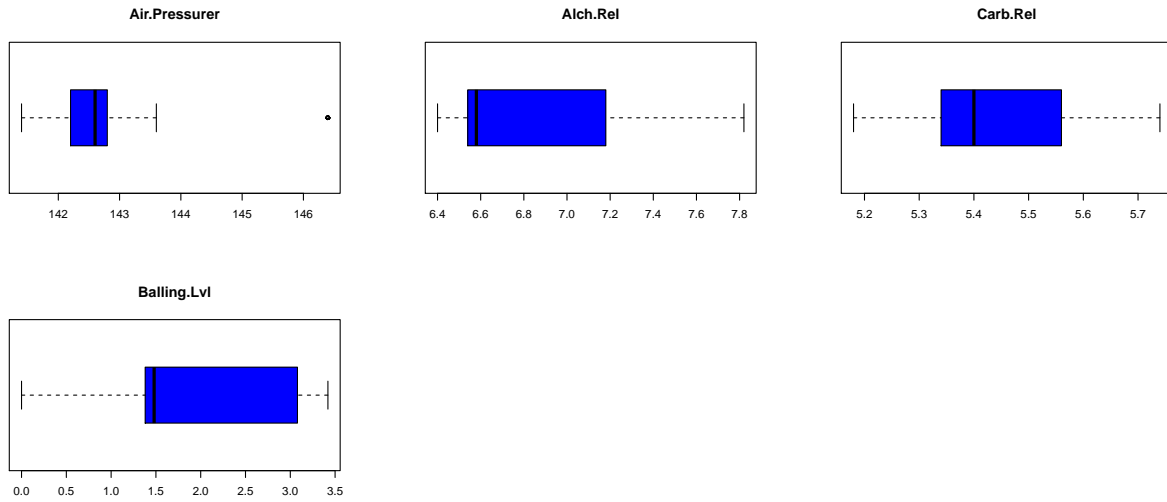
par(mfrow = c(3, 3))
for(i in 2:33) {
  if(i == 26) next # skipping the PH column, which is a 26th column position.

