Data624 - Project2

Amanda Arce, Jatin Jain, Amit Kapoor

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Contents

Overview

ABC Beverage has new regulations in place and the leadership team requires the data scientists team to understand the manufacturing process, the predictive factors and be able to report to them predictive model of PH. The selection of model depends upon various factors like model accuracy, data relevance, cross validation etc.

R packages

We will use `r` for data modeling. All packages used for data exploration, visualization, preparation and modeling are listed in Code Appendix.

Data Exploration

We will first get the historical dataset, provided in excel and use it to analyze and eventually predict the PH of beverages.

Data summary

There are 31 predictor variables that are numeric and 1 predictor variable `Brand Code` which is factor. The training dataset has 2,571 observations.

```
## Rows: 2,571
## Columns: 33
## $ `Brand Code`        <fct> B, A, B, A, A, A, A, B, B, B, B, B, B, B, B, B, C,~
## $ `Carb Volume`       <dbl> 5.340000, 5.426667, 5.286667, 5.440000, 5.486667, ~
## $ `Fill Ounces`       <dbl> 23.96667, 24.00667, 24.06000, 24.00667, 24.31333, ~
## $ `PC Volume`         <dbl> 0.2633333, 0.2386667, 0.2633333, 0.2933333, 0.1113~
## $ `Carb Pressure`     <dbl> 68.2, 68.4, 70.8, 63.0, 67.2, 66.6, 64.2, 67.6, 64~
## $ `Carb Temp`         <dbl> 141.2, 139.6, 144.8, 132.6, 136.8, 138.4, 136.8, 1~
## $ PSC                 <dbl> 0.104, 0.124, 0.090, NA, 0.026, 0.090, 0.128, 0.15~
## $ `PSC Fill`          <dbl> 0.26, 0.22, 0.34, 0.42, 0.16, 0.24, 0.40, 0.34, 0.~
## $ `PSC CO2`           <dbl> 0.04, 0.04, 0.16, 0.04, 0.12, 0.04, 0.04, 0.04, 0.~
## $ `Mnf Flow`          <dbl> -100, -100, -100, -100, -100, -100, -100, -100, -1~
## $ `Carb Pressure1`    <dbl> 118.8, 121.6, 120.2, 115.2, 118.4, 119.6, 122.2, 1~
## $ `Fill Pressure`     <dbl> 46.0, 46.0, 46.0, 46.4, 45.8, 45.6, 51.8, 46.8, 46~
## $ `Hyd Pressure1`     <dbl> 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,~
## $ `Hyd Pressure2`     <dbl> NA, NA, NA, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,~
## $ `Hyd Pressure3`     <dbl> NA, NA, NA, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,~
## $ `Hyd Pressure4`     <dbl> 118, 106, 82, 92, 92, 116, 124, 132, 90, 108, 94, ~
## $ `Filler Level`      <dbl> 121.2, 118.6, 120.0, 117.8, 118.6, 120.2, 123.4, 1~
## $ `Filler Speed`      <dbl> 4002, 3986, 4020, 4012, 4010, 4014, NA, 1004, 4014~
## $ Temperature         <dbl> 66.0, 67.6, 67.0, 65.6, 65.6, 66.2, 65.8, 65.2, 65~
## $ `Usage cont`        <dbl> 16.18, 19.90, 17.76, 17.42, 17.68, 23.82, 20.74, 1~
## $ `Carb Flow`         <dbl> 2932, 3144, 2914, 3062, 3054, 2948, 30, 684, 2902,~
## $ Density             <dbl> 0.88, 0.92, 1.58, 1.54, 1.54, 1.52, 0.84, 0.84, 0.~
## $ MFR                 <dbl> 725.0, 726.8, 735.0, 730.6, 722.8, 738.8, NA, NA, ~
## $ Balling             <dbl> 1.398, 1.498, 3.142, 3.042, 3.042, 2.992, 1.298, 1~
## $ `Pressure Vacuum`   <dbl> -4.0, -4.0, -3.8, -4.4, -4.4, -4.4, -4.4, -4.4, -4~
## $ PH                  <dbl> 8.36, 8.26, 8.94, 8.24, 8.26, 8.32, 8.40, 8.38, 8.~
## $ `Oxygen Filler`     <dbl> 0.022, 0.026, 0.024, 0.030, 0.030, 0.024, 0.066, 0~
## $ `Bowl Setpoint`     <dbl> 120, 120, 120, 120, 120, 120, 120, 120, 120, 120, ~
## $ `Pressure Setpoint` <dbl> 46.4, 46.8, 46.6, 46.0, 46.0, 46.0, 46.0, 46.0, 46~
## $ `Air Pressurer`     <dbl> 142.6, 143.0, 142.0, 146.2, 146.2, 146.6, 146.2, 1~
## $ `Alch Rel`          <dbl> 6.58, 6.56, 7.66, 7.14, 7.14, 7.16, 6.54, 6.52, 6.~
## $ `Carb Rel`          <dbl> 5.32, 5.30, 5.84, 5.42, 5.44, 5.44, 5.38, 5.34, 5.~
## $ `Balling Lvl`       <dbl> 1.48, 1.56, 3.28, 3.04, 3.04, 3.02, 1.44, 1.44, 1.~
```

```
##                      n    mean      sd  median     min     max   range  skew
## Brand Code*       2451    2.51    1.00    2.00    1.00    4.00    3.00  0.38
## Carb Volume       2561    5.37    0.11    5.35    5.04    5.70    0.66  0.39
## Fill Ounces       2533   23.97    0.09   23.97   23.63   24.32    0.69 -0.02
```

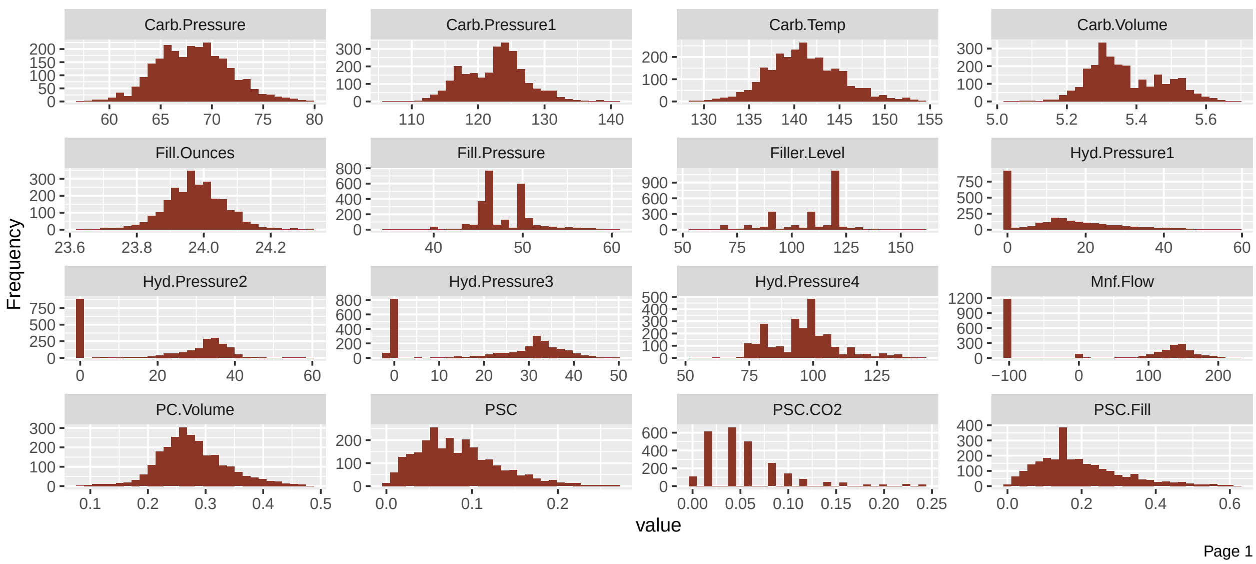
```
## PC Volume         2532    0.28    0.06    0.27    0.08    0.48    0.40  0.34
## Carb Pressure     2544   68.19    3.54   68.20   57.00   79.40   22.40  0.18
## Carb Temp         2545  141.09    4.04  140.80  128.60  154.00   25.40  0.25
## PSC               2538    0.08    0.05    0.08    0.00    0.27    0.27  0.85
## PSC Fill          2548    0.20    0.12    0.18    0.00    0.62    0.62  0.93
## PSC CO2           2532    0.06    0.04    0.04    0.00    0.24    0.24  1.73
## Mnf Flow          2569   24.57  119.48   65.20 -100.20  229.40  329.60  0.00
## Carb Pressure1    2539  122.59    4.74  123.20  105.60  140.20   34.60  0.05
## Fill Pressure     2549   47.92    3.18   46.40   34.60   60.40   25.80  0.55
## Hyd Pressure1     2560   12.44   12.43   11.40   -0.80   58.00   58.80  0.78
## Hyd Pressure2     2556   20.96   16.39   28.60    0.00   59.40   59.40 -0.30
## Hyd Pressure3     2556   20.46   15.98   27.60   -1.20   50.00   51.20 -0.32
## Hyd Pressure4     2541   96.29   13.12   96.00   52.00  142.00   90.00  0.55
## Filler Level      2551  109.25   15.70  118.40   55.80  161.20  105.40 -0.85
## Filler Speed      2514 3687.20  770.82 3982.00  998.00 4030.00 3032.00 -2.87
## Temperature       2557   65.97    1.38   65.60   63.60   76.20   12.60  2.39
## Usage cont        2566   20.99    2.98   21.79   12.08   25.90   13.82 -0.54
## Carb Flow         2569 2468.35 1073.70 3028.00   26.00 5104.00 5078.00 -0.99
## Density           2570    1.17    0.38    0.98    0.24    1.92    1.68  0.53
## MFR               2359  704.05   73.90  724.00   31.40  868.60  837.20 -5.09
## Balling           2570    2.20    0.93    1.65   -0.17    4.01    4.18  0.59
## Pressure Vacuum   2571   -5.22    0.57   -5.40   -6.60   -3.60    3.00  0.53
## PH                2567    8.55    0.17    8.54    7.88    9.36    1.48 -0.29
## Oxygen Filler     2559    0.05    0.05    0.03    0.00    0.40    0.40  2.66
## Bowl Setpoint     2569  109.33   15.30  120.00   70.00  140.00   70.00 -0.97
## Pressure Setpoint 2559   47.62    2.04   46.00   44.00   52.00    8.00  0.20
## Air Pressurer     2571  142.83    1.21  142.60  140.80  148.20    7.40  2.25
## Alch Rel          2562    6.90    0.51    6.56    5.28    8.62    3.34  0.88
## Carb Rel          2561    5.44    0.13    5.40    4.96    6.06    1.10  0.50
## Balling Lvl       2570    2.05    0.87    1.48    0.00    3.66    3.66  0.59
##                   kurtosis
## Brand Code*          -1.06
## Carb Volume          -0.47
## Fill Ounces           0.86
## PC Volume             0.67
## Carb Pressure        -0.01
## Carb Temp             0.24
## PSC                   0.65
## PSC Fill              0.77
## PSC CO2               3.73
## Mnf Flow             -1.87
## Carb Pressure1        0.14
## Fill Pressure         1.41
## Hyd Pressure1        -0.14
## Hyd Pressure2        -1.56
## Hyd Pressure3        -1.57
## Hyd Pressure4         0.63
## Filler Level          0.05
## Filler Speed          6.71
## Temperature          10.16
## Usage cont           -1.02
## Carb Flow            -0.58
## Density              -1.20
## MFR                  30.46
```

