Data624\_group1\_Project2

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# Business Case

A new regulations by the FDA forces the ABC company to understand our manufacturing process as it relates to the pH of the bevrages we produced. To this effect, a predictive model has been commissioned by the Production manager to better understand the predictive factors and report on the predictive model of pH.

## Business Considrations

* VB- To be determined, level of accuracy, complexity, … based on our models results\*

## Deliverables

* A Executive level report of the findings
* A Detail tecnical reports to be reviewed by an outside consultant

## Thecnical Considerations

The team is opeating under a ver tight deadline, the deliverables have to be remitted on 05/22/2018. Since the team is operating remotely in various location, the following tools were adopted to enhanced efficient communication;

* Slack was used for daily communication during the project and for quick access to code and documentation.
* GoToMeeting was utilized for regular touch point meetings and on as needed basis.
* Github was used for version control management and to ensure each team member had access to the latest version of the project documentation
* R was used to perform analysis, R code can be found in Appendix A for Technical report

**Team Members**  
Prashant Bhuyan (Team Leader)  
Bruce Hao  
Cheryl Bowersox  
Chris Estevez  
Valerie Briot

#Please update Data explorer to below version  
pack\_URL= "https://cran.r-project.org/src/contrib/Archive/DataExplorer/DataExplorer\_0.4.0.tar.gz"  
if (!require("DataExplorer")) install.packages(pack\_URL, repos=NULL, type='source')  
  
library(psych) # EDA, describe function   
library(tidyverse) #  
library(knitr) #  
library(VIM) # correlation  
library(caret) # correlation, model building  
library(corrplot) # Correlation  
library(mice) # Imputation  
library(MASS) # BoxCox Transformation  
library("usdm")  
library(forecast) # alternate transform  
library(ranger) # Random Forest Model  
  
library(parallel) # Parallel processing for model building  
library(doParallel) # Parallel processing for model building  
  
library(randomForest) # Get Tree, model interpretation  
  
rm(pack\_URL)

# Data Set

The analysis will be performed on historical data. For reproducibility of the results, the data was loaded to and accessed from a Github repository.

#set file name - to be change by github link#  
beverages\_filename <- "https://raw.githubusercontent.com/vbriot28/Data624\_Group1\_FinalProject/master/StudentData.csv"  
  
# Load Trainning Data Set  
beverages <-read.csv(beverages\_filename, header=TRUE, sep=",",stringsAsFactors = F)  
  
#From DataExplorer  
data\_list <- list(beverages)  
  
PlotStr(data\_list, type="r")  
  
rm(data\_list)

dim(beverages)

## [1] 2571 33

summary(beverages)

## 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.:0.23917   
## Mode :character Median :5.347 Median :23.97 Median :0.27133   
## Mean :5.370 Mean :23.97 Mean :0.27712   
## 3rd Qu.:5.453 3rd Qu.:24.03 3rd Qu.:0.31200   
## Max. :5.700 Max. :24.32 Max. :0.47800   
## NA's :10 NA's :38 NA's :39   
## Carb.Pressure Carb.Temp PSC PSC.Fill   
## Min. :57.00 Min. :128.6 Min. :0.00200 Min. :0.0000   
## 1st Qu.:65.60 1st Qu.:138.4 1st Qu.:0.04800 1st Qu.:0.1000   
## Median :68.20 Median :140.8 Median :0.07600 Median :0.1800   
## Mean :68.19 Mean :141.1 Mean :0.08457 Mean :0.1954   
## 3rd Qu.:70.60 3rd Qu.:143.8 3rd Qu.:0.11200 3rd Qu.:0.2600   
## Max. :79.40 Max. :154.0 Max. :0.27000 Max. :0.6200   
## NA's :27 NA's :26 NA's :33 NA's :23   
## 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 : 65.20 Median :123.2 Median :46.40   
## Mean :0.05641 Mean : 24.57 Mean :122.6 Mean :47.92   
## 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   
## NA's :39 NA's :2 NA's :32 NA's :22   
## Hyd.Pressure1 Hyd.Pressure2 Hyd.Pressure3 Hyd.Pressure4   
## Min. :-0.80 Min. : 0.00 Min. :-1.20 Min. : 52.00   
## 1st Qu.: 0.00 1st Qu.: 0.00 1st Qu.: 0.00 1st Qu.: 86.00   
## Median :11.40 Median :28.60 Median :27.60 Median : 96.00   
## Mean :12.44 Mean :20.96 Mean :20.46 Mean : 96.29   
## 3rd Qu.:20.20 3rd Qu.:34.60 3rd Qu.:33.40 3rd Qu.:102.00   
## Max. :58.00 Max. :59.40 Max. :50.00 Max. :142.00   
## NA's :11 NA's :15 NA's :15 NA's :30   
## Filler.Level Filler.Speed Temperature Usage.cont   
## Min. : 55.8 Min. : 998 Min. :63.60 Min. :12.08   
## 1st Qu.: 98.3 1st Qu.:3888 1st Qu.:65.20 1st Qu.:18.36   
## Median :118.4 Median :3982 Median :65.60 Median :21.79   
## Mean :109.3 Mean :3687 Mean :65.97 Mean :20.99   
## 3rd Qu.:120.0 3rd Qu.:3998 3rd Qu.:66.40 3rd Qu.:23.75   
## Max. :161.2 Max. :4030 Max. :76.20 Max. :25.90   
## NA's :20 NA's :57 NA's :14 NA's :5   
## Carb.Flow Density MFR Balling   
## Min. : 26 Min. :0.240 Min. : 31.4 Min. :-0.170   
## 1st Qu.:1144 1st Qu.:0.900 1st Qu.:706.3 1st Qu.: 1.496   
## Median :3028 Median :0.980 Median :724.0 Median : 1.648   
## Mean :2468 Mean :1.174 Mean :704.0 Mean : 2.198   
## 3rd Qu.:3186 3rd Qu.:1.620 3rd Qu.:731.0 3rd Qu.: 3.292   
## Max. :5104 Max. :1.920 Max. :868.6 Max. : 4.012   
## NA's :2 NA's :1 NA's :212 NA's :1   
## Pressure.Vacuum PH Oxygen.Filler Bowl.Setpoint   
## Min. :-6.600 Min. :7.880 Min. :0.00240 Min. : 70.0   
## 1st Qu.:-5.600 1st Qu.:8.440 1st Qu.:0.02200 1st Qu.:100.0   
## Median :-5.400 Median :8.540 Median :0.03340 Median :120.0   
## Mean :-5.216 Mean :8.546 Mean :0.04684 Mean :109.3   
## 3rd Qu.:-5.000 3rd Qu.:8.680 3rd Qu.:0.06000 3rd Qu.:120.0   
## Max. :-3.600 Max. :9.360 Max. :0.40000 Max. :140.0   
## NA's :4 NA's :12 NA's :2   
## Pressure.Setpoint Air.Pressurer Alch.Rel Carb.Rel   
## Min. :44.00 Min. :140.8 Min. :5.280 Min. :4.960   
## 1st Qu.:46.00 1st Qu.:142.2 1st Qu.:6.540 1st Qu.:5.340   
## Median :46.00 Median :142.6 Median :6.560 Median :5.400   
## Mean :47.62 Mean :142.8 Mean :6.897 Mean :5.437   
## 3rd Qu.:50.00 3rd Qu.:143.0 3rd Qu.:7.240 3rd Qu.:5.540   
## Max. :52.00 Max. :148.2 Max. :8.620 Max. :6.060   
## NA's :12 NA's :9 NA's :10   
## Balling.Lvl   
## Min. :0.00   
## 1st Qu.:1.38   
## Median :1.48   
## Mean :2.05   
## 3rd Qu.:3.14   
## Max. :3.66   
## NA's :1

object.size(beverages)

## 642096 bytes

The dataset is comprised of 33 variables and 2571 observations. At first glance, it is clear that some variables have missing values that will need to be addressed. All the variables beside Brand.code are numeric.

# Data Exploration and Statistic Measures

The purpose of the data exploration and statistic measures phase is to understand the data to determine how to process the dataset for modelling.

## Descriptive Statistics

Descriptive statistics were calculated to examine the basic features of the data.

#Calculate mean missing values per variable  
missing\_values <- beverages %>%   
 summarize\_all(funs(sum(is.na(.))))  
  
missing\_values\_ratio <- beverages %>%   
 summarize\_all(funs(sum(is.na(.)) / length(.)\*100))  
  
#Use Describe Package to calculate Descriptive Statistic  
(beverages\_d <- describe(beverages, na.rm=TRUE, interp=FALSE, skew=TRUE, ranges=TRUE, trim=.1, type=3, check=TRUE, fast=FALSE, quant=c(.25,.75), IQR=TRUE))

## vars n mean sd median trimmed mad min  
## Brand.Code\* 1 2571 NaN NA NA NaN NA Inf  
## Carb.Volume 2 2561 5.37 0.11 5.35 5.37 0.11 5.04  
## Fill.Ounces 3 2533 23.97 0.09 23.97 23.98 0.08 23.63  
## PC.Volume 4 2532 0.28 0.06 0.27 0.27 0.05 0.08  
## Carb.Pressure 5 2544 68.19 3.54 68.20 68.12 3.56 57.00  
## Carb.Temp 6 2545 141.09 4.04 140.80 140.99 3.85 128.60  
## PSC 7 2538 0.08 0.05 0.08 0.08 0.05 0.00  
## PSC.Fill 8 2548 0.20 0.12 0.18 0.18 0.12 0.00  
## PSC.CO2 9 2532 0.06 0.04 0.04 0.05 0.03 0.00  
## Mnf.Flow 10 2569 24.57 119.48 65.20 21.07 169.02 -100.20  
## Carb.Pressure1 11 2539 122.59 4.74 123.20 122.54 4.45 105.60  
## Fill.Pressure 12 2549 47.92 3.18 46.40 47.71 2.37 34.60  
## Hyd.Pressure1 13 2560 12.44 12.43 11.40 10.84 16.90 -0.80  
## Hyd.Pressure2 14 2556 20.96 16.39 28.60 21.05 13.34 0.00  
## Hyd.Pressure3 15 2556 20.46 15.98 27.60 20.51 13.94 -1.20  
## Hyd.Pressure4 16 2541 96.29 13.12 96.00 95.45 11.86 52.00  
## Filler.Level 17 2551 109.25 15.70 118.40 111.04 9.19 55.80  
## Filler.Speed 18 2514 3687.20 770.82 3982.00 3919.99 47.44 998.00  
## Temperature 19 2557 65.97 1.38 65.60 65.80 0.89 63.60  
## Usage.cont 20 2566 20.99 2.98 21.79 21.25 3.19 12.08  
## Carb.Flow 21 2569 2468.35 1073.70 3028.00 2601.14 326.17 26.00  
## Density 22 2570 1.17 0.38 0.98 1.15 0.15 0.24  
## MFR 23 2359 704.05 73.90 724.00 718.16 15.42 31.40  
## Balling 24 2570 2.20 0.93 1.65 2.13 0.37 -0.17  
## Pressure.Vacuum 25 2571 -5.22 0.57 -5.40 -5.25 0.59 -6.60  
## PH 26 2567 8.55 0.17 8.54 8.55 0.18 7.88  
## Oxygen.Filler 27 2559 0.05 0.05 0.03 0.04 0.02 0.00  
## Bowl.Setpoint 28 2569 109.33 15.30 120.00 111.35 0.00 70.00  
## Pressure.Setpoint 29 2559 47.62 2.04 46.00 47.60 0.00 44.00  
## Air.Pressurer 30 2571 142.83 1.21 142.60 142.58 0.59 140.80  
## Alch.Rel 31 2562 6.90 0.51 6.56 6.84 0.06 5.28  
## Carb.Rel 32 2561 5.44 0.13 5.40 5.43 0.12 4.96  
## Balling.Lvl 33 2570 2.05 0.87 1.48 1.98 0.21 0.00  
## max range skew kurtosis se IQR Q0.25  
## Brand.Code\* -Inf -Inf NA NA NA NA NA  
## Carb.Volume 5.70 0.66 0.39 -0.47 0.00 0.16 5.29  
## Fill.Ounces 24.32 0.69 -0.02 0.86 0.00 0.11 23.92  
## PC.Volume 0.48 0.40 0.34 0.67 0.00 0.07 0.24  
## Carb.Pressure 79.40 22.40 0.18 -0.01 0.07 5.00 65.60  
## Carb.Temp 154.00 25.40 0.25 0.24 0.08 5.40 138.40  
## PSC 0.27 0.27 0.85 0.65 0.00 0.06 0.05  
## PSC.Fill 0.62 0.62 0.93 0.77 0.00 0.16 0.10  
## PSC.CO2 0.24 0.24 1.73 3.73 0.00 0.06 0.02  
## Mnf.Flow 229.40 329.60 0.00 -1.87 2.36 240.80 -100.00  
## Carb.Pressure1 140.20 34.60 0.05 0.14 0.09 6.40 119.00  
## Fill.Pressure 60.40 25.80 0.55 1.41 0.06 4.00 46.00  
## Hyd.Pressure1 58.00 58.80 0.78 -0.14 0.25 20.20 0.00  
## Hyd.Pressure2 59.40 59.40 -0.30 -1.56 0.32 34.60 0.00  
## Hyd.Pressure3 50.00 51.20 -0.32 -1.57 0.32 33.40 0.00  
## Hyd.Pressure4 142.00 90.00 0.55 0.63 0.26 16.00 86.00  
## Filler.Level 161.20 105.40 -0.85 0.05 0.31 21.70 98.30  
## Filler.Speed 4030.00 3032.00 -2.87 6.71 15.37 110.00 3888.00  
## Temperature 76.20 12.60 2.39 10.16 0.03 1.20 65.20  
## Usage.cont 25.90 13.82 -0.54 -1.02 0.06 5.39 18.36  
## Carb.Flow 5104.00 5078.00 -0.99 -0.58 21.18 2042.00 1144.00  
## Density 1.92 1.68 0.53 -1.20 0.01 0.72 0.90  
## MFR 868.60 837.20 -5.09 30.46 1.52 24.70 706.30  
## Balling 4.01 4.18 0.59 -1.39 0.02 1.80 1.50  
## Pressure.Vacuum -3.60 3.00 0.53 -0.03 0.01 0.60 -5.60  
## PH 9.36 1.48 -0.29 0.06 0.00 0.24 8.44  
## Oxygen.Filler 0.40 0.40 2.66 11.09 0.00 0.04 0.02  
## Bowl.Setpoint 140.00 70.00 -0.97 -0.06 0.30 20.00 100.00  
## Pressure.Setpoint 52.00 8.00 0.20 -1.60 0.04 4.00 46.00  
## Air.Pressurer 148.20 7.40 2.25 4.73 0.02 0.80 142.20  
## Alch.Rel 8.62 3.34 0.88 -0.85 0.01 0.70 6.54  
## Carb.Rel 6.06 1.10 0.50 -0.29 0.00 0.20 5.34  
## Balling.Lvl 3.66 3.66 0.59 -1.49 0.02 1.76 1.38  
## Q0.75  
## Brand.Code\* NA  
## Carb.Volume 5.45  
## Fill.Ounces 24.03  
## PC.Volume 0.31  
## Carb.Pressure 70.60  
## Carb.Temp 143.80  
## PSC 0.11  
## PSC.Fill 0.26  
## PSC.CO2 0.08  
## Mnf.Flow 140.80  
## Carb.Pressure1 125.40  
## Fill.Pressure 50.00  
## Hyd.Pressure1 20.20  
## Hyd.Pressure2 34.60  
## Hyd.Pressure3 33.40  
## Hyd.Pressure4 102.00  
## Filler.Level 120.00  
## Filler.Speed 3998.00  
## Temperature 66.40  
## Usage.cont 23.75  
## Carb.Flow 3186.00  
## Density 1.62  
## MFR 731.00  
## Balling 3.29  
## Pressure.Vacuum -5.00  
## PH 8.68  
## Oxygen.Filler 0.06  
## Bowl.Setpoint 120.00  
## Pressure.Setpoint 50.00  
## Air.Pressurer 143.00  
## Alch.Rel 7.24  
## Carb.Rel 5.54  
## Balling.Lvl 3.14