  if (is.numeric(Ins_eval_cap[,i])) {
    boxplot(Ins_eval_cap[,i], main = names(Ins_eval_cap[i]), col = 4, horizontal = TRUE)
  }
}

```







The outliers were capped and now we see that several fields Carb.Volume, PSC.FILL, PSC.C02, Mnf.Flow, Hyd.Pressure1, Hyd.Pressure2, Hyd.Pressure3, Usage.cont, Carb.Flow, Density, Balling, Bowl.Setpoint, Pressure.Setpoint, Alch.Rel, Carb.Rel, Balling.Lvl have high variance.

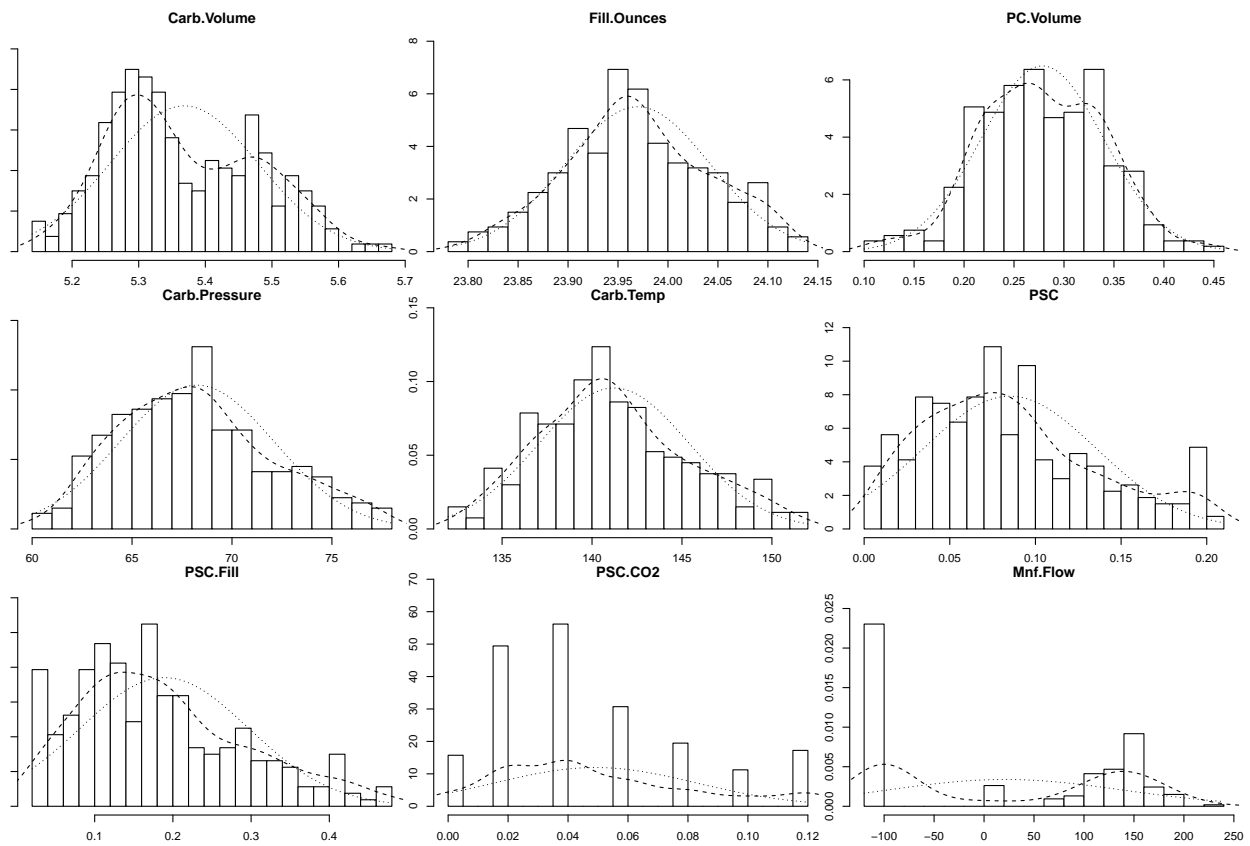
We'll do the boxplots differently, with ggplot, to check if there are any differences.

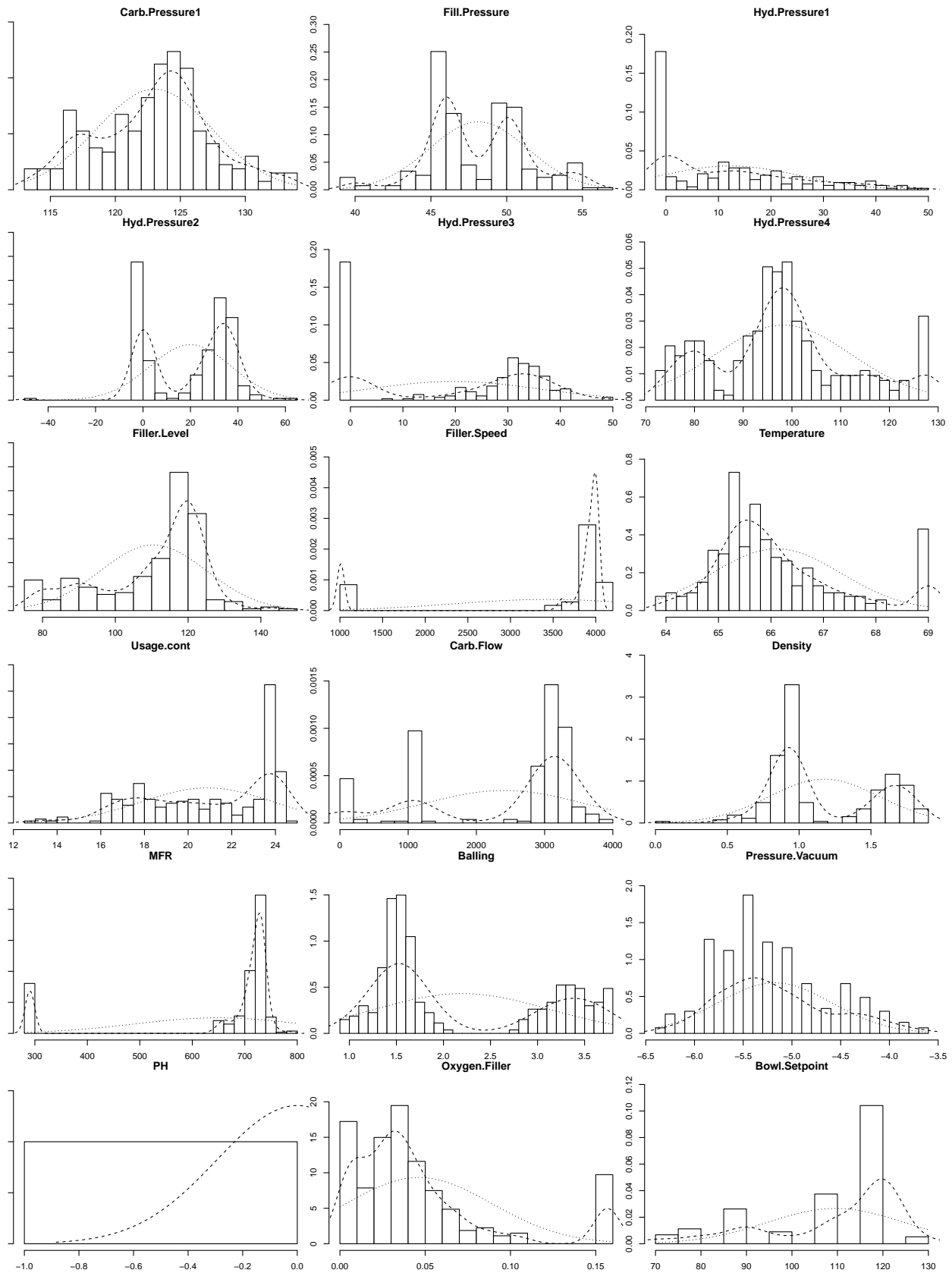


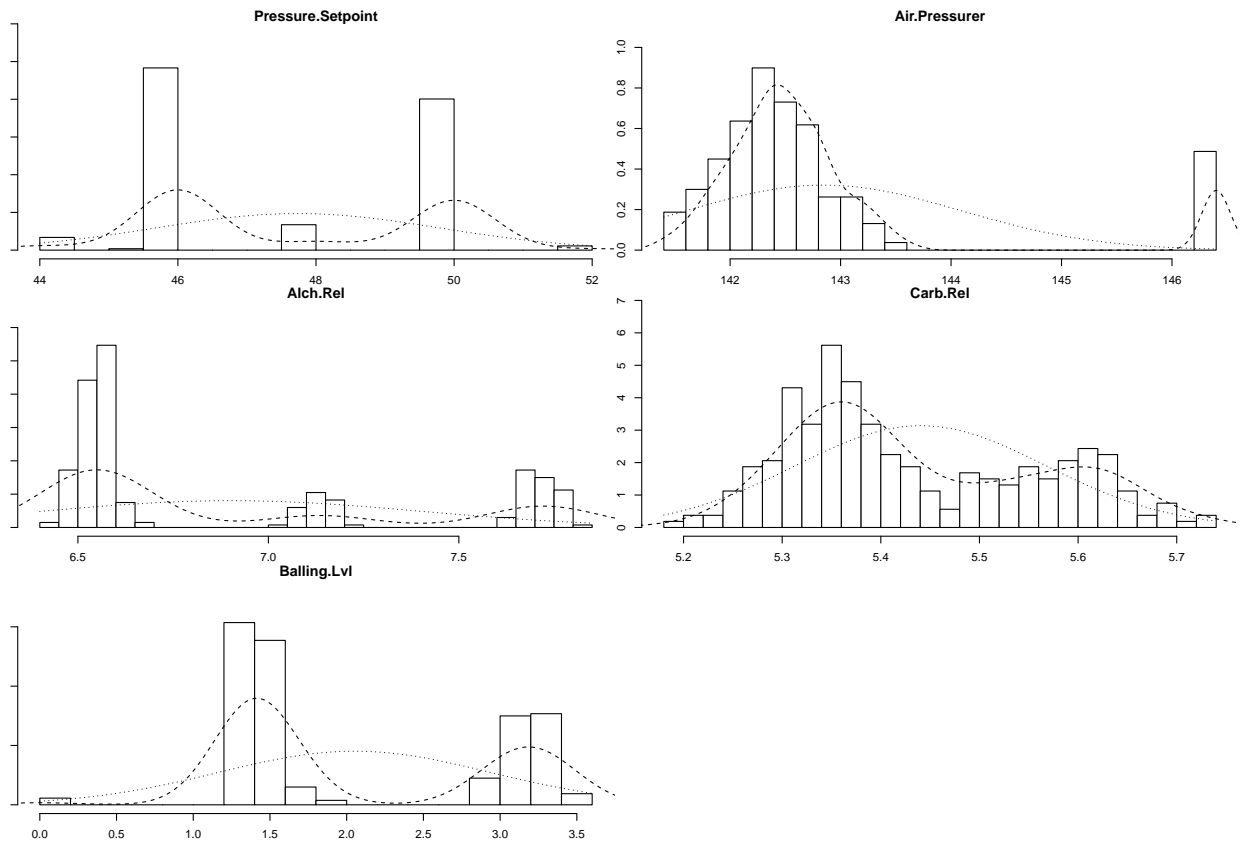
## Histograms

Histograms tell us how the data is distributed in the dataset (numeric fields).