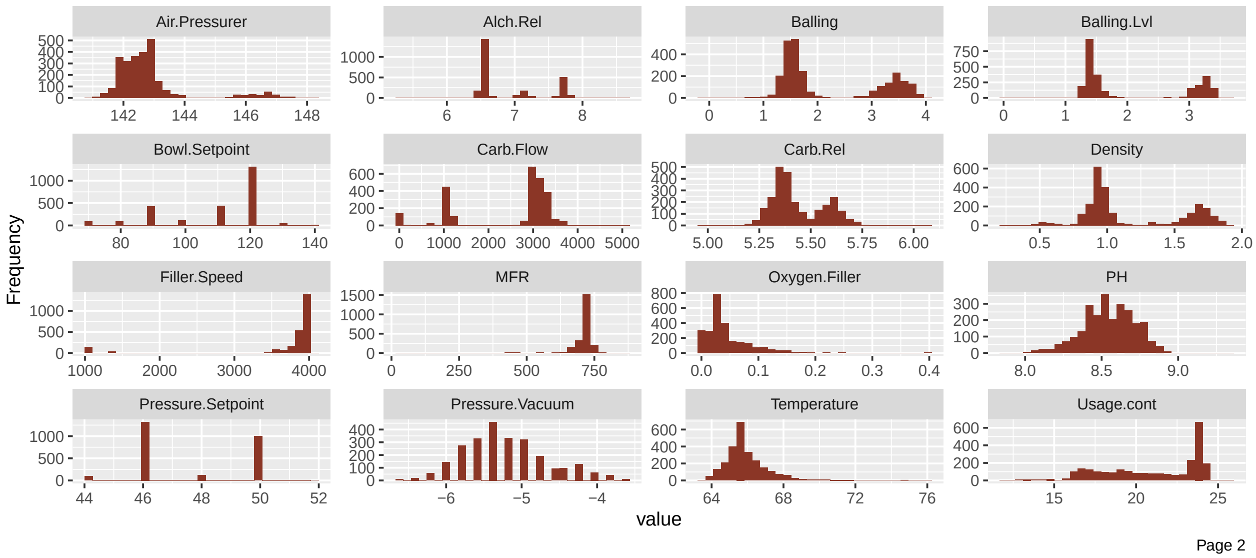
```
## Balling                 -1.39
## Pressure Vacuum         -0.03
## PH                       0.06
## Oxygen Filler           11.09
## Bowl Setpoint           -0.06
## Pressure Setpoint       -1.60
## Air Pressurer            4.73
## Alch Rel                -0.85
## Carb Rel                -0.29
## Balling Lvl             -1.49
```

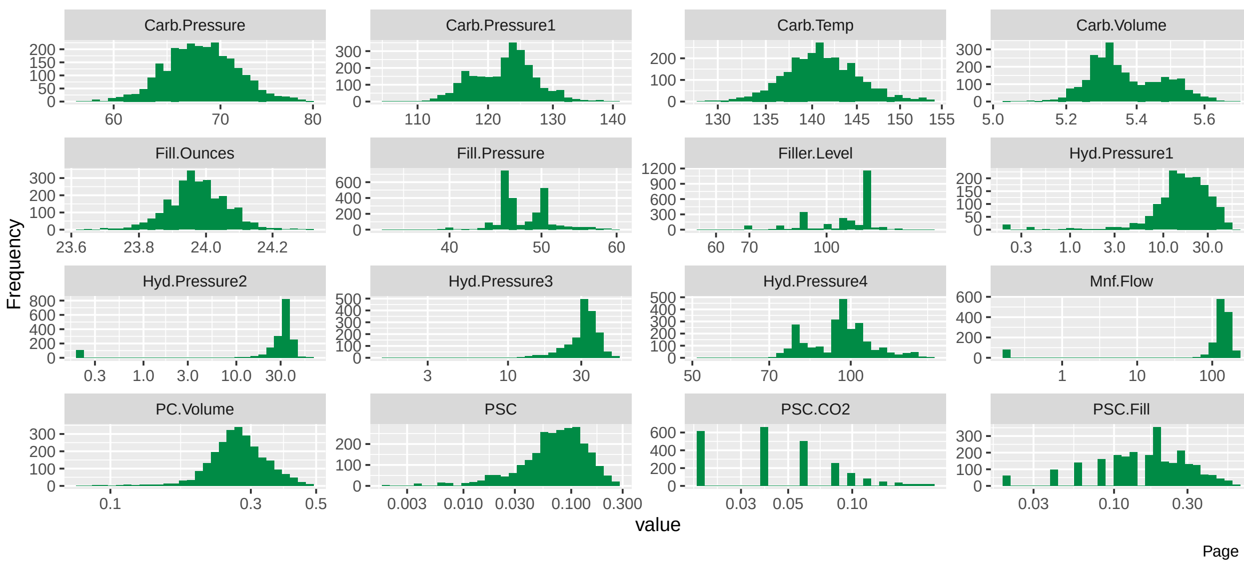
Based of above description, we can see the dataset has missing values so it would need imputation. The predictors `Oxygen Filler`, `MFR`, `Filler Speed` and `Temperature` seems highly skewed and would require transformation. This could be seen in below histogram plots as well.

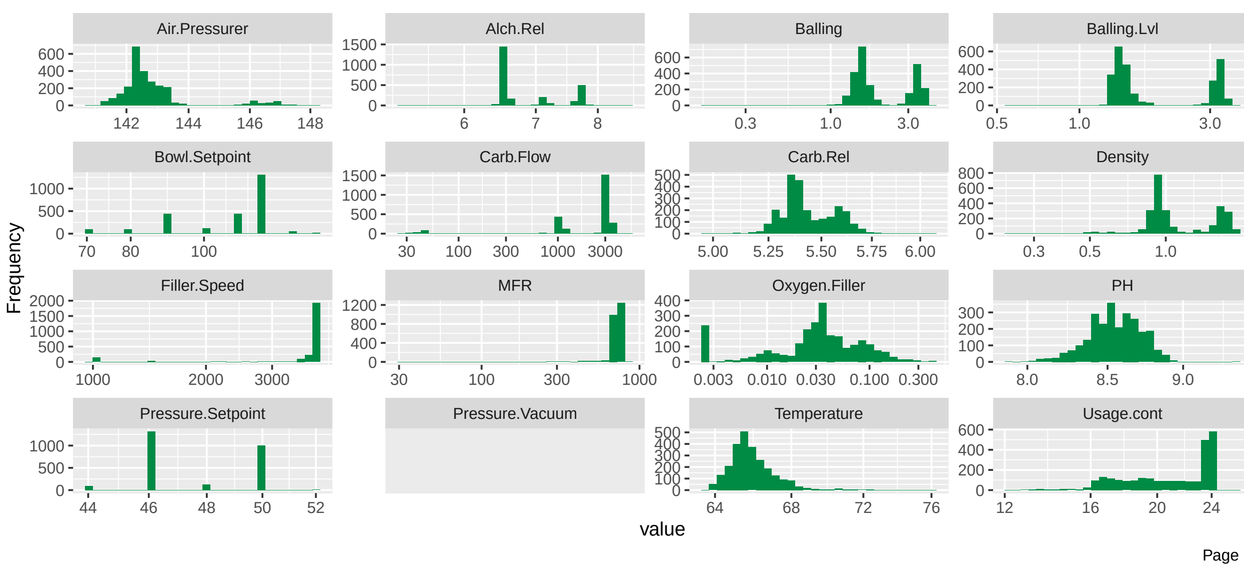
Variables Distribution

Below we have shown the distribution of dataset variables. There are 2 sets of histograms; the one in red is natural distribution and the ones in green are logarithmic disctribution




Air.Pressurer
Alch.Rel
Balling
Balling.Lvl
Bowl.Setpoint
Carb.Flow
Carb.Rel
Density
Filler.Speed
MFR
Oxygen.Filler
PH
Pressure.Setpoint
Pressure.Vacuum
Temperature
Usage.cont
Frequency
value
Page 2

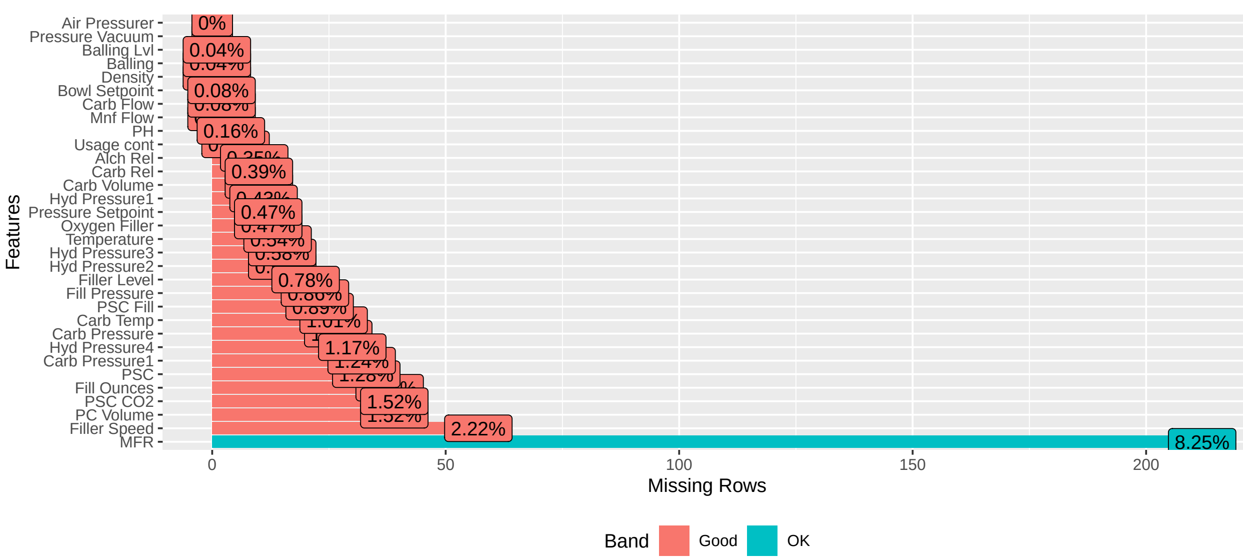

Carb.Pressure
Carb.Pressure1
Carb.Temp
Carb.Volume
Fill.Ounces
Fill.Pressure
Filler.Level
Hyd.Pressure1
Hyd.Pressure2
Hyd.Pressure3
Hyd.Pressure4
Mnf.Flow
PC.Volume
PSC
PSC.CO2
PSC.Fill
Frequency
value
Page 1


