

# FIT5149 - Applied Data Analysis

## S1 2009 Assessment #1

### Predicting the Critical Temperature of a Superconductor

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# 1 Introduction

## 1.1 Background

Superconductivity is a phenomenon of exactly zero electrical resistance and expulsion of magnetic flux fields occurring in certain materials, called superconductors, when cooled below a characteristic critical temperature. One of the applications is in the Magnetic Resonance Imaging (MRI) systems which is widely performed by health care professionals for detailed internal body imaging.

Predicting the critical temperature ( $T_c$ ) of a superconductor is still an open problem in the scientific community. In the past, simple empirical rules based on experiments have guided researchers in synthesizing superconducting materials for many years. Nowadays, features (or predictors) based on the superconductor's elemental properties can be generated and used to predict  $T_c$ .

In this task, we are going to analyze superconductor data from the Superconducting Material Database maintained by Japan's National Institute for Materials Science (NIMS). The aim is to build statistical models that can predict  $T_c$  based on the material's chemical properties.

## 1.2 Data Preparation

The dataset for this assessment is from the Superconducting Material Database maintained by Japan's National Institute for Materials Science (NIMS) and processed by [Hamidieh \[2018\]](#). There are two datasets namely train.csv and unique\_m.csv. The first dataset contains a large list of superconductors, their critical temperatures and other variables, meanwhile the later contains the chemical formula of each corresponding material.

### 1.2.1 Superconducting Material Dataset

In this subsection, we will load the **train.csv** dataset and print the dimension of the dataset.

```
# Loading the dataset
data <- read.csv(file="superconduct//train.csv", header=TRUE, sep=",")
head(data)

##   number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1                  4      88.94447      57.86269
## 2                  5      92.72921      58.51842
## 3                  4      88.94447      57.88524
## 4                  4      88.94447      57.87397
## 5                  4      88.94447      57.84014
## 6                  4      88.94447      57.79504
##   gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1      66.36159      36.11661      1.181795
## 2     73.13279      36.39660      1.449309
## 3     66.36159      36.12251      1.181795
## 4     66.36159      36.11956      1.181795
## 5     66.36159      36.11072      1.181795
## 6     66.36159      36.09893      1.181795
##   wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1      1.0623955      122.9061      31.79492
## 2      1.0577551      122.9061      36.16194
## 3      0.9759805      122.9061      35.74110
## 4      1.0222909      122.9061      33.76801
```

```

## 5          1.1292237      122.9061      27.84874
## 6          1.2252028      122.9061      20.68746
##   std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie gmean_fie
## 1          51.96883      53.62253    775.425    1010.269   718.1529
## 2          47.09463      53.97987    766.440    1010.613   720.6055
## 3          51.96883      53.65627    775.425    1010.820   718.1529
## 4          51.96883      53.63940    775.425    1010.544   718.1529
## 5          51.96883      53.58877    775.425    1009.717   718.1529
## 6          51.96883      53.52115    775.425    1008.614   718.1529
##   wtd_gmean_fie entropy_fie wtd_entropy_fie range_fie wtd_range_fie
## 1          938.0168     1.305967    0.7914878   810.6      735.9857
## 2          938.7454     1.544145    0.8070782   810.6      743.1643
## 3          939.0090     1.305967    0.7736202   810.6      743.1643
## 4          938.5128     1.305967    0.7832067   810.6      739.5750
## 5          937.0256     1.305967    0.8052296   810.6      728.8071
## 6          935.0463     1.305967    0.8247426   810.6      714.4500
##   std_fie wtd_std_fie mean_atomic_radius wtd_mean_atomic_radius
## 1          323.8118     355.5630    160.25      105.5143
## 2          290.1830     354.9635    161.20      104.9714
## 3          323.8118     354.8042    160.25      104.6857
## 4          323.8118     355.1839    160.25      105.1000
## 5          323.8118     356.3193    160.25      106.3429
## 6          323.8118     357.8246    160.25      108.0000
##   gmean_atomic_radius wtd_gmean_atomic_radius entropy_atomic_radius
## 1          136.1260     84.52842    1.259244
## 2          141.4652     84.37017    1.508328
## 3          136.1260     84.21457    1.259244
## 4          136.1260     84.37135    1.259244
## 5          136.1260     84.84344    1.259244
## 6          136.1260     85.47701    1.259244
##   wtd_entropy_atomic_radius range_atomic_radius wtd_range_atomic_radius
## 1          1.207040     205        42.91429
## 2          1.204115     205        50.57143
## 3          1.132547     205        49.31429
## 4          1.173033     205        46.11429
## 5          1.261194     205        36.51429
## 6          1.331339     205        23.71429
##   std_atomic_radius wtd_std_atomic_radius mean_Density wtd_mean_Density
## 1          75.23754     69.23557    4654.357    2961.502
## 2          67.32132     68.00882    5821.486    3021.017
## 3          75.23754     67.79771    4654.357    2999.159
## 4          75.23754     68.52166    4654.357    2980.331
## 5          75.23754     70.63445    4654.357    2923.845
## 6          75.23754     73.32413    4654.357    2848.531
##   gmean_Density wtd_gmean_Density entropy_Density wtd_entropy_Density
## 1          724.9532     53.54381    1.033129    0.8145982
## 2          1237.0951    54.09572    1.314442    0.9148022
## 3          724.9532     53.97402    1.033129    0.7603052
## 4          724.9532     53.75849    1.033129    0.7888885
## 5          724.9532     53.11703    1.033129    0.8598109
## 6          724.9532     52.27364    1.033129    0.9323687
##   range_Density wtd_range_Density std_Density wtd_std_Density
## 1          8958.571     1579.583    3306.163    3572.597
## 2          10488.571    1667.383    3767.403    3632.649

```

```

## 3      8958.571      1667.383      3306.163      3592.019
## 4      8958.571      1623.483      3306.163      3582.371
## 5      8958.571      1491.783      3306.163      3552.669
## 6      8958.571      1316.183      3306.163      3511.262
##   mean_ElectronAffinity wtd_mean_ElectronAffinity gmean_ElectronAffinity
## 1          81.8375      111.7271      60.12318
## 2          90.8900      112.3164      69.83331
## 3          81.8375      112.2136      60.12318
## 4          81.8375      111.9704      60.12318
## 5          81.8375      111.2407      60.12318
## 6          81.8375      110.2679      60.12318
##   wtd_gmean_ElectronAffinity entropy_ElectronAffinity
## 1          99.41468     1.159687
## 2          101.16640     1.427997
## 3          101.08215     1.159687
## 4          100.24495     1.159687
## 5          97.77472     1.159687
## 6          94.57550     1.159687
##   wtd_entropy_ElectronAffinity range_ElectronAffinity
## 1          0.7873817    127.05
## 2          0.8386665    127.05
## 3          0.7860067    127.05
## 4          0.7869005    127.05
## 5          0.7873962    127.05
## 6          0.7844615    127.05
##   wtd_range_ElectronAffinity std_ElectronAffinity wtd_std_ElectronAffinity
## 1          80.98714     51.43371     42.55840
## 2          81.20786     49.43817     41.66762
## 3          81.20786     51.43371     41.63988
## 4          81.09750     51.43371     42.10234
## 5          80.76643     51.43371     43.45206
## 6          80.32500     51.43371     45.17068
##   mean_FusionHeat wtd_mean_FusionHeat gmean_FusionHeat
## 1          6.9055       3.846857     3.479475
## 2          7.7844       3.796857     4.403790
## 3          6.9055       3.822571     3.479475
## 4          6.9055       3.834714     3.479475
## 5          6.9055       3.871143     3.479475
## 6          6.9055       3.919714     3.479475
##   wtd_gmean_FusionHeat entropy_FusionHeat wtd_entropy_FusionHeat
## 1          1.040986     1.088575     0.9949982
## 2          1.035251     1.374977     1.0730938
## 3          1.037439     1.088575     0.9274794
## 4          1.039211     1.088575     0.9640310
## 5          1.044545     1.088575     1.0449695
## 6          1.051699     1.088575     1.1118503
##   range_FusionHeat wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
## 1          12.878       1.744571     4.599064     4.666920
## 2          12.878       1.595714     4.473363     4.603000
## 3          12.878       1.757143     4.599064     4.649635
## 4          12.878       1.744571     4.599064     4.658301
## 5          12.878       1.744571     4.599064     4.684014
## 6          12.878       1.744571     4.599064     4.717642
##   mean_ThermalConductivity wtd_mean_ThermalConductivity

```

```

## 1          107.7566           61.01519
## 2          172.2053           61.37233
## 3          107.7566           60.94376
## 4          107.7566           60.97947
## 5          107.7566           61.08662
## 6          107.7566           61.22947
##   gmean_ThermalConductivity wtd_gmean_ThermalConductivity
## 1              7.062488          0.6219795
## 2             16.064228          0.6197346
## 3             7.062488          0.6190947
## 4             7.062488          0.6205354
## 5             7.062488          0.6248777
## 6             7.062488          0.6307148
##   entropy_ThermalConductivity wtd_entropy_ThermalConductivity
## 1            0.3081480          0.2628483
## 2            0.8474042          0.5677061
## 3            0.3081480          0.2504774
## 4            0.3081480          0.2570451
## 5            0.3081480          0.2728199
## 6            0.3081480          0.2882356
##   range_ThermalConductivity wtd_range_ThermalConductivity
## 1            399.9734          57.12767
## 2            429.9734          51.41338
## 3            399.9734          57.12767
## 4            399.9734          57.12767
## 5            399.9734          57.12767
## 6            399.9734          57.12767
##   std_ThermalConductivity wtd_std_ThermalConductivity mean_Valence
## 1            168.8542          138.5172          2.25
## 2            198.5546          139.6309          2.00
## 3            168.8542          138.5406          2.25
## 4            168.8542          138.5289          2.25
## 5            168.8542          138.4937          2.25
## 6            168.8542          138.4466          2.25
##   wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
## 1            2.257143          2.213364          2.219783          1.368922
## 2            2.257143          1.888175          2.210679          1.557113
## 3            2.271429          2.213364          2.232679          1.368922
## 4            2.264286          2.213364          2.226222          1.368922
## 5            2.242857          2.213364          2.206963          1.368922
## 6            2.214286          2.213364          2.181543          1.368922
##   wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
## 1            1.066221           1           1.085714          0.4330127
## 2            1.047221           2           1.128571          0.6324555
## 3            1.029175           1           1.114286          0.4330127
## 4            1.048834           1           1.100000          0.4330127
## 5            1.096052           1           1.057143          0.4330127
## 6            1.141474           1           1.000000          0.4330127
##   wtd_std_Valence critical_temp
## 1            0.4370588          29
## 2            0.4686063          26
## 3            0.4446966          19
## 4            0.4409521          22
## 5            0.4288095          23

```

```
## 6      0.4103259      23
```

```
cat("Total Rows: ",dim(data)[1])
```

```
## Total Rows: 21263
```

```
cat("\nTotal Columns: ",dim(data)[2])
```

```
##  
## Total Columns: 82
```

The **train.csv** has 21263 rows and 82 columns.