```
for(i in seq(from = 2, to = length(Ins_eval_cap), by = 9)) {  
  if(i <= 27) {  
    multi.hist(Ins_eval_cap[i:(i + 8)])  
  } else {  
    multi.hist(Ins_eval_cap[i:(i + 4)])  
  }  
}
```







We can ignore PH, which is target column, where zeros were forced in.

Observing the above histograms, I decided the critical skewness, needing BoxCox transformation, to be 0.75 or higher. Based on this critical value, I am creating a vector `transform_cols2`, which'll contain the column names of skewed columns.

The columns, whose skewness exceed the critical value of 0.75, are printed below.

```
transform_cols2 <- c()

for(i in seq(from = 2, to = length(Ins_eval_cap), by = 1)) {
  if(i == 26) next # skipping the PH column, which is a 26th column position.

  if(abs(skewness(Ins_eval_cap[, i])) >= 1) {
    transform_cols2 <- append(transform_cols2, names(Ins_eval_cap[i]))
    print(paste0(names(Ins_eval_cap[i]), ": ", skewness(Ins_eval_cap[, i])))
  }
}
```

```
## [1] "Filler.Speed: -1.73167358616647"
## [1] "MFR: -1.76232670134858"
## [1] "Oxygen.Filler: 1.55180608681166"
## [1] "Bowl.Setpoint: -1.1242132435293"
## [1] "Air.Pressurer: 2.13701548204288"
```

Many of these histograms are skewed. So, following the recommendations of “Applied Statistical Learning” (page 105, 2nd para), I’ll apply Box-Cox transformation to remove the skewness.

```

lambda <- NULL
data_imputed_3 <- Ins_eval_cap

for (i in 1:length(transform_cols2)) {
  lambda[transform_cols2[i]] <- BoxCox.lambda(abs(Ins_eval_cap[, transform_cols2[i]]))

  data_imputed_3[c(transform_cols2[i])] <- BoxCox(Ins_eval_cap[transform_cols2[i]], lambda[transform_cols2[i]])
}

```

Now, we don't need to observe the histograms all over again. It will suffice to see the skewness. We observe that skewness of most or all of the columns reduced and some even reduced to less than 1.

```

for(i in seq(from = 2, to = length(data_imputed_3), by = 1)) {
  if(i == 26) next # skipping the PH column, which is a 26th column position.

  if(abs(skewness(data_imputed_3[, i])) >= 1) {
    print(paste0(names(data_imputed_3[i]), ": ", skewness(data_imputed_3[, i])))
  }
}

```

```

## [1] "Filler.Speed: -1.6934044682825"
## [1] "MFR: -1.69890061556103"
## [1] "Air.Pressurer: 2.11038285372631"

```

## Categorical variables

Now, we'll explore the Categorical variables.

```
cat('Brand.Code:')
```

```
## Brand.Code:
```

```
table(data_imputed_3$Brand.Code)
```

```
##  
##      A      B      C      D  
##    8  35 129  31  64
```

Observation: In Brand.Code column, 120 rows are empty. So, we'll impute them with "X".