Air.Pressurer
Alch.Rel
Balling
Balling.Lvl
Bowl.Setpoint
Carb.Flow
Carb.Rel
Density
Filler.Speed
MFR
Oxygen.Filler
PH
Pressure.Setpoint
Pressure.Vacuum
Temperature
Usage.cont
Frequency
value
Page 2

Missing Data

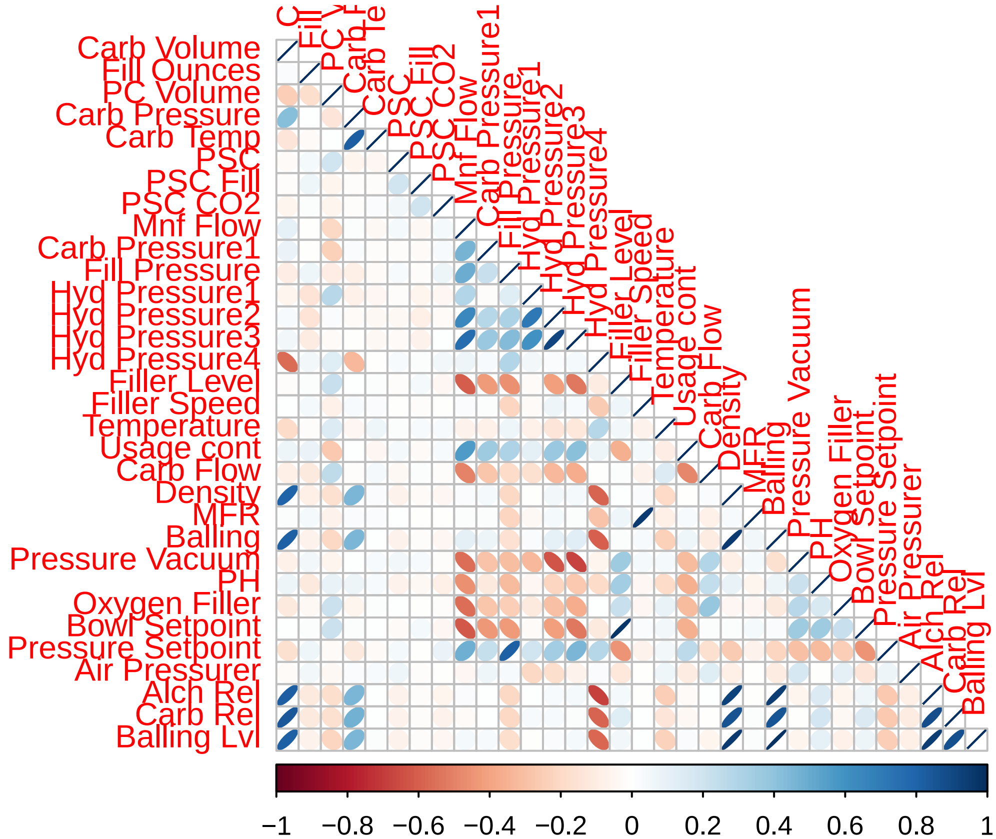
The summary and following graphs show the missing data in training dataset. The plot below shows more than 8% data is missing for `MFR` variable. Next feature that has missing data is `Filler Speed` which shows more than 2% missing data. The missing data will be handled through imputation.

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



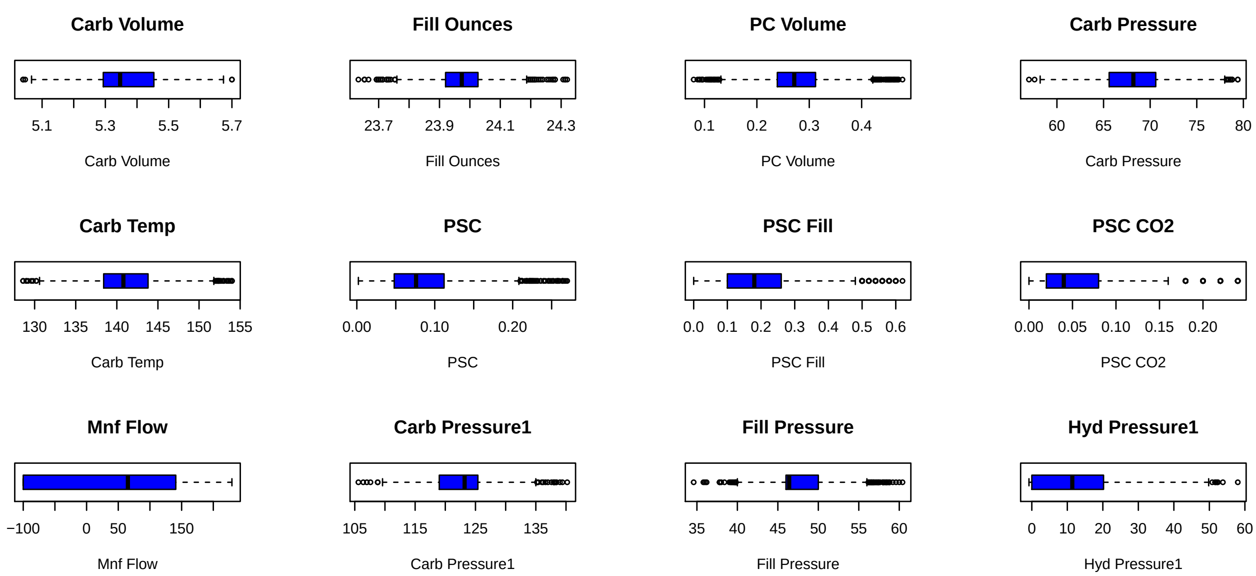
Correlation

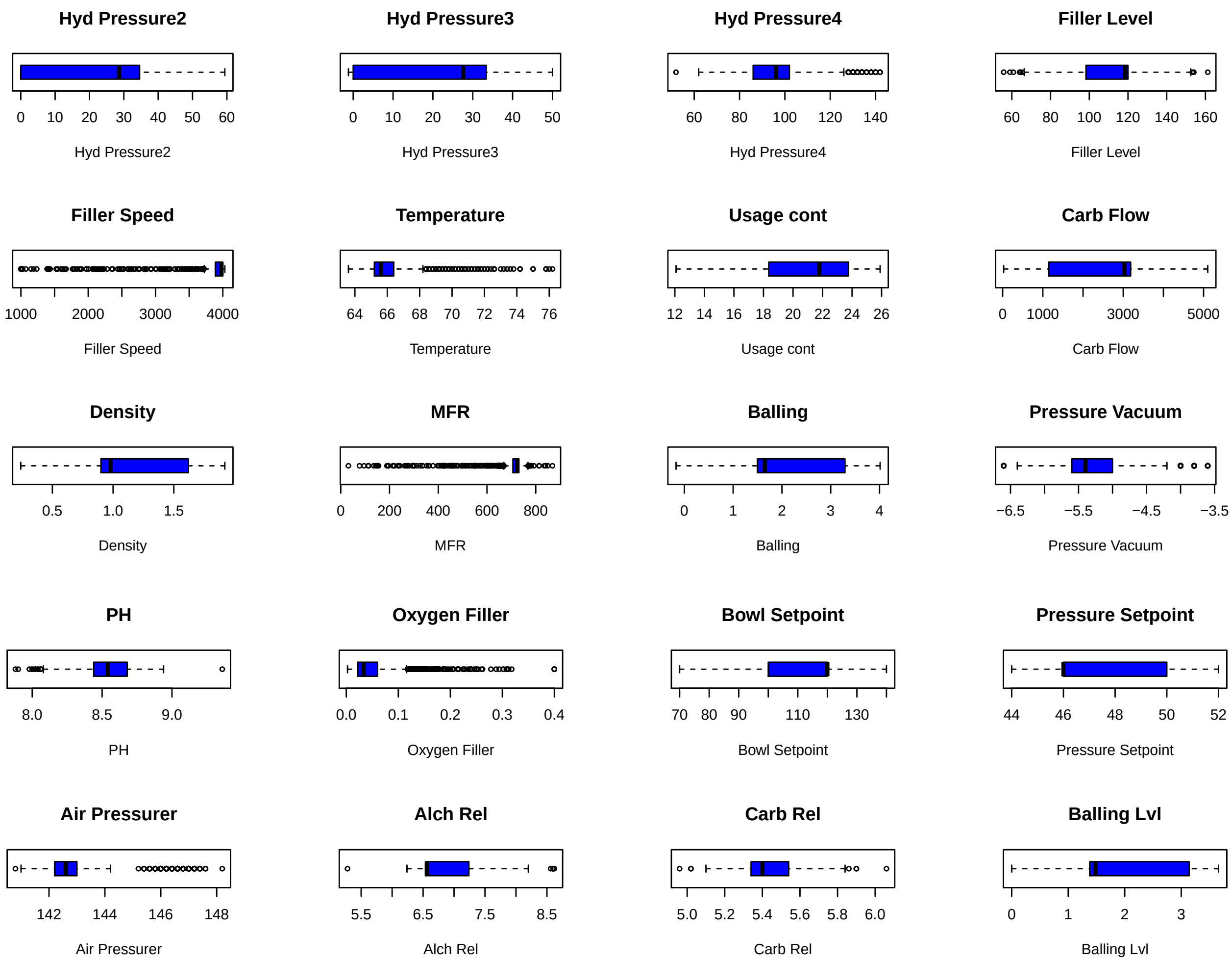
below plot shows the correlation among numeric variables in the dataset. We can see few variables are highly correlated. We will handle the pairwise predictors that has correlation above 0.90 in data preparation section.



Outliers

In this section we will check the outliers in the data. An outlier is an observation that lies an unusual distance from other values in a random sample.These outlier could impact predictions so will be handled through imputation





Data Preparation

Handling missing and outliers

The very first in data preparation we will perform is handling missing data and outliers through imputation. We will use mice package to perform imputation here. MICE (Multivariate Imputation via Chained Equations) is one of the commonly used package for this activity. It creates multiple imputations for multivariate missing data. Also we will perform `nearZeroVar` to see if a variable has very little change or variation and not useful for prediction. If we founf any predictor variable satisfying this condition we would remove it.

Create Dummy Variables

The variable Brand Code is a categorical variable, having 4 classes (A, B, C, and D). For modeling, we got to convert into set of dummy variables. We will use `dummyVars` function for this purpose that creates a full set of dummy variables.

Correlation

Next step is to remove highly correlated predictor variables. we will use the cutoff as 0.90 here.

Preprocess using transformation

In this step we will use caret `preprocess` method using transformation as `YeoJohnson` which applies Yeo-Johnson transformation, like a BoxCox, but values can be negative as well.

Training and Test Partition

Finally in this step for data preparation we will partition the training dataset for training and validation using `createDataPartition` method from `caret` package. We will reserve 75% for training and rest 25% for validation purpose.