beverages\_d$missing <- t(missing\_values)  
beverages\_d$miss\_ratio <- t(round(missing\_values\_ratio,4))  
  
beverages\_d <- beverages\_d %>%   
 dplyr::select(n, missing, miss\_ratio, mean, sd, min, max, skew, kurtosis, median, IQR, Q0.25, Q0.75)  
  
kable(beverages\_d)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | n | missing | miss\_ratio | mean | sd | min | max | skew | kurtosis | median | IQR | Q0.25 | Q0.75 |
| Brand.Code\* | 2571 | 0 | 0.0000 | NaN | NA | Inf | -Inf | NA | NA | NA | NA | NA | NA |
| Carb.Volume | 2561 | 10 | 0.3890 | 5.3701978 | 0.1063852 | 5.0400000 | 5.700 | 0.3922121 | -0.4669916 | 5.3466667 | 0.1600000 | 5.2933333 | 5.453333 |
| Fill.Ounces | 2533 | 38 | 1.4780 | 23.9747546 | 0.0875299 | 23.6333333 | 24.320 | -0.0215452 | 0.8624714 | 23.9733333 | 0.1066667 | 23.9200000 | 24.026667 |
| PC.Volume | 2532 | 39 | 1.5169 | 0.2771187 | 0.0606953 | 0.0793333 | 0.478 | 0.3396269 | 0.6699690 | 0.2713333 | 0.0728333 | 0.2391667 | 0.312000 |
| Carb.Pressure | 2544 | 27 | 1.0502 | 68.1895755 | 3.5382039 | 57.0000000 | 79.400 | 0.1822162 | -0.0138046 | 68.2000000 | 5.0000000 | 65.6000000 | 70.600000 |
| Carb.Temp | 2545 | 26 | 1.0113 | 141.0949234 | 4.0373861 | 128.6000000 | 154.000 | 0.2468280 | 0.2375822 | 140.8000000 | 5.4000000 | 138.4000000 | 143.800000 |
| PSC | 2538 | 33 | 1.2835 | 0.0845737 | 0.0492690 | 0.0020000 | 0.270 | 0.8491445 | 0.6480498 | 0.0760000 | 0.0640000 | 0.0480000 | 0.112000 |
| PSC.Fill | 2548 | 23 | 0.8946 | 0.1953689 | 0.1177817 | 0.0000000 | 0.620 | 0.9334450 | 0.7691466 | 0.1800000 | 0.1600000 | 0.1000000 | 0.260000 |
| PSC.CO2 | 2532 | 39 | 1.5169 | 0.0564139 | 0.0430387 | 0.0000000 | 0.240 | 1.7288937 | 3.7250025 | 0.0400000 | 0.0600000 | 0.0200000 | 0.080000 |
| Mnf.Flow | 2569 | 2 | 0.0778 | 24.5689373 | 119.4811263 | -100.2000000 | 229.400 | 0.0041430 | -1.8697072 | 65.2000000 | 240.8000000 | -100.0000000 | 140.800000 |
| Carb.Pressure1 | 2539 | 32 | 1.2447 | 122.5863726 | 4.7428819 | 105.6000000 | 140.200 | 0.0543587 | 0.1418265 | 123.2000000 | 6.4000000 | 119.0000000 | 125.400000 |
| Fill.Pressure | 2549 | 22 | 0.8557 | 47.9221656 | 3.1775457 | 34.6000000 | 60.400 | 0.5471107 | 1.4067532 | 46.4000000 | 4.0000000 | 46.0000000 | 50.000000 |
| Hyd.Pressure1 | 2560 | 11 | 0.4278 | 12.4375781 | 12.4332538 | -0.8000000 | 58.000 | 0.7798043 | -0.1426463 | 11.4000000 | 20.2000000 | 0.0000000 | 20.200000 |
| Hyd.Pressure2 | 2556 | 15 | 0.5834 | 20.9610329 | 16.3863066 | 0.0000000 | 59.400 | -0.3019570 | -1.5592984 | 28.6000000 | 34.6000000 | 0.0000000 | 34.600000 |
| Hyd.Pressure3 | 2556 | 15 | 0.5834 | 20.4584507 | 15.9757236 | -1.2000000 | 50.000 | -0.3189061 | -1.5745834 | 27.6000000 | 33.4000000 | 0.0000000 | 33.400000 |
| Hyd.Pressure4 | 2541 | 30 | 1.1669 | 96.2888627 | 13.1225594 | 52.0000000 | 142.000 | 0.5459786 | 0.6340041 | 96.0000000 | 16.0000000 | 86.0000000 | 102.000000 |
| Filler.Level | 2551 | 20 | 0.7779 | 109.2523716 | 15.6984241 | 55.8000000 | 161.200 | -0.8482847 | 0.0460488 | 118.4000000 | 21.7000000 | 98.3000000 | 120.000000 |
| Filler.Speed | 2514 | 57 | 2.2170 | 3687.1988862 | 770.8200208 | 998.0000000 | 4030.000 | -2.8700359 | 6.7059692 | 3982.0000000 | 110.0000000 | 3888.0000000 | 3998.000000 |
| Temperature | 2557 | 14 | 0.5445 | 65.9675401 | 1.3827783 | 63.6000000 | 76.200 | 2.3869732 | 10.1612904 | 65.6000000 | 1.2000000 | 65.2000000 | 66.400000 |
| Usage.cont | 2566 | 5 | 0.1945 | 20.9929618 | 2.9779364 | 12.0800000 | 25.900 | -0.5353253 | -1.0170230 | 21.7900000 | 5.3950000 | 18.3600000 | 23.755000 |
| Carb.Flow | 2569 | 2 | 0.0778 | 2468.3542234 | 1073.6964743 | 26.0000000 | 5104.000 | -0.9877287 | -0.5826893 | 3028.0000000 | 2042.0000000 | 1144.0000000 | 3186.000000 |
| Density | 2570 | 1 | 0.0389 | 1.1736498 | 0.3775269 | 0.2400000 | 1.920 | 0.5260149 | -1.1992070 | 0.9800000 | 0.7200000 | 0.9000000 | 1.620000 |
| MFR | 2359 | 212 | 8.2458 | 704.0492582 | 73.8983094 | 31.4000000 | 868.600 | -5.0917729 | 30.4558939 | 724.0000000 | 24.7000000 | 706.3000000 | 731.000000 |
| Balling | 2570 | 1 | 0.0389 | 2.1977696 | 0.9310914 | -0.1700000 | 4.012 | 0.5939224 | -1.3855651 | 1.6480000 | 1.7960000 | 1.4960000 | 3.292000 |
| Pressure.Vacuum | 2571 | 0 | 0.0000 | -5.2161027 | 0.5699933 | -6.6000000 | -3.600 | 0.5256608 | -0.0313126 | -5.4000000 | 0.6000000 | -5.6000000 | -5.000000 |
| PH | 2567 | 4 | 0.1556 | 8.5456486 | 0.1725162 | 7.8800000 | 9.360 | -0.2906437 | 0.0644294 | 8.5400000 | 0.2400000 | 8.4400000 | 8.680000 |
| Oxygen.Filler | 2559 | 12 | 0.4667 | 0.0468426 | 0.0466436 | 0.0024000 | 0.400 | 2.6603955 | 11.0882098 | 0.0334000 | 0.0380000 | 0.0220000 | 0.060000 |
| Bowl.Setpoint | 2569 | 2 | 0.0778 | 109.3265862 | 15.3031541 | 70.0000000 | 140.000 | -0.9743842 | -0.0564212 | 120.0000000 | 20.0000000 | 100.0000000 | 120.000000 |
| Pressure.Setpoint | 2559 | 12 | 0.4667 | 47.6153966 | 2.0390474 | 44.0000000 | 52.000 | 0.2031970 | -1.6012622 | 46.0000000 | 4.0000000 | 46.0000000 | 50.000000 |
| Air.Pressurer | 2571 | 0 | 0.0000 | 142.8339946 | 1.2119170 | 140.8000000 | 148.200 | 2.2521053 | 4.7336291 | 142.6000000 | 0.8000000 | 142.2000000 | 143.000000 |
| Alch.Rel | 2562 | 9 | 0.3501 | 6.8974161 | 0.5052753 | 5.2800000 | 8.620 | 0.8836378 | -0.8506221 | 6.5600000 | 0.7000000 | 6.5400000 | 7.240000 |
| Carb.Rel | 2561 | 10 | 0.3890 | 5.4367825 | 0.1287183 | 4.9600000 | 6.060 | 0.5032472 | -0.2949480 | 5.4000000 | 0.2000000 | 5.3400000 | 5.540000 |
| Balling.Lvl | 2570 | 1 | 0.0389 | 2.0500078 | 0.8703089 | 0.0000000 | 3.660 | 0.5858456 | -1.4858636 | 1.4800000 | 1.7600000 | 1.3800000 | 3.140000 |

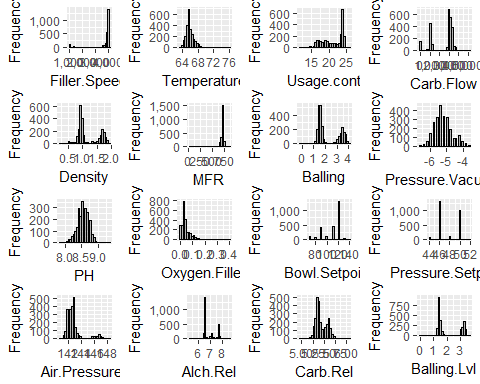
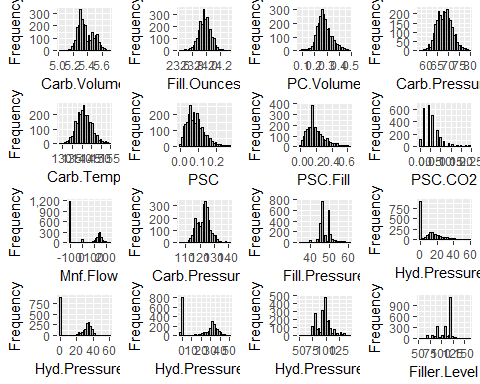
rm(beverages\_d,missing\_values,missing\_values\_ratio)

From the skewness coefficient, we observed that some variables may have a right skewed distribution (PSC.CO2, Temperature, Oxygen.Filler, Air.Pressurer) or a left skewed distribution (Filler.Speed, MFR). As we observed prior, we have missing values for some of the variables, we will need to take this into considerations.

## Analysis of predictors

We will now examined each predictor to understand their distribution and determine whether any transformation is required.

# from DataExplorer Package  
  
DataExplorer::HistogramContinuous(beverages)

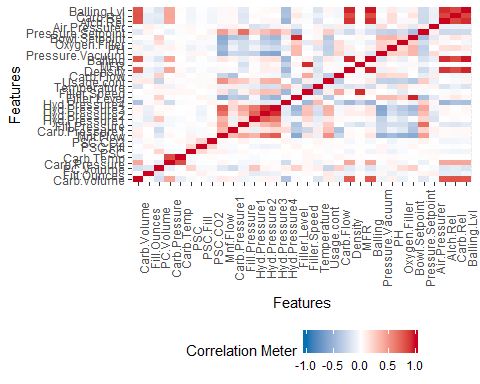


## Variable to Variable Analysis

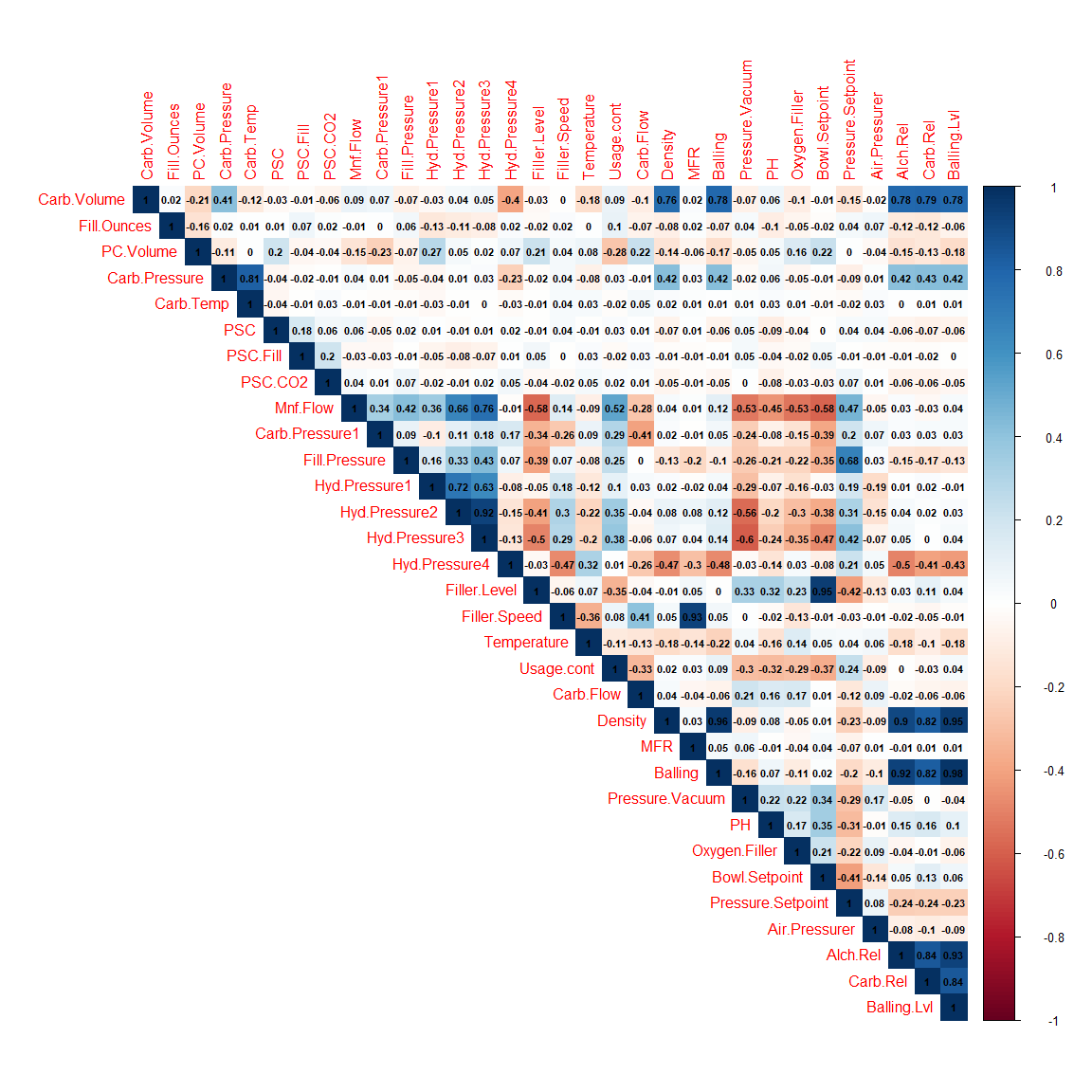
### Correlation Analysis

The correlation matrix shown below highlights correlations among several predictor variables.