### 1.2.2 Element Dataset

In this subsection, we will load the **unique\_m.csv** dataset and print the dimension of the dataset.

```
# Loading the dataset  
chemical <- read.csv(file="superconduct//unique_m.csv", header=TRUE, sep=",")  
head(chemical)
```

```
##   H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar K Ca Sc Ti V Cr Mn Fe Co  
## 1 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 2 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 3 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 4 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 5 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 6 0 0 0 0 0 0 0 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
##   Ni Cu Zn Ga Ge As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb  
## 1 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 2 0 0.9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 3 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 4 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 5 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 6 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
##   Te I Xe Cs Ba La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu Hf Ta W  
## 1 0 0 0 0 0.20 1.80 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 2 0 0 0 0 0.10 1.90 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 3 0 0 0 0 0.10 1.90 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 4 0 0 0 0 0.15 1.85 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 5 0 0 0 0 0.30 1.70 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
## 6 0 0 0 0 0.50 1.50 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
##   Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn critical_temp material  
## 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29 Ba0.2La1.8Cu104  
## 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26 Ba0.1La1.9Ag0.1Cu0.904  
## 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19 Ba0.1La1.9Cu104  
## 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22 Ba0.15La1.85Cu104  
## 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23 Ba0.3La1.7Cu104  
## 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23 Ba0.5La1.5Cu104
```

```

cat("Total Rows: ",dim(chemical)[1])

## Total Rows: 21263

cat("\nTotal Columns: ",dim(chemical)[2])

## 
## Total Columns: 88

```

The `unique_m.csv` has 21263 rows and 88 columns

## 1.3 Data Description

### 1.3.1 Superconducting Material Dataset

In this subsection, we will describe the meaning of each column and its datatype of the superconducting material dataset.

```

# Description of the Superconducting Material Dataset
str(data)

## 'data.frame': 21263 obs. of 82 variables:
## $ number_of_elements : int 4 5 4 4 4 4 4 4 4 ...
## $ mean_atomic_mass   : num 88.9 92.7 88.9 88.9 88.9 ...
## $ wtd_mean_atomic_mass: num 57.9 58.5 57.9 57.9 57.8 ...
## $ gmean_atomic_mass  : num 66.4 73.1 66.4 66.4 66.4 ...
## $ wtd_gmean_atomic_mass: num 36.1 36.4 36.1 36.1 36.1 ...
## $ entropy_atomic_mass: num 1.18 1.45 1.18 1.18 1.18 ...
## $ wtd_entropy_atomic_mass: num 1.062 1.058 0.976 1.022 1.129 ...
## $ range_atomic_mass   : num 123 123 123 123 123 ...
## $ wtd_range_atomic_mass: num 31.8 36.2 35.7 33.8 27.8 ...
## $ std_atomic_mass     : num 52 47.1 52 52 52 ...
## $ wtd_std_atomic_mass: num 53.6 54 53.7 53.6 53.6 ...
## $ mean_fie             : num 775 766 775 775 775 ...
## $ wtd_mean_fie         : num 1010 1011 1011 1011 1010 ...
## $ gmean_fie            : num 718 721 718 718 718 ...
## $ wtd_gmean_fie        : num 938 939 939 939 937 ...
## $ entropy_fie          : num 1.31 1.54 1.31 1.31 1.31 ...
## $ wtd_entropy_fie      : num 0.791 0.807 0.774 0.783 0.805 ...
## $ range_fie             : num 811 811 811 811 811 ...
## $ wtd_range_fie         : num 736 743 743 740 729 ...
## $ std_fie               : num 324 290 324 324 324 ...
## $ wtd_std_fie           : num 356 355 355 355 356 ...
## $ mean_atomic_radius    : num 160 161 160 160 160 ...
## $ wtd_mean_atomic_radius: num 106 105 105 105 106 ...
## $ gmean_atomic_radius   : num 136 141 136 136 136 ...
## $ wtd_gmean_atomic_radius: num 84.5 84.4 84.2 84.4 84.8 ...
## $ entropy_atomic_radius: num 1.26 1.51 1.26 1.26 1.26 ...
## $ wtd_entropy_atomic_radius: num 1.21 1.2 1.13 1.17 1.26 ...
## $ range_atomic_radius    : int 205 205 205 205 205 ...
## $ wtd_range_atomic_radius: num 42.9 50.6 49.3 46.1 36.5 ...

```

```

## $ std_atomic_radius : num 75.2 67.3 75.2 75.2 75.2 ...
## $ wtd_std_atomic_radius : num 69.2 68 67.8 68.5 70.6 ...
## $ mean_Density : num 4654 5821 4654 4654 4654 ...
## $ wtd_mean_Density : num 2962 3021 2999 2980 2924 ...
## $ gmean_Density : num 725 1237 725 725 725 ...
## $ wtd_gmean_Density : num 53.5 54.1 54 53.8 53.1 ...
## $ entropy_Density : num 1.03 1.31 1.03 1.03 1.03 ...
## $ wtd_entropy_Density : num 0.815 0.915 0.76 0.789 0.86 ...
## $ range_Density : num 8959 10489 8959 8959 8959 ...
## $ wtd_range_Density : num 1580 1667 1667 1623 1492 ...
## $ std_Density : num 3306 3767 3306 3306 3306 ...
## $ wtd_std_Density : num 3573 3633 3592 3582 3553 ...
## $ mean_ElectronAffinity : num 81.8 90.9 81.8 81.8 81.8 ...
## $ wtd_mean_ElectronAffinity : num 112 112 112 112 111 ...
## $ gmean_ElectronAffinity : num 60.1 69.8 60.1 60.1 60.1 ...
## $ wtd_gmean_ElectronAffinity : num 99.4 101.2 101.1 100.2 97.8 ...
## $ entropy_ElectronAffinity : num 1.16 1.43 1.16 1.16 1.16 ...
## $ wtd_entropy_ElectronAffinity : num 0.787 0.839 0.786 0.787 0.787 ...
## $ range_ElectronAffinity : num 127 127 127 127 127 ...
## $ wtd_range_ElectronAffinity : num 81 81.2 81.2 81.1 80.8 ...
## $ std_ElectronAffinity : num 51.4 49.4 51.4 51.4 51.4 ...
## $ wtd_std_ElectronAffinity : num 42.6 41.7 41.6 42.1 43.5 ...
## $ mean_FusionHeat : num 6.91 7.78 6.91 6.91 6.91 ...
## $ wtd_mean_FusionHeat : num 3.85 3.8 3.82 3.83 3.87 ...
## $ gmean_FusionHeat : num 3.48 4.4 3.48 3.48 3.48 ...
## $ wtd_gmean_FusionHeat : num 1.04 1.04 1.04 1.04 1.04 ...
## $ entropy_FusionHeat : num 1.09 1.37 1.09 1.09 1.09 ...
## $ wtd_entropy_FusionHeat : num 0.995 1.073 0.927 0.964 1.045 ...
## $ range_FusionHeat : num 12.9 12.9 12.9 12.9 12.9 ...
## $ wtd_range_FusionHeat : num 1.74 1.6 1.76 1.74 1.74 ...
## $ std_FusionHeat : num 4.6 4.47 4.6 4.6 4.6 ...
## $ wtd_std_FusionHeat : num 4.67 4.6 4.65 4.66 4.68 ...
## $ mean_ThermalConductivity : num 108 172 108 108 108 ...
## $ wtd_mean_ThermalConductivity : num 61 61.4 60.9 61 61.1 ...
## $ gmean_ThermalConductivity : num 7.06 16.06 7.06 7.06 7.06 ...
## $ wtd_gmean_ThermalConductivity : num 0.622 0.62 0.619 0.621 0.625 ...
## $ entropy_ThermalConductivity : num 0.308 0.847 0.308 0.308 0.308 ...
## $ wtd_entropy_ThermalConductivity : num 0.263 0.568 0.25 0.257 0.273 ...
## $ range_ThermalConductivity : num 400 430 400 400 400 ...
## $ wtd_range_ThermalConductivity : num 57.1 51.4 57.1 57.1 57.1 ...
## $ std_ThermalConductivity : num 169 199 169 169 169 ...
## $ wtd_std_ThermalConductivity : num 139 140 139 139 138 ...
## $ mean_Valence : num 2.25 2 2.25 2.25 2.25 ...
## $ wtd_mean_Valence : num 2.26 2.26 2.27 2.26 2.24 ...
## $ gmean_Valence : num 2.21 1.89 2.21 2.21 2.21 ...
## $ wtd_gmean_Valence : num 2.22 2.21 2.23 2.23 2.21 ...
## $ entropy_Valence : num 1.37 1.56 1.37 1.37 1.37 ...
## $ wtd_entropy_Valence : num 1.07 1.05 1.03 1.05 1.1 ...
## $ range_Valence : int 1 2 1 1 1 1 1 1 ...
## $ wtd_range_Valence : num 1.09 1.13 1.11 1.1 1.06 ...
## $ std_Valence : num 0.433 0.632 0.433 0.433 0.433 ...
## $ wtd_std_Valence : num 0.437 0.469 0.445 0.441 0.429 ...
## $ critical_temp : num 29 26 19 22 23 23 11 33 36 31 ...

```

From the above information, it can be seen that all variables are numeric variables and each record contains number\_of\_element, eight main properties (Atomic Mass, First Ionization Energy, Atomic Radius, Density, Electron Affinity, Fusion Heat, Thermal Conductivity, Valence) and the critical\_temp. For each main property, ten features are extracted: Mean, Weighted mean, Geometric mean, Weighted geometric mean, Entropy, Weighted entropy, Range, Weighted range. Standard deviation, Weighted standard deviation. Here, the details of each property will be explained

- **number\_of\_elements:** number of element needed to produce a particular material. For example, the number of elements for  $Ba0.2La1.8Cu1O_4$  is 4 which are Ba, La, Cu, and O.
- **Atomic Mass:** the mass of an atom
- **First Ionization Energy:** the energy required to remove one mole of the most loosely held electrons from one mole of gaseous atoms to produce 1 mole of gaseous ions each with a charge of 1+
- **Atomic Radius:** a measure of the size of its atoms, usually the mean or typical distance from the center of the nucleus to the boundary of the surrounding shells of electrons.
- **Density:** the density of the nucleus of an atom
- **Electron Affinity:** the amount of energy released or spent when an electron is added to a neutral atom or molecule in the gaseous state to form a negative ion
- **Fusion Heat:** the change in its enthalpy resulting from providing energy, typically heat, to a specific quantity of the substance to change its state from a solid to a liquid, at constant pressure
- **Thermal Conductivity:** a measure of its ability to conduct heat
- **Valence:** a measure of its combining power with other atoms when it forms chemical compounds or molecules
- **critical\_temp:** the temperature at which the electrical resistivity of a metal drops to zero

All the definitions are taken from external resource [[Wikipedia, 2019](#)].

As described above, ten features are extracted from each of the eight main properties. Here, the details of extraction process will be provided.

$$Mean(\mu) = \frac{1}{n} \sum_{i=1}^n t_i$$

$$Weighted Mean(v) = \sum_{i=1}^n p_i t_i$$

$$Geometric Mean = \sqrt[n]{\prod_{i=1}^n t_i}$$

$$Weighted Geometric Mean = \prod_{i=1}^n t_i^{p_i}$$

$$Entropy = - \sum_{i=1}^n w_i \ln(w_i)$$

$$Weighted Entropy = - \sum_{i=1}^n z_i \ln(z_i)$$

$$Range = t_{max} - t_{min}$$

$$Weighted Range = p_{max} t_{max} - p_{min} t_{min}$$

$$Standard Deviation = \sqrt{\frac{1}{n} \sum_{i=1}^n (t_i - \mu)^2}$$

$$Weighted Standard Deviation = \sqrt{\frac{1}{n} \sum_{i=1}^n p_i (t_i - \mu)^2}$$

Where:

$t_i$  : thermal conductivity coefficients of element i

$p_i$  : the ratio of element i in the corresponding material

$w_i$  : the fractions of total thermal conductivities

$z_i$  : intermediate value based on  $p_i$  and  $w_i$

$t_{max}$  : the maximum thermal conductivity coefficient

$t_{min}$  : the minimum thermal conductivity coefficient

$p_{max}$  : the ratio of the element with maximum thermal conductivity coefficient

$p_{min}$  : the ratio of the element with minimum thermal conductivity coefficient

In order to ease the exploration and analysis processes, we will store the index and name of the properties for later use.

```
# Store the index of each main property for later use
data_index <- list(1, c(2:11), c(12:21), c(22:31), c(32:41), c(42:51), c(52:61), c(62:71),
c(72:81), 82)

property_name <- c("Number of Elements", "Atomic Mass", "First Ionization Energy",
"Atomic Radius", "Density", "Electron Affinity", "Fusion Heat",
"Thermal Conductivity", "Valence", "Critical Temperature")
```