Build Models

Linear Regression

Simple Linear Regression

We will start with Simple Linear Regression model. It will include all the predictor variables in training dataset.

```
##
## Call:
## lm(formula = y.train ~ ., data = X.train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.50865 -0.08187  0.01030  0.08869  0.82191
##
## Coefficients: (1 not defined because of singularities)
##                     Estimate Std. Error t value Pr(>|t|)
## (Intercept)       -7.448e+02  4.113e+03  -0.181  0.85633
## Brand.Code.A      -5.371e-02  1.773e-02  -3.030  0.00248 **
## Brand.Code.B       4.502e-02  2.794e-02   1.611  0.10729
## Brand.Code.C      -8.575e-02  2.891e-02  -2.966  0.00305 **
## Brand.Code.D              NA         NA      NA       NA
## Carb.Volume       -5.906e-02  9.057e-02  -0.652  0.51443
## Fill.Ounces       -2.363e-03  9.073e-04  -2.605  0.00927 **
## PC.Volume         -2.143e-01  9.730e-02  -2.202  0.02777 *
## Carb.Pressure      2.425e-01  6.661e-01   0.364  0.71593
## Carb.Temp          1.481e+03  8.134e+03   0.182  0.85554
## PSC               -4.662e-02  6.751e-02  -0.691  0.48992
## PSC.Fill          -7.216e-02  5.804e-02  -1.243  0.21393
## PSC.CO2           -1.478e-01  7.517e-02  -1.966  0.04948 *
## Mnf.Flow          -6.253e-04  5.385e-05 -11.612  < 2e-16 ***
## Carb.Pressure1     8.485e-02  1.007e-02   8.426  < 2e-16 ***
## Fill.Pressure      2.690e+00  8.374e-01   3.212  0.00134 **
## Hyd.Pressure2      7.293e-03  1.229e-03   5.932 3.54e-09 ***
## Hyd.Pressure4      5.719e-02  1.123e-01   0.509  0.61070
## Temperature       -1.270e-02  2.553e-03  -4.976 7.06e-07 ***
## Usage.cont        -8.134e-03  1.341e-03  -6.068 1.56e-09 ***
## Carb.Flow          9.961e-07  4.356e-07   2.287  0.02232 *
## MFR               -5.603e-05  3.119e-05  -1.797  0.07255 .
## Pressure.Vacuum    9.796e-05  1.700e-04   0.576  0.56451
## Oxygen.Filler     -2.461e-01  7.787e-02  -3.160  0.00160 **
## Bowl.Setpoint      2.408e-03  3.106e-04   7.752 1.46e-14 ***
```

```
## Pressure.Setpoint -7.424e-03  2.266e-03  -3.276  0.00107 **
## Air.Pressurer      4.131e-04  2.784e-03   0.148  0.88205
## Alch.Rel           6.044e-02  2.220e-02   2.722  0.00654 **
## Carb.Rel           4.822e-03  5.215e-02   0.092  0.92634
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.1359 on 1902 degrees of freedom
## Multiple R-squared:  0.3875, Adjusted R-squared:  0.3788
## F-statistic: 44.56 on 27 and 1902 DF,  p-value: < 2.2e-16
```

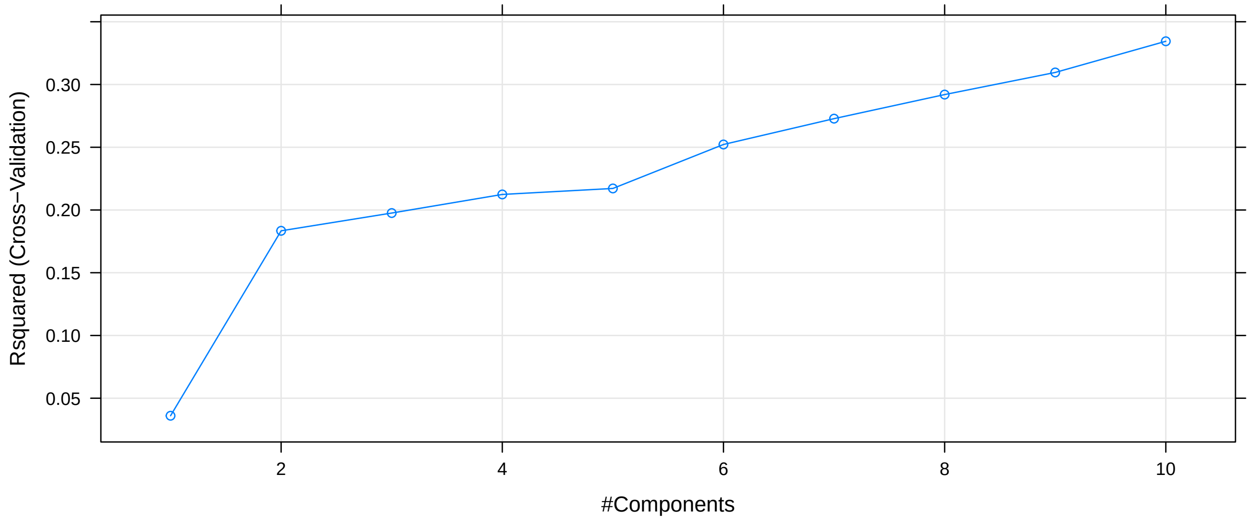
We can see that Simple Linear Regression model only covers 38% of variability of data. Next we will check for better models which covers better variability, RMSE and MAE. We can consider this Simple regression as a benchmark model among others we are going to check.

Partial Least Squares

Partial least squares (PLS) is an alternative to ordinary least squares (OLS) regression. It reduces the predictors to a smaller set of uncorrelated components and then performs least squares regression on these components, instead of on the original data. PLS finds linear combinations of the predictors called components. PLS finds components that attempts to maximally summarize the variation of the predictors while at the same time attempts these components to have maximum correlation with the response.

```
## Partial Least Squares
##
## 1930 samples
##   28 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   ncomp  RMSE       Rsquared    MAE
##    1     0.1695850  0.03602419  0.1357999
##    2     0.1557700  0.18341292  0.1233261
##    3     0.1545817  0.19755922  0.1216561
##    4     0.1532406  0.21239112  0.1210109
##    5     0.1528414  0.21716670  0.1205175
##    6     0.1491851  0.25219747  0.1167355
##    7     0.1471796  0.27279224  0.1153866
##    8     0.1450812  0.29197059  0.1140281
##    9     0.1431131  0.30960456  0.1118836
##   10     0.1405086  0.33444735  0.1097224
##
## Rsquared was used to select the optimal model using the largest value.
## The final value used for the model was ncomp = 10.
```

```
##    ncomp
## 10    10
```




```
##   ncomp      RMSE  Rsquared
## 1    10 0.1405086 0.3344473
```

```
##    Rsquared      RMSE
## 1 0.3344473 0.1405086
```

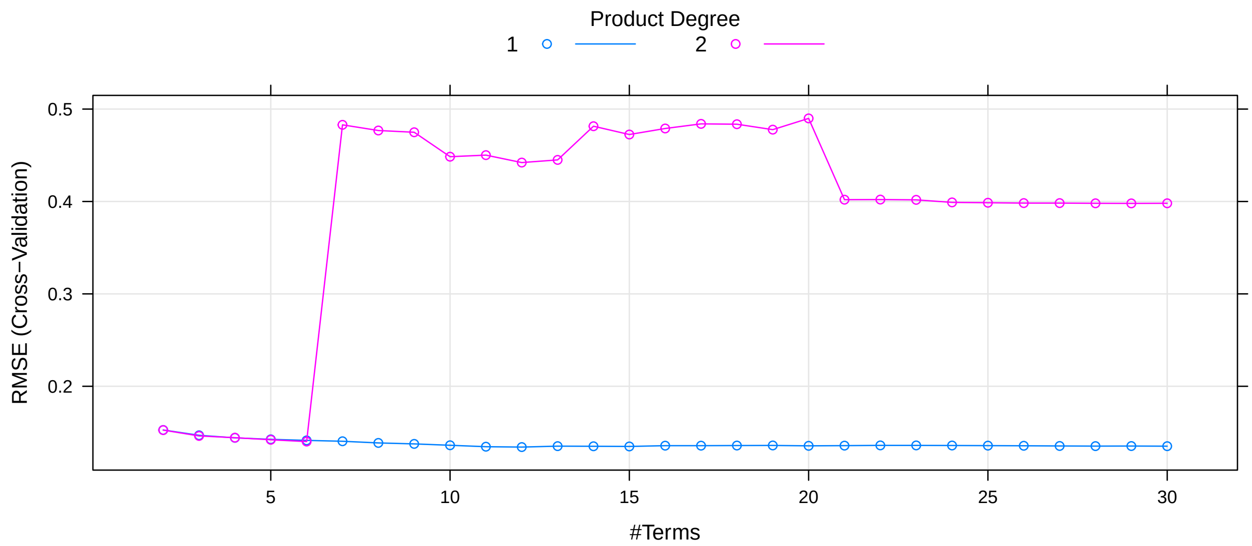
Rsquared was used to select the optimal model using the largest value. The final value used for the model was ncomp = 10 which corresponds to best tune model. In this case we see that R^2 is 0.33 so only covers 33% variability in data but it produces small RMSE.

Non Linear Regression

MARS

MARS creates a piecewise linear model which provides an intuitive stepping block into non-linearity after grasping the concept of multiple linear regression. MARS provided a convenient approach to capture the nonlinear relationships in the data by assessing cutpoints (knots) similar to step functions. The procedure assesses each data point for each predictor as a knot and creates a linear regression model with the candidate features

```
##    nprune degree
## 11     12      1
```




```
## Call: earth(x=data.frame[1930,28], y=c(8.36,8.26,8.9...), keepxy=TRUE,
##             degree=1, nprune=12)
##
##                                coefficients
## (Intercept)                       8.5433911
## Brand.Code.C                     -0.1187748
## h(0.199353-Mnf.Flow)              0.0011789
## h(19.8091-Carb.Pressure1)        -0.0845067
## h(2.1938-Hyd.Pressure2)          -0.0196752
## h(Temperature-65)                -0.0307466
## h(Temperature-68.4)               0.0443562
## h(Usage.cont-22.2)               -0.0443013
## h(Pressure.Vacuum- -63.7021)     -0.0031964
## h(Bowl.Setpoint-90)               0.0024596
## h(7.16-Alch.Rel)                  0.1127772
## h(Alch.Rel-7.16)                  0.1804968
##
## Selected 12 of 32 terms, and 9 of 28 predictors (nprune=12)
## Termination condition: RSq changed by less than 0.001 at 32 terms
## Importance: Mnf.Flow, Brand.Code.C, Alch.Rel, Usage.cont, Carb.Pressure1, ...
## Number of terms at each degree of interaction: 1 11 (additive model)
## GCV 0.0178492    RSS 33.63279    GRSq 0.3998146    RSq 0.4134266
```

```
##   Rsquared      RMSE
## 1 0.337374 0.1404835
```