# From DataExplorer Package  
#plot\_correlation(beverages, use = "pairwise.complete.obs")  
DataExplorer::CorrelationContinuous(beverages, use = "pairwise.complete.obs")



cor\_mx =cor(beverages%>% dplyr::select(-Brand.Code) ,use="pairwise.complete.obs", method = "pearson")  
  
corrplot(cor\_mx, method = "color",type = "upper", order = "original", number.cex = .7,addCoef.col = "black", #Add coefficient of correlation  
 tl.srt = 90,# Text label color and rotation  
 diag = TRUE)# hide correlation coefficient on the principal diagonal



rm(cor\_mx)

This section will test the predictor variables to determine if there is correlation among them. Variance inflaction factor (VIF) is used to detect multicollinearity, specifically among the entire set of predictors versus within pairs of variables.

Testing for collinearity among the predictor variables, we see that none of the numeric predictor variables appear to have a problem with collinearity based on their low VIF scores.

# from VIM Package  
beverages\_predictors <- dplyr::select(beverages, -PH)  
  
numeric\_fields <- dplyr::select\_if(beverages\_predictors, is.numeric)[, 3:15]  
  
usdm::vifcor(numeric\_fields)

## 1 variables from the 13 input variables have collinearity problem:   
##   
## Hyd.Pressure3   
##   
## After excluding the collinear variables, the linear correlation coefficients ranges between:   
## min correlation ( Fill.Pressure ~ PSC.Fill ): 0.001947733   
## max correlation ( Carb.Temp ~ Carb.Pressure ): 0.8233431   
##   
## ---------- VIFs of the remained variables --------   
## Variables VIF  
## 1 PC.Volume 1.340747  
## 2 Carb.Pressure 4.043068  
## 3 Carb.Temp 3.731096  
## 4 PSC 1.120366  
## 5 PSC.Fill 1.093121  
## 6 PSC.CO2 1.053359  
## 7 Mnf.Flow 2.404566  
## 8 Carb.Pressure1 1.312199  
## 9 Fill.Pressure 1.291768  
## 10 Hyd.Pressure1 2.586587  
## 11 Hyd.Pressure2 3.752048  
## 12 Hyd.Pressure4 1.325928

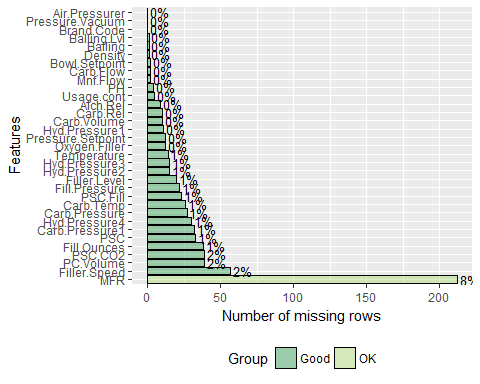
rm(beverages\_predictors,numeric\_fields)

# Data Transformation

## Missing Values

We have some observed some predictors with missing values however no predictors are missing more than 8% of data and no rows are missing more than ?? of data. We will feel confortable with imputing the missing data.

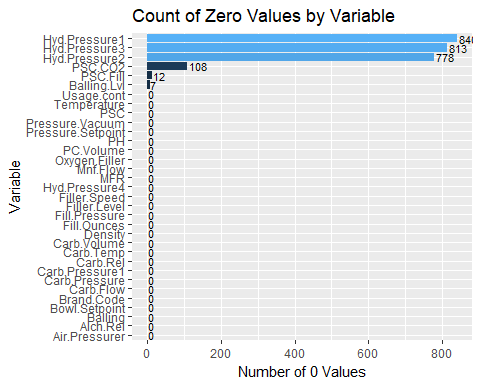
# From Data Explorer   
PlotMissing(beverages)



## Examination of Zero values

Some cases, a zero values are actually representative of missing data, is this the case here?

df <- setNames(data.frame(colSums(beverages==0, na.rm = T)), 'Count')  
   
df$Variable <- rownames(df)  
  
rownames(df) <- NULL  
  
df %>% dplyr::filter(!Variable %in% c("Brand.code")) %>%   
ggplot(aes(x=reorder(Variable, Count), y=Count, fill=Count)) +  
 geom\_bar(stat="identity") + coord\_flip() + guides(fill=FALSE) +  
 xlab("Variable") + ylab("Number of 0 Values") +   
 ggtitle("Count of Zero Values by Variable") +  
 geom\_text(aes(label=Count), vjust=.5, hjust=-.1,position= position\_dodge(width=0.5),size=3, color="black")



rm(df)

We had observed the high number of 0 values for variables; Hyd.Pressure1, Hyd.Pressure2, and Hyd.Pressure3 and we will add a dummy variable to flag such data. Also, based on correlation coefficient, we will probably drop Hyd.Pressure3.

Brand.code has a proportion of its data that is unspecify, we will flag these records with a “U’, for”unknown“.

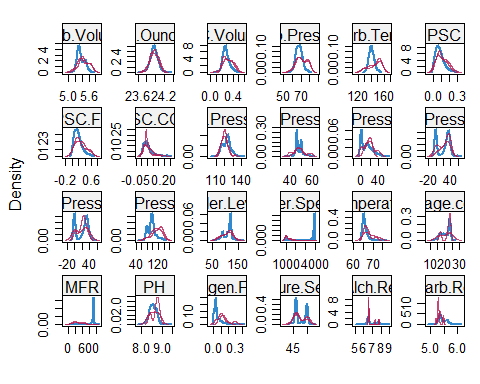
## Data Imputation

Since we have a limited amount of missing values accross predictors, we will impute the data. We will use the mice package.

# Replace \*BLANK Brand.Code with "U"  
  
beverages$Brand.Code[beverages$Brand.Code==""]= "U"  
  
summary(beverages$Brand.Code)

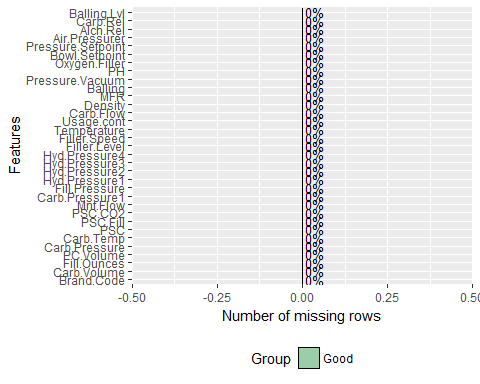
## Length Class Mode   
## 2571 character character

mice\_imputes =mice(beverages, m = 2, maxit = 2, print = FALSE,seed = 143)  
densityplot(mice\_imputes)



The imputed density distribution is indicated in red.

# Applied the imputed values V1  
beverages\_v1 =complete(mice\_imputes)  
  
# Plot missing values  
PlotMissing(beverages\_v1)



rm(mice\_imputes)

We have addressed the missing values. We will continue to possible problem with predictors by investigation possible near-zero variances predictors.

## Near-Zero Variance Predictors

By default, a predictor is classified as near-zero variance if the percentage of unique values in the samples is less than 10% and when the frequency ratio mentioned above is greater than 19 (95/5).

These default values can be changed by setting the arguments uniqueCut and freqCut.

# From Caret package  
#  
x = nearZeroVar(beverages\_v1, saveMetrics = TRUE)  
  
#str(x, vec.len = 2)  
  
x[x[,"zeroVar"] > 0, ]

## [1] freqRatio percentUnique zeroVar nzv   
## <0 rows> (or 0-length row.names)

x[x[,"nzv"] > 0, ]

## freqRatio percentUnique zeroVar nzv  
## Hyd.Pressure1 31.22222 9.529366 FALSE TRUE

rm(x)

Since Hyd.Pressure1 is the only variable with near zero variance and the percentate is very close to cut-off, we will not drop this variables.

## Features Creation

**Invalid data or bimodal distributions**

Based on the histograms above, it’s clear that some variables have bimodal distributions or a large number of records with what appear to be invalid data, for example, Mnf.Flow and the Hyd.Pressure variables. While some models may be able to deal with such data without modification, other models may not. As such, se will create dummy variables to flag which distribution a given record belongs to within each variable.

beverages\_v2 = beverages\_v1 %>%  
 mutate(Mnf.Flow.lt0 = if\_else(Mnf.Flow < 0, 1, 0)) %>%   
 mutate(Hyd.Pressure1.lte0 = if\_else(Hyd.Pressure1 <= 0 ,1, 0)) %>%   
 mutate(Hyd.Pressure2.lte0 = if\_else(Hyd.Pressure2 <= 0, 1, 0)) %>% #remove Hyd.Pressure3 since variable dropped  
 mutate(Filler.Speed.lt2500 = if\_else(Filler.Speed < 2500, 1, 0)) %>%   
 mutate(Carb.Flow.lt2500 = if\_else(Carb.Flow < 2000, 1, 0)) %>%   
 mutate(Balling.lt.2.5 = if\_else(Balling < 2.5, 1, 0))

## Dropping predictors

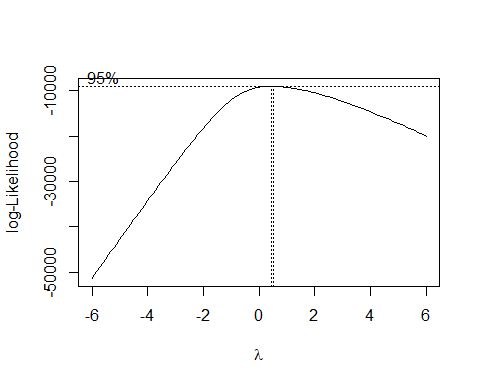
Based on the correlation results we are proposing the drop the following predictors: Density, Balling.Lvl, Carb.Rel, Alch.Rel, and Hyd.Pressure3.

# Drop some predictors due to high correlation   
beverages\_v2$Density <- NULL  
beverages\_v2$Balling.Lvl <- NULL  
beverages\_v2$Carb.Rel <- NULL  
beverages\_v2$Alch.Rel <- NULL  
beverages\_v2$Hyd.Pressure3 <- NULL

## Data Transformation

We have observed significant skewness for the following variables: PSC and Oxygen.Filler. We are proposing to apply boxcox tranformation to these variables.

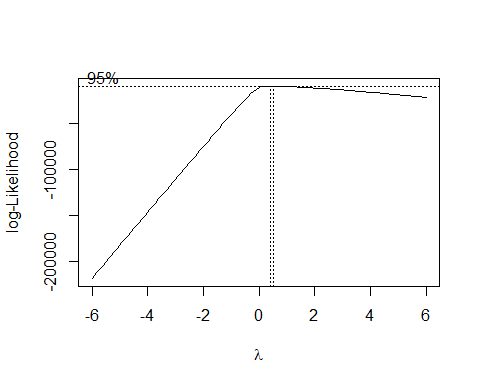
# Copy our data set  
beverages\_v3 <- beverages\_v2  
offset <- 0.0000001  
  
# PSC  
Box = boxcox(beverages\_v3$PSC ~ 1, # Transform PSC Column as a single vector  
 lambda = seq(-6,6,0.1) # Try values -6 to 6 by 0.1  
 )



Cox = data.frame(Box$x, Box$y) # Create a data frame with the results  
  
Cox2 = Cox[with(Cox, order(-Cox$Box.y)),] # Order the new data frame by decreasing y  
  
Cox2[1,] # Display the lambda with the greatest

## Box.x Box.y  
## 66 0.5 -9024.124

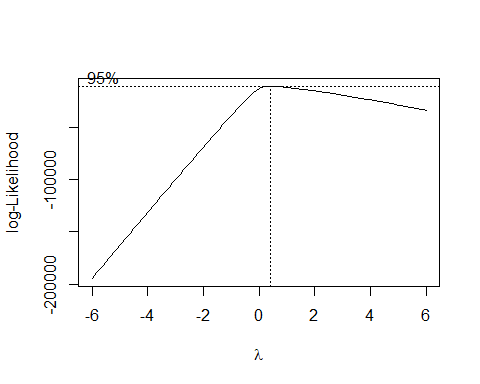
# log likelihood  
  
  
lambda.PSC = Cox2[1, "Box.x"] # Extract that lambda  
  
#------------------------------#  
  
#PSC.FILL  
beverages\_v3$PSC.Fill <- beverages\_v3$PSC.Fill + offset  
  
Box = boxcox(beverages\_v3$PSC.Fill ~ 1, # Transform PSC Column as a single vector  
 lambda = seq(-6,6,0.1) # Try values -6 to 6 by 0.1  
 )



Cox = data.frame(Box$x, Box$y) # Create a data frame with the results  
  
Cox2 = Cox[with(Cox, order(-Cox$Box.y)),] # Order the new data frame by decreasing y  
  
Cox2[1,] # Display the lambda with the greatest

## Box.x Box.y  
## 66 0.5 -9175.448

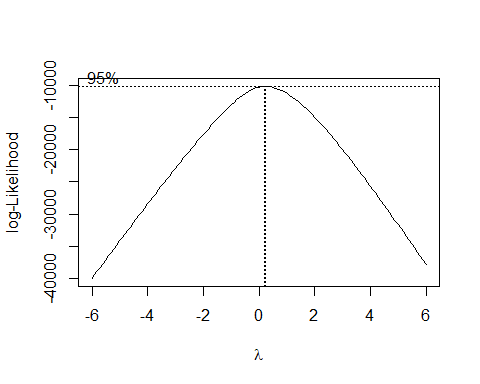
# log likelihood  
  
  
lambda.PSC\_Fill = Cox2[1, "Box.x"] # Extract that lambda  
  
#------------------------------#  
  
#PSC.CO2  
beverages\_v3$PSC.CO2 <- beverages\_v3$PSC.CO2 + offset  
  
Box = boxcox(beverages\_v3$PSC.CO2 ~ 1, # Transform PSC Column as a single vector  
 lambda = seq(-6,6,0.1) # Try values -6 to 6 by 0.1  
 )



Cox = data.frame(Box$x, Box$y) # Create a data frame with the results  
  
Cox2 = Cox[with(Cox, order(-Cox$Box.y)),] # Order the new data frame by decreasing y  
  
Cox2[1,] # Display the lambda with the greatest

## Box.x Box.y  
## 65 0.4 -10243.13

# log likelihood  
  
  
lambda.PSC\_CO2 = Cox2[1, "Box.x"] # Extract that lambda  
  
#------------------------------#  
  
#Oxygen.Filler  
Box = boxcox(beverages\_v3$Oxygen.Filler ~ 1, # Transform PSC Column as a single vector  
 lambda = seq(-6,6,0.1) # Try values -6 to 6 by 0.1  
 )



Cox = data.frame(Box$x, Box$y) # Create a data frame with the results  
  
Cox2 = Cox[with(Cox, order(-Cox$Box.y)),] # Order the new data frame by decreasing y  
  
Cox2[1,] # Display the lambda with the greatest

## Box.x Box.y  
## 63 0.2 -10203.42

# log likelihood  
  
  
lambda.Oxygen\_Filler = Cox2[1, "Box.x"] # Extract that lambda  
  
  
rm(offset)

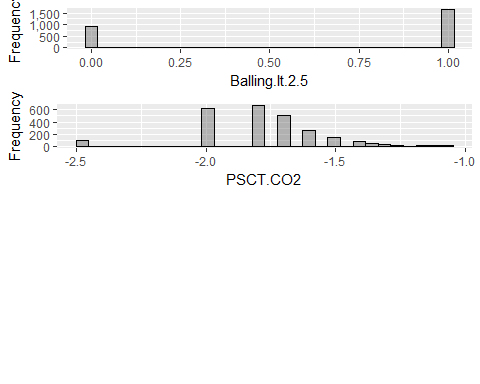
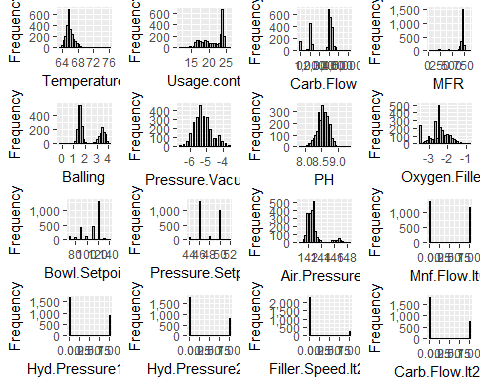
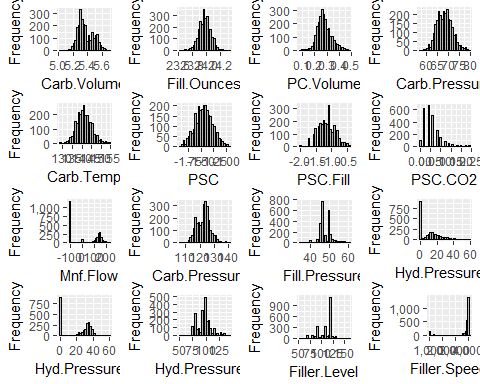
The R code to produce the lambda value is not working. I believe is due to the object being a list.