### 1.3.2 Element Dataset

In this subsection, we will describe the meaning of each column and its datatype of the element dataset.

```
# Description of the Element Dataset
str(chemical)
```

```
## 'data.frame': 21263 obs. of 88 variables:
##   $ H : num 0 0 0 0 0 0 0 0 0 ...
##   $ He : int 0 0 0 0 0 0 0 0 0 ...
##   $ Li : num 0 0 0 0 0 0 0 0 0 ...
##   $ Be : num 0 0 0 0 0 0 0 0 0 ...
##   $ B : num 0 0 0 0 0 0 0 0 0 ...
##   $ C : num 0 0 0 0 0 0 0 0 0 ...
##   $ N : num 0 0 0 0 0 0 0 0 0 ...
##   $ O : num 4 4 4 4 4 4 4 4 4 ...
##   $ F : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ne : int 0 0 0 0 0 0 0 0 0 ...
##   $ Na : num 0 0 0 0 0 0 0 0 0 ...
##   $ Mg : num 0 0 0 0 0 0 0 0 0 ...
##   $ Al : num 0 0 0 0 0 0 0 0 0 ...
##   $ Si : num 0 0 0 0 0 0 0 0 0 ...
##   $ P : num 0 0 0 0 0 0 0 0 0 ...
##   $ S : num 0 0 0 0 0 0 0 0 0 ...
##   $ Cl : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ar : int 0 0 0 0 0 0 0 0 0 ...
##   $ K : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ca : num 0 0 0 0 0 0 0 0 0 ...
##   $ Sc : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ti : num 0 0 0 0 0 0 0 0 0 ...
##   $ V : num 0 0 0 0 0 0 0 0 0 ...
##   $ Cr : num 0 0 0 0 0 0 0 0 0 ...
##   $ Mn : num 0 0 0 0 0 0 0 0 0 ...
##   $ Fe : num 0 0 0 0 0 0 0 0 0 ...
##   $ Co : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ni : num 0 0 0 0 0 0 0 0 0 ...
##   $ Cu : num 1 0.9 1 1 1 1 1 1 1 ...
##   $ Zn : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ga : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ge : num 0 0 0 0 0 0 0 0 0 ...
##   $ As : num 0 0 0 0 0 0 0 0 0 ...
##   $ Se : num 0 0 0 0 0 0 0 0 0 ...
##   $ Br : num 0 0 0 0 0 0 0 0 0 ...
##   $ Kr : int 0 0 0 0 0 0 0 0 0 ...
##   $ Rb : num 0 0 0 0 0 0 0 0 0 ...
##   $ Sr : num 0 0 0 0 0 0 0 0.1 0.15 0.2 ...
##   $ Y : num 0 0 0 0 0 0 0 0 0 ...
##   $ Zr : num 0 0 0 0 0 0 0 0 0 ...
##   $ Nb : num 0 0 0 0 0 0 0 0 0 ...
##   $ Mo : num 0 0 0 0 0 0 0 0 0 ...
##   $ Tc : num 0 0 0 0 0 0 0 0 0 ...
##   $ Ru : num 0 0 0 0 0 0 0 0 0 ...
##   $ Rh : num 0 0 0 0 0 0 0 0 0 ...
##   $ Pd : num 0 0 0 0 0 0 0 0 0 ...
```

```

## $ Ag      : num  0 0.1 0 0 0 0 0 0 0 0 ...
## $ Cd      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ In      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Sn      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Sb      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Te      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ I       : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Xe      : int   0 0 0 0 0 0 0 0 0 0 ...
## $ Cs      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Ba      : num  0.2 0.1 0.1 0.15 0.3 0.5 1 0 0 0 ...
## $ La      : num  1.8 1.9 1.9 1.85 1.7 1.5 1 1.9 1.85 1.8 ...
## $ Ce      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Pr      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Nd      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Pm      : int   0 0 0 0 0 0 0 0 0 0 ...
## $ Sm      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Eu      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Gd      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Tb      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Dy      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Ho      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Er      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Tm      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Yb      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Lu      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Hf      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Ta      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ W       : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Re      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Os      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Ir      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Pt      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Au      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Hg      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Tl      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Pb      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Bi      : num  0 0 0 0 0 0 0 0 0 0 ...
## $ Po      : int   0 0 0 0 0 0 0 0 0 0 ...
## $ At      : int   0 0 0 0 0 0 0 0 0 0 ...
## $ Rn      : int   0 0 0 0 0 0 0 0 0 0 ...
## $ critical_temp: num  29 26 19 22 23 23 11 33 36 31 ...
## $ material : Factor w/ 15542 levels "Ag0.002A10.998",...: 518 509 512 504 528 592 950 11890 11880
```

From the above information, it can be seen that from column 1 to 82 are the chemical elements, whereas column critical\_temp is the temperature at which the electrical resistivity of a metal drops to zero and the last column is the material that is formed from the corresponding elements. In addition, only one variable (material) is factor variable, all other variables are numeric variables.

**Since this dataset only contains the chemical formula for the corresponding material, we will not use this dataset for the rest of this project**

## 2 Data Exploration

In this section we will perform Exploratory Data Analysis (EDA). In general, this section will contain descriptive, correlation and distribution analysis as well as data transformation. However, before that, we need to split the dataset into train and test datasets with proportion (80:20).

```
set.seed(seed)

ind <- createDataPartition(data$critical_temp, p = .8, list = FALSE)

# Split data into train and test
train.data <- data[ind,]
test.data <- data[-ind,]
```

### 2.1 Descriptive Analysis

In this subsection, we will do some descriptive analysis on the dataset.

```
# Display the Statistics Summary
round(describe(train.data), 3)
```

##	vars	n	mean	sd	median	trimmed
## number_of_elements	1	17011	4.12	1.45	4.00	4.11
## mean_atomic_mass	2	17011	87.62	29.70	85.03	85.87
## wtd_mean_atomic_mass	3	17011	73.02	33.47	60.76	68.44
## gmean_atomic_mass	4	17011	71.33	31.04	66.36	67.66
## wtd_gmean_atomic_mass	5	17011	58.53	36.65	39.92	52.04
## entropy_atomic_mass	6	17011	1.17	0.37	1.20	1.19
## wtd_entropy_atomic_mass	7	17011	1.06	0.40	1.15	1.09
## range_atomic_mass	8	17011	115.85	54.84	122.91	119.09
## wtd_range_atomic_mass	9	17011	33.19	27.00	26.53	28.64
## std_atomic_mass	10	17011	44.43	20.09	45.13	45.40
## wtd_std_atomic_mass	11	17011	41.52	20.07	44.29	42.16
## mean_fie	12	17011	769.55	87.42	765.32	763.08
## wtd_mean_fie	13	17011	870.62	143.35	890.71	879.43
## gmean_fie	14	17011	737.45	78.38	728.06	730.20
## wtd_gmean_fie	15	17011	832.94	119.87	857.82	839.86
## entropy_fie	16	17011	1.30	0.38	1.36	1.33
## wtd_entropy_fie	17	17011	0.93	0.34	0.92	0.92
## range_fie	18	17011	572.29	309.44	764.10	593.30
## wtd_range_fie	19	17011	483.30	224.85	514.69	494.99
## std_fie	20	17011	215.50	109.81	266.00	221.59
## wtd_std_fie	21	17011	224.07	127.92	258.63	233.18
## mean_atomic_radius	22	17011	158.04	20.11	160.25	159.05
## wtd_mean_atomic_radius	23	17011	134.73	28.86	125.94	132.32
## gmean_atomic_radius	24	17011	144.52	22.11	142.81	144.29
## wtd_gmean_atomic_radius	25	17011	120.98	35.91	113.17	117.52
## entropy_atomic_radius	26	17011	1.27	0.38	1.33	1.29
## wtd_entropy_atomic_radius	27	17011	1.13	0.41	1.25	1.17
## range_atomic_radius	28	17011	139.33	67.33	171.00	146.85
## wtd_range_atomic_radius	29	17011	51.26	35.12	42.81	45.57
## std_atomic_radius	30	17011	51.56	22.90	58.66	53.73

```

## wtd_std_atomic_radius          31 17011   52.35   25.34   60.16   54.74
## mean_Density                  32 17011 6121.60 2845.72 5329.09 5681.00
## wtd_mean_Density              33 17011 5268.57 3218.68 4289.34 4710.98
## gmean_Density                 34 17011 3464.00 3702.06 1339.97 2833.75
## wtd_gmean_Density              35 17011 3114.23 3972.46 1510.88 2427.45
## entropy_Density                36 17011   1.07   0.34   1.09   1.10
## wtd_entropy_Density            37 17011   0.86   0.32   0.89   0.88
## range_Density                  38 17011 8694.20 4108.80 8958.57 8599.88
## wtd_range_Density              39 17011 2896.07 2394.68 2082.15 2463.40
## std_Density                   40 17011 3428.20 1677.65 3303.28 3323.50
## wtd_std_Density                41 17011 3329.68 1613.73 3629.11 3316.20
## mean_ElectronAffinity          42 17011   76.78   27.64   73.10   74.42
## wtd_mean_ElectronAffinity      43 17011   92.66   32.24  102.97  93.58
## gmean_ElectronAffinity         44 17011   54.28   28.98   51.47  50.97
## wtd_gmean_ElectronAffinity     45 17011   72.38   31.60   73.15  71.50
## entropy_ElectronAffinity       46 17011   1.07   0.34   1.14   1.10
## wtd_entropy_ElectronAffinity    47 17011   0.77   0.29   0.78   0.78
## range_ElectronAffinity         48 17011 120.69   58.27  127.05 118.80
## wtd_range_ElectronAffinity     49 17011   59.25   28.65   71.15  59.74
## std_ElectronAffinity           50 17011   48.89   21.59   51.13  48.38
## wtd_std_ElectronAffinity        51 17011   44.38   20.21   48.07  44.59
## mean_FusionHeat                52 17011   14.31   11.39   9.30  11.99
## wtd_mean_FusionHeat             53 17011   13.86   14.38   8.32  10.94
## gmean_FusionHeat                54 17011   10.16   10.18   5.28  8.16
## wtd_gmean_FusionHeat             55 17011   10.16   13.24   4.91  7.62
## entropy_FusionHeat              56 17011   1.09   0.38   1.11  1.12
## wtd_entropy_FusionHeat            57 17011   0.92   0.37   1.00  0.94
## range_FusionHeat                 58 17011   21.08   20.32  12.88 16.86
## wtd_range_FusionHeat              59 17011   8.20   11.43   3.40  5.88
## std_FusionHeat                  60 17011   8.29   8.66   4.95  6.36
## wtd_std_FusionHeat                61 17011   7.69   7.28   5.50  6.21
## mean_ThermalConductivity        62 17011 89.76  38.44  96.50  90.01
## wtd_mean_ThermalConductivity     63 17011 81.49  45.20  73.83  77.01
## gmean_ThermalConductivity        64 17011 29.86  34.13  14.29  23.02
## wtd_gmean_ThermalConductivity     65 17011 27.28  40.22  6.10  19.06
## entropy_ThermalConductivity      66 17011   0.73   0.33   0.74  0.73
## wtd_entropy_ThermalConductivity    67 17011   0.54   0.32   0.55  0.52
## range_ThermalConductivity        68 17011 251.29 158.56 399.80 261.80
## wtd_range_ThermalConductivity     69 17011 61.92  42.80  56.56  57.79
## std_ThermalConductivity          70 17011 99.05  60.03 135.78 101.43
## wtd_std_ThermalConductivity       71 17011 96.36  63.61 114.19 97.55
## mean_Valence                    72 17011   3.20   1.04   2.83  3.06
## wtd_mean_Valence                  73 17011   3.15   1.19   2.61  2.99
## gmean_Valence                   74 17011   3.06   1.04   2.62  2.90
## wtd_gmean_Valence                  75 17011   3.05   1.17   2.43  2.88
## entropy_Valence                  76 17011   1.30   0.39   1.37  1.32
## wtd_entropy_Valence                 77 17011   1.05   0.38   1.17  1.08
## range_Valence                     78 17011   2.04   1.24   2.00  1.97
## wtd_range_Valence                  79 17011   1.48   0.98   1.06  1.33
## std_Valence                      80 17011   0.84   0.48   0.80  0.82
## wtd_std_Valence                   81 17011   0.67   0.46   0.50  0.64
## critical_temp                     82 17011 34.44  34.25  20.00 30.35
##                               mad   min    max  range skew
##                               1.48  1.00   9.00   8.00  0.01