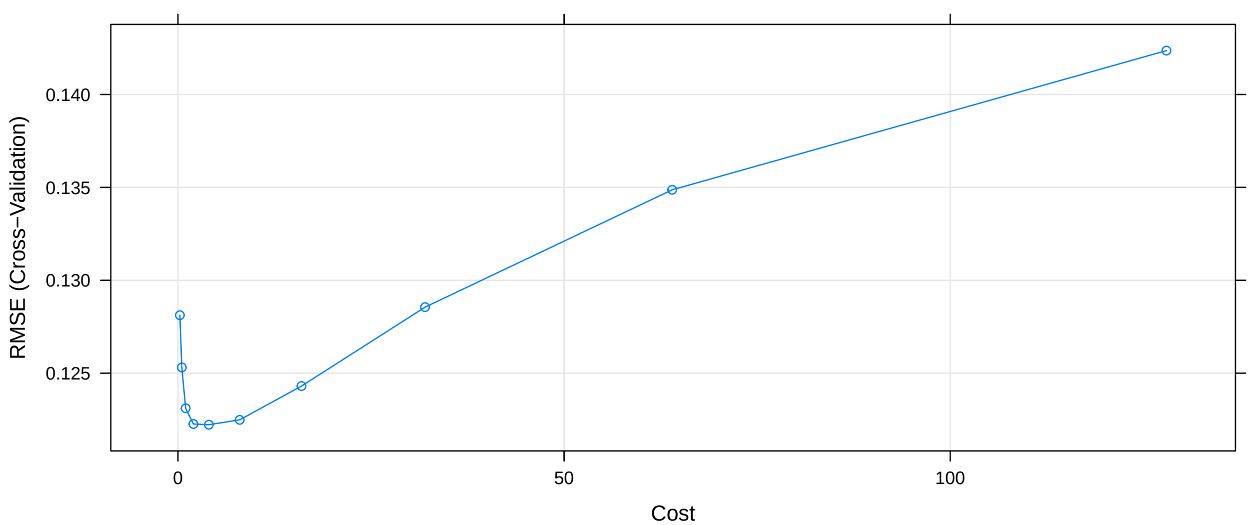
RMSE was used to select the optimal model using the smallest value. The final values used for the model were nprune = 12 and degree = 1 which corresponds to best tune model. In this case we see that R^2 is 0.33 so only covers 33% variability in data but it also produces small RMSE.

Support Vector Machines

The objective of the support vector machine algorithm is to find a hyperplane in an N-dimensional space (N being the number of features) that classifies the data points. Hyperplanes are decision boundaries to classify the data points. Data points that falls on either side of the hyperplane can be qualified for different classes. Support vectors are data points that are closer to the hyperplane and effect the position and orientation of the hyperplane. Using these support vectors, we do maximize the margin of the classifier.

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 1930 samples
##   28 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   C       RMSE       Rsquared   MAE
##     0.25  0.1281215  0.4579577  0.09713141
##     0.50  0.1253089  0.4791453  0.09426183
##     1.00  0.1231103  0.4955504  0.09220593
##     2.00  0.1222647  0.5021667  0.09130259
##     4.00  0.1222248  0.5026551  0.09101076
##     8.00  0.1224871  0.5032033  0.09123477
##    16.00  0.1243066  0.4963536  0.09255112
##    32.00  0.1285533  0.4780063  0.09605588
##    64.00  0.1348701  0.4507836  0.10107242
##   128.00  0.1423623  0.4203709  0.10632568
##
## Tuning parameter 'sigma' was held constant at a value of 0.02339058
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were sigma = 0.02339058 and C = 4.
```

```
## Length  Class   Mode
##      1   ksvm     S4
```




```
##    Rsquared      RMSE
## 1 0.5026551 0.1222248
```

RMSE was used to select the optimal model using the smallest value. The final values used for the model were sigma = 0.02339058 and C = 4. We see an improvement here in R^2 value which is 0.50 so this model covers 50% variability in the data and RMSE is smallest as well among the models used so far.

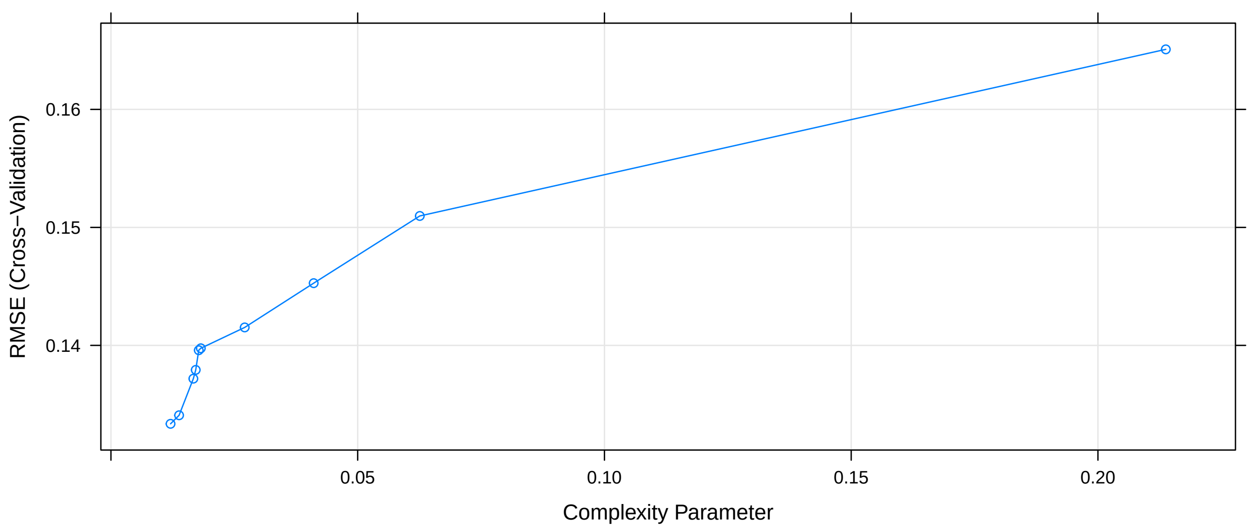
Trees

Single Tree

Regression trees partition a data set into smaller groups and then fit a simple model for each subgroup. Basic regression trees partition the data into smaller groups that are more homogenous against the response. To achieve outcome consistency, regression trees determine the predictor to split on and value of the split, the depth or complexity of the tree and the prediction equation in the terminal nodes

```
## CART
##
## 1930 samples
##   28 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   cp          RMSE       Rsquared   MAE
##   0.01207650  0.1333503  0.4028576  0.1044068
##   0.01380773  0.1340749  0.3955543  0.1053418
##   0.01669720  0.1371790  0.3668106  0.1080092
##   0.01718055  0.1379191  0.3599851  0.1087860
##   0.01779192  0.1395878  0.3461880  0.1103633
##   0.01820999  0.1397537  0.3446394  0.1103571
##   0.02710422  0.1415195  0.3281409  0.1121354
##   0.04108223  0.1452717  0.2904693  0.1150555
##   0.06257960  0.1509679  0.2330729  0.1184916
##   0.21375175  0.1650893  0.1676081  0.1313650
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was cp = 0.0120765.
```

```
##          cp
## 1 0.0120765
```




```
##    Rsquared      RMSE
## 1 0.4028576 0.1333503
```

RMSE was used to select the optimal model using the smallest value. The final value used for the model was cp = 0.0120765. We see R^2 value is 0.40 so this model covers 40% variability in the data and RMSE as 0.133. The Rsquared value is comparatively low as compared to previous best value.

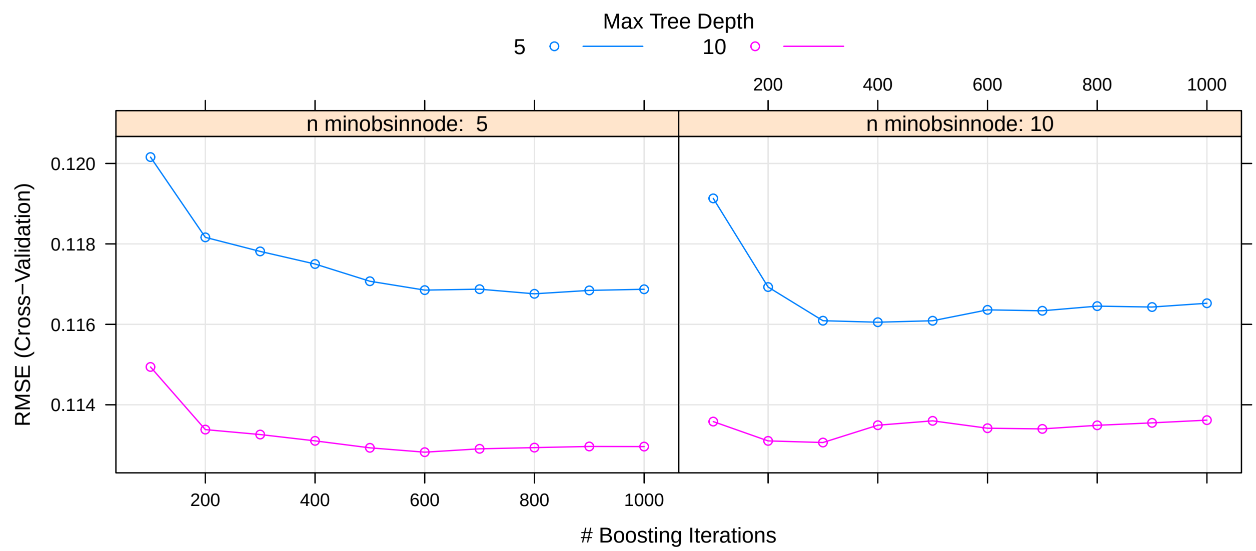
Boosted Tree

Boosting algorithms are influenced by learning theory. Boosting algorithm seeks to improve the prediction power by training a sequence of weak models where each of them compensates the weaknesses of its predecessors. The trees in boosting are dependent on past trees, have minimum depth and do not contribute equally to the final model. It requires usto specify a weak model (e.g. regression, shallow decision trees etc) and then improves it.