The lambda for predictor PSC is 0.5 The lambda for predictor PSC.FIL is 0.5 The lambad for predictor PSC.CO2 is 0.4 The lambda for predictor Oxygen.Filler is 0.2

# Transform the original data  
beverages\_v3$PSC = (beverages\_v3$PSC ^ lambda.PSC - 1)/lambda.PSC   
beverages\_v3$PSC.Fill = (beverages\_v3$PSC.Fill ^ lambda.PSC\_Fill - 1)/lambda.PSC\_Fill   
beverages\_v3$PSCT.CO2 = (beverages\_v3$PSC.CO2 ^ lambda.PSC\_CO2 - 1)/lambda.PSC\_CO2   
beverages\_v3$Oxygen.Filler = (beverages\_v3$Oxygen.Filler ^ lambda.Oxygen\_Filler - 1)/lambda.Oxygen\_Filler  
  
  
#rm(Box,Cox,Cox2,lambda.Oxygen\_Filler,lambda.PSC\_CO2,lambda.PSC\_Fill,lambda.PSC)

These complete the transformation on the data set, any additional tranfomations will be performed in the building model phase as they will be model dependent.

HistogramContinuous(beverages\_v3)



#?HistogramContinuous()

## Categorical Response (Ph)

Our goal is to build a model that accurately predicts pH levels given a large number of factors. Based on pH values of common substances (<https://en.wikipedia.org/wiki/PH>), values below 8 indicate higher levels of acidity than pH values above 8. Since we have many factors that may influence alkalinity but not many observations, we chose to use a random forest model to classify observations.

The model is built using data that has been imputed of missing values. Further, blank spaces in the variable Brand.Code were replaced with ‘U’ for known. Highly correlated variables were dropped and the data was also transformed to address problems related to skewness in the distribution of certain variables.

Since the minimum pH value in our data is 7.88 and most pH values are greater than 8 with a mean value of 8.546 and a max value of 9.360, we have bucketed values below or equal to 8.5 as “Neutral” and values above 8.5 as “Alkaline”. As such, our goal is to accurately predict whether or not a beverage is more likely to be alkaline or neutral given a plethora of potentially influential factors.

In the original data, we have 2,571 observations. In order to create a predictive model, we will split the data into training and test sets based on a 70/30 percent split. After splitting the data, we have 1,799 observations across 39 factors in the training data and 772 observations across 39 factors in the test data.

beverages\_v4 <- beverages\_v1  
  
beverages\_v4$PH <- ifelse(beverages\_v4$PH <= 8.5, "Neutral", "Alkaline")  
beverages\_v4$PH <- factor(beverages\_v4$PH )  
beverages\_v4$Brand.Code <- factor(beverages\_v4$Brand.Code)

# Model Buidlings

We will explore and build various model to identify the most significant variable that influence the pH and be able to predict pH values.

## Data Splitting

We have 4 versions of the data set that we will use to based our models. Additional transformations such as scaling and centering may be also applied at the time of model building;

* version 1; Imputed data set, with brand.code missing values (Blank) impuated as ‘U’
* version 2; based on version 1, with additional feagures and dropped highly correlated variables
* version 3; based on version 2, with box-cox transformations applied to very skewed variables
* version 4: based on version 1, with converting PH to categorical variable (Neutral, Alkaline)

# Where Imputed data is the dataset such as beverages\_v1  
set.seed(143)   
sample = sample.int(n = nrow(beverages), size = floor(.70\*nrow(beverages)), replace = F)  
  
beverages\_v1\_train = beverages\_v1[sample, ]  
beverages\_v1\_test = beverages\_v1[-sample,]  
  
beverages\_v2\_train = beverages\_v2[sample, ]  
beverages\_v2\_test = beverages\_v2[-sample,]  
  
beverages\_v3\_train = beverages\_v3[sample, ]  
beverages\_v3\_test = beverages\_v3[-sample,]  
  
beverages\_v4\_train = beverages\_v4[sample, ]  
beverages\_v4\_test = beverages\_v4[-sample,]  
  
rm(beverages\_v1,beverages\_v2,beverages\_v3,beverages\_v4,beverages,sample)

# Set-up parallel Enviroment to increase performance  
Mycluster =makeCluster(detectCores()-1)  
registerDoParallel(Mycluster)  
  
myControl = trainControl(method = 'cv', number = 5,   
 verboseIter = FALSE, savePredictions = TRUE,allowParallel = T)

## GLM

# first, start with a general linear model   
set.seed(143)  
GLM\_M1\_Data1 = train(PH ~ ., data = beverages\_v1\_train , metric = 'RMSE', method = 'glm',preProcess = c('center', 'scale'), trControl = myControl)  
GLM\_M1\_Data1

## Generalized Linear Model   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results:  
##   
## RMSE Rsquared MAE   
## 0.1321942 0.4198535 0.1016524

set.seed(143)  
GLM\_M2\_Data2 = train(PH ~ ., data = beverages\_v2\_train , metric = 'RMSE', method = 'glm', trControl = myControl)  
GLM\_M2\_Data2

## Generalized Linear Model   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results:  
##   
## RMSE Rsquared MAE   
## 0.1327388 0.4153035 0.1039857

set.seed(143)  
GLM\_M3\_Data3 = train(PH ~ ., data = beverages\_v3\_train, metric = 'RMSE', method = 'glm', trControl = myControl)  
GLM\_M3\_Data3

## Generalized Linear Model   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results:  
##   
## RMSE Rsquared MAE   
## 0.1328461 0.4143476 0.1042366

## glmnet

# next, we'll try a glmnet model which combines lasso and ridge regression   
set.seed(143)  
glmnet\_M1\_Data1 = train(PH ~ ., data = beverages\_v1\_train , metric = 'RMSE', method = 'glmnet',preProcess = c('center', 'scale'), trControl = myControl)  
glmnet\_M1\_Data1

## glmnet   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## alpha lambda RMSE Rsquared MAE   
## 0.10 0.0001599694 0.1321682 0.4200101 0.1016777  
## 0.10 0.0015996935 0.1322468 0.4191405 0.1020003  
## 0.10 0.0159969354 0.1344230 0.4028236 0.1050963  
## 0.55 0.0001599694 0.1321767 0.4198747 0.1017159  
## 0.55 0.0015996935 0.1326398 0.4157909 0.1026923  
## 0.55 0.0159969354 0.1391558 0.3693005 0.1092707  
## 1.00 0.0001599694 0.1321877 0.4197298 0.1017613  
## 1.00 0.0015996935 0.1331279 0.4118142 0.1033393  
## 1.00 0.0159969354 0.1439824 0.3318423 0.1128677  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were alpha = 0.1 and lambda  
## = 0.0001599694.

set.seed(143)  
glmnet\_M2\_Data2 = train(PH ~ ., data = beverages\_v2\_train , metric = 'RMSE', method = 'glmnet', trControl = myControl)  
glmnet\_M2\_Data2

## glmnet   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## alpha lambda RMSE Rsquared MAE   
## 0.10 0.0001672247 0.1326933 0.4155451 0.1038747  
## 0.10 0.0016722466 0.1328820 0.4135047 0.1038632  
## 0.10 0.0167224659 0.1343540 0.4025188 0.1051299  
## 0.55 0.0001672247 0.1326944 0.4154579 0.1038483  
## 0.55 0.0016722466 0.1333793 0.4090589 0.1041986  
## 0.55 0.0167224659 0.1386539 0.3740453 0.1086213  
## 1.00 0.0001672247 0.1326960 0.4153719 0.1038397  
## 1.00 0.0016722466 0.1336176 0.4071727 0.1044491  
## 1.00 0.0167224659 0.1439849 0.3307979 0.1127147  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were alpha = 0.1 and lambda  
## = 0.0001672247.

set.seed(143)  
glmnet\_M3\_Data3 = train(PH ~ ., data = beverages\_v3\_train, metric = 'RMSE', method = 'glmnet', trControl = myControl)  
glmnet\_M3\_Data3

## glmnet   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## alpha lambda RMSE Rsquared MAE   
## 0.10 0.0001672247 0.1327977 0.4145988 0.1041364  
## 0.10 0.0016722466 0.1329433 0.4128907 0.1040781  
## 0.10 0.0167224659 0.1343872 0.4021404 0.1052213  
## 0.55 0.0001672247 0.1328009 0.4144859 0.1041151  
## 0.55 0.0016722466 0.1333806 0.4089906 0.1043980  
## 0.55 0.0167224659 0.1386158 0.3743946 0.1085942  
## 1.00 0.0001672247 0.1328006 0.4144030 0.1040986  
## 1.00 0.0016722466 0.1336274 0.4070431 0.1046215  
## 1.00 0.0167224659 0.1439831 0.3308204 0.1127133  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were alpha = 0.1 and lambda  
## = 0.0001672247.

## ranger

# random forest just for fun  
set.seed(143)  
ranger\_M1\_Data1 = train(PH ~ ., data = beverages\_v1\_train, metric = 'RMSE', method = 'ranger',preProcess = c('center', 'scale'),trControl = myControl)  
ranger\_M1\_Data1

## Random Forest   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## mtry splitrule RMSE Rsquared MAE   
## 2 variance 0.1148168 0.6082763 0.08645160  
## 2 extratrees 0.1191566 0.5732928 0.09119231  
## 18 variance 0.1022603 0.6658250 0.07395862  
## 18 extratrees 0.1016529 0.6675300 0.07357492  
## 35 variance 0.1025035 0.6570685 0.07348070  
## 35 extratrees 0.1000349 0.6754776 0.07205404  
##   
## Tuning parameter 'min.node.size' was held constant at a value of 5  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were mtry = 35, splitrule =  
## extratrees and min.node.size = 5.

set.seed(143)  
ranger\_M2\_Data2 = train(PH ~ ., data = beverages\_v2\_train, metric = 'RMSE', method = 'ranger',trControl = myControl)  
ranger\_M2\_Data2

## Random Forest   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## mtry splitrule RMSE Rsquared MAE   
## 2 variance 0.1183735 0.5767453 0.09000200  
## 2 extratrees 0.1219389 0.5435630 0.09361688  
## 19 variance 0.1042656 0.6494408 0.07637783  
## 19 extratrees 0.1036684 0.6506936 0.07604484  
## 36 variance 0.1046413 0.6425340 0.07615347  
## 36 extratrees 0.1021818 0.6590873 0.07477257  
##   
## Tuning parameter 'min.node.size' was held constant at a value of 5  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were mtry = 36, splitrule =  
## extratrees and min.node.size = 5.

set.seed(143)  
ranger\_M3\_Data3 = train(PH ~ ., data = beverages\_v3\_train, metric = 'RMSE', method = 'ranger',trControl = myControl)  
ranger\_M3\_Data3

## Random Forest   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## mtry splitrule RMSE Rsquared MAE   
## 2 variance 0.1191127 0.5698374 0.09056467  
## 2 extratrees 0.1222293 0.5412470 0.09392975  
## 19 variance 0.1042516 0.6498560 0.07627652  
## 19 extratrees 0.1041126 0.6479240 0.07647817  
## 37 variance 0.1047951 0.6413251 0.07615708  
## 37 extratrees 0.1024866 0.6571123 0.07519137  
##   
## Tuning parameter 'min.node.size' was held constant at a value of 5  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were mtry = 37, splitrule =  
## extratrees and min.node.size = 5.

## PLS

Since we observed correlation between the predictors variables, we will consider building a Partial Least Square model.

set.seed(143)  
pls\_M1\_Data1 = train(PH ~ ., data = beverages\_v1\_train, metric = 'RMSE', method ='pls', preProcess = c('center', 'scale'), tunelength = 15, trControl = myControl)  
pls\_M1\_Data1

## Partial Least Squares   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## ncomp RMSE Rsquared MAE   
## 1 0.1494403 0.2581107 0.1177883  
## 2 0.1403749 0.3456090 0.1099254  
## 3 0.1378683 0.3686338 0.1086210  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was ncomp = 3.

set.seed(143)  
pls\_M2\_Data2 = train(PH ~ ., data = beverages\_v2\_train, metric = 'RMSE', method ='pls', tunelength = 15, trControl = myControl)  
pls\_M2\_Data2

## Partial Least Squares   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## ncomp RMSE Rsquared MAE   
## 1 0.1705840 0.03468439 0.1360308  
## 2 0.1691324 0.04868677 0.1352213  
## 3 0.1536504 0.21647890 0.1197444  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was ncomp = 3.

set.seed(143)  
pls\_M3\_Data3 = train(PH ~ ., data = beverages\_v3\_train, metric = 'RMSE', method ='pls', tunelength = 15, trControl = myControl)  
pls\_M3\_Data3

## Partial Least Squares   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## ncomp RMSE Rsquared MAE   
## 1 0.1705840 0.03468441 0.1360308  
## 2 0.1691324 0.04868680 0.1352213  
## 3 0.1536504 0.21647873 0.1197445  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was ncomp = 3.