```

## mean_atomic_mass	20.16	6.94	208.98	202.04	0.77
## wtd_mean_atomic_mass	18.34	6.94	208.98	202.04	1.50
## gmean_atomic_mass	15.06	5.68	208.98	203.29	1.47
## wtd_gmean_atomic_mass	15.03	3.19	208.98	205.79	1.70
## entropy_atomic_mass	0.36	0.00	1.98	1.98	-0.78
## wtd_entropy_atomic_mass	0.38	0.00	1.94	1.94	-0.63
## range_atomic_mass	61.12	0.00	207.97	207.97	-0.38
## wtd_range_atomic_mass	16.11	0.00	205.59	205.59	2.46
## std_atomic_mass	19.46	0.00	101.02	101.02	-0.36
## wtd_std_atomic_mass	17.37	0.00	101.02	101.02	-0.31
## mean_fie	53.84	375.50	1313.10	937.60	1.01
## wtd_mean_fie	173.71	375.50	1313.10	937.60	-0.30
## gmean_fie	54.43	375.50	1313.10	937.60	1.20
## wtd_gmean_fie	126.74	375.50	1313.10	937.60	-0.32
## entropy_fie	0.39	0.00	2.16	2.16	-0.80
## wtd_entropy_fie	0.22	0.00	2.04	2.04	-0.03
## range_fie	68.94	0.00	1304.50	1304.50	-0.46
## wtd_range_fie	273.18	0.00	1049.39	1049.39	-0.29
## std_fie	79.01	0.00	499.67	499.67	-0.46
## wtd_std_fie	136.15	0.00	477.81	477.81	-0.41
## mean_atomic_radius	15.49	48.00	298.00	250.00	-0.56
## wtd_mean_atomic_radius	28.75	48.00	298.00	250.00	0.57
## gmean_atomic_radius	15.68	48.00	298.00	250.00	0.10
## wtd_gmean_atomic_radius	39.61	48.00	298.00	250.00	0.56
## entropy_atomic_radius	0.36	0.00	2.14	2.14	-0.75
## wtd_entropy_atomic_radius	0.35	0.00	1.89	1.89	-0.80
## range_atomic_radius	50.41	0.00	256.00	256.00	-0.69
## wtd_range_atomic_radius	22.48	0.00	240.16	240.16	1.66
## std_atomic_radius	18.72	0.00	115.50	115.50	-0.75
## wtd_std_atomic_radius	25.83	0.00	91.50	91.50	-0.65
## mean_Density	1589.71	1.43	22590.00	22588.57	2.09
## wtd_mean_Density	2012.49	1.43	22590.00	22588.57	2.13
## gmean_Density	1078.96	1.43	22590.00	22588.57	1.65
## wtd_gmean_Density	2157.55	1.43	22590.00	22588.57	1.65
## entropy_Density	0.34	0.00	1.95	1.95	-0.80
## wtd_entropy_Density	0.29	0.00	1.70	1.70	-0.61
## range_Density	2355.01	0.00	22588.57	22588.57	0.38
## wtd_range_Density	909.78	0.00	22434.16	22434.16	3.31
## std_Density	905.60	0.00	10724.37	10724.37	0.85
## wtd_std_Density	706.39	0.00	10410.93	10410.93	0.45
## mean_ElectronAffinity	16.89	1.50	296.70	295.20	1.08
## wtd_mean_ElectronAffinity	19.70	1.50	296.70	295.20	-0.23
## gmean_ElectronAffinity	25.55	1.50	296.70	295.20	1.33
## wtd_gmean_ElectronAffinity	28.34	1.50	296.70	295.20	0.40
## entropy_ElectronAffinity	0.32	0.00	1.77	1.77	-0.92
## wtd_entropy_ElectronAffinity	0.17	0.00	1.68	1.68	-0.24
## range_ElectronAffinity	20.68	0.00	349.00	349.00	0.92
## wtd_range_ElectronAffinity	18.84	0.00	218.70	218.70	0.12
## std_ElectronAffinity	9.67	0.00	162.90	162.90	0.56
## wtd_std_ElectronAffinity	11.75	0.00	169.08	169.08	0.46
## mean_FusionHeat	3.76	0.22	105.00	104.78	2.58
## wtd_mean_FusionHeat	5.67	0.22	105.00	104.78	2.78
## gmean_FusionHeat	2.67	0.22	105.00	104.78	2.77
## wtd_gmean_FusionHeat	5.46	0.22	105.00	104.78	2.52

## entropy_FusionHeat	0.40	0.00	2.03	2.03	-0.58
## wtd_entropy_FusionHeat	0.34	0.00	1.75	1.75	-0.58
## range_FusionHeat	5.07	0.00	104.78	104.78	2.75
## wtd_range_FusionHeat	2.58	0.00	102.39	102.39	4.25
## std_FusionHeat	1.66	0.00	51.63	51.63	2.84
## wtd_std_FusionHeat	1.82	0.00	51.68	51.68	2.87
## mean_ThermalConductivity	29.41	0.03	332.50	332.47	0.22
## wtd_mean_ThermalConductivity	35.50	0.03	406.96	406.93	1.35
## gmean_ThermalConductivity	10.81	0.03	317.88	317.86	2.36
## wtd_gmean_ThermalConductivity	8.12	0.02	376.03	376.01	2.58
## entropy_ThermalConductivity	0.38	0.00	1.63	1.63	-0.12
## wtd_entropy_ThermalConductivity	0.40	0.00	1.61	1.61	0.31
## range_ThermalConductivity	0.47	0.00	429.97	429.97	-0.24
## wtd_range_ThermalConductivity	45.77	0.00	401.44	401.44	1.39
## std_ThermalConductivity	50.03	0.00	213.50	213.50	-0.23
## wtd_std_ThermalConductivity	79.63	0.00	213.30	213.30	-0.09
## mean_Valence	0.86	1.00	7.00	6.00	1.00
## wtd_mean_Valence	0.79	1.00	7.00	6.00	0.90
## gmean_Valence	0.66	1.00	7.00	6.00	1.17
## wtd_gmean_Valence	0.55	1.00	7.00	6.00	1.02
## entropy_Valence	0.41	0.00	2.14	2.14	-0.78
## wtd_entropy_Valence	0.32	0.00	1.95	1.95	-0.74
## range_Valence	1.48	0.00	6.00	6.00	0.45
## wtd_range_Valence	0.37	0.00	6.99	6.99	1.55
## std_Valence	0.54	0.00	3.00	3.00	0.42
## wtd_std_Valence	0.37	0.00	3.00	3.00	0.64
## critical_temp	25.43	0.00	185.00	185.00	0.86
##		kurtosis	se		
## number_of_elements	-0.68	0.01			
## mean_atomic_mass	2.03	0.23			
## wtd_mean_atomic_mass	2.83	0.26			
## gmean_atomic_mass	3.31	0.24			
## wtd_gmean_atomic_mass	2.91	0.28			
## entropy_atomic_mass	0.31	0.00			
## wtd_entropy_atomic_mass	-0.20	0.00			
## range_atomic_mass	-0.68	0.42			
## wtd_range_atomic_mass	8.39	0.21			
## std_atomic_mass	-0.45	0.15			
## wtd_std_atomic_mass	-0.52	0.15			
## mean_fie	2.88	0.67			
## wtd_mean_fie	-1.23	1.10			
## gmean_fie	3.30	0.60			
## wtd_gmean_fie	-0.91	0.92			
## entropy_fie	0.41	0.00			
## wtd_entropy_fie	0.86	0.00			
## range_fie	-1.13	2.37			
## wtd_range_fie	-1.11	1.72			
## std_fie	-0.97	0.84			
## wtd_std_fie	-1.43	0.98			
## mean_atomic_radius	1.50	0.15			
## wtd_mean_atomic_radius	-0.59	0.22			
## gmean_atomic_radius	1.19	0.17			
## wtd_gmean_atomic_radius	-0.91	0.28			
## entropy_atomic_radius	0.39	0.00			

## wtd_entropy_atomic_radius	-0.09	0.00
## range_atomic_radius	-0.92	0.52
## wtd_range_atomic_radius	2.94	0.27
## std_atomic_radius	-0.50	0.18
## wtd_std_atomic_radius	-0.86	0.19
## mean_Density	6.06	21.82
## wtd_mean_Density	6.16	24.68
## gmean_Density	3.12	28.38
## wtd_gmean_Density	3.40	30.46
## entropy_Density	0.61	0.00
## wtd_entropy_Density	0.42	0.00
## range_Density	1.15	31.50
## wtd_range_Density	15.55	18.36
## std_Density	2.07	12.86
## wtd_std_Density	2.03	12.37
## mean_ElectronAffinity	2.87	0.21
## wtd_mean_ElectronAffinity	0.62	0.25
## gmean_ElectronAffinity	2.84	0.22
## wtd_gmean_ElectronAffinity	0.87	0.24
## entropy_ElectronAffinity	0.51	0.00
## wtd_entropy_ElectronAffinity	0.97	0.00
## range_ElectronAffinity	3.27	0.45
## wtd_range_ElectronAffinity	0.74	0.22
## std_ElectronAffinity	2.35	0.17
## wtd_std_ElectronAffinity	3.10	0.16
## mean_FusionHeat	9.63	0.09
## wtd_mean_FusionHeat	10.70	0.11
## gmean_FusionHeat	13.70	0.08
## wtd_gmean_FusionHeat	9.79	0.10
## entropy_FusionHeat	0.04	0.00
## wtd_entropy_FusionHeat	-0.21	0.00
## range_FusionHeat	7.58	0.16
## wtd_range_FusionHeat	25.58	0.09
## std_FusionHeat	8.19	0.07
## wtd_std_FusionHeat	9.20	0.06
## mean_ThermalConductivity	1.42	0.30
## wtd_mean_ThermalConductivity	3.97	0.35
## gmean_ThermalConductivity	7.92	0.26
## wtd_gmean_ThermalConductivity	10.06	0.31
## entropy_ThermalConductivity	-0.63	0.00
## wtd_entropy_ThermalConductivity	-0.85	0.00
## range_ThermalConductivity	-1.76	1.22
## wtd_range_ThermalConductivity	4.32	0.33
## std_ThermalConductivity	-1.64	0.46
## wtd_std_ThermalConductivity	-1.65	0.49
## mean_Valence	0.14	0.01
## wtd_mean_Valence	-0.34	0.01
## gmean_Valence	0.50	0.01
## wtd_gmean_Valence	-0.07	0.01
## entropy_Valence	0.16	0.00
## wtd_entropy_Valence	0.07	0.00
## range_Valence	-0.55	0.01
## wtd_range_Valence	2.43	0.01
## std_Valence	-0.34	0.00

```

## wtd_std_Valence           -0.37  0.00
## critical_temp              -0.53  0.26

```

From the Summary result, some observations can be extracted. Here is the details.

### Number of Element

- The number of elements for each material varies from 1 to 9, however the median is 4 and mean is 4.115 which means that the majority of the materials has less than equal to 5.

### Atomic Mass

- There is a large range for almost all the features except entropy\_atomic\_mass and wtd\_entropy\_atomic\_mass.
- mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, and wtd\_range\_atomic\_mass have Right Skewed Distribution whereas the others have Left Skewed Distribution
- mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, and wtd\_gmean\_atomic\_mass have a quite similar characteristics of data, whereas entropy\_atomic\_mass has a quite similar characteristics of data with wtd\_entropy\_atomic\_mass.

### First Ionization Energy

- There is a large range for almost all the features except entropy\_fie and wtd\_entropy\_fie.
- mean\_fie and gmean\_fie have Right Skewed Distribution whereas the others have Left Skewed Distribution
- mean\_fie has a similar characteristics of data with gmean\_fie
- wtd\_mean\_fie and wtd\_gmean\_fie have a similar characteristics data.

### Atomic Radius

- mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, and wtd\_gmean\_atomic\_radius have a same range.
- wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, and wtd\_range\_atomic\_radius have Right Skewed Distribution whereas the others tend to have Left Skewed Distribution.
- mean\_atomic\_radius has a similar statistics information with gmean\_atomic\_radius
- wtd\_mean\_atomic\_radius and wtd\_gmean\_atomic\_radius have a similar statistics information

### Density

- mean\_Density, wtd\_mean\_Density, gmean\_Density and range\_Density have a same range of value.
- entropy\_Density and wtd\_entropy\_Density have Left Skewed Distribution, whereas the others tend to have Right Skewed Distribution

### Electron Affinity

- mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, and wtd\_gmean\_ElectronAffinity have a same range of value
- wtd\_mean\_ElectronAffinity, entropy\_ElectronAffinity and wtd\_entropy\_ElectronAffinity have Left Skewed Distribution, whereas the others tend to have Right Skewed Distribution

### Fusion Heat

- mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, and wtd\_gmean\_FusionHeat have a same range of value
- entropy\_FusionHeat and wtd\_entropy\_FusionHeat have Left Skewed Distribution, whereas the others tend to have Right Skewed Distribution

## Thermal Conductivity

- mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, and gmean\_ThermalConductivity have a same minimum value but not the maximum value.
- wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, and wtd\_range\_ThermalConductivity have Right Skewed Distribution, whereas the others tend to have a approximately normal distribution (not exactly)

## Valence

- mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, and wtd\_gmean\_Valence have a same range of value
- entropy\_Valence and wtd\_entropy\_Valence have Left Skewed Distribution, whereas the others tend to have Right Skewed Distribution

## Critical Temperature

- The range of crital\_temp is 185, however, the standard deviation is 34.254 and mean is 34.421 which means this feature has Right Skewed Distribution.

From all the above analysis, we know that most of the variables have skewed distribution, therefore, we might need to perform data transformation in the future step. In addition, we also know that the range of entropy related variables is very small compared to the other variables, therefore, we might need to do scaling in the model development section.