```
## Stochastic Gradient Boosting
##
## 1930 samples
##   28 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   interaction.depth  n.minobsinnode  n.trees  RMSE       Rsquared   MAE
##    5                  5               100     0.1201589  0.5146306  0.09207892
##    5                  5               200     0.1181629  0.5292995  0.08948714
##    5                  5               300     0.1178137  0.5332979  0.08884903
##    5                  5               400     0.1175003  0.5368565  0.08843330
##    5                  5               500     0.1170720  0.5410113  0.08774659
##    5                  5               600     0.1168508  0.5432174  0.08755074
##    5                  5               700     0.1168744  0.5432030  0.08758473
##    5                  5               800     0.1167593  0.5443230  0.08744776
##    5                  5               900     0.1168440  0.5440714  0.08756333
##    5                  5              1000     0.1168717  0.5444031  0.08748994
##    5                 10               100     0.1191319  0.5228682  0.09129258
##    5                 10               200     0.1169277  0.5393692  0.08910966
##    5                 10               300     0.1160904  0.5467017  0.08774226
##    5                 10               400     0.1160526  0.5473892  0.08782760
##    5                 10               500     0.1160895  0.5472092  0.08763751
##    5                 10               600     0.1163602  0.5457502  0.08766444
##    5                 10               700     0.1163370  0.5469193  0.08780567
##    5                 10               800     0.1164528  0.5466926  0.08801583
##    5                 10               900     0.1164304  0.5470955  0.08798276
##    5                 10              1000     0.1165244  0.5467362  0.08792449
##   10                  5               100     0.1149405  0.5552740  0.08711143
##   10                  5               200     0.1133828  0.5668386  0.08549391
##   10                  5               300     0.1132601  0.5674924  0.08523105
##   10                  5               400     0.1131027  0.5689499  0.08534686
##   10                  5               500     0.1129297  0.5704178  0.08511479
##   10                  5               600     0.1128214  0.5713018  0.08518070
##   10                  5               700     0.1129052  0.5708420  0.08517432
##   10                  5               800     0.1129350  0.5707847  0.08513301
##   10                  5               900     0.1129632  0.5705997  0.08512540
##   10                  5              1000     0.1129606  0.5706867  0.08507831
##   10                 10               100     0.1135823  0.5656884  0.08625103
##   10                 10               200     0.1131019  0.5700441  0.08536386
```

```
##    10                  10                300      0.1130614  0.5710046  0.08495719
##    10                  10                400      0.1134918  0.5682695  0.08524655
##    10                  10                500      0.1136005  0.5675580  0.08535124
##    10                  10                600      0.1134173  0.5689492  0.08540763
##    10                  10                700      0.1134000  0.5693393  0.08532770
##    10                  10                800      0.1134899  0.5686146  0.08543362
##    10                  10                900      0.1135501  0.5682792  0.08553778
##    10                  10               1000      0.1136177  0.5678470  0.08556643
##
## Tuning parameter 'shrinkage' was held constant at a value of 0.1
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were n.trees = 600, interaction.depth =
##  10, shrinkage = 0.1 and n.minobsinnode = 5.
```

```
##    n.trees interaction.depth shrinkage n.minobsinnode
## 26     600                10       0.1              5
```




```
##    Rsquared     RMSE
## 1 0.5469193 0.116337
```

Tuning parameter 'shrinkage' was held constant at a value of 0.1. RMSE was used to select the optimal model using the smallest value. The final values used for the model were n.trees = 600, interaction.depth = 10, shrinkage = 0.1 and n.minobsinnode = 5. The R^2 and RMSE are 0.54 and 0.11 respectively on training data. This is the best Rsquared so far.

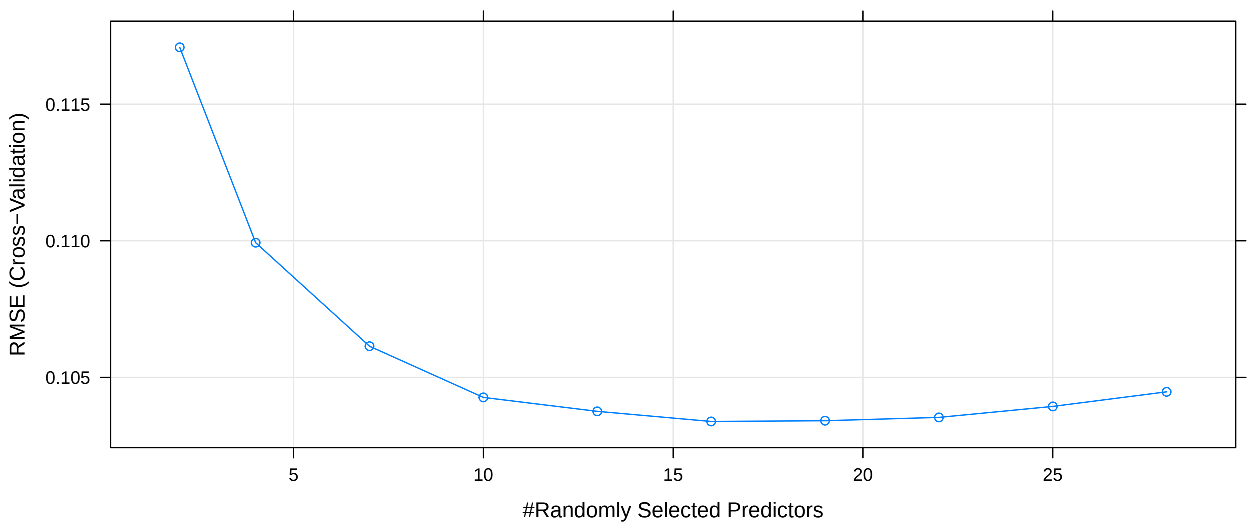
Random Forest

Random forest consists of a large number of individual decision trees that work as an ensemble. Each model in the ensemble is used to generate a prediction for a new sample and these predictions are then averaged to give the forest's prediction. Since the algorithm randomly selects predictors at each split, tree correlation gets reduces as compared to bagging. In random forest algorithm, we first select the number of models to build and theen loop through this number and train a tree model. Once done then avearage the predictions to get overall prediction. In random forests, trees are created independently, each tree is created having maximum depth and each tree contributes equally in the final model.

```
## Random Forest
##
## 1930 samples
```

```
##   28 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   mtry  RMSE       Rsquared   MAE
##    2    0.1170800  0.5833714  0.09028846
##    4    0.1099305  0.6240126  0.08329171
##    7    0.1061407  0.6419264  0.07955917
##   10    0.1042662  0.6505196  0.07754109
##   13    0.1037564  0.6514222  0.07669700
##   16    0.1033861  0.6513098  0.07623180
##   19    0.1034130  0.6491251  0.07593447
##   22    0.1035350  0.6469633  0.07567737
##   25    0.1039367  0.6423775  0.07573747
##   28    0.1044708  0.6374838  0.07603538
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was mtry = 16.
```

```
##   mtry
## 6   16
```



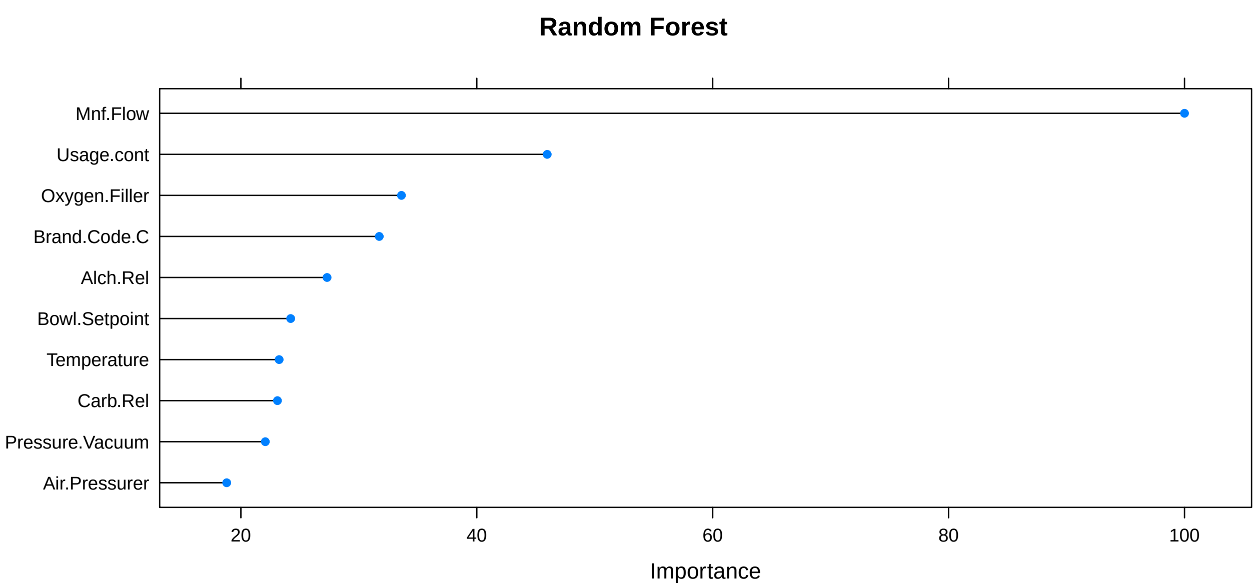

```
##    Rsquared      RMSE
## 1 0.6513098 0.1033861
```

RMSE was used to select the optimal model using the smallest value. The final value used for the model was mtry = 16. It has R^2 as 0.65 and RMSE as 0.10. Both these values are best among the models used so far.

Lets see the informative variables found by Random Forest models. we will use `varImp` method to find these variables.

```
## rf variable importance
##
##   only 20 most important variables shown (out of 28)
##
```

```
##                   Overall
## Mnf.Flow          100.000
## Usage.cont         45.970
## Oxygen.Filler      33.613
## Brand.Code.C       31.732
## Alch.Rel           27.308
## Bowl.Setpoint      24.221
## Temperature        23.245
## Carb.Rel           23.100
## Pressure.Vacuum    22.072
## Air.Pressurer      18.798
## Carb.Flow          17.838
## Carb.Pressure1     17.346
## MFR                13.262
## PC.Volume          10.958
## Fill.Pressure       9.119
## Carb.Volume         8.747
## Hyd.Pressure2       8.268
## Fill.Ounces         7.433
## PSC                 6.693
## Hyd.Pressure4       5.604
```



From above plot, it is evident `Mnf.Flow` is the most informative variable for PH response variable.

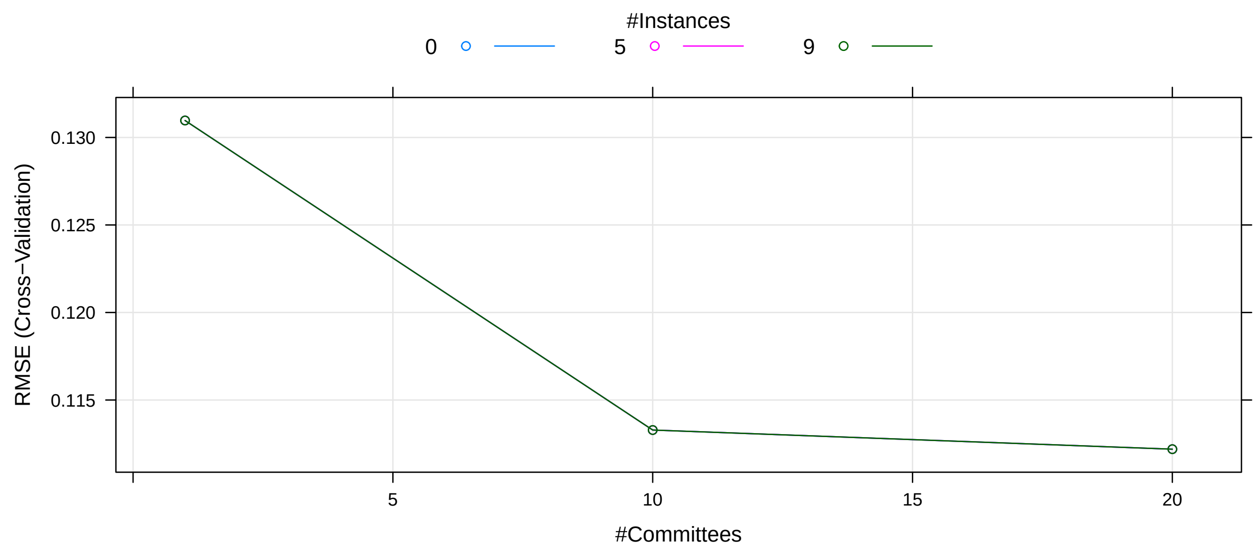
Cubist

Cubist is a rule-based model. A tree is built where the terminal leaves contain linear regression models. These models are based upon the predictors used in previous splits along with intermediate models. The tree is reduced to a set of rules which initially are paths from the top of the tree to the bottom. Rules are eliminated via pruning or combined and the candidate variables for the models are the predictors that were pruned away. .