## SVM

set.seed(143)  
svmRadial\_M1\_Data1 =train(PH~.,beverages\_v1\_train, metric = 'RMSE', method = "svmRadial",preProc =c("center", "scale"),tuneLength = 14, trControl = myControl)  
svmRadial\_M1\_Data1

## Support Vector Machines with Radial Basis Function Kernel   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## C RMSE Rsquared MAE   
## 0.25 0.1271623 0.4763276 0.09440391  
## 0.50 0.1237651 0.4996104 0.09135600  
## 1.00 0.1203705 0.5237636 0.08824463  
## 2.00 0.1177148 0.5422556 0.08548582  
## 4.00 0.1160196 0.5542984 0.08379616  
## 8.00 0.1157321 0.5578480 0.08375405  
## 16.00 0.1173556 0.5510887 0.08532832  
## 32.00 0.1209362 0.5333375 0.08834497  
## 64.00 0.1264312 0.5071734 0.09295419  
## 128.00 0.1339292 0.4748267 0.09843867  
## 256.00 0.1413222 0.4466638 0.10391393  
## 512.00 0.1458019 0.4293654 0.10746593  
## 1024.00 0.1476611 0.4221392 0.10865742  
## 2048.00 0.1476611 0.4221392 0.10865742  
##   
## Tuning parameter 'sigma' was held constant at a value of 0.01892239  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were sigma = 0.01892239 and C = 8.

set.seed(143)  
svmRadial\_M2\_Data2 =train(PH~.,beverages\_v2\_train, metric = 'RMSE', method = "svmRadial",tuneLength = 14, trControl = myControl)  
svmRadial\_M2\_Data2

## Support Vector Machines with Radial Basis Function Kernel   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## C RMSE Rsquared MAE   
## 0.25 0.1266025 0.4790584 0.09407358  
## 0.50 0.1240029 0.4962984 0.09161310  
## 1.00 0.1211552 0.5161218 0.08903764  
## 2.00 0.1190476 0.5308862 0.08701478  
## 4.00 0.1174062 0.5430372 0.08576343  
## 8.00 0.1177581 0.5424166 0.08617114  
## 16.00 0.1189869 0.5385996 0.08746447  
## 32.00 0.1224791 0.5220192 0.09017677  
## 64.00 0.1272165 0.5005933 0.09363698  
## 128.00 0.1350334 0.4651577 0.09944323  
## 256.00 0.1450232 0.4250946 0.10690726  
## 512.00 0.1523229 0.3972286 0.11217570  
## 1024.00 0.1563843 0.3830348 0.11491475  
## 2048.00 0.1587342 0.3766594 0.11665990  
##   
## Tuning parameter 'sigma' was held constant at a value of 0.018282  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were sigma = 0.018282 and C = 4.

set.seed(143)  
svmRadial\_M3\_Data3 =train(PH~.,beverages\_v3\_train, metric = 'RMSE', method = "svmRadial",tuneLength = 14, trControl = myControl)  
svmRadial\_M3\_Data3

## Support Vector Machines with Radial Basis Function Kernel   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## C RMSE Rsquared MAE   
## 0.25 0.1270587 0.4752379 0.09442825  
## 0.50 0.1243818 0.4933657 0.09170709  
## 1.00 0.1215350 0.5134861 0.08906423  
## 2.00 0.1195646 0.5269365 0.08746778  
## 4.00 0.1180271 0.5382430 0.08653561  
## 8.00 0.1180227 0.5401329 0.08624021  
## 16.00 0.1190728 0.5382667 0.08744345  
## 32.00 0.1231344 0.5185287 0.09067732  
## 64.00 0.1277064 0.4976801 0.09401868  
## 128.00 0.1360166 0.4596066 0.10049839  
## 256.00 0.1463599 0.4181806 0.10841813  
## 512.00 0.1528888 0.3935027 0.11342022  
## 1024.00 0.1556328 0.3859861 0.11575868  
## 2048.00 0.1568338 0.3823311 0.11670405  
##   
## Tuning parameter 'sigma' was held constant at a value of 0.01751442  
## RMSE was used to select the optimal model using the smallest value.  
## The final values used for the model were sigma = 0.01751442 and C = 8.

#plot(svmRadial\_M1\_Data1, scales = list(x=list(log=2)))

## rf

control\_forest = trainControl(method="repeatedcv", number=5, repeats=2, search="random", allowParallel = T)  
mtry = sqrt(ncol(beverages\_v1\_train))  
  
  
set.seed(143)  
rf\_M1\_Data1 = train(PH~., data=beverages\_v1\_train, metric = 'RMSE' , method="rf", tuneLength=5, importance=T, trControl=control\_forest)  
rf\_M1\_Data1

## Random Forest   
##   
## 1799 samples  
## 32 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold, repeated 2 times)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440, 1440, ...   
## Resampling results across tuning parameters:  
##   
## mtry RMSE Rsquared MAE   
## 1 0.1269387 0.5384941 0.09774909  
## 3 0.1113403 0.6259804 0.08295917  
## 15 0.1027157 0.6647482 0.07437338  
## 26 0.1019036 0.6644823 0.07329716  
## 34 0.1024474 0.6573263 0.07334071  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was mtry = 26.

mtry = sqrt(ncol(beverages\_v2\_train))  
  
set.seed(143)  
rf\_M2\_Data2 = train(PH~., data=beverages\_v2\_train, metric = 'RMSE' , method="rf", tuneLength=5, importance=T, trControl=control\_forest)  
rf\_M2\_Data2

## Random Forest   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold, repeated 2 times)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440, 1440, ...   
## Resampling results across tuning parameters:  
##   
## mtry RMSE Rsquared MAE   
## 1 0.1331093 0.4799951 0.10315811  
## 3 0.1140147 0.6009601 0.08581825  
## 15 0.1049859 0.6458754 0.07681567  
## 27 0.1045193 0.6441318 0.07603646  
## 35 0.1052487 0.6376317 0.07636096  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was mtry = 27.

mtry = sqrt(ncol(beverages\_v3\_train))  
set.seed(143)  
rf\_M3\_Data3 = train(PH~., data=beverages\_v3\_train, metric = 'RMSE' , method="rf", tuneLength=5, importance=T, trControl=control\_forest)  
rf\_M3\_Data3

## Random Forest   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold, repeated 2 times)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440, 1440, ...   
## Resampling results across tuning parameters:  
##   
## mtry RMSE Rsquared MAE   
## 1 0.1337708 0.4727309 0.10364403  
## 3 0.1145820 0.5973462 0.08648148  
## 16 0.1049238 0.6463335 0.07683496  
## 28 0.1046783 0.6431562 0.07605231  
## 36 0.1049284 0.6394810 0.07609281  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was mtry = 28.

rm(control\_forest,mtry)

## knn

set.seed(143)  
knn\_M1\_Data1 <- train(PH ~ .,  
 method = "knn",  
 tuneGrid = expand.grid(k = 1:10),  
 trControl = myControl,  
 metric = "RMSE",  
 data = beverages\_v1\_train,preProc =c("center", "scale"))  
knn\_M1\_Data1

## k-Nearest Neighbors   
##   
## 1799 samples  
## 32 predictor  
##   
## Pre-processing: centered (35), scaled (35)   
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## k RMSE Rsquared MAE   
## 1 0.1552863 0.3519753 0.10524865  
## 2 0.1354010 0.4441269 0.09628802  
## 3 0.1288917 0.4719160 0.09184895  
## 4 0.1256230 0.4900061 0.09103044  
## 5 0.1239321 0.4978780 0.09017747  
## 6 0.1244458 0.4922766 0.09122504  
## 7 0.1240195 0.4953110 0.09169746  
## 8 0.1244070 0.4920447 0.09218550  
## 9 0.1244541 0.4919942 0.09257184  
## 10 0.1244123 0.4917993 0.09265990  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was k = 5.

set.seed(143)  
knn\_M2\_Data2 <- train(PH ~ .,  
 method = "knn",  
 tuneGrid = expand.grid(k = 1:10),  
 trControl = myControl,  
 metric = "RMSE",  
 data = beverages\_v2\_train)  
knn\_M2\_Data2

## k-Nearest Neighbors   
##   
## 1799 samples  
## 33 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## k RMSE Rsquared MAE   
## 1 0.1683200 0.2859914 0.1144311  
## 2 0.1500658 0.3327492 0.1058868  
## 3 0.1418583 0.3653536 0.1021784  
## 4 0.1401030 0.3694645 0.1028647  
## 5 0.1401516 0.3633672 0.1033130  
## 6 0.1393636 0.3643894 0.1034378  
## 7 0.1400595 0.3562528 0.1038978  
## 8 0.1398343 0.3550924 0.1045687  
## 9 0.1405531 0.3466922 0.1052976  
## 10 0.1408672 0.3423547 0.1057476  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was k = 6.

set.seed(143)  
knn\_M3\_Data3 <- train(PH ~ .,  
 method = "knn",  
 tuneGrid = expand.grid(k = 1:10),  
 trControl = myControl,  
 metric = "RMSE",  
 data = beverages\_v3\_train)  
knn\_M3\_Data3

## k-Nearest Neighbors   
##   
## 1799 samples  
## 34 predictor  
##   
## No pre-processing  
## Resampling: Cross-Validated (5 fold)   
## Summary of sample sizes: 1439, 1439, 1439, 1439, 1440   
## Resampling results across tuning parameters:  
##   
## k RMSE Rsquared MAE   
## 1 0.1678809 0.2883229 0.1142200  
## 2 0.1501421 0.3320212 0.1059035  
## 3 0.1419641 0.3647402 0.1022868  
## 4 0.1400958 0.3695812 0.1028442  
## 5 0.1401539 0.3633406 0.1033219  
## 6 0.1393665 0.3643136 0.1034634  
## 7 0.1400607 0.3562888 0.1039153  
## 8 0.1398256 0.3552039 0.1045193  
## 9 0.1405340 0.3468925 0.1052685  
## 10 0.1408292 0.3426671 0.1056854  
##   
## RMSE was used to select the optimal model using the smallest value.  
## The final value used for the model was k = 6.

## Random Forest Classification

Using the ‘randomForest’ and ‘caret’ packages, we applied k-fold cross validation on the training set, fitting the random forest model to 10 random samples of the training set and taking the average.

Control\_rf\_c = trainControl(method = "cv", number = 10, allowParallel = TRUE, verboseIter = FALSE)  
  
set.seed(143)  
  
rf\_M4\_Data4 = train(PH ~ ., data = beverages\_v4\_train, method = "rf", prox = FALSE, trControl = Control\_rf\_c)  
rf\_M4\_Data4

## Random Forest   
##   
## 1799 samples  
## 32 predictor  
## 2 classes: 'Alkaline', 'Neutral'   
##   
## No pre-processing  
## Resampling: Cross-Validated (10 fold)   
## Summary of sample sizes: 1619, 1620, 1619, 1619, 1619, 1619, ...   
## Resampling results across tuning parameters:  
##   
## mtry Accuracy Kappa   
## 2 0.8110199 0.6098046  
## 18 0.8215633 0.6354398  
## 35 0.8215447 0.6367609  
##   
## Accuracy was used to select the optimal model using the largest value.  
## The final value used for the model was mtry = 18.

rm(Control\_rf\_c)

stopCluster(Mycluster)  
registerDoSEQ()

From the results of the cross validated model above, we can see that model accuracy was above 80 percent. From the confusion matrix below, we can see that overall accuracy of the model was 82.64 percent with a 95 percent confidence interval between 79.78 percent and 85.25 percent, sensitivity of 90.57 percent and specificity of 69.01 percent.

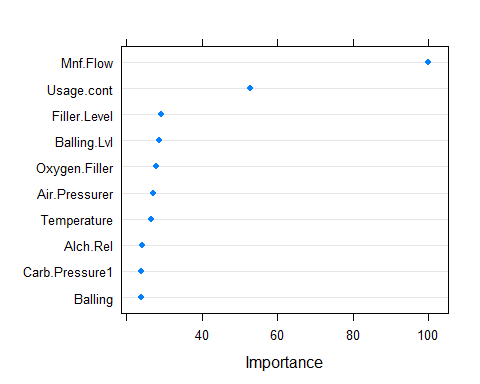
test <- predict( rf\_M4\_Data4, newdata = beverages\_v4\_test)  
cf <- confusionMatrix(data = test, beverages\_v4\_test$PH)  
print(cf, digits = 4)

## Confusion Matrix and Statistics  
##   
## Reference  
## Prediction Alkaline Neutral  
## Alkaline 408 68  
## Neutral 58 238  
##   
## Accuracy : 0.8368   
## 95% CI : (0.8088, 0.8622)  
## No Information Rate : 0.6036   
## P-Value [Acc > NIR] : <2e-16   
##   
## Kappa : 0.657   
## Mcnemar's Test P-Value : 0.4227   
##   
## Sensitivity : 0.8755   
## Specificity : 0.7778   
## Pos Pred Value : 0.8571   
## Neg Pred Value : 0.8041   
## Prevalence : 0.6036   
## Detection Rate : 0.5285   
## Detection Prevalence : 0.6166   
## Balanced Accuracy : 0.8267   
##   
## 'Positive' Class : Alkaline   
##

# Concept importance for model  
varImp(rf\_M4\_Data4, top = 10)

## rf variable importance  
##   
## only 20 most important variables shown (out of 35)  
##   
## Overall  
## Mnf.Flow 100.00  
## Usage.cont 52.94  
## Filler.Level 29.34  
## Balling.Lvl 28.60  
## Oxygen.Filler 27.96  
## Air.Pressurer 27.02  
## Temperature 26.60  
## Alch.Rel 24.33  
## Carb.Pressure1 24.03  
## Balling 23.89  
## Hyd.Pressure3 23.89  
## Filler.Speed 21.83  
## Carb.Flow 20.92  
## Brand.CodeC 20.64  
## PC.Volume 20.64  
## Bowl.Setpoint 19.70  
## Density 18.26  
## Pressure.Vacuum 17.89  
## Carb.Rel 17.42  
## Fill.Pressure 17.34

dotPlot(varImp(rf\_M4\_Data4), top=10)



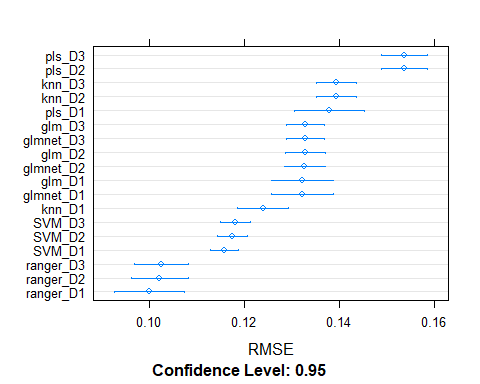
# Model Selection, Insterpretation, & Evaluation

## Selecting Best Model

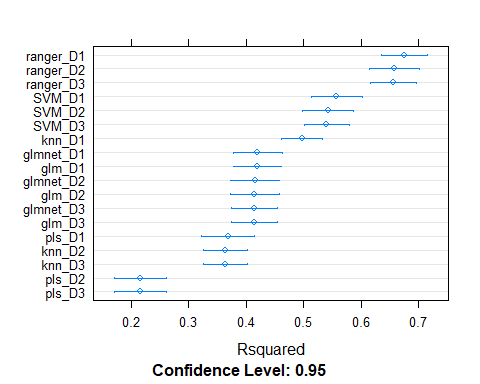
We have build various models, linear regression ones and nonlinear regression ones. We will now evaluate each on the test data sets. Best on the results, we will select the best performing model. The following criteria will be considered for the selection:

* Accuracy (how accurately the model performed, evaluated using RMSE and MAE)
* Rsquared
* MAE
* Scalability (as measure by run time)
* Interpretability

# compare models  
models\_list = list("glm\_D1" = GLM\_M1\_Data1, "glm\_D2" = GLM\_M2\_Data2, "glm\_D3" = GLM\_M3\_Data3,   
 "glmnet\_D1" = glmnet\_M1\_Data1, "glmnet\_D2" = glmnet\_M2\_Data2, "glmnet\_D3" = glmnet\_M3\_Data3,   
 "ranger\_D1"= ranger\_M1\_Data1, "ranger\_D2" = ranger\_M2\_Data2, "ranger\_D3" = ranger\_M3\_Data3,   
 "pls\_D1"= pls\_M1\_Data1, "pls\_D2" = pls\_M2\_Data2, "pls\_D3" = pls\_M3\_Data3,   
 "SVM\_D1" = svmRadial\_M1\_Data1, "SVM\_D2" = svmRadial\_M2\_Data2, "SVM\_D3" = svmRadial\_M3\_Data3,   
 # "rf\_D1" = rf\_M1\_Data1, "rf\_D2" = rf\_M2\_Data2, "rf\_D3" = rf\_M3\_Data3,  
 "knn\_D1" = knn\_M1\_Data1, "knn\_D2" = knn\_M2\_Data2, "knn\_D3" = knn\_M3\_Data3)  
  
resamps = resamples(models\_list)   
  
dotplot(resamps, metric = 'RMSE')



dotplot(resamps, metric = 'Rsquared')



summary(resamps)