```
Ins_eval_cap_imputed <- data_imputed_3 %>% mutate(Brand.Code = ifelse((Brand.Code == ""), "X", Brand.Code))  
cat("Brand.Code: ")
```

```
## Brand.Code:
```

```
table(Ins_eval_cap_imputed$Brand.Code)
```

```
##  
##      A      B      C      D      X  
##    35 129  31  64    8
```

## Correlations

At this point the data is prepared. So, we'll explore the top correlated variables.

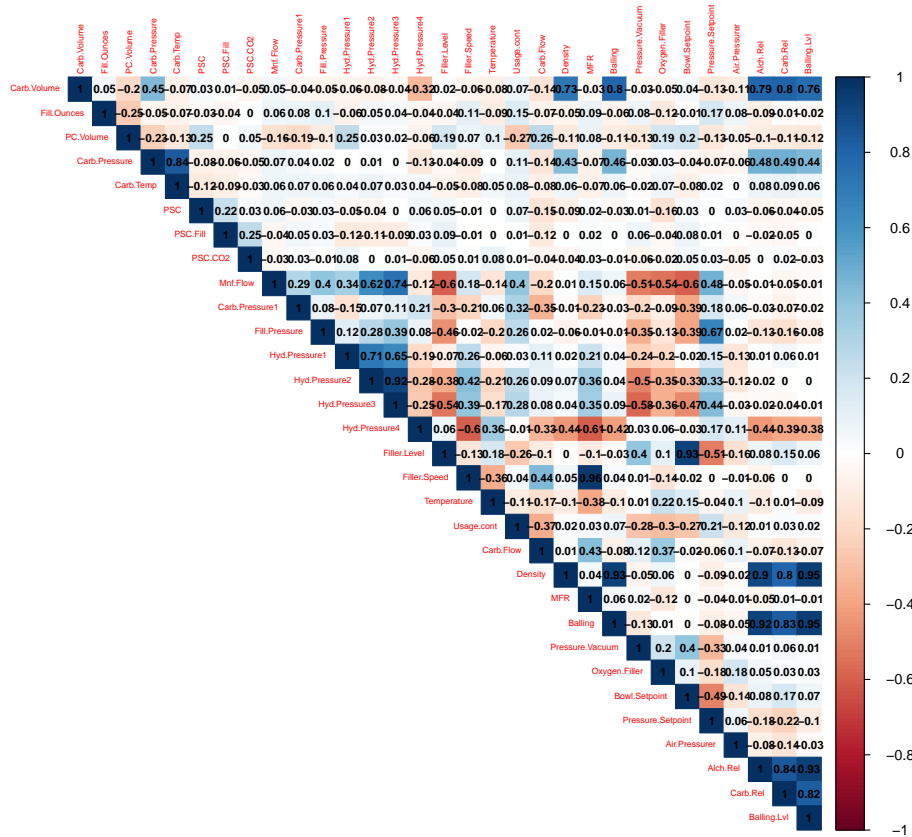
For the purpose of correlation, we'll remove the only non-numeric field Brand.Code, out of the correlation.

Now, we'll look at the correlation matrix of the variables.

```
Ins_cap_corr <- subset(Ins_eval_cap_imputed, select = -c(Brand.Code, PH))

cor_mx = cor(Ins_cap_corr, use = "pairwise.complete.obs", method = "pearson")

corrplot(cor_mx, method = "color", type = "upper", order = "original", number.cex = .7, addCoef.col = "black",
          tl.srt = 90, # Text label color and rotation
          diag = TRUE, # hide correlation coefficient on the principal diagonal
          tl.cex = 0.5)
```



At this point exploration, preparation and pair-wise correlations of **StudentEvaluation.csv** are done. So, I'll begin the building process.

## Models

### Splitting Test and Train

We will use 80/20 split to create Test and Train data from our Ins\_train\_cap\_imputed file. Since our dataset is not that large, we want to have as much training data available for modeling as possible.

```

set.seed(300)
trainingRows <- createDataPartition(Ins_train_cap_imputed$PH, p = 0.8, list = FALSE)
Ins_train <- Ins_train_cap_imputed[trainingRows, ]
Ins_test <- Ins_train_cap_imputed[-trainingRows, ]

Ins_train_Y <- subset( Ins_train, select = PH )
Ins_train_X <- subset( Ins_train, select = -PH )
Ins_test_Y <- subset( Ins_test, select = PH )
Ins_test_X <- subset( Ins_test, select = -PH )

```

## Linear Models

First we are going to try to use linear models to predict the relationship between our predictors and PH values, assuming that the relationship shows a constant rate of change. We do not have very high hopes for these models since there are a lot of limitations associated with Linear Models - in the real world, the data is rarely linearly separable.

### GLM Model

First, we will try Generalized Linear model. The GLM generalizes linear regression by allowing the linear model to be related to the response variable via a link function and by allowing the magnitude of the variance of each measurement to be a function of its predicted value.

```

set.seed(300)
lmFit1 = train(PH ~ ., data = Ins_train,
               metric = 'RMSE',
               method = 'glm',
               preProcess = c('center', 'scale'),
               trControl = trainControl(method = 'cv', number = 5, savePredictions = TRUE)
)

lmFit1_pred <- predict(lmFit1, Ins_test_X)

lmFit1

```

```

## Generalized Linear Model
##
## 2058 samples
## 32 predictor
##
## Pre-processing: centered (35), scaled (35)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 1645, 1646, 1648, 1648, 1645
## Resampling results:
##
## RMSE      Rsquared    MAE
## 0.130516  0.4012911  0.102511

```

The GLM R-Squared value is not very high - 0.40, meaning that the model explains 40% of variability in the data. RMSE for GLM is 0.135.

## PLS Model

Next, we will try Partial Least Squares model. PLS finds a linear regression model by projecting the predicted variables and the observable variables to a new space. If the correlation among predictors is high, then the partial least squares squares might be a better option. PLS might also be better if the number of predictors may be greater than the number of observations.