```
## Cubist
##
## 1930 samples
##   28 predictor
```

```
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 1737, 1737, 1737, 1737, 1737, 1737, ...
## Resampling results across tuning parameters:
##
##   committees  neighbors  RMSE       Rsquared   MAE
##    1          0          0.1309689  0.4563136  0.09299230
##    1          5          0.1309689  0.4563136  0.09299230
##    1          9          0.1309689  0.4563136  0.09299230
##   10          0          0.1132853  0.5698369  0.08344530
##   10          5          0.1132853  0.5698369  0.08344530
##   10          9          0.1132853  0.5698369  0.08344530
##   20          0          0.1121916  0.5786100  0.08294355
##   20          5          0.1121916  0.5786100  0.08294355
##   20          9          0.1121916  0.5786100  0.08294355
##
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were committees = 20 and neighbors = 0.
```

```
##   committees neighbors
## 7         20         0
```




```
##   Rsquared      RMSE
## 1  0.57861 0.1121916
```

RMSE was used to select the optimal model using the smallest value. The best tune for the cubist model which resulted in the smallest root mean squared error was with 20 committees. It had RMSE = 0.112, and $R^2 = 0.578$. So far, it covered 57% of the variability in the data than all other variables and with the low RMSE.

Select Model

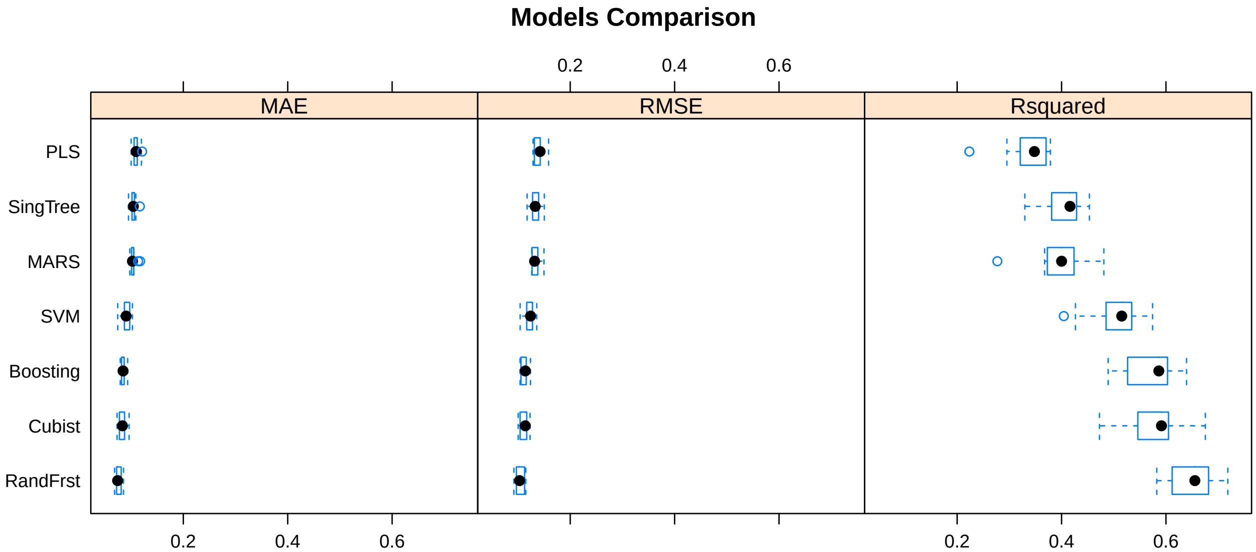
To select the best model for making predictions for evaluation data, we will look at 3 parameters.

- R^2, which shows the variance explained by given model.
- RMSE (Root Mean Squared Error), which is the std deviation of the residuals.

- MAE (Mean Absolute Error), which is avg of all absoulte errors.

Here we will summarize the resamplling to compare the above 3 values among all the models followed by checking the prediction on validation data which we reserved earlier during data partition.

```
##
## Call:
## summary.resamples(object = resamples(list(PLS = pls_model, MARS =
##  mars_model, SVM = svm_model, RandFrst = rf_model, Cubist =
##  cubist_model, SingTree = st_model, Boosting = gbm_model)))
##
## Models: PLS, MARS, SVM, RandFrst, Cubist, SingTree, Boosting
## Number of resamples: 10
##
## MAE
##                Min.    1st Qu.     Median       Mean    3rd Qu.       Max. NA's
## PLS      0.10007430 0.10632857 0.10955896 0.10972243 0.11147862 0.12102507    0
## MARS     0.09755457 0.10103709 0.10257144 0.10430716 0.10479898 0.11728296    0
## SVM      0.07431813 0.08783748 0.09039245 0.09101076 0.09603653 0.10257755    0
## RandFrst 0.06831115 0.07221768 0.07417746 0.07623180 0.08048781 0.08547669    0
## Cubist   0.07304460 0.07819699 0.08336354 0.08294355 0.08680539 0.09616592    0
## SingTree 0.09505792 0.10204748 0.10426442 0.10440681 0.10611650 0.11670546    0
## Boosting 0.07920377 0.08203256 0.08455857 0.08518070 0.08656302 0.09338149    0
##
## RMSE
##                Min.    1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## PLS      0.12877712 0.13210324 0.1422288 0.1405086 0.1425127 0.1585968    0
## MARS     0.12621745 0.12681807 0.1317765 0.1341767 0.1372495 0.1497212    0
## SVM      0.10408448 0.11689184 0.1240176 0.1222248 0.1274946 0.1358440    0
## RandFrst 0.09204647 0.09706146 0.1029516 0.1033861 0.1112461 0.1148481    0
## Cubist   0.10031577 0.10550214 0.1139246 0.1121916 0.1163640 0.1230009    0
## SingTree 0.11741724 0.12900263 0.1329154 0.1333503 0.1380354 0.1503560    0
## Boosting 0.10388119 0.10737048 0.1139532 0.1128214 0.1154602 0.1238834    0
##
## Rsquared
##               Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## PLS      0.2234196 0.3216855 0.3480238 0.3344473 0.3671433 0.3786303    0
## MARS     0.2770408 0.3734935 0.4001130 0.3951300 0.4217082 0.4810568    0
## SVM      0.4043236 0.4854691 0.5152359 0.5026551 0.5327833 0.5743832    0
## RandFrst 0.5824412 0.6175968 0.6553779 0.6513098 0.6796676 0.7184821    0
## Cubist   0.4726667 0.5517988 0.5914461 0.5786100 0.6037048 0.6754578    0
## SingTree 0.3296664 0.3836444 0.4161688 0.4028576 0.4281188 0.4533947    0
## Boosting 0.4892704 0.5377983 0.5863510 0.5713018 0.6007364 0.6394236    0
```



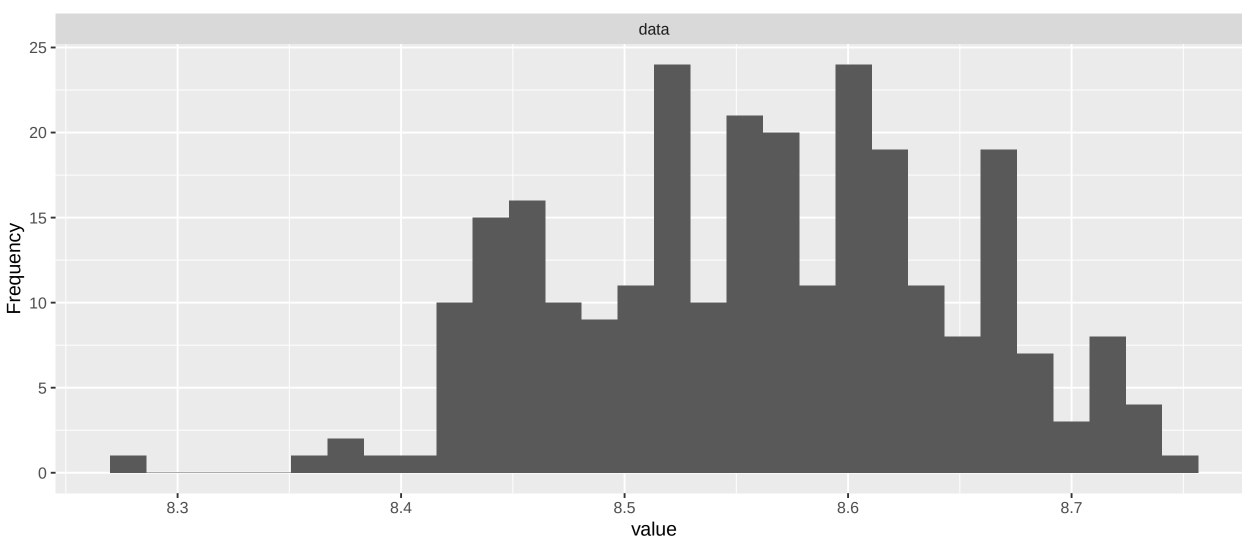