##   
## Call:  
## summary.resamples(object = resamps)  
##   
## Models: glm\_D1, glm\_D2, glm\_D3, glmnet\_D1, glmnet\_D2, glmnet\_D3, ranger\_D1, ranger\_D2, ranger\_D3, pls\_D1, pls\_D2, pls\_D3, SVM\_D1, SVM\_D2, SVM\_D3, knn\_D1, knn\_D2, knn\_D3   
## Number of resamples: 5   
##   
## MAE   
## Min. 1st Qu. Median Mean 3rd Qu.  
## glm\_D1 0.09666894 0.09942818 0.10199874 0.10165235 0.10299856  
## glm\_D2 0.10102661 0.10223363 0.10447857 0.10398573 0.10557358  
## glm\_D3 0.10147052 0.10211471 0.10429855 0.10423661 0.10626413  
## glmnet\_D1 0.09663290 0.09954874 0.10193387 0.10167772 0.10302650  
## glmnet\_D2 0.10065809 0.10216259 0.10443190 0.10387471 0.10523665  
## glmnet\_D3 0.10110529 0.10213228 0.10427775 0.10413636 0.10587722  
## ranger\_D1 0.06786358 0.07040292 0.07101260 0.07205404 0.07494206  
## ranger\_D2 0.07129082 0.07329099 0.07353123 0.07477257 0.07660736  
## ranger\_D3 0.07163892 0.07375833 0.07402880 0.07519137 0.07733681  
## pls\_D1 0.10437163 0.10693019 0.10831682 0.10862104 0.10853792  
## pls\_D2 0.11767023 0.11779981 0.11818900 0.11974444 0.12134258  
## pls\_D3 0.11767028 0.11779984 0.11818904 0.11974447 0.12134259  
## SVM\_D1 0.08213192 0.08245333 0.08308356 0.08375405 0.08523859  
## SVM\_D2 0.08461577 0.08530356 0.08619329 0.08576343 0.08628458  
## SVM\_D3 0.08365267 0.08554557 0.08699018 0.08624021 0.08728870  
## knn\_D1 0.08647778 0.08762407 0.08943733 0.09017747 0.09360185  
## knn\_D2 0.10080556 0.10267460 0.10373148 0.10343780 0.10478704  
## knn\_D3 0.10086111 0.10281217 0.10373148 0.10346342 0.10479630  
## Max. NA's  
## glm\_D1 0.10716736 0  
## glm\_D2 0.10661626 0  
## glm\_D3 0.10703516 0  
## glmnet\_D1 0.10724661 0  
## glmnet\_D2 0.10688432 0  
## glmnet\_D3 0.10728927 0  
## ranger\_D1 0.07604905 0  
## ranger\_D2 0.07914248 0  
## ranger\_D3 0.07919399 0  
## pls\_D1 0.11494863 0  
## pls\_D2 0.12372057 0  
## pls\_D3 0.12372060 0  
## SVM\_D1 0.08586286 0  
## SVM\_D2 0.08641993 0  
## SVM\_D3 0.08772396 0  
## knn\_D1 0.09374630 0  
## knn\_D2 0.10519034 0  
## knn\_D3 0.10511606 0  
##   
## RMSE   
## Min. 1st Qu. Median Mean 3rd Qu. Max.  
## glm\_D1 0.12621266 0.12781745 0.13327061 0.1321942 0.1343726 0.1392976  
## glm\_D2 0.12830641 0.12998963 0.13447989 0.1327388 0.1347217 0.1361965  
## glm\_D3 0.12907229 0.12977273 0.13420197 0.1328461 0.1351756 0.1360080  
## glmnet\_D1 0.12607353 0.12790057 0.13320295 0.1321682 0.1343930 0.1392709  
## glmnet\_D2 0.12811704 0.12998409 0.13440741 0.1326933 0.1344478 0.1365103  
## glmnet\_D3 0.12888018 0.12978222 0.13419480 0.1327977 0.1348079 0.1363235  
## ranger\_D1 0.09439369 0.09520722 0.09902175 0.1000349 0.1028925 0.1086594  
## ranger\_D2 0.09691783 0.09898420 0.10053759 0.1021818 0.1062923 0.1081773  
## ranger\_D3 0.09778360 0.09926945 0.10073966 0.1024866 0.1059522 0.1086880  
## pls\_D1 0.13207873 0.13496768 0.13623735 0.1378683 0.1383636 0.1476942  
## pls\_D2 0.15002937 0.15183945 0.15294128 0.1536504 0.1533633 0.1600786  
## pls\_D3 0.15002936 0.15183948 0.15294132 0.1536504 0.1533633 0.1600786  
## SVM\_D1 0.11414350 0.11450657 0.11474578 0.1157321 0.1152596 0.1200051  
## SVM\_D2 0.11390861 0.11586534 0.11775419 0.1174062 0.1192320 0.1202709  
## SVM\_D3 0.11495380 0.11607523 0.11806490 0.1180227 0.1199672 0.1210523  
## knn\_D1 0.11860654 0.12054109 0.12441642 0.1239321 0.1278198 0.1282764  
## knn\_D2 0.13580898 0.13761135 0.13780790 0.1393636 0.1415940 0.1439956  
## knn\_D3 0.13581806 0.13761213 0.13782806 0.1393665 0.1415940 0.1439801  
## NA's  
## glm\_D1 0  
## glm\_D2 0  
## glm\_D3 0  
## glmnet\_D1 0  
## glmnet\_D2 0  
## glmnet\_D3 0  
## ranger\_D1 0  
## ranger\_D2 0  
## ranger\_D3 0  
## pls\_D1 0  
## pls\_D2 0  
## pls\_D3 0  
## SVM\_D1 0  
## SVM\_D2 0  
## SVM\_D3 0  
## knn\_D1 0  
## knn\_D2 0  
## knn\_D3 0  
##   
## Rsquared   
## Min. 1st Qu. Median Mean 3rd Qu. Max. NA's  
## glm\_D1 0.3754037 0.4092567 0.4221824 0.4198535 0.4236080 0.4688166 0  
## glm\_D2 0.3760839 0.3887926 0.4116245 0.4153035 0.4494463 0.4505704 0  
## glm\_D3 0.3781507 0.3901476 0.4083413 0.4143476 0.4440705 0.4510277 0  
## glmnet\_D1 0.3750825 0.4083490 0.4224277 0.4200101 0.4240016 0.4701898 0  
## glmnet\_D2 0.3759551 0.3887307 0.4139908 0.4155451 0.4468962 0.4521526 0  
## glmnet\_D3 0.3778683 0.3899859 0.4110299 0.4145988 0.4456483 0.4484614 0  
## ranger\_D1 0.6386150 0.6534604 0.6729665 0.6754776 0.6939372 0.7184088 0  
## ranger\_D2 0.6096241 0.6447042 0.6577528 0.6590873 0.6837220 0.6996338 0  
## ranger\_D3 0.6127104 0.6429981 0.6539811 0.6571123 0.6824112 0.6934609 0  
## pls\_D1 0.3383685 0.3416709 0.3466076 0.3686338 0.3971515 0.4193703 0  
## pls\_D2 0.1618021 0.1996063 0.2342121 0.2164789 0.2347790 0.2519949 0  
## pls\_D3 0.1618017 0.1996060 0.2342120 0.2164787 0.2347789 0.2519950 0  
## SVM\_D1 0.5111507 0.5339595 0.5633987 0.5578480 0.5786375 0.6020936 0  
## SVM\_D2 0.5038734 0.5065026 0.5521155 0.5430372 0.5736115 0.5790830 0  
## SVM\_D3 0.5003738 0.5196611 0.5376545 0.5401329 0.5691793 0.5737960 0  
## knn\_D1 0.4475560 0.5060286 0.5085413 0.4978780 0.5090711 0.5181928 0  
## knn\_D2 0.3242176 0.3467361 0.3687084 0.3643894 0.3785921 0.4036930 0  
## knn\_D3 0.3240750 0.3467935 0.3684318 0.3643136 0.3785749 0.4036930 0

We will now compute a matrix for summarize all the models and metrics. We will evaluate the models on the test data and compare the results.

predictAndMeasure <- function(model, model.label, testData, ytest, score\_interpretability, grid = NULL) {  
   
 #mesure prediction time  
 ptm <- proc.time()  
 # Predict Model on Test Date set  
 pred <- predict(model, testData)  
 tm <- proc.time() - ptm  
   
 post<- postResample(pred = pred, obs = ytest)  
 RMSE.test <- c(post[[1]])  
 RSquared.test <- c(post[[2]])  
 MAE.test <- c(post[[3]])  
   
 perf.grid = NULL  
 if (is.null(grid)) {   
 perf.grid = data.frame(predictor = c(model.label) , RMSE = RMSE.test , RSquared = RSquared.test, MAE = MAE.test, time = c(tm[[3]]), interpretability = c(score\_interpretability))  
 } else {  
 .grid = data.frame(predictor = c(model.label) , RMSE = RMSE.test , RSquared = RSquared.test, MAE = MAE.test, time = c(tm[[3]]), interpretability = c(score\_interpretability))  
 perf.grid = rbind(grid, .grid)  
 }  
   
 perf.grid  
}  
  
  
#Prediction for glm   
performance.grid <- predictAndMeasure (GLM\_M1\_Data1, "glm\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=NULL)  
performance.grid <- predictAndMeasure (GLM\_M2\_Data2, "glm\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (GLM\_M3\_Data3, "glm\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for glmnet  
performance.grid <- predictAndMeasure (glmnet\_M1\_Data1, "glmnet\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (glmnet\_M2\_Data2, "glmnet\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (glmnet\_M3\_Data3, "glmnet\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for ranger  
performance.grid <- predictAndMeasure (ranger\_M1\_Data1, "ranger\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (ranger\_M2\_Data2, "ranger\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (ranger\_M3\_Data3, "ranger\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for pls  
performance.grid <- predictAndMeasure (pls\_M1\_Data1, "PLS\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (pls\_M2\_Data2, "PLS\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (pls\_M3\_Data3, "PLS\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for SVM  
performance.grid <- predictAndMeasure (svmRadial\_M1\_Data1, "SVM\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (svmRadial\_M2\_Data2, "SVM\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (svmRadial\_M3\_Data3, "SVM\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for rf  
performance.grid <- predictAndMeasure (rf\_M1\_Data1, "rf\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (rf\_M2\_Data2, "rf\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (rf\_M3\_Data3, "rf\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
#Prediction for knn  
performance.grid <- predictAndMeasure (knn\_M1\_Data1, "knn\_D1", beverages\_v1\_test, beverages\_v1\_test$PH, 3, grid=performance.grid)  
performance.grid <- predictAndMeasure (knn\_M2\_Data2, "knn\_D2", beverages\_v2\_test, beverages\_v2\_test$PH, 2, grid=performance.grid)  
performance.grid <- predictAndMeasure (knn\_M3\_Data3, "knn\_D3", beverages\_v3\_test, beverages\_v3\_test$PH, 1, grid=performance.grid)  
  
  
kable(performance.grid[order(performance.grid$RMSE, decreasing=F),])

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | predictor | RMSE | RSquared | MAE | time | interpretability |
| 7 | ranger\_D1 | 0.0939969 | 0.7032532 | 0.0696673 | 0.06 | 3 |
| 16 | rf\_D1 | 0.0967080 | 0.6879884 | 0.0718421 | 0.23 | 3 |
| 9 | ranger\_D3 | 0.0977129 | 0.6765406 | 0.0728909 | 0.07 | 1 |
| 8 | ranger\_D2 | 0.0982740 | 0.6727468 | 0.0728900 | 0.35 | 2 |
| 17 | rf\_D2 | 0.1006485 | 0.6599316 | 0.0747288 | 0.05 | 2 |
| 18 | rf\_D3 | 0.1010058 | 0.6561546 | 0.0748624 | 0.05 | 1 |
| 13 | SVM\_D1 | 0.1170556 | 0.5343906 | 0.0861389 | 0.13 | 3 |
| 15 | SVM\_D3 | 0.1175400 | 0.5305444 | 0.0881589 | 0.19 | 1 |
| 14 | SVM\_D2 | 0.1192273 | 0.5150016 | 0.0890344 | 0.13 | 2 |
| 19 | knn\_D1 | 0.1192457 | 0.5140818 | 0.0883048 | 0.08 | 3 |
| 4 | glmnet\_D1 | 0.1356713 | 0.3705383 | 0.1050806 | 0.05 | 3 |
| 1 | glm\_D1 | 0.1356927 | 0.3705787 | 0.1051352 | 0.08 | 3 |
| 5 | glmnet\_D2 | 0.1376930 | 0.3537371 | 0.1068528 | 0.06 | 2 |
| 2 | glm\_D2 | 0.1379206 | 0.3522181 | 0.1069320 | 0.04 | 2 |
| 6 | glmnet\_D3 | 0.1381452 | 0.3500481 | 0.1072481 | 0.02 | 1 |
| 3 | glm\_D3 | 0.1383895 | 0.3484315 | 0.1073678 | 0.00 | 1 |
| 20 | knn\_D2 | 0.1415026 | 0.3352160 | 0.1059370 | 0.11 | 2 |
| 21 | knn\_D3 | 0.1416439 | 0.3343843 | 0.1060579 | 0.08 | 1 |
| 10 | PLS\_D1 | 0.1423358 | 0.3062500 | 0.1109452 | 0.00 | 3 |
| 11 | PLS\_D2 | 0.1559200 | 0.1733901 | 0.1248626 | 0.05 | 2 |
| 12 | PLS\_D3 | 0.1559200 | 0.1733898 | 0.1248626 | 0.01 | 1 |

From the summary table, we observed that the random forest models (ranger\_D1 and rf\_D1) are better performing based on RMSE, MAE, and RSquared values. They are both built on a data set with no transformation which allow for better interpretability of the model.

The model is meant to be “productionalized” and application will be built to monitor the manufarturing process, this will require the model to be scalable and operate on large amount of data. Due to this requirement, we will select rf\_D1 model.