```
set.seed(300)
lmFit2 = train(PH ~ ., data = Ins_train,
               metric = 'RMSE',
               method = 'pls',
               preprocess = c('center', 'scale'),
               trControl = trainControl(method = 'cv', number = 5, savePredictions = TRUE)
)

lmFit2_pred <- predict(lmFit2, Ins_test_X)

lmFit2
```

```
## Partial Least Squares
##
## 2058 samples
## 32 predictor
##
## Pre-processing: centered (35), scaled (35)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 1645, 1646, 1648, 1648, 1645
## Resampling results across tuning parameters:
##
##  ncomp  RMSE      Rsquared  MAE
##  1      0.1462555  0.2468770  0.1164412
##  2      0.1387162  0.3227460  0.1096007
##  3      0.1357027  0.3523941  0.1079358
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was ncomp = 3.
```

The PLS R-Squared value is not very high - 0.37, meaning that the model explains 37% of variability in the data. RMSE for PLS is 0.132.

## Ridge Model

Next, we will try some penalized models, we will start with a Ridge model. Ridge regression adds a penalty on the sum of the squared regression parameters.

```
set.seed(300)
ridgeGrid <- data.frame(lambda = seq(0, .1, length = 15))
ridgeRegFit <- train(x = Ins_train_X[, -1], y = Ins_train_Y$PH,
                    method = "ridge",
                    tuneGrid = ridgeGrid,
                    trControl = trainControl(method = "cv", number = 10),
                    preProc = c("center", "scale"))
```



```

    )
ridgeRegFit

## Ridge Regression
##
## 2058 samples
## 31 predictor
##
## Pre-processing: centered (31), scaled (31)
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1851, 1852, 1852, 1853, 1852, 1852, ...
## Resampling results across tuning parameters:
##
##   lambda      RMSE      Rsquared    MAE
## 0.000000000 0.1357570 0.3526654 0.1058840
## 0.007142857 0.1356996 0.3527490 0.1059281
## 0.014285714 0.1357660 0.3519846 0.1060283
## 0.021428571 0.1358495 0.3511184 0.1061402
## 0.028571429 0.1359385 0.3502213 0.1062551
## 0.035714286 0.1360298 0.3493107 0.1063743
## 0.042857143 0.1361220 0.3483955 0.1064905
## 0.050000000 0.1362144 0.3474818 0.1066042
## 0.057142857 0.1363063 0.3465737 0.1067151
## 0.064285714 0.1363975 0.3456745 0.1068218
## 0.071428571 0.1364877 0.3447861 0.1069237
## 0.078571429 0.1365769 0.3439101 0.1070195
## 0.085714286 0.1366650 0.3430473 0.1071109
## 0.092857143 0.1367520 0.3421983 0.1072005
## 0.100000000 0.1368379 0.3413633 0.1072865
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was lambda = 0.007142857.

```

```
ridge_pred <- predict(ridgeRegFit, Ins_test_X)
```

The Ridge R-Squared value is not very high - 0.376, meaning that the model explains 38% of variability in the data. RMSE for Ridge is 0.132.

## ENET Model

Next, we will try ENET model. Elastic net model has both ridge penalties and lasso penalties.

```

df1_enet <- train(x = as.matrix(Ins_train_X[,-1]),
                  y = Ins_train_Y$PH,
                  method='enet',
                  metric='RMSE',
                  trControl = trainControl(method = 'cv', number = 5, savePredictions = TRUE))

df1_enet

```

```
## Elasticnet
```

```
##
## 2058 samples
## 31 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 1645, 1646, 1646, 1649, 1646
## Resampling results across tuning parameters:
##
##  lambda  fraction  RMSE      Rsquared  MAE
##  0e+00   0.050     0.1559944  0.2011812  0.1258371
##  0e+00   0.525     0.1362108  0.3475361  0.1066165
##  0e+00   1.000     0.1355580  0.3535090  0.1055971
##  1e-04   0.050     0.1560215  0.2008990  0.1258614
##  1e-04   0.525     0.1362236  0.3474297  0.1066316
##  1e-04   1.000     0.1355544  0.3535331  0.1055981
##  1e-01   0.050     0.1606700  0.1979930  0.1301814
##  1e-01   0.525     0.1398222  0.3134469  0.1105084
##  1e-01   1.000     0.1366982  0.3422300  0.1072176
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were fraction = 1 and lambda = 1e-04.
```

```
enet_pred <- predict(df1_enet, Ins_test_X)
```

The ENet R-Squared value is not very high - 0.319, meaning that the model explains 32% of variability in the data. RMSE for Enet is 0.144.

## Comparing Linear Models

As expected, it doesn't look like either of the linear models has a good performance based on their R-squared and RMSE values, but let's compare those and see which model performs best.

```
z<- rbind(
  postResample(pred = lmFit1_pred, obs = Ins_test_Y$PH),
  postResample(pred = lmFit2_pred, obs = Ins_test_Y$PH),
  postResample(pred = ridge_pred, obs = Ins_test_Y$PH),
  postResample(pred = enet_pred, obs = Ins_test_Y$PH)
)

data.frame(z,row.names = c('GLM', 'PLS', 'RIDGE', 'ENET'))
```

```
##          RMSE  Rsquared      MAE
## GLM    0.1244260 0.4362877 0.0990657
## PLS    0.1309578 0.3747149 0.1057584
## RIDGE  0.1280518 0.4028059 0.1005767
## ENET   0.1281544 0.4017962 0.1004734
```

The best linear model based on the highest R-Squared and lowest RSME value is GLM.

## Non-Linear Models

Next we will try several Non-Linear models: multivariate adaptive regression splines (MARS), support vector machines (SVMs), and K-nearest neighbors (KNNs). We expect these models to perform better than Linear Models. We will look at Tree models separately.

### MARS Model

We will continue modeling by tuning and evaluating a MARS model. MARS uses surrogate features instead of the original predictors.