For the next step, we will visualize the value of each column through boxplot visualisation.

```
# Boxplot visualisation for the number of elements
boxplot(train.data[,1], type="l", cex.main = 0.8, col = 'lightblue', ylab="Value")
```

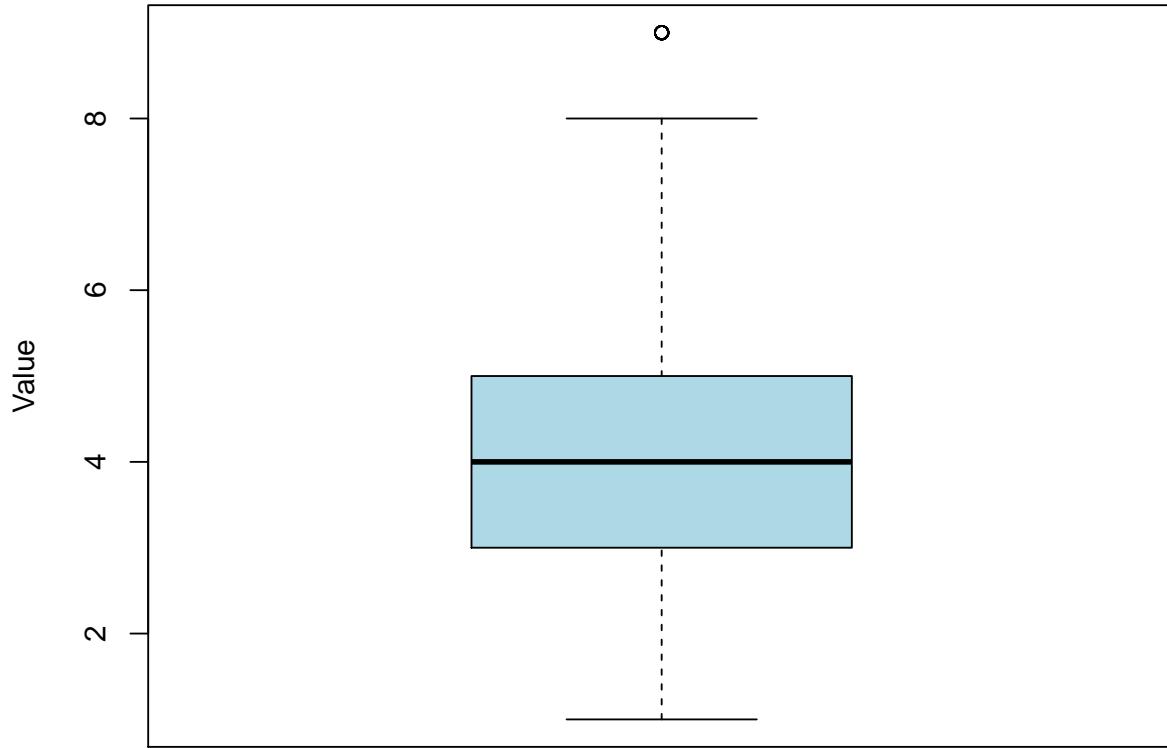


Figure 1: Number of Element Boxplot

From Figure 1, the median of number of elements is 4 and there is only a few materials that has 9 number of elements.

```
# Boxplot visualisation for the eight main properties
i <- 2
for(col in data_index[2:9]){
  boxplot(train.data[,col], type="l", cex.main = 0.8,
          col = 'lightblue', ylab="Value", xaxt = "n")
  axis(1, at = c(1:10), labels = names(train.data)[(10*i - 18):(10*i - 9)], cex.axis = 0.5)
  i <- i+1
  cat('\n\n')
}
```