## Interpretation of selected model

# variable importance   
varImp(rf\_M1\_Data1)

## rf variable importance  
##   
## only 20 most important variables shown (out of 35)  
##   
## Overall  
## Mnf.Flow 100.00  
## Brand.CodeC 80.66  
## Pressure.Vacuum 64.61  
## Oxygen.Filler 59.63  
## Air.Pressurer 52.38  
## Alch.Rel 51.74  
## Balling.Lvl 49.53  
## Carb.Rel 46.71  
## Hyd.Pressure3 45.36  
## Temperature 44.65  
## Carb.Pressure1 41.28  
## Filler.Speed 40.04  
## Carb.Flow 37.19  
## Usage.cont 36.56  
## Density 36.05  
## Bowl.Setpoint 31.30  
## Balling 29.54  
## Hyd.Pressure2 27.83  
## Hyd.Pressure1 26.55  
## Carb.Volume 24.78

# decision tree of final random forest model   
getTree(rf\_M1\_Data1$finalModel, labelVar = T)

## left daughter right daughter split var split point status  
## 1 2 3 Mnf.Flow -49.9000000 -3  
## 2 4 5 Brand.CodeC 0.5000000 -3  
## 3 6 7 Brand.CodeD 0.5000000 -3  
## 4 8 9 Air.Pressurer 143.3000000 -3  
## 5 10 11 Oxygen.Filler 0.2330000 -3  
## 6 12 13 Balling.Lvl 1.3900000 -3  
## 7 14 15 Hyd.Pressure3 32.9000000 -3  
## 8 16 17 Density 0.9700000 -3  
## 9 18 19 Carb.Pressure1 123.9000000 -3  
## 10 20 21 Oxygen.Filler 0.0710000 -3  
## 11 0 0 <NA> 0.0000000 -1  
## 12 22 23 Air.Pressurer 143.3000000 -3  
## 13 24 25 Filler.Speed 3907.0000000 -3  
## 14 26 27 MFR 650.4000000 -3  
## 15 28 29 Usage.cont 23.3500000 -3  
## 16 30 31 Temperature 65.9000000 -3  
## 17 32 33 Filler.Speed 4005.0000000 -3  
## 18 34 35 Air.Pressurer 146.7000000 -3  
## 19 36 37 PSC.Fill 0.2700000 -3  
## 20 38 39 Carb.Flow 2985.0000000 -3  
## 21 40 41 Hyd.Pressure2 17.7000000 -3  
## 22 42 43 Carb.Volume 5.3433333 -3  
## 23 44 45 Bowl.Setpoint 105.0000000 -3  
## 24 46 47 MFR 641.8000000 -3  
## 25 48 49 Carb.Rel 5.2500000 -3  
## 26 50 51 Temperature 65.6000000 -3  
## 27 52 53 Filler.Speed 3964.0000000 -3  
## 28 54 55 Mnf.Flow 133.1000000 -3  
## 29 56 57 Carb.Pressure1 124.3000000 -3  
## 30 58 59 Oxygen.Filler 0.1390000 -3  
## 31 60 61 Filler.Speed 3985.0000000 -3  
## 32 62 63 Filler.Speed 3993.0000000 -3  
## 33 64 65 Filler.Level 117.3000000 -3  
## 34 66 67 Filler.Speed 4019.0000000 -3  
## 35 68 69 Balling 1.3730000 -3  
## 36 70 71 Brand.CodeB 0.5000000 -3  
## 37 0 0 <NA> 0.0000000 -1  
## 38 72 73 MFR 738.7000000 -3  
## 39 74 75 Air.Pressurer 142.7000000 -3  
## 40 76 77 PC.Volume 0.3216667 -3  
## 41 78 79 MFR 702.1000000 -3  
## 42 80 81 Hyd.Pressure2 42.8000000 -3  
## 43 82 83 Carb.Pressure1 126.4000000 -3  
## 44 84 85 Carb.Volume 5.2833333 -3  
## 45 86 87 Pressure.Vacuum -5.3000000 -3  
## 46 88 89 Usage.cont 24.0500000 -3  
## 47 90 91 Carb.Rel 5.5300000 -3  
## 48 92 93 Carb.Pressure 67.9000000 -3  
## 49 94 95 Balling 2.2310000 -3  
## 50 96 97 PSC 0.0270000 -3  
## 51 98 99 Carb.Volume 5.5566667 -3  
## 52 100 101 Alch.Rel 7.1000000 -3  
## 53 102 103 Fill.Ounces 23.9100000 -3  
## 54 104 105 Pressure.Vacuum -5.6000000 -3  
## 55 106 107 Hyd.Pressure1 6.9000000 -3  
## 56 108 109 Usage.cont 24.1800000 -3  
## 57 110 111 Pressure.Setpoint 48.0000000 -3  
## 58 112 113 Fill.Pressure 45.9000000 -3  
## 59 114 115 Carb.Pressure1 116.9000000 -3  
## 60 116 117 Fill.Ounces 24.0600000 -3  
## 61 118 119 Usage.cont 20.1100000 -3  
## 62 120 121 Pressure.Vacuum -5.3000000 -3  
## 63 122 123 Pressure.Vacuum -5.1000000 -3  
## 64 0 0 <NA> 0.0000000 -1  
## 65 124 125 Carb.Volume 5.5166667 -3  
## 66 126 127 Filler.Level 119.9000000 -3  
## 67 0 0 <NA> 0.0000000 -1  
## 68 0 0 <NA> 0.0000000 -1  
## 69 128 129 Filler.Level 121.3000000 -3  
## 70 130 131 PSC 0.0780000 -3  
## 71 0 0 <NA> 0.0000000 -1  
## 72 132 133 Carb.Volume 5.3033333 -3  
## 73 0 0 <NA> 0.0000000 -1  
## 74 134 135 Density 0.8900000 -3  
## 75 0 0 <NA> 0.0000000 -1  
## 76 136 137 MFR 736.3000000 -3  
## 77 138 139 Fill.Ounces 23.9900000 -3  
## 78 140 141 Carb.Rel 5.3900000 -3  
## 79 142 143 Balling.Lvl 1.3200000 -3  
## 80 144 145 Carb.Rel 5.4500000 -3  
## 81 0 0 <NA> 0.0000000 -1  
## 82 146 147 Hyd.Pressure4 95.0000000 -3  
## 83 148 149 Filler.Speed 3995.0000000 -3  
## 84 0 0 <NA> 0.0000000 -1  
## 85 150 151 Carb.Volume 5.3233333 -3  
## 86 152 153 Oxygen.Filler 0.0071000 -3  
## 87 0 0 <NA> 0.0000000 -1  
## 88 154 155 Usage.cont 23.5900000 -3  
## 89 156 157 Carb.Rel 5.3700000 -3  
## 90 158 159 Filler.Level 86.5000000 -3  
## 91 160 161 Hyd.Pressure1 30.0000000 -3  
## 92 0 0 <NA> 0.0000000 -1  
## 93 0 0 <NA> 0.0000000 -1  
## 94 162 163 Carb.Rel 5.3500000 -3  
## 95 164 165 Carb.Flow 3307.0000000 -3  
## 96 0 0 <NA> 0.0000000 -1  
## 97 166 167 Mnf.Flow 87.7000000 -3  
## 98 0 0 <NA> 0.0000000 -1  
## 99 168 169 PSC 0.0510000 -3  
## 100 0 0 <NA> 0.0000000 -1  
## 101 170 171 Oxygen.Filler 0.0339000 -3  
## 102 0 0 <NA> 0.0000000 -1  
## 103 172 173 Carb.Flow 1065.0000000 -3  
## 104 174 175 Hyd.Pressure2 23.6000000 -3  
## 105 176 177 Carb.Pressure1 125.5000000 -3  
## 106 178 179 Carb.Pressure1 126.0000000 -3  
## 107 180 181 PC.Volume 0.2493333 -3  
## 108 182 183 Filler.Level 110.9000000 -3  
## 109 0 0 <NA> 0.0000000 -1  
## 110 184 185 Fill.Ounces 23.9433333 -3  
## 111 186 187 Filler.Speed 3904.0000000 -3  
## 112 188 189 Alch.Rel 6.5700000 -3  
## 113 190 191 Carb.Pressure1 111.7000000 -3  
## 114 0 0 <NA> 0.0000000 -1  
## 115 0 0 <NA> 0.0000000 -1  
## 116 192 193 Hyd.Pressure4 131.0000000 -3  
## 117 194 195 Carb.Pressure1 115.5000000 -3  
## 118 196 197 Carb.Rel 5.4300000 -3  
## 119 198 199 Carb.Pressure 65.2000000 -3  
## 120 200 201 PSC.Fill 0.1500000 -3  
## 121 202 203 Carb.Rel 5.5300000 -3  
## 122 0 0 <NA> 0.0000000 -1  
## 123 204 205 Temperature 65.2000000 -3  
## 124 206 207 PC.Volume 0.2676667 -3  
## 125 208 209 Carb.Rel 5.5900000 -3  
## 126 210 211 Fill.Pressure 49.0000000 -3  
## 127 212 213 Carb.Volume 5.3366667 -3  
## 128 214 215 PSC.Fill 0.1200000 -3  
## 129 0 0 <NA> 0.0000000 -1  
## 130 216 217 Usage.cont 22.3000000 -3  
## 131 0 0 <NA> 0.0000000 -1  
## 132 218 219 Usage.cont 17.2700000 -3  
## 133 220 221 PC.Volume 0.2976667 -3  
## 134 222 223 Oxygen.Filler 0.0530000 -3  
## 135 224 225 Carb.Flow 3064.0000000 -3  
## 136 226 227 MFR 174.6000000 -3  
## 137 0 0 <NA> 0.0000000 -1  
## 138 228 229 MFR 734.3000000 -3  
## 139 230 231 PSC.CO2 0.1500000 -3  
## 140 232 233 PSC.Fill 0.1200000 -3  
## 141 0 0 <NA> 0.0000000 -1  
## 142 0 0 <NA> 0.0000000 -1  
## 143 234 235 Hyd.Pressure2 27.3000000 -3  
## 144 236 237 Carb.Pressure 70.9000000 -3  
## 145 238 239 Oxygen.Filler 0.0305000 -3  
## 146 240 241 Carb.Temp 137.8000000 -3  
## 147 242 243 Filler.Level 90.9000000 -3  
## 148 244 245 Usage.cont 23.9100000 -3  
## 149 0 0 <NA> 0.0000000 -1  
## 150 246 247 Alch.Rel 6.5700000 -3  
## 151 248 249 Carb.Pressure 65.8000000 -3  
## 152 0 0 <NA> 0.0000000 -1  
## 153 250 251 PSC.Fill 0.1400000 -3  
## 154 252 253 Air.Pressurer 141.9000000 -3  
## 155 254 255 PSC.Fill 0.1500000 -3  
## 156 256 257 Hyd.Pressure4 120.0000000 -3  
## 157 0 0 <NA> 0.0000000 -1  
## 158 258 259 Fill.Ounces 24.0600000 -3  
## 159 260 261 Hyd.Pressure3 35.4000000 -3  
## 160 262 263 Hyd.Pressure3 33.7000000 -3  
## 161 0 0 <NA> 0.0000000 -1  
## 162 264 265 Temperature 64.7000000 -3  
## 163 266 267 Carb.Volume 5.4633333 -3  
## 164 268 269 Alch.Rel 7.7000000 -3  
## 165 270 271 MFR 730.1000000 -3  
## 166 0 0 <NA> 0.0000000 -1  
## 167 272 273 Carb.Temp 144.9000000 -3  
## 168 0 0 <NA> 0.0000000 -1  
## 169 0 0 <NA> 0.0000000 -1  
## 170 274 275 Hyd.Pressure3 30.5000000 -3  
## 171 276 277 Filler.Level 88.8000000 -3  
## 172 0 0 <NA> 0.0000000 -1  
## 173 278 279 Filler.Level 120.3000000 -3  
## 174 0 0 <NA> 0.0000000 -1  
## 175 0 0 <NA> 0.0000000 -1  
## 176 0 0 <NA> 0.0000000 -1  
## 177 280 281 Hyd.Pressure1 7.8000000 -3  
## 178 282 283 Mnf.Flow 142.4000000 -3  
## 179 0 0 <NA> 0.0000000 -1  
## 180 0 0 <NA> 0.0000000 -1  
## 181 0 0 <NA> 0.0000000 -1  
## 182 284 285 Carb.Pressure 67.9000000 -3  
## 183 286 287 PSC.Fill 0.2100000 -3  
## 184 288 289 PSC.Fill 0.1700000 -3  
## 185 290 291 Density 1.3400000 -3  
## 186 0 0 <NA> 0.0000000 -1  
## 187 292 293 Air.Pressurer 142.5000000 -3  
## 188 294 295 Carb.Pressure 71.6000000 -3  
## 189 0 0 <NA> 0.0000000 -1  
## 190 0 0 <NA> 0.0000000 -1  
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## 752 8.300000  
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## 754 8.185000  
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## 758 8.498182  
## 759 8.446829  
## 760 8.400000  
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## 763 8.556667  
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## 765 8.438095  
## 766 8.397692  
## 767 8.356000  
## 768 8.348889  
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## 773 8.471429  
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## 780 8.400000  
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## 782 8.371429  
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## 790 8.740000  
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## 792 8.680000  
## 793 8.737143  
## 794 8.790000  
## 795 8.726667  
## 796 8.768090  
## 797 8.706000  
## 798 8.682857  
## 799 8.540000  
## 800 8.820000  
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## 802 8.680000  
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## 804 8.715200  
## 805 8.780000  
## 806 8.660000  
## 807 8.572000  
## 808 8.400000  
## 809 8.460000  
## 810 8.505833  
## 811 8.551429  
## 812 8.633333  
## 813 8.660000  
## 814 8.593333  
## 815 8.630000  
## 816 8.560000  
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## 820 8.665000  
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## 823 8.640000  
## 824 8.776667  
## 825 8.833333  
## 826 8.740000  
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## 828 8.720000  
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## 830 8.700000  
## 831 8.676000  
## 832 8.706667  
## 833 8.745000  
## 834 8.720000  
## 835 8.700000  
## 836 8.680000  
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## 838 8.486667  
## 839 8.580000  
## 840 8.574286  
## 841 8.528889  
## 842 8.435556  
## 843 8.393333  
## 844 8.605455  
## 845 8.570000  
## 846 8.511220  
## 847 8.646667  
## 848 8.680000  
## 849 8.540000  
## 850 8.460000  
## 851 8.388000  
## 852 8.380000  
## 853 8.420000  
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## 857 8.428889  
## 858 8.460000  
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## 861 8.382000  
## 862 8.260000  
## 863 8.314286  
## 864 8.368000  
## 865 8.420000  
## 866 8.180000  
## 867 8.200000  
## 868 8.480000  
## 869 8.530000  
## 870 8.439459  
## 871 8.515000  
## 872 8.540000  
## 873 8.560000  
## 874 8.480000  
## 875 8.431111  
## 876 8.422000  
## 877 8.382500  
## 878 8.364444  
## 879 8.280000  
## 880 8.340000  
## 881 8.420000  
## 882 8.560000  
## 883 8.560000  
## 884 8.456667  
## 885 8.560000  
## 886 8.620000  
## 887 8.582500  
## 888 8.633333  
## 889 8.680000  
## 890 8.382857  
## 891 8.360000  
## 892 8.580000  
## 893 8.600000  
## 894 8.726667  
## 895 8.652000  
## 896 8.713333  
## 897 8.743636  
## 898 8.740000  
## 899 8.797143  
## 900 8.866667  
## 901 8.764651  
## 902 8.720000  
## 903 8.580000  
## 904 8.700000  
## 905 8.640000  
## 906 8.840000  
## 907 8.840000  
## 908 8.711304  
## 909 8.760000  
## 910 8.509565  
## 911 8.420000  
## 912 8.540000  
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## 921 8.755000  
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## 930 8.493333  
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## 932 8.470000  
## 933 8.425714  
## 934 8.405000  
## 935 8.370000  
## 936 8.600000  
## 937 8.620000  
## 938 8.452000  
## 939 8.519444  
## 940 8.475000  
## 941 8.440000  
## 942 8.420000  
## 943 8.440000  
## 944 8.365714  
## 945 8.420000  
## 946 8.370000  
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## 948 8.600000  
## 949 8.180000  
## 950 8.460000  
## 951 8.488000  
## 952 8.540000  
## 953 8.436667  
## 954 8.380000  
## 955 8.437500  
## 956 8.460000  
## 957 8.417778  
## 958 8.398000  
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## 962 8.345714  
## 963 8.300000  
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## 971 8.380000  
## 972 8.360000  
## 973 8.360000  
## 974 8.740000  
## 975 8.760000  
## 976 8.780000  
## 977 8.804000  
## 978 8.752581  
## 979 8.795833  
## 980 8.703333  
## 981 8.753333  
## 982 8.704444  
## 983 8.736000  
## 984 8.488000  
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## 986 8.776000  
## 987 8.806667  
## 988 8.360000  
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## 992 8.520000  
## 993 8.471429  
## 994 8.576000  
## 995 8.600000  
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## 999 8.420000  
## 1000 8.600000  
## 1001 8.600000  
## 1002 8.528000  
## 1003 8.376000  
## 1004 8.615000  
## 1005 8.513824  
## 1006 8.360000  
## 1007 8.380000  
## 1008 8.313333  
## 1009 8.280000  
## 1010 8.462500  
## 1011 8.429286  
## 1012 8.460000  
## 1013 8.434286  
## 1014 8.400000  
## 1015 8.420000  
## 1016 8.382857  
## 1017 8.433333  
## 1018 8.400000  
## 1019 8.348000  
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## 1024 8.480000  
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## 1028 8.740000  
## 1029 8.740000  
## 1030 8.756000  
## 1031 8.650000  
## 1032 8.821333  
## 1033 8.753333  
## 1034 8.720000  
## 1035 8.695000  
## 1036 8.709333  
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## 1039 8.512500  
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## 1044 8.511045  
## 1045 8.700000  
## 1046 8.320000  
## 1047 8.300000  
## 1048 8.480000  
## 1049 8.456667  
## 1050 8.423200  
## 1051 8.480000  
## 1052 8.440000  
## 1053 8.424000  
## 1054 8.420000  
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## 1063 8.784706  
## 1064 8.720000  
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## 1068 8.715556  
## 1069 8.700000  
## 1070 8.518182  
## 1071 8.500000  
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## 1080 8.428571  
## 1081 8.395000  
## 1082 8.700000  
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## 1086 8.800000  
## 1087 8.460000  
## 1088 8.726154  
## 1089 8.772941  
## 1090 8.777500  
## 1091 8.900000  
## 1092 8.920000  
## 1093 8.821538  
## 1094 8.700000  
## 1095 8.720000  
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## 1098 8.500000  
## 1099 8.520000  
## 1100 8.513684  
## 1101 8.586667  
## 1102 8.470000  
## 1103 8.380000  
## 1104 8.436000  
## 1105 8.410000  
## 1106 8.440000  
## 1107 8.440000  
## 1108 8.460000  
## 1109 8.460000  
## 1110 8.720000  
## 1111 8.800000  
## 1112 8.785714  
## 1113 8.713333  
## 1114 8.740000  
## 1115 8.794545  
## 1116 8.836667  
## 1117 8.808571  
## 1118 8.720000  
## 1119 8.720000  
## 1120 8.520000  
## 1121 8.520000  
## 1122 8.519600  
## 1123 8.471429  
## 1124 8.490000  
## 1125 8.460000  
## 1126 8.440000  
## 1127 8.425000  
## 1128 8.400000  
## 1129 8.420000  
## 1130 8.460000  
## 1131 8.460000  
## 1132 8.760000  
## 1133 8.714286  
## 1134 8.813333  
## 1135 8.765000  
## 1136 8.780000  
## 1137 8.802857  
## 1138 8.800000  
## 1139 8.844000  
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## 1141 8.800000  
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## 1144 8.520000  
## 1145 8.520000  
## 1146 8.525581  
## 1147 8.482857  
## 1148 8.460000  
## 1149 8.486667  
## 1150 8.440000  
## 1151 8.440000  
## 1152 8.760000  
## 1153 8.709474  
## 1154 8.795000  
## 1155 8.850000  
## 1156 8.750000  
## 1157 8.780000  
## 1158 8.820000  
## 1159 8.800000  
## 1160 8.492000  
## 1161 8.530000  
## 1162 8.420000  
## 1163 8.493333  
## 1164 8.440000  
## 1165 8.440000  
## 1166 8.722500  
## 1167 8.700000  
## 1168 8.120000  
## 1169 8.800000  
## 1170 8.531892  
## 1171 8.460000  
## 1172 8.500000  
## 1173 8.480000  
## 1174 8.440000  
## 1175 8.440000  
## 1176 8.740000  
## 1177 8.720000  
## 1178 8.695556  
## 1179 8.720000  
## 1180 8.522857  
## 1181 8.543750  
## 1182 8.440000  
## 1183 8.440000  
## 1184 8.760000  
## 1185 8.720000  
## 1186 8.680000  
## 1187 8.700000  
## 1188 8.560000  
## 1189 8.518947  
## 1190 8.540000  
## 1191 8.570000  
## 1192 8.580000  
## 1193 8.720000  
## 1194 8.700000  
## 1195 8.700000  
## 1196 8.500000  
## 1197 8.522500  
## 1198 8.500000  
## 1199 8.543077  
## 1200 8.540000  
## 1201 8.520000  
## 1202 8.540000  
## 1203 8.560000  
## 1204 8.520000  
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## 1213 8.520000  
## 1214 8.540000  
## 1215 8.540000