```
set.seed(200)
marsGrid <- expand.grid(.degree = 1:2, .nprune = 2:20)
marsTune <- train(x = Ins_train_X,
                  y = Ins_train_Y$PH,
                  method = "earth",
                  preProc=c("center", "scale"),
                  tuneGrid= marsGrid,
                  trControl = trainControl(method = "cv"))

## Loading required package: earth

## Warning: package 'earth' was built under R version 3.6.3

## Loading required package: Formula

## Warning: package 'Formula' was built under R version 3.6.3

## Loading required package: plotmo

## Warning: package 'plotmo' was built under R version 3.6.3

## Loading required package: plotrix

## Warning: package 'plotrix' was built under R version 3.6.3

##
## Attaching package: 'plotrix'

## The following object is masked from 'package:psych':
##
##   rescale

## Loading required package: TeachingDemos

## Warning: package 'TeachingDemos' was built under R version 3.6.3

##
## Attaching package: 'plotmo'
```

```
## The following object is masked from 'package:urca':
##
##      plotres
```

Evaluating MARS model's performance:

```
marsPred = predict(marsTune, newdata = Ins_test_X)
postResample(pred = marsPred, obs = Ins_test_Y$PH)
```

```
##      RMSE    Rsquared      MAE
## 0.11636907 0.50852879 0.09003745
```

The MARS R-Squared value is 0.506, meaning that the model explains 51% of variability in the data. RMSE for MARS is 0.122.

## SVM Model

The next model we will tune and evaluate is SVM model - I will use pre-process to center and scale the data and will use tune length of 10. The benefit of SVM are that, since the squared residuals are not used, large outliers have a limited effect on the regression equation. Second, samples that the model fits well have no effect on the regression equation.

```
set.seed(200)
svmTuned = train(x = Ins_train_X[,-1],
                 y = Ins_train_Y$PH,
                 method="svmRadial",
                 preProc=c("center", "scale"),
                 tuneLength=10,
                 trControl = trainControl(method = "repeatedcv"))

svmTuned
```

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 2058 samples
## 31 predictor
##
## Pre-processing: centered (31), scaled (31)
## Resampling: Cross-Validated (10 fold, repeated 1 times)
## Summary of sample sizes: 1853, 1852, 1851, 1852, 1852, ...
## Resampling results across tuning parameters:
##
##  C          RMSE          Rsquared    MAE
##  0.25 0.1272464 0.4384177 0.09572176
##  0.50 0.1241135 0.4624993 0.09248300
##  1.00 0.1218636 0.4807283 0.09013977
##  2.00 0.1200089 0.4963205 0.08879083
##  4.00 0.1189986 0.5061337 0.08822828
##  8.00 0.1197453 0.5048866 0.08880997
## 16.00 0.1216411 0.4984268 0.09016625
## 32.00 0.1254165 0.4817496 0.09350822
## 64.00 0.1307583 0.4570976 0.09822049
```

```
## 128.00 0.1365759 0.4318984 0.10286652
##
## Tuning parameter 'sigma' was held constant at a value of 0.02246471
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were sigma = 0.02246471 and C = 4.
```

```
SVMPred = predict(svmTuned, newdata = Ins_test_X[,-1])
postResample(pred = SVMPred, obs = Ins_test_Y$PH)
```

```
## RMSE Rsquared MAE
## 0.1162560 0.5143944 0.0829104
```

The SVM R-Squared value is 0.432, meaning that the model explains 43% of variability in the data. RMSE for SVM is 0.133.

## KNN Model

The next Non-Linear model we will tune and evaluate is KNN model. The KNN approach predicts a new sample using the K-closest samples from the training set.

```
set.seed(333)
knnModel <- train(x = Ins_train_X[,-1],
                  y = Ins_train_Y$PH,
                  method = "knn",
                  preProc = c("center", "scale"),
                  tuneLength = 10)
knnModel
```

```
## k-Nearest Neighbors
##
## 2058 samples
## 31 predictor
##
## Pre-processing: centered (31), scaled (31)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 2058, 2058, 2058, 2058, 2058, ...
## Resampling results across tuning parameters:
##
## k RMSE Rsquared MAE
## 5 0.1371224 0.3712314 0.10169027
## 7 0.1337001 0.3882396 0.09992491
## 9 0.1324302 0.3941617 0.09953493
## 11 0.1314058 0.4007852 0.09914991
## 13 0.1313228 0.4006225 0.09949358
## 15 0.1311343 0.4021223 0.09962376
## 17 0.1311953 0.4018486 0.10012350
## 19 0.1313681 0.4004091 0.10054008
## 21 0.1316230 0.3986019 0.10098786
## 23 0.1320249 0.3952025 0.10153718
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 15.
```

Evaluating the model's performance:

```
knnPred <- predict(knnModel, newdata = Ins_test_X[,-1])
postResample(pred = knnPred, obs = Ins_test_Y$PH)
```

```
##          RMSE   Rsquared         MAE
## 0.12086455 0.47755052 0.09114263
```

The SVM R-Squared value is 0.416, meaning that the model explains 42% of variability in the data. RMSE for SVM is 0.135.

## Comparing Non-Linear Models

It looks like non-linear models are performing better than the linear models based on their R-squared values, but let's compare those and see which model performs best.

```
z<- rbind(
  postResample(pred = marsPred, obs = Ins_test_Y$PH),
  postResample(pred = SVMPred, obs = Ins_test_Y$PH),
  postResample(pred = knnPred, obs = Ins_test_Y$PH)
)

data.frame(z,row.names = c('MARS', 'SVM', 'KNN'))
```

```
##          RMSE   Rsquared         MAE
## MARS 0.1163691 0.5085288 0.09003745
## SVM  0.1162560 0.5143944 0.08291040
## KNN  0.1208645 0.4775505 0.09114263
```

The best non-linear model based on the highest R-Squared and lowest RSME value is MARS

## Tree Models

We will now try some Tree models. Decision tree analysis involves making a tree-shaped diagram to chart out a course of action or a statistical probability analysis. It is used to break down complex problems or branches. Each branch of the decision tree could be a possible outcome.