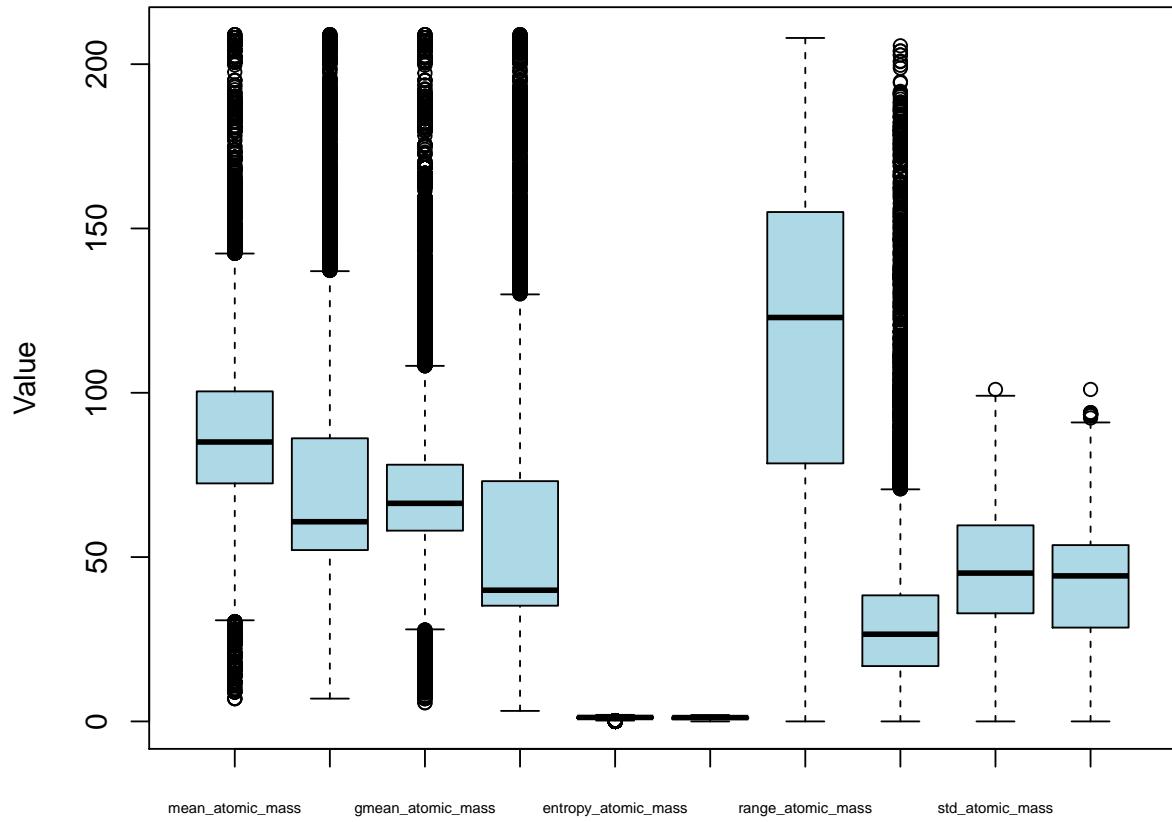


Figure 2: Atomic Mass Boxplot

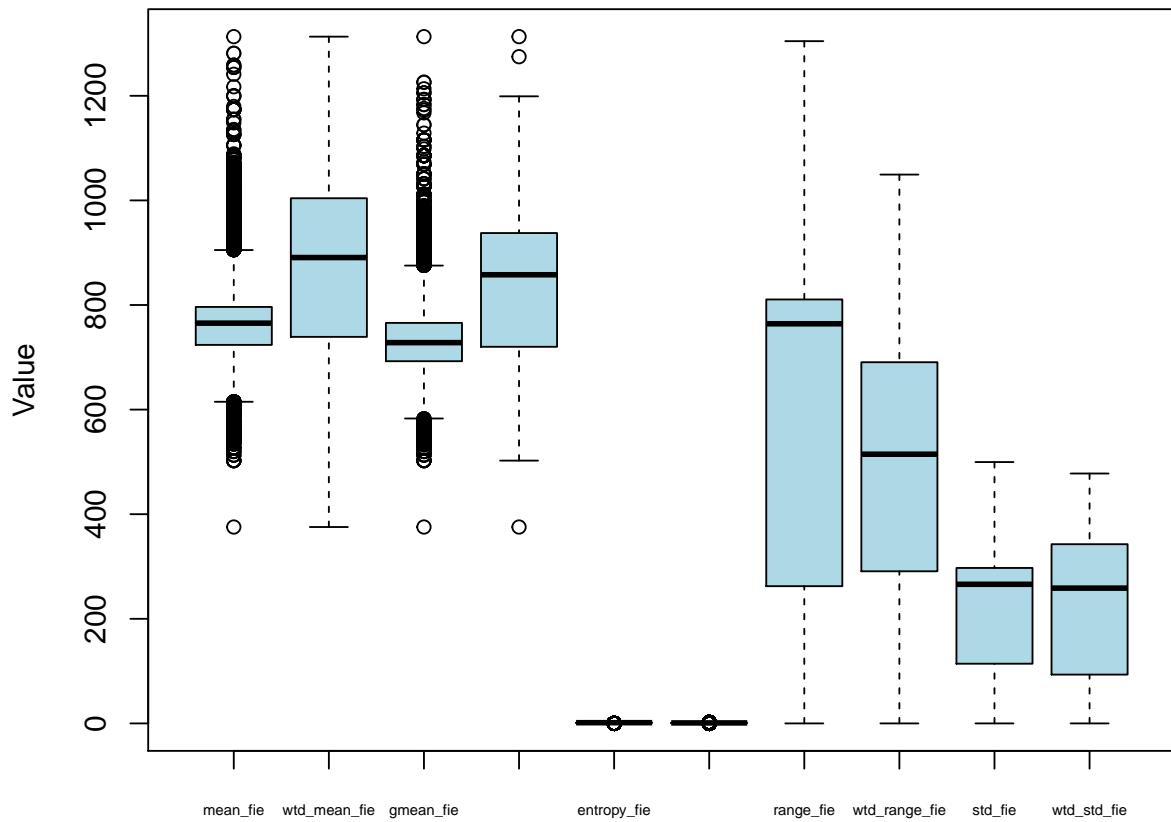


Figure 3: First Ionization Energy Boxplot

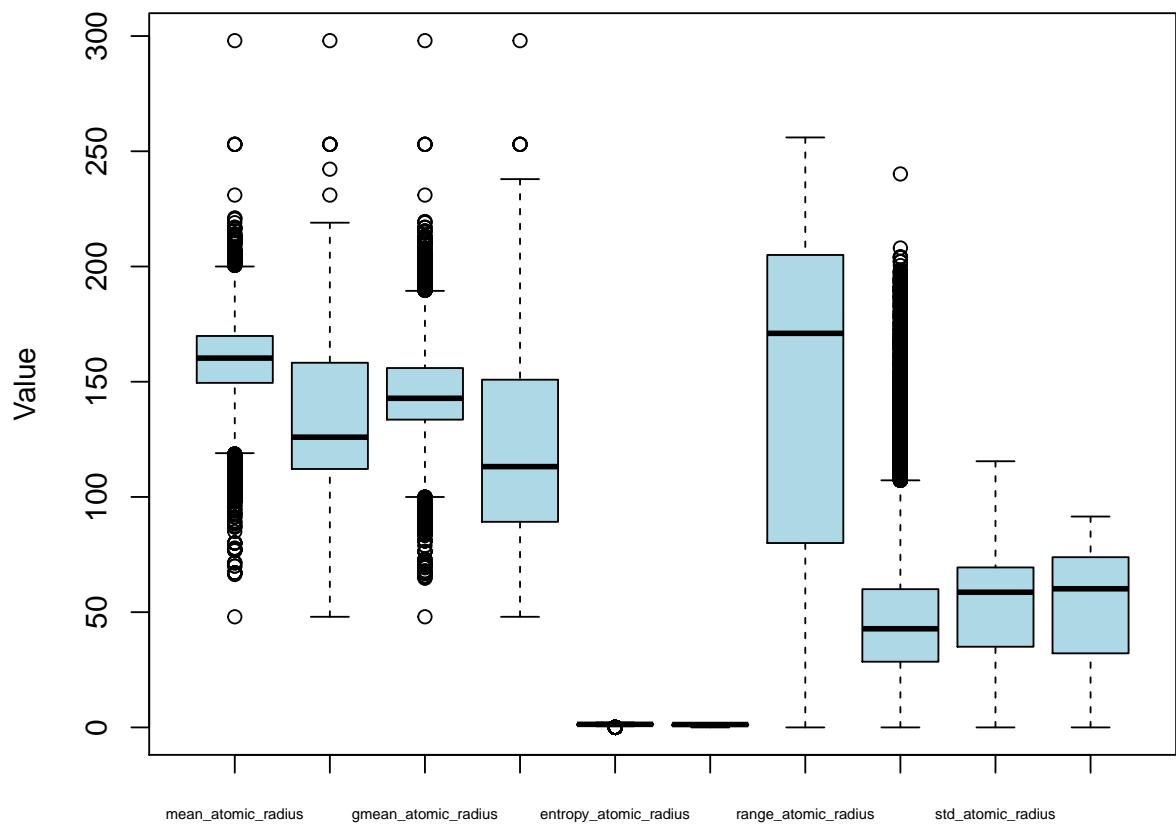


Figure 4: Atomic Radius Boxplot

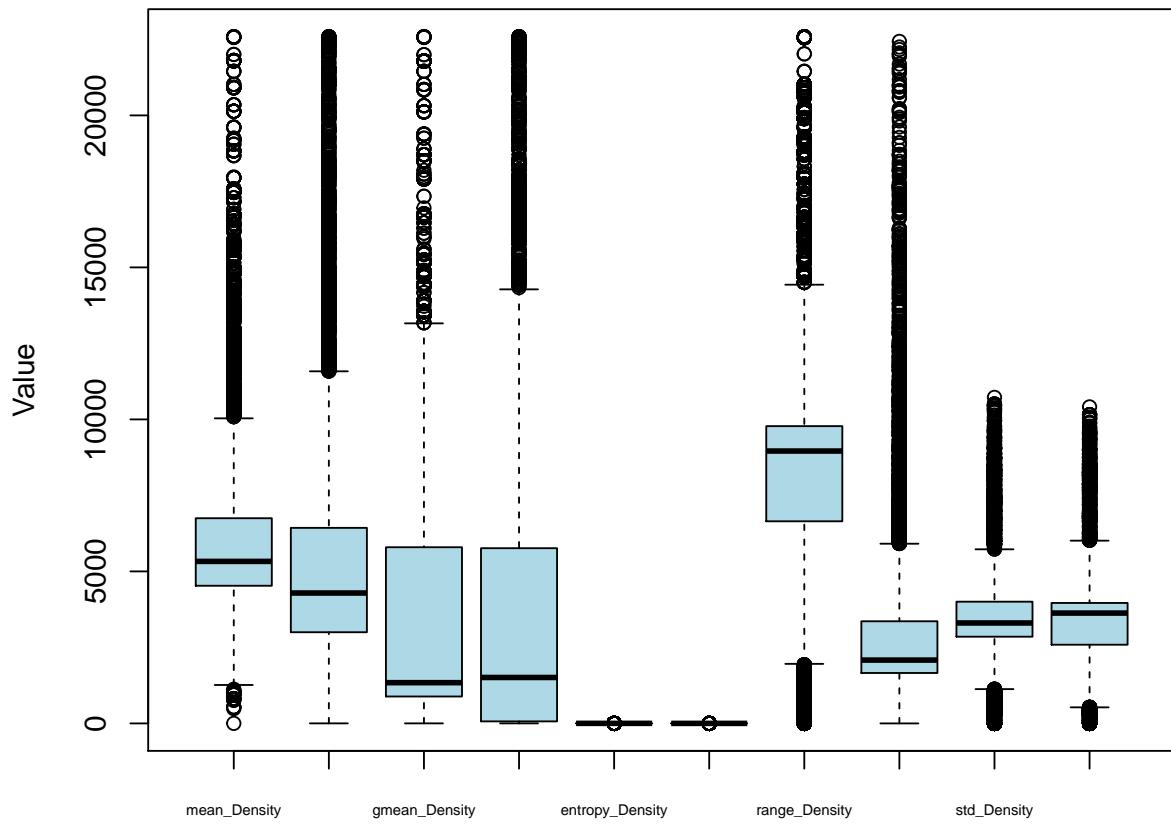


Figure 5: Density Boxplot

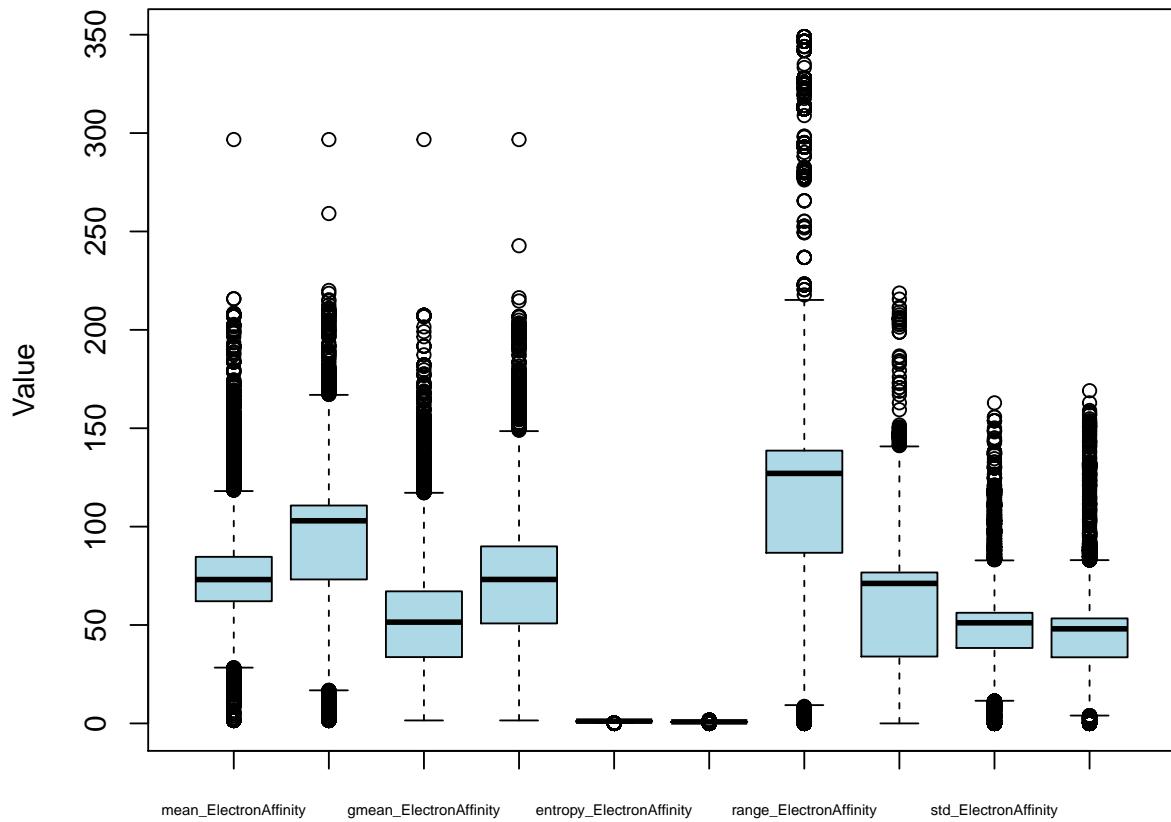


Figure 6: Electron Affinity Boxplot

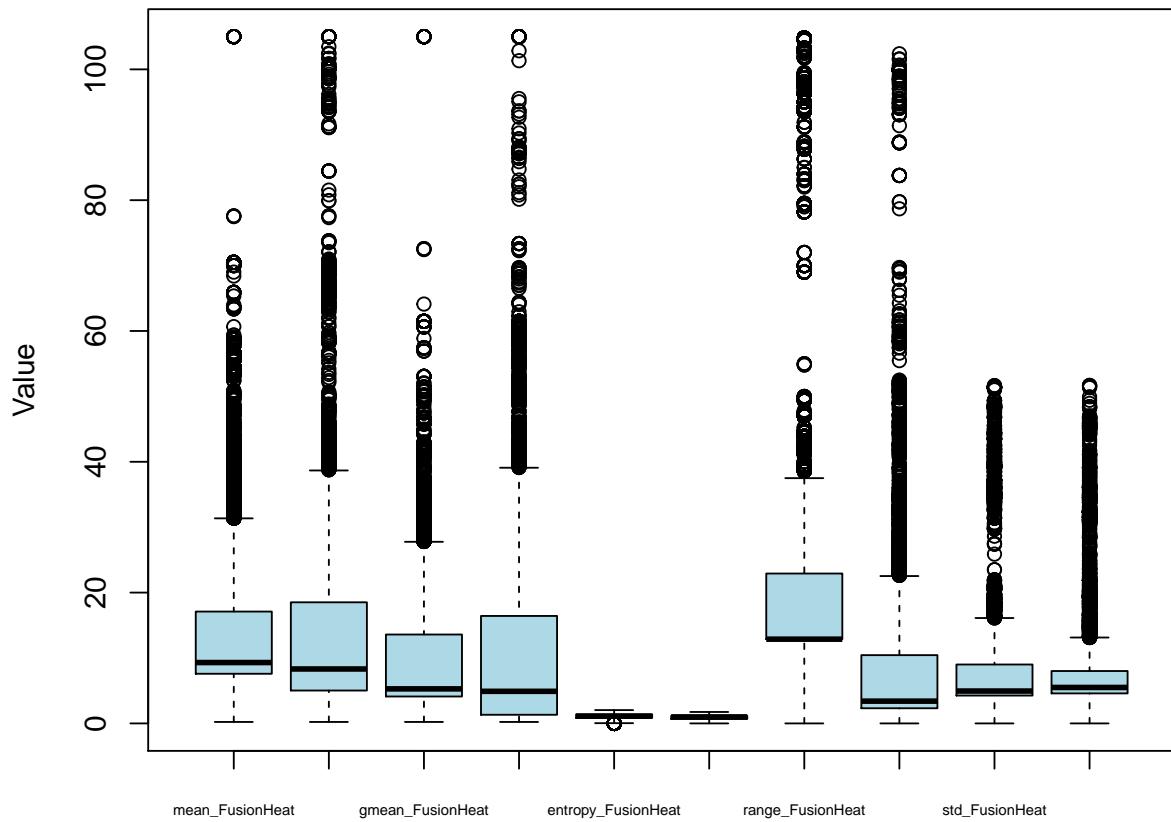


Figure 7: Fusion Heat Boxplot

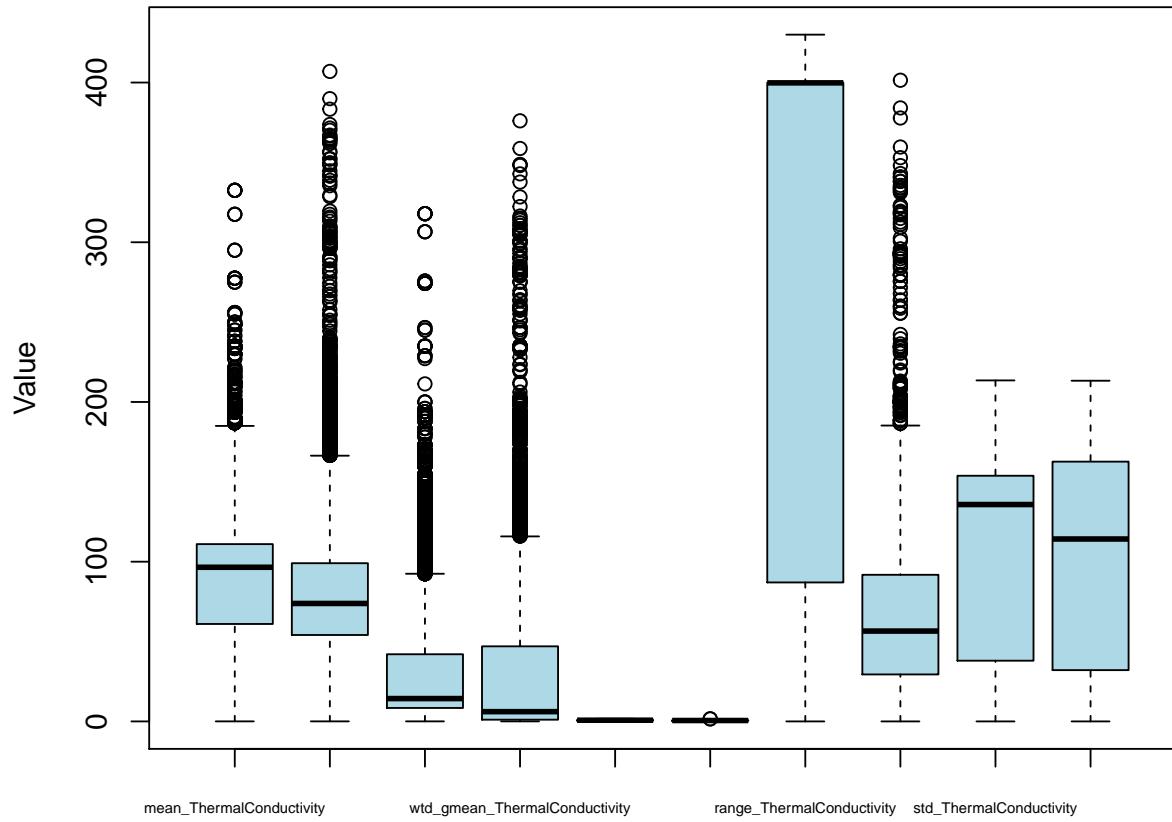


Figure 8: Thermal Conductivity Boxplot

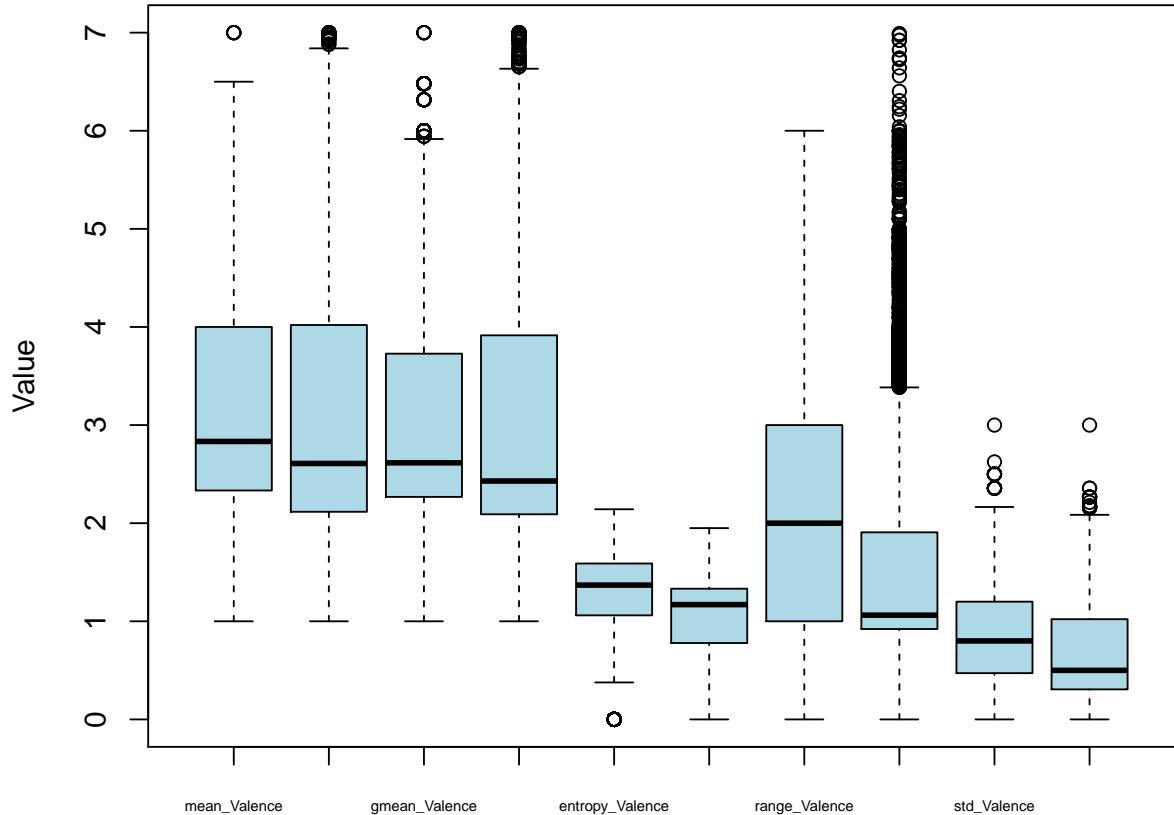


Figure 9: Valence Boxplot

From the above figures, we can see that

- For each property, the entropy and weighted entropy have different range of values, this makes sense since they are the entropy.
- All property have similar pattern of distribution, except First Ionization Energy and Valence.
- The majority of the variables have a very skewed distribution, this is why in the future step we need to perform data transformation.

```
# Boxplot visualisation for the critical temperature
boxplot(train.data[,82], type="l", cex.main = 0.8, col = 'lightblue', ylab="Value")
```

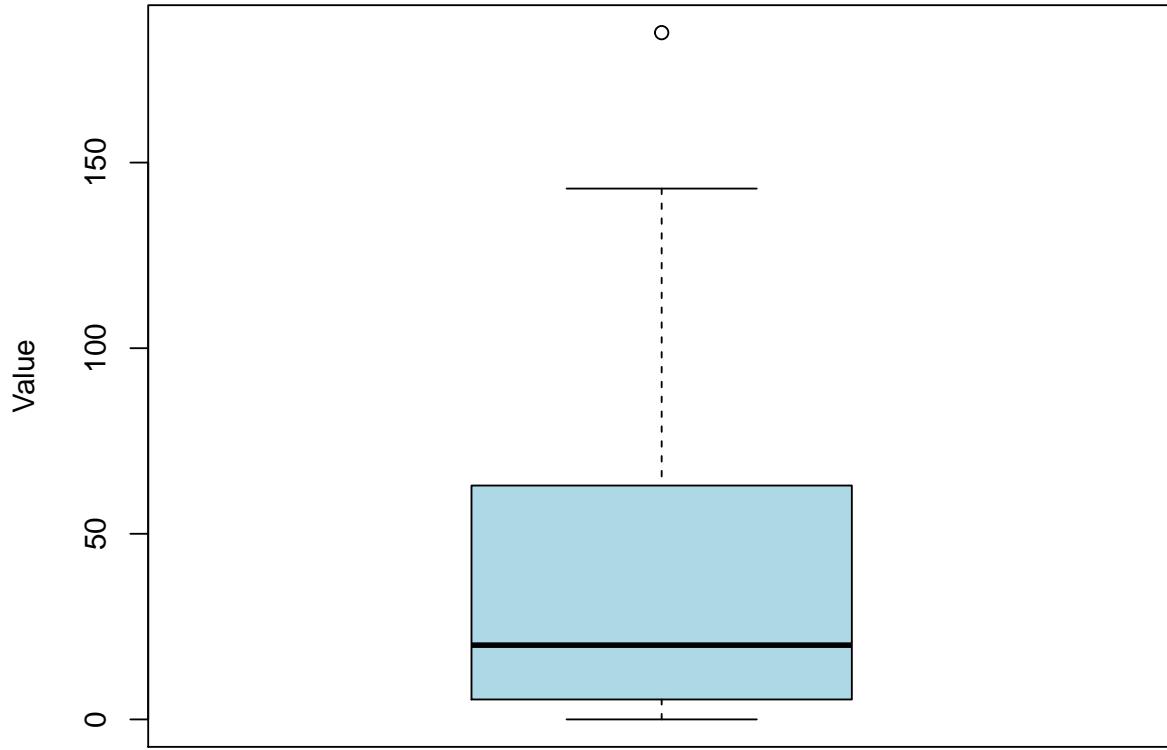


Figure 10: Critical Temperature Boxplot

From Figure 10, we can see that the median of critical temperature is 20 and there is a few value which is greater than 150. In addition, the distribution of critical temparature is Right Skewed, this can be seen from the boxplot visualisation.

## 2.2 Correlation Analysis

In this subsection, we will do some correlation analysis. First, we will plot the correlation matrix between features.

```
# Correlation Matrix
corrmatrix <- cor(train.data)

# Correlation Matrix Function based on P-Value
cor.mtest <- function(mat, conf.level){
  mat <- as.matrix(mat)
  n <- ncol(mat)
```

```

p.mat <- lowCI.mat <- uppCI.mat <- matrix(NA, n, n)
diag(p.mat) <- 0
diag(lowCI.mat) <- diag(uppCI.mat) <- 1
for(i in 1:(n-1)){
  for(j in (i+1):n){
    tmp <- cor.test(mat[,i], mat[,j], conf.level = conf.level)
    p.mat[i,j] <- p.mat[j,i] <- tmp$p.value
    lowCI.mat[i,j] <- lowCI.mat[j,i] <- tmp$conf.int[1]
    uppCI.mat[i,j] <- uppCI.mat[j,i] <- tmp$conf.int[2]
  }
}
return(list(p.mat, lowCI.mat, uppCI.mat))
}

```

```

# Correlation Matrix with 0.001 p-value
res1 <- cor.mtest(corrmatrix, 0.999)
col1 <- colorRampPalette(brewer.pal(9, "BrBG"))

# Visualize the correlation matrix
corrplot(cor(train.data), method = "square", order = "original", tl.col = "black",
         tl.cex = 0.25, p.mat = res1[[1]], sig.level = 0.001, insig = "pch",
         pch.cex = 0.3, col = col1(100))

```

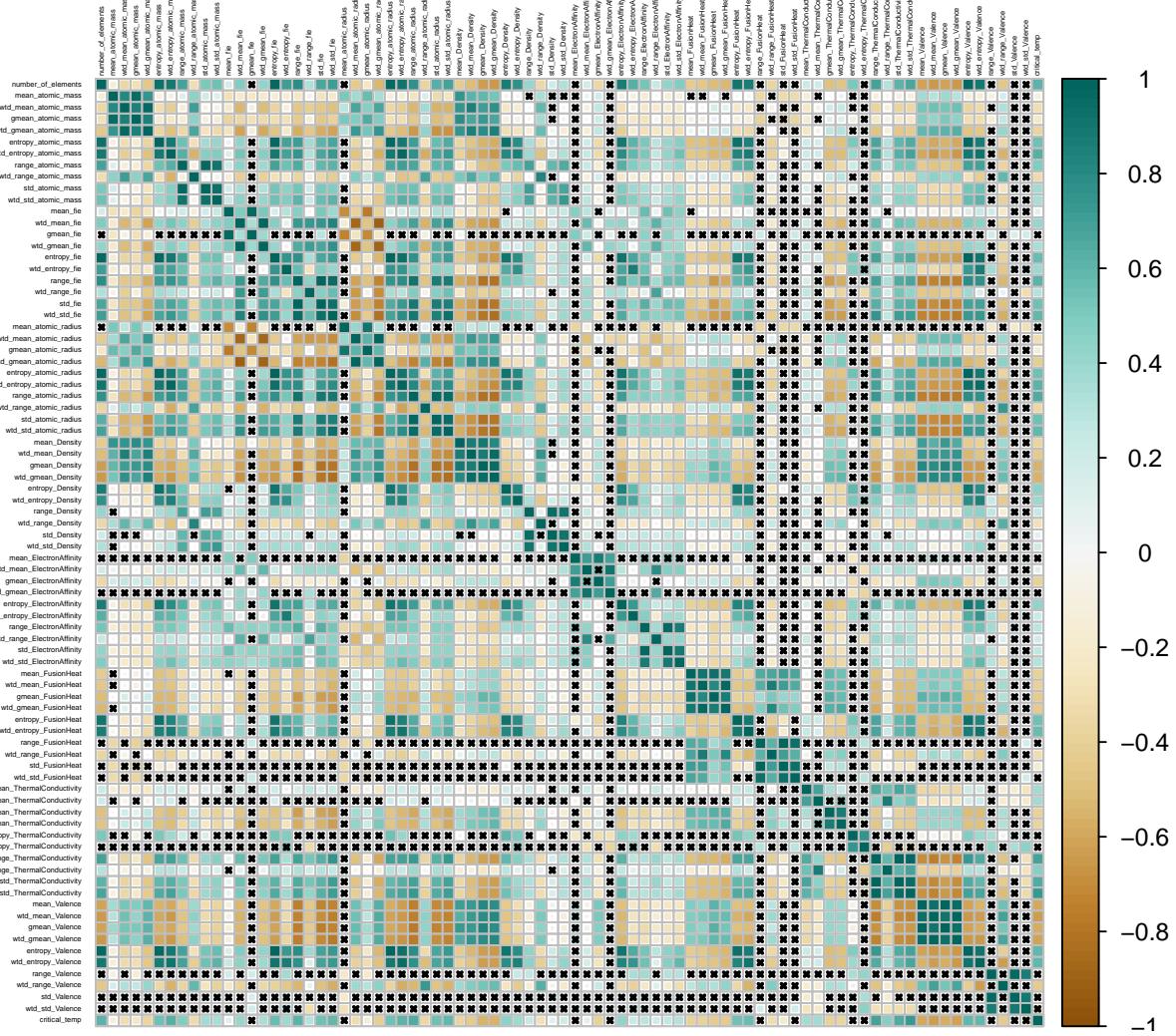


Figure 11: Correlation Matrix

```
cor(train.data$entropy_fie, train.data$critical_temp)
```

```
## [1] 0.5674736
```

From Figure 11, we can gain some informations as follows.

- **number\_of\_elements** has positive correlation with entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **number\_of\_elements** has negative correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence

- **number\_of\_elements** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **mean\_atomic\_mass** has positive correlation with wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, mean\_atomic\_radius, gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density
- **mean\_atomic\_mass** has no correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_mean\_atomic\_mass** has positive correlation with mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **wtd\_mean\_atomic\_mass** has negative correlation with wtd\_mean\_fie, wtd\_gmean\_fie, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius
- **wtd\_mean\_atomic\_mass** has no correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **gmean\_atomic\_mass** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, mean\_atomic\_radius, gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density,

gmean\_Density, wtd\_gmean\_Density, gmean\_Valence

- **gmean\_atomic\_mass** has negative correlation with std\_atomic\_radius
- **gmean\_atomic\_mass** has no correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_gmean\_atomic\_mass** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **wtd\_gmean\_atomic\_mass** has negative correlation with wtd\_mean\_fie, wtd\_gmean\_fie, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius
- **wtd\_gmean\_atomic\_mass** has no correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, entropy\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **entropy\_atomic\_mass** has positive correlation with number\_of\_elements, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **entropy\_atomic\_mass** has negative correlation with gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **entropy\_atomic\_mass** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius,

- wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_entropy\_atomic\_mass** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, range\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **wtd\_entropy\_atomic\_mass** has negative correlation with wtd\_range\_atomic\_mass, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_entropy\_atomic\_mass** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **range\_atomic\_mass** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
  - **range\_atomic\_mass** has negative correlation with wtd\_gmean\_Density
  - **range\_atomic\_mass** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_range\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **wtd\_range\_atomic\_mass** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, wtd\_range\_Valence
  - **wtd\_range\_atomic\_mass** has negative correlation with wtd\_entropy\_atomic\_mass
  - **wtd\_range\_atomic\_mass** has no correlation with number\_of\_elements, mean\_atomic\_mass, gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass,

mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie,  
 wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density,  
 std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, std\_Valence, wtd\_std\_Valence, criti-  
 cal\_temp