```
##                RMSE  Rsquared        MAE
## PLS      0.1371313 0.3722429 0.10861129
## MARS     0.1302255 0.4347408 0.10245641
## SVM      0.1175582 0.5395039 0.08694041
## SingTree 0.1314174 0.4238484 0.10420760
## RandFrst 0.1004640 0.6737302 0.07310555
## Boosting 0.1113162 0.5897395 0.08321032
## Cubist   0.1029136 0.6505194 0.07567148
```

We can see here Random Forest performed the best among all the models tried considering the 3 metrics Rsquared, RMSE and MAE, we identified earlier.

Prediction

Based on the analysis so far, it is confirmed that the Random Forest model is the optimal model. we will now use it tp predict PH values of evaluation dataset and then write it in csv.

Here are the predicted values of PH for evaluation dataset.



Conclusion

After extracting the data from the given files, we did first perform data exploration which helped us to find missing data, correlation among the variables and outliers. Next we performed steps for data preparation that included handling missing and outliers through mice, creating dummy vars for a categorical variable Brand Code, remove highly correlated variables, transform data for Normality and finally data partition of 75% and 25% for training and validation respectively. We then trained various models using linear regression, non linear and Trees model. We finally founf the optimal model as Random Forest for predicting PH values for evaluation data.

We notice that all the values predicted are greater than 8. This value translates that the beverage made is alkaline. At the start of this study, we were not known about the nature of the ABC Beverage company i.e. what type of beverage manufacturer it was. But from this study we can conclude that this company mainly produces alkaline beverages like water, tea, fruit drinks and all.

References

- Applied Predictive Modeling. Max Kuhn and Kjell Johnson
- https://machinelearningmastery.com/pre-process-your-dataset-in-r/
- https://www.analyticsvidhya.com/blog/2016/03/tutorial-powerful-packages-imputing-missing-values/
- https://newalbanysmiles.com/ph-values-of-common-beverages/

Code Appendix

```
knitr::opts_chunk$set(echo=FALSE, error=FALSE, warning=FALSE, message=FALSE, fig.align="center", fig.wi
# Libraries
library(readxl)
library(tidyverse)
library(caret)
library(doParallel)
library(DataExplorer)
library(psych)
library(mice)
library(MASS)
library(caret)
library(AppliedPredictiveModeling)
library(lars)
library(pls)
library(earth)
library(Cubist)
library(randomForest)
library(DT)

set.seed(624)
# download training data from git repo
temp.file <- tempfile(fileext = ".xlsx")
download.file(url="https://github.com/DATA624-PredictiveAnalytics-Project2/Project2/blob/main/StudentDa
              destfile = temp.file,
              mode = "wb",
              quiet = TRUE)

# read excel for training data
```

```
train.df <- read_excel(temp.file, skip=0)

# download testing data from git repo
download.file(url="https://github.com/DATA624-PredictiveAnalytics-Project2/Project2/blob/main/StudentEva
              destfile = temp.file,
              mode = "wb",
              quiet = TRUE)

# read excel for testing data
test.df <- read_excel(temp.file, skip=0)


# transform Brand.code to factor
train.df$`Brand Code` = as.factor(train.df$`Brand Code`)
test.df$`Brand Code` = as.factor(test.df$`Brand Code`)
glimpse(train.df)
describe(train.df) %>% dplyr::select(-vars, -trimmed, -mad, -se)
plot_histogram(train.df, geom_histogram_args = list("fill" = "tomato4"))
# log histograms
plot_histogram(train.df, scale_x = "log10", geom_histogram_args = list("fill" = "springgreen4"))
colSums(is.na(train.df))
plot_missing(train.df[-1])
forcorr <- train.df[complete.cases(train.df),-1]
corrplot::corrplot(cor(forcorr), method = 'ellipse', type = 'lower')

# boxplot
par(mfrow = c(3,4))
for(i in colnames(train.df[-1])){
boxplot(train.df[,i], xlab = names(train.df[i]),
  main = names(train.df[i]), col="blue", horizontal = T)
}
set.seed(317)

# Training set
train.df.clean <- mice(data.frame(train.df), method = 'rf', m=2, maxit = 2, print=FALSE)
train.df.clean <- complete(train.df.clean)

nzv_preds <- nearZeroVar(train.df.clean)
train.df.clean <- train.df.clean[,-nzv_preds]
set.seed(317)

# Testing set
test.df.clean <- mice(data.frame(test.df), method = 'rf', m=2, maxit = 2, print=FALSE)
test.df.clean <- complete(test.df.clean)
set.seed(317)
dum.brandcode <- dummyVars(PH ~ Brand.Code, data = train.df.clean)
dum.train.predict <- predict(dum.brandcode, train.df.clean)
train.df.clean <- cbind(dum.train.predict, train.df.clean) %>% dplyr::select(-Brand.Code)
set.seed(317)
dum.brandcode <- dummyVars( ~ Brand.Code, data = test.df.clean)
dum.test.predict <- predict(dum.brandcode, test.df.clean)
test.df.clean <- cbind(dum.test.predict, test.df.clean) %>% dplyr::select(-Brand.Code)
highCorr <- findCorrelation(cor(train.df.clean), 0.90)
```

```
train.df.clean <- train.df.clean[, -highCorr]
set.seed(317)
preproc_traindf <- preProcess(train.df.clean, method = "YeoJohnson")
train.df.clean <- predict(preproc_traindf, train.df.clean)
set.seed(317)
preproc_testdf <- preProcess(test.df.clean, method = "YeoJohnson")
test.df.clean <- predict(preproc_testdf, test.df.clean)
set.seed(317)

partition <- createDataPartition(train.df.clean$PH, p=0.75, list = FALSE)

# training/validation partition for independent variables
X.train <- train.df.clean[partition, ] %>% dplyr::select(-PH)
X.test <- train.df.clean[-partition, ] %>% dplyr::select(-PH)

# training/validation partition for dependent variable PH
y.train <- train.df.clean$PH[partition]
y.test <- train.df.clean$PH[-partition]
set.seed(317)

lm_model <- lm(y.train ~ ., data = X.train)
summary(lm_model)
set.seed(317)

# tune pls model
pls_model <- train(x=X.train,
                 y=y.train,
                 method="pls",
                 metric="Rsquared",
                 tuneLength=10,
                 trControl=trainControl(method = "cv")
                 )

pls_model
pls_model$bestTune
plot(pls_model)
pls_model$results %>%
  filter(ncomp == pls_model$bestTune$ncomp) %>%
  dplyr::select(ncomp,RMSE,Rsquared)
data.frame(Rsquared=pls_model[["results"]][["Rsquared"]][as.numeric(rownames(pls_model$bestTune))],
           RMSE=pls_model[["results"]][["RMSE"]][as.numeric(rownames(pls_model$bestTune))])
set.seed(317)
marsGrid <- expand.grid(.degree=1:2, .nprune=2:30)
mars_model <- train(x=X.train,
                    y=y.train,
                    method = "earth",
                    tuneGrid = marsGrid,
                    trControl = trainControl(method = "cv"))

# final parameters
mars_model$bestTune
# plot RMSE
plot(mars_model)
```

```
summary(mars_model$finalModel)
data.frame(Rsquared=mars_model[["results"]][["Rsquared"]][as.numeric(rownames(mars_model$bestTune))],
           RMSE=mars_model[["results"]][["RMSE"]][as.numeric(rownames(mars_model$bestTune))])
set.seed(317)
svm_model <- train(x=X.train,
                   y=y.train,
                   method = "svmRadial",
                   tuneLength = 10,
                   trControl = trainControl(method = "cv"))

svm_model
summary(svm_model$finalModel)
# plot RMSE
plot(svm_model)
data.frame(Rsquared=svm_model[["results"]][["Rsquared"]][as.numeric(rownames(svm_model$bestTune))],
           RMSE=svm_model[["results"]][["RMSE"]][as.numeric(rownames(svm_model$bestTune))])
set.seed(317)

st_model <- train(x=X.train,
                  y=y.train,
                  method = "rpart",
                  tuneLength = 10,
                  trControl = trainControl(method = "cv"))

st_model
st_model$bestTune
# plot RMSE
plot(st_model)
data.frame(Rsquared=st_model[["results"]][["Rsquared"]][as.numeric(rownames(st_model$bestTune))],
           RMSE=st_model[["results"]][["RMSE"]][as.numeric(rownames(st_model$bestTune))])
set.seed(317)

# boosting regression trees via stochastic gradient boosting machines

gbmGrid <- expand.grid(interaction.depth = c(5,10),
                       n.trees = seq(100, 1000, by = 100),
                       shrinkage = 0.1,
                       n.minobsinnode = c(5,10))

gbm_model <- train(x=X.train,
                   y=y.train,
                   method = "gbm",
                   tuneGrid = gbmGrid,
                   trControl = trainControl(method = "cv"),
                   verbose = FALSE)

gbm_model
gbm_model$bestTune
plot(gbm_model)
data.frame(Rsquared=gbm_model[["results"]][["Rsquared"]][as.numeric(rownames(gbm_model$bestTune))],
           RMSE=gbm_model[["results"]][["RMSE"]][as.numeric(rownames(gbm_model$bestTune))])
set.seed(317)
```

```
rf_model <- train(x=X.train,
                  y=y.train,
                  method = "rf",
                  tuneLength = 10,
                  trControl = trainControl(method = "cv"))

rf_model
rf_model$bestTune
plot(rf_model)
data.frame(Rsquared=rf_model[["results"]][["Rsquared"]][as.numeric(rownames(rf_model$bestTune))],
           RMSE=rf_model[["results"]][["RMSE"]][as.numeric(rownames(rf_model$bestTune))])
varImp(rf_model)
plot(varImp(rf_model), top=10, main="Random Forest")
set.seed(317)

cubist_model <- train(x=X.train,
                      y=y.train,
                      method = "cubist",
                      tuneLength = 10,
                      trControl = trainControl(method = "cv"))

cubist_model
cubist_model$bestTune
plot(cubist_model)
data.frame(Rsquared=cubist_model[["results"]][["Rsquared"]][as.numeric(rownames(cubist_model$bestTune))]
           RMSE=cubist_model[["results"]][["RMSE"]][as.numeric(rownames(cubist_model$bestTune))])
set.seed(317)
summary(resamples(list(PLS=pls_model, MARS=mars_model, SVM=svm_model, RandFrst=rf_model,  Cubist=cubist_
bwplot(resamples(list(PLS=pls_model, MARS=mars_model, SVM=svm_model, RandFrst=rf_model,  Cubist=cubist_
set.seed(317)

pls_pred <- predict(pls_model, newdata = X.test)
mars_pred <- predict(mars_model, newdata = X.test)
svm_pred <- predict(svm_model, newdata = X.test)
rf_pred <- predict(rf_model, newdata = X.test)
cubist_pred <- predict(cubist_model, newdata = X.test)
st_pred<- predict(st_model, newdata = X.test)
gbm_pred <- predict(gbm_model, newdata = X.test)

data.frame(rbind(PLS=postResample(pred=pls_pred,obs = y.test),
                 MARS=postResample(pred=mars_pred,obs = y.test),
                 SVM=postResample(pred=svm_pred,obs = y.test),
                 SingTree=postResample(pred=st_pred,obs = y.test),
                 RandFrst=postResample(pred=rf_pred,obs = y.test),
                 Boosting=postResample(pred=gbm_pred,obs = y.test),
                 Cubist=postResample(pred=cubist_pred,obs = y.test)))
set.seed(317)

# remove PH from evaluation data
test.df.clean <- test.df.clean %>% dplyr::select(-PH)

# predict final PH values
test.df.clean$PH <- predict(rf_model, newdata = test.df.clean)
```

```r
plot_histogram(test.df.clean$PH)
write.csv(test.df.clean$PH, "StudentEvaluations_PHPredictions.csv")
```