### Random Forest

First, we will try a Random Forest Model, these model achieves variance reduction by selecting strong, complex learners that exhibit low bias. Because each learner is selected independently of all previous learners, random forests is robust to a noisy response.

```
suppressWarnings(library(randomForest))
```

```
## randomForest 4.6-14
```

```
## Type rfNews() to see new features/changes/bug fixes.
```

```
##
## Attaching package: 'randomForest'

## The following object is masked from 'package:psych':
##
##      outlier

## The following object is masked from 'package:gridExtra':
##
##      combine

## The following object is masked from 'package:dplyr':
##
##      combine

## The following object is masked from 'package:ggplot2':
##
##      margin
```

```
set.seed(333)
RF_model <- randomForest(x = Ins_train_X[,-1],
                        y = Ins_train_Y$PH,
                        importance = TRUE,
                        ntree = 700
                        )

RFPred <- predict(RF_model, newdata = Ins_test_X[,-1])
postResample(pred = RFPred, obs = Ins_test_Y$PH)
```

```
##      RMSE   Rsquared      MAE
## 0.09392728 0.70008130 0.06799525
```

The Random Forest R-Squared value is 0.641, meaning that the model explains 64% of variability in the data. RMSE for Random Forest is 0.109.

## Boosted trees

Next, we will try a Boosted Tree Model. The basic principles of gradient boosting are as follows: given a loss function (e.g., squared error for regression) and a weak learner (e.g., regression trees), the algorithm seeks to find an additive model that minimizes the loss function.

```
suppressWarnings(library(gbm))
```

```
## Loaded gbm 2.1.8
```

```
set.seed(333)
gbmGrid <- expand.grid(.interaction.depth = seq(1, 5, by = 2),
                      .n.trees = seq(300, 1000, by = 100),
                      .shrinkage = c(0.05, 0.1),
                      .n.minobsinnode = 5)
```

```
gbmTune <- suppressWarnings(train(Ins_train_X[,-1], Ins_train_Y$PH,
                                method = "gbm",
                                tuneGrid = gbmGrid,
                                verbose = FALSE)
                                )

GBM_Pred <- predict(gbmTune, newdata = Ins_test_X[,-1])
postResample(pred = GBM_Pred, obs = Ins_test_Y$PH)
```

```
##          RMSE    Rsquared        MAE
## 0.09686779 0.65934518 0.07174660
```

The Boosted Tree R-Squared value is 0.578, meaning that the model explains 58% of variability in the data. RMSE for Boosted Tree is 0.114.

## Single Tree

Next, we will try a Single Tree Model. Basic regression trees partition the data into smaller groups that are more homogenous with respect to the response.

```
set.seed(333)
rpartTune <- train(Ins_train_X, Ins_train_Y$PH,
                  method = "rpart2",
                  tuneLength = 10,
                  trControl = trainControl(method = "cv"))

ST_Pred <- predict(rpartTune, newdata = Ins_test_X)
postResample(pred = ST_Pred, obs = Ins_test_Y$PH)
```

```
##          RMSE    Rsquared        MAE
## 0.12101384 0.46763842 0.09201532
```

The Basic Regression Tree R-Squared value is 0.459, meaning that the model explains 46% of variability in the data. RMSE for Basic Regression Tree is 0.129.

## Cubist

Next, we will try a Cubist Model. Cubist is a rule-based model. A tree is grown where the terminal leaves contain linear regression models. These models are based on the predictors used in previous splits. Also, there are intermediate linear models at each step of the tree.

```
suppressWarnings(library(Cubist))
set.seed(333)

cubistMod <- cubist(Ins_train_X,
                  Ins_train_Y$PH,
                  committees = 6
                  )
```

```
## Warning in cubist.default(Ins_train_X, Ins_train_Y$PH, committees = 6): NAs
## introduced by coercion
```



```
cubistModPred <- predict(cubistMod, newdata = Ins_test_X)
postResample(pred = cubistModPred, obs = Ins_test_Y$PH)
```

```
##          RMSE   Rsquared      MAE
## 0.10649471 0.63787710 0.07413891
```

The Cubist R-Squared value is 0.671, meaning that the model explains 67% of variability in the data. RMSE for Cubist is 0.101.

## Bagged Trees

Finally, we will try Bagged Trees Model. Bagging effectively reduces the variance of a prediction through its aggregation process.

```
set.seed(333)
suppressWarnings(library(ipred))

baggedTree <- ipredbagg(Ins_train_Y$PH, Ins_train_X)

baggedTreePred <- predict(baggedTree, newdata = Ins_test_X)
postResample(pred = baggedTreePred, obs = Ins_test_Y$PH)
```

```
##          RMSE   Rsquared      MAE
## 0.11078774 0.55770116 0.08685231
```

The Bagged R-Squared value is 0.523, meaning that the model explains 53% of variability in the data. RMSE for Bagged Tree is 0.122.