# revisit glmnet model to compare coefficient values with random forest splits   
myControl <- trainControl(method = 'cv', number = 5, verboseIter = FALSE, savePredictions = TRUE)  
  
model\_glmnet = train(PH ~ ., data = beverages\_v1\_train, metric = 'RMSE', method = 'glmnet',   
 preProcess = c('center', 'scale'), trControl = myControl)  
  
coef(model\_glmnet$finalModel, model\_glmnet$bestTune$lambda)

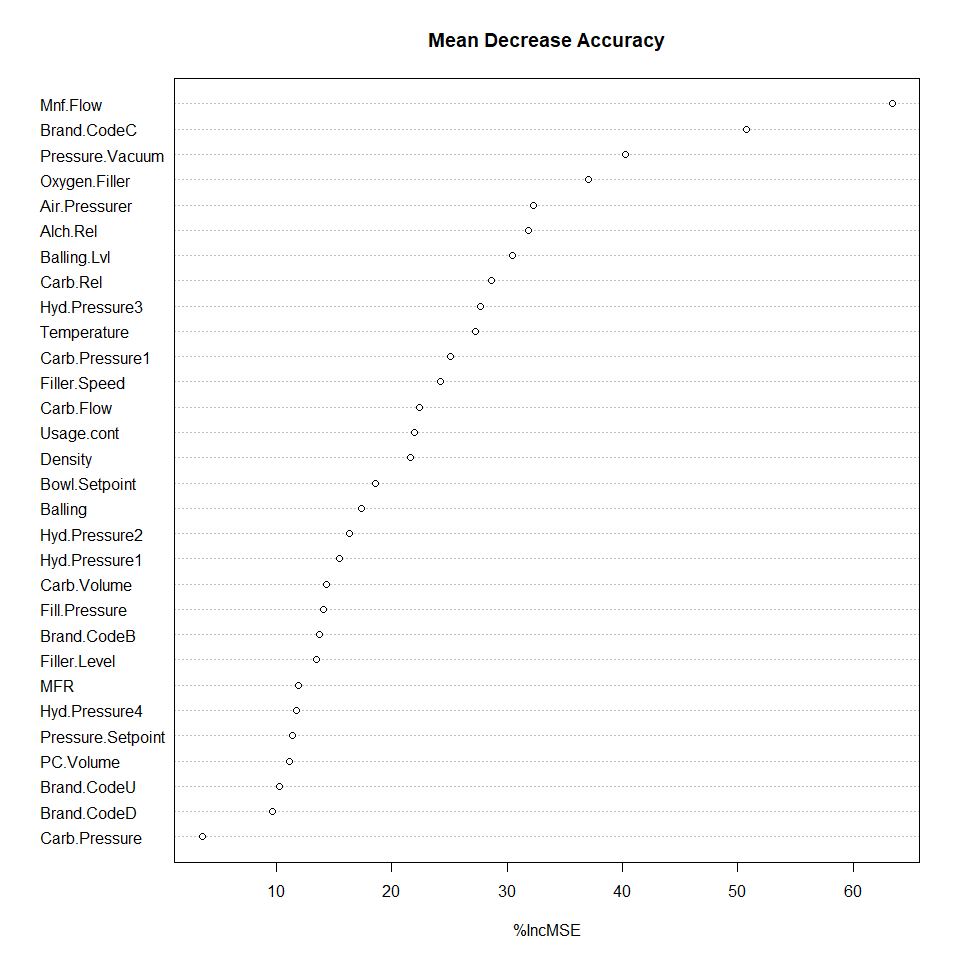
## 36 x 1 sparse Matrix of class "dgCMatrix"  
## 1  
## (Intercept) 8.5425680934  
## Brand.CodeB 0.0387439580  
## Brand.CodeC -0.0214470730  
## Brand.CodeD 0.0168660330  
## Brand.CodeU -0.0031507530  
## Carb.Volume -0.0069102324  
## Fill.Ounces -0.0064728090  
## PC.Volume -0.0086349925  
## Carb.Pressure 0.0042024483  
## Carb.Temp -0.0004410234  
## PSC -0.0067630474  
## PSC.Fill 0.0004887432  
## PSC.CO2 -0.0093595276  
## Mnf.Flow -0.0833512790  
## Carb.Pressure1 0.0334238213  
## Fill.Pressure 0.0059565543  
## Hyd.Pressure1 0.0015061320  
## Hyd.Pressure2 -0.0133821510  
## Hyd.Pressure3 0.0462655396  
## Hyd.Pressure4 -0.0049424662  
## Filler.Level -0.0030960208  
## Filler.Speed 0.0125569647  
## Temperature -0.0199411911  
## Usage.cont -0.0235922599  
## Carb.Flow 0.0096585625  
## Density -0.0351709812  
## MFR -0.0167306418  
## Balling -0.0255499223  
## Pressure.Vacuum -0.0052203278  
## Oxygen.Filler -0.0086074139  
## Bowl.Setpoint 0.0357194663  
## Pressure.Setpoint -0.0168456678  
## Air.Pressurer -0.0009366253  
## Alch.Rel 0.0284011130  
## Carb.Rel .   
## Balling.Lvl 0.0479795428

The model’s decision tree is consistent with the the variable importance output. The first node of the tree is Mnf.Flow with a split point of about -50, which seems to be separating valid vs. invalid (-100) Mnf.Flow values. The records with invalid Mnf.Flow values seem to have higher pH values.

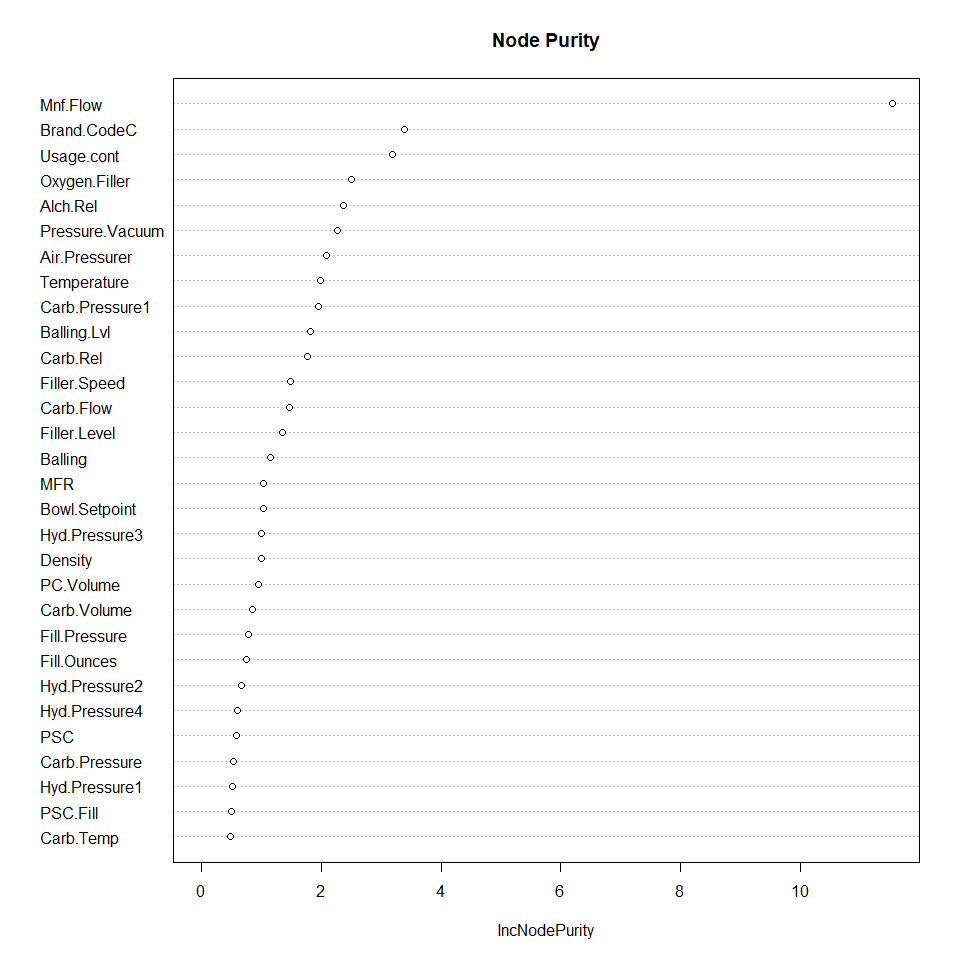
The first node on the left branch is Brand.Code4, which equates to Brand.Code “C”. Here, it seems that records with Brand.Code “C” have lower pH values. The first node on the right branch is Brand.Code5, which equates to Brand.Code “D” and is associated with higher pH values.

These positive/negative associations between pH and the important variables are consistent with the coefficients from an earlier glmnet model, which while not as accurate in terms of RMSE does produce much more interpretable results. On a centered and scaled basis, the variables that most increased pH were Balling.Lvl and Carb.Pressure1, and the variables that most decreased pH were Mnf.Flow and Brand.Code “C”.

varImpPlot(rf\_M1\_Data1$finalModel, type = 1, main = "Mean Decrease Accuracy") # graph 1 MSE



varImpPlot(rf\_M1\_Data1$finalModel, type = 2, main = "Node Purity") # graph 2 RSS



Graph1 above shows that if a variable is assigned values by random permutation, how much the mean squared error (MSE) will increase. In this case, if you randomly permute Mnf.Flow, MSE will increase by 60% on average.

Graph2 above shows Node purity which is measured by the Gini index which is the difference between residual sum of squares (RSS) before and after the split on that particular variable. So, IncNodePurity measures decrease in node impurities from splitting on the variable, averaged across all trees.

## Evaluation

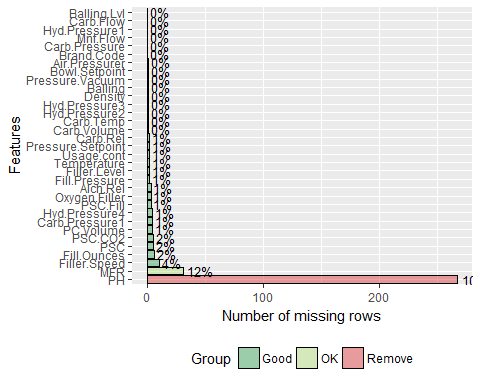
### Evaluation Data set and required tranformations

We will load the evaluation data set and performed the necessary data transformation to run our selected model.

#set file name - to be change by github link#  
beverages\_filename\_eval<- "https://raw.githubusercontent.com/vbriot28/Data624\_Group1\_FinalProject/master/StudentEvaluation-%20TO%20PREDICT.csv"  
  
# Load Evaluation Data Set  
beverages\_eval <-read.csv(beverages\_filename\_eval, header=TRUE, sep=",",stringsAsFactors = F)

Based on our selected model, we only need to impute the data and converting any “unspecified” Brand code as “U”, we will first check whether this is a required steps but checking for missing data.

PlotMissing(beverages\_eval)



We will impute the missing values for all our predictors.

beverages\_eval$Brand.Code[beverages\_eval$Brand.Code==""]= "U"  
  
beverages\_eval\_predictor <-beverages\_eval  
beverages\_eval\_predictor$PH <- NULL  
  
mice\_imputes\_eval <- mice(beverages\_eval\_predictor, m = 2, maxit = 2, print = FALSE,seed = 143)  
  
beverages\_eval\_v1 <- complete(mice\_imputes\_eval)  
  
beverages\_eval\_v1 <- cbind(beverages\_eval\_v1, beverages\_eval$PH)

We will now predict PH using our selected model, the result will be written in a .csv file.

prediction\_rf <- predict(rf\_M1\_Data1, beverages\_eval\_v1)  
  
write.csv(prediction\_rf, file = "prediction\_rf1.csv")

# Conclusing

# References:

**EDA**  
<https://cran.r-project.org/web/packages/DataExplorer/vignettes/dataexplorer-intro.html>

**Data Transformation**  
<https://www.r-bloggers.com/near-zero-variance-predictors-should-we-remove-them/> <http://rcompanion.org/handbook/I_12.html>

**Model Selection** <https://rpubs.com/Isaac/caret_reg>