## Comparing Tree Models

It looks like Tree Models are performing better than non-linear models and linear models based on their R-squared values, but let's compare those and see which model performs best.

```
z<- rbind(
  postResample(pred = RFPred, obs = Ins_test_Y$PH),
  postResample(pred = GBM_Pred, obs = Ins_test_Y$PH),
  postResample(pred = ST_Pred, obs = Ins_test_Y$PH),
  postResample(pred = cubistModPred, obs = Ins_test_Y$PH),
  postResample(pred = baggedTreePred, obs = Ins_test_Y$PH)
)
```

```
data.frame(z,row.names = c('Random Forrest', 'Boosted Trees', 'Single Tree', 'Cubist', 'Bagged Tree'))
```

```
##          RMSE   Rsquared      MAE
## Random Forrest 0.09392728 0.7000813 0.06799525
## Boosted Trees  0.09686779 0.6593452 0.07174660
## Single Tree    0.12101384 0.4676384 0.09201532
## Cubist         0.10649471 0.6378771 0.07413891
## Bagged Tree    0.11078774 0.5577012 0.08685231
```

Based on the combination of R-Squared and RMSE values for all models we tried - the best Model is Cubist - that's what we will use for our predictions. Random Forest model also has vevry good performance compared to all the other models we tuned and evaluated. Overall, Tree models are performing better that Linear and other Non-Linear Models based on RMSE and R-Squared values.

Here is the list of most relevant variables in this Cubist model:

```
varImp(cubistMod)
```

##	Overall
## Mnf.Flow	85.5
## Pressure.Vacuum	49.5
## Brand.Code	19.0
## Oxygen.Filler	41.5
## Alch.Rel	46.5
## Balling.Lvl	45.0
## Bowl.Setpoint	34.0
## Balling	50.5
## Filler.Speed	35.0
## Carb.Rel	35.5
## Air.Pressurer	8.0
## Usage.cont	22.0
## Carb.Pressure1	27.0
## Carb.Flow	22.0
## Filler.Level	17.5
## Carb.Volume	14.5
## Temperature	30.0
## PC.Volume	7.5
## Hyd.Pressure1	17.5
## Density	32.5
## Hyd.Pressure2	22.0
## Hyd.Pressure3	28.5
## MFR	19.5
## Pressure.Setpoint	12.0
## Hyd.Pressure4	11.5
## Carb.Pressure	10.5
## Carb.Temp	10.0
## Fill.Pressure	5.0
## Fill.Ounces	2.5
## PSC.Fill	2.5
## PSC.CO2	1.0
## PSC	1.0

## Predictions

Now that we have identified the best model, we can use our evaluation data to make PH predictions and output predictions to an excel readable format. We are adding predicted PH values to our Evaluation data set.

```
final_predictions <- predict(cubistMod, newdata=Ins_eval_cap_imputed)
Ins_eval_cap_imputed$PH <- final_predictions
final_predictions_df <- data.frame(Ins_eval_cap_imputed)
head(final_predictions_df)
```

##	Brand.Code	Carb.Volume	Fill.Ounces	PC.Volume	Carb.Pressure	Carb.Temp	PSC
## 1	D	5.480000	24.03333	0.2700000	65.4	134.6	0.1934
## 2	A	5.393333	23.95333	0.2266667	63.2	135.0	0.0420
## 3	B	5.293333	23.92000	0.3033333	66.4	140.4	0.0680
## 4	B	5.266667	23.94000	0.1860000	64.8	139.0	0.0040
## 5	B	5.406667	24.09800	0.1600000	69.4	142.2	0.0400
## 6	B	5.286667	24.10667	0.2120000	73.4	147.2	0.0780
##	PSC.Fill	PSC.CO2	Mnf.Flow	Carb.Pressure1	Fill.Pressure	Hyd.Pressure1	
## 1	0.40	0.04	-100	116.6	46.0	0	
## 2	0.22	0.08	-100	118.8	46.2	0	
## 3	0.10	0.02	-100	120.2	45.8	0	
## 4	0.20	0.02	-100	124.8	40.0	0	
## 5	0.30	0.06	-100	115.0	51.4	0	
## 6	0.22	0.00	-100	118.6	46.4	0	
##	Hyd.Pressure2	Hyd.Pressure3	Hyd.Pressure4	Filler.Level	Filler.Speed		
## 1	0	0	96	129.4	7939410.7		
## 2	0	0	112	120.0	8043319.4		
## 3	0	0	98	119.4	8035302.4		
## 4	0	0	128	120.2	509801.6		
## 5	0	0	94	116.0	8067394.3		
## 6	0	0	94	120.4	8035302.4		
##	Temperature	Usage.cont	Carb.Flow	Density	MFR	Balling	Pressure.Vacuum
## 1	66.0	21.66	2950	0.88	264578.30	1.398	-3.8
## 2	65.6	17.60	2916	1.50	270575.24	2.942	-4.4
## 3	65.6	24.18	3056	0.90	269840.31	1.448	-4.2
## 4	69.0	18.12	28	0.74	42207.14	1.056	-4.0
## 5	66.4	21.32	3214	0.88	282620.39	1.398	-4.0
## 6	66.6	18.00	3064	0.84	267787.82	1.298	-3.8
##	PH	Oxygen.Filler	Bowl.Setpoint	Pressure.Setpoint	Air.Pressurer	Alch.Rel	
## 1	8.868498	-3.778093	8446.705	45.2	0.9930600	6.56	
## 2	8.765560	-3.473941	7197.162	46.0	0.9932421	7.14	
## 3	8.612129	-3.053945	7197.162	46.0	0.9932421	6.52	
## 4	8.913590	-1.843651	7197.162	46.0	0.9932421	6.48	
## 5	8.641433	-2.484414	7197.162	50.0	0.9932421	6.50	
## 6	8.492193	-2.728801	7197.162	46.0	0.9932421	6.50	
##	Carb.Rel	Balling.Lvl					
## 1	5.34	1.48					
## 2	5.58	3.04					
## 3	5.34	1.46					
## 4	5.50	1.48					
## 5	5.38	1.46					
## 6	5.42	1.44					

```
write_csv(final_predictions_df, "PH_Result.csv")
```