- **std\_atomic\_mass** has positive correlation with number\_of\_elements, range\_atomic\_mass,  
 wtd\_std\_atomic\_mass, entropy\_fie, range\_fie, std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius,  
 range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, range\_Density, std\_Density,  
 wtd\_std\_Density, wtd\_entropy\_FusionHeat, entropy\_Valence, wtd\_entropy\_Valence
- **std\_atomic\_mass** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
 gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
 wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie,  
 wtd\_range\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, wtd\_range\_Density,  
 mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity,  
 entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity,  
 std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat,  
 gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
 std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
 gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence,  
 wtd\_std\_Valence, critical\_temp
- **wtd\_std\_atomic\_mass** has positive correlation with number\_of\_elements, range\_atomic\_mass,  
 std\_atomic\_mass, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius,  
 range\_Density, std\_Density, wtd\_std\_Density, entropy\_ElectronAffinity, wtd\_entropy\_FusionHeat,  
 entropy\_Valence, wtd\_entropy\_Valence
- **wtd\_std\_atomic\_mass** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
 gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
 wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie,  
 wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, wtd\_range\_Density,  
 mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity,  
 wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity,  
 wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat,  
 wtd\_gmean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
 std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,

gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

- **mean\_fie** has positive correlation with gmean\_fie, wtd\_gmean\_fie, std\_fie, range\_ElectronAffinity, std\_ElectronAffinity
- **mean\_fie** has negative correlation with mean\_atomic\_radius, gmean\_atomic\_radius
- **mean\_fie** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, wtd\_std\_fie, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_mean\_fie** has positive correlation with wtd\_entropy\_atomic\_mass, wtd\_gmean\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_mean\_ElectronAffinity, wtd\_range\_ElectronAffinity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity
- **wtd\_mean\_fie** has negative correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **wtd\_mean\_fie** has no correlation with number\_of\_elements, mean\_atomic\_mass, gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, wtd\_mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **gmean\_fie** has positive correlation with mean\_fie
- **gmean\_fie** has negative correlation with mean\_atomic\_radius, gmean\_atomic\_radius
- **gmean\_fie** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density,

wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence,  
 wtd\_std\_Valence, critical\_temp

- **wtd\_gmean\_fie** has positive correlation with mean\_fie, wtd\_mean\_fie, range\_fie, wtd\_range\_fie,  
 std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, wtd\_mean\_ElectronAffinity, wtd\_range\_ElectronAffinity, range\_ThermalConductivity
- **wtd\_gmean\_fie** has negative correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass,  
 wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density
- **wtd\_gmean\_fie** has no correlation with number\_of\_elements, mean\_atomic\_mass, gmean\_atomic\_mass,  
 entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass,  
 std\_atomic\_mass, wtd\_std\_atomic\_mass, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, mean\_atomic\_radius,  
 gmean\_atomic\_radius, entropy\_atomic\_radius, mean\_Density, entropy\_Density, wtd\_entropy\_Density,  
 range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity,  
 gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity,  
 range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity,  
 mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence,  
 wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence,  
 critical\_temp
- **entropy\_fie** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
 range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_entropy\_fie, range\_fie,  
 std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius,  
 std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity,  
 wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity,  
 entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence,  
 critical\_temp
- **entropy\_fie** has negative correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence,  
 wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **entropy\_fie** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass,  
 wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie,  
 wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_range\_atomic\_radius, mean\_Density, range\_Density, wtd\_range\_Density, std\_Density,  
 wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
 range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_entropy\_fie** has positive correlation with number\_of\_elements, entropy\_atomic\_mass,

- wtd\_entropy\_atomic\_mass, range\_atomic\_mass, entropy\_fie, range\_fie, entropy\_atomic\_radius,  
wtd\_entropy\_atomic\_radius, range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, en-  
tropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity,  
entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_Valence, wtd\_entropy\_Valence
- **wtd\_entropy\_fie** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,  
wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie,  
std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius,  
mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density,  
wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity,  
gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity,  
mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat,  
range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,  
wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity,  
entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity,  
wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity,  
mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence,  
wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **range\_fie** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie,  
entropy\_fie, wtd\_entropy\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius,  
range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, en-  
tropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity,  
wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity,  
std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence,  
critical\_temp
  - **range\_fie** has negative correlation with wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius,  
wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density,  
gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity,  
mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **range\_fie** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass,  
wtd\_range\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius,  
wtd\_range\_atomic\_radius, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density,  
wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat,  
range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,  
wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_range\_fie** has positive correlation with wtd\_mean\_fie, wtd\_gmean\_fie, wtd\_std\_fie,  
wtd\_std\_atomic\_radius, wtd\_range\_ElectronAffinity, range\_ThermalConductivity, std\_ThermalConductivity
  - **wtd\_range\_fie** has negative correlation with wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius
  - **wtd\_range\_fie** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass,  
mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, mean\_atomic\_radius,  
gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius,  
wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density,  
wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density,  
std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat,  
gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat,  
range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,

- wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **std\_fie** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **std\_fie** has negative correlation with wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
  - **std\_fie** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_range\_atomic\_mass, gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_std\_fie** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **wtd\_std\_fie** has negative correlation with wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_std\_fie** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **mean\_atomic\_radius** has positive correlation with mean\_atomic\_mass, gmean\_atomic\_mass, gmean\_atomic\_radius
  - **mean\_atomic\_radius** has negative correlation with mean\_fie, gmean\_fie
  - **mean\_atomic\_radius** has no correlation with number\_of\_elements, wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius,

- wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_mean\_atomic\_radius** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **wtd\_mean\_atomic\_radius** has negative correlation with wtd\_mean\_fie, wtd\_gmean\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_range\_ElectronAffinity
  - **wtd\_mean\_atomic\_radius** has no correlation with number\_of\_elements, mean\_atomic\_mass, gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, entropy\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **gmean\_atomic\_radius** has positive correlation with mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, gmean\_Density, wtd\_gmean\_Density
  - **gmean\_atomic\_radius** has negative correlation with mean\_fie, gmean\_fie, std\_fie
  - **gmean\_atomic\_radius** has no correlation with number\_of\_elements, wtd\_mean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

wtd\_std\_Valence, critical\_temp

- **wtd\_gmean\_atomic\_radius** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **wtd\_gmean\_atomic\_radius** has negative correlation with number\_of\_elements, wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_range\_ElectronAffinity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence
- **wtd\_gmean\_atomic\_radius** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, entropy\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **entropy\_atomic\_radius** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **entropy\_atomic\_radius** has negative correlation with gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **entropy\_atomic\_radius** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_entropy\_atomic\_radius** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **wtd\_entropy\_atomic\_radius** has negative correlation with wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity,

- wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
- **wtd\_entropy\_atomic\_radius** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **range\_atomic\_radius** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **range\_atomic\_radius** has negative correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **range\_atomic\_radius** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_range\_atomic\_radius** has positive correlation with wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_gmean\_Density, wtd\_range\_Density, wtd\_range\_Valence
  - **wtd\_range\_atomic\_radius** has negative correlation with wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_entropy\_Valence
  - **wtd\_range\_atomic\_radius** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **std\_atomic\_radius** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius,

- wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity,  
wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity,  
entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **std\_atomic\_radius** has negative correlation with wtd\_mean\_atomic\_mass, gmean\_atomic\_mass,  
wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density,  
wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_ThermalConductivity, mean\_Valence,  
wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
  - **std\_atomic\_radius** has no correlation with mean\_atomic\_mass, wtd\_range\_atomic\_mass,  
mean\_fie, gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius,  
wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density,  
std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity,  
std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat,  
gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_std\_atomic\_radius** has positive correlation with number\_of\_elements, entropy\_atomic\_mass,  
wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass,  
wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, en-  
tropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
entropy\_Density, entropy\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat,  
wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity,  
entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **wtd\_std\_atomic\_radius** has negative correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass,  
wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density,  
wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat,  
gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_std\_atomic\_radius** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass,  
wtd\_range\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, mean\_atomic\_radius,  
gmean\_atomic\_radius, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density,  
wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity,  
std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
range\_Valence, std\_Valence, wtd\_std\_Valence
  - **mean\_Density** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius,  
gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density,  
wtd\_gmean\_Density, wtd\_range\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence,  
wtd\_gmean\_Valence
  - **mean\_Density** has negative correlation with range\_fie, std\_fie, wtd\_std\_fie, range\_atomic\_radius,  
std\_atomic\_radius, wtd\_std\_atomic\_radius
  - **mean\_Density** has no correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie,  
gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius,  
entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density,  
wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity,  
wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity,  
wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity,  
wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat,  
wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat,

wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

- **wtd\_mean\_Density** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **wtd\_mean\_Density** has negative correlation with number\_of\_elements, wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, range\_ThermalConductivity, std\_ThermalConductivity, entropy\_Valence
- **wtd\_mean\_Density** has no correlation with entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, wtd\_std\_ThermalConductivity, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **gmean\_Density** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
- **gmean\_Density** has negative correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **gmean\_Density** has no correlation with range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_gmean\_Density** has positive correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_range\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence

- **wtd\_gmean\_Density** has negative correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **wtd\_gmean\_Density** has no correlation with std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
- **entropy\_Density** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
- **entropy\_Density** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_entropy\_Density** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
- **wtd\_entropy\_Density** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence,

- range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **range\_Density** has positive correlation with range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, std\_Density, wtd\_std\_Density
  - **range\_Density** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, wtd\_range\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **wtd\_range\_Density** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_mean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_range\_Density** has no correlation with number\_of\_elements, mean\_atomic\_mass, gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **std\_Density** has positive correlation with range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, range\_Density, wtd\_std\_Density
  - **std\_Density** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, wtd\_range\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat

- entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
 std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
 gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence,  
 wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_std\_Density** has positive correlation with range\_atomic\_mass, std\_atomic\_mass,  
 wtd\_std\_atomic\_mass, range\_Density, std\_Density
  - **wtd\_std\_Density** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
 gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass,  
 wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie,  
 wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius,  
 wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density,  
 entropy\_Density, wtd\_entropy\_Density, wtd\_range\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity,  
 gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity,  
 range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity,  
 mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat,  
 entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
 std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
 gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence,  
 wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **mean\_ElectronAffinity** has positive correlation with wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity
  - **mean\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass,  
 wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,  
 wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie,  
 wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius,  
 wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density,  
 entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density,  
 wtd\_std\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence,  
 wtd\_std\_Valence, critical\_temp
  - **wtd\_mean\_ElectronAffinity** has positive correlation with wtd\_mean\_fie, wtd\_gmean\_fie,  
 mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity
  - **wtd\_mean\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass,  
 wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,  
 wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie,

- std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **gmean\_ElectronAffinity** has positive correlation with mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, mean\_Valence, wtd\_mean\_Valence
  - **gmean\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
  - **wtd\_gmean\_ElectronAffinity** has positive correlation with mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity
  - **wtd\_gmean\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

critical\_temp

- **entropy\_ElectronAffinity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, wtd\_entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
- **entropy\_ElectronAffinity** has negative correlation with gmean\_Density, wtd\_gmean\_Density, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **entropy\_ElectronAffinity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, mean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_entropy\_ElectronAffinity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, entropy\_Valence, wtd\_entropy\_Valence
- **wtd\_entropy\_ElectronAffinity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **range\_ElectronAffinity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, mean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_Valence, wtd\_entropy\_Valence
- **range\_ElectronAffinity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity,

- entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity ,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_range\_ElectronAffinity** has positive correlation with wtd\_mean\_fie, wtd\_gmean\_fie,  
 wtd\_range\_fie, wtd\_mean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity
  - **wtd\_range\_ElectronAffinity** has negative correlation with wtd\_mean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius
  - **wtd\_range\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass,  
 wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,  
 wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie,  
 wtd\_std\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius,  
 range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius,  
 mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density,  
 wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density,  
 mean\_ElectronAffinity, gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity,  
 range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence,  
 wtd\_std\_Valence, critical\_temp
  - **std\_ElectronAffinity** has positive correlation with mean\_fie, range\_fie, std\_fie, range\_ElectronAffinity,  
 wtd\_std\_ElectronAffinity
  - **std\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass,  
 wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,  
 wtd\_std\_atomic\_mass, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie,  
 wtd\_range\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius,  
 wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density,  
 wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity,  
 gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat,  
 wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat,  
 wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,  
 wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity,  
 entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity,  
 wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity,  
 mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence,  
 wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence,  
 critical\_temp
  - **wtd\_std\_ElectronAffinity** has positive correlation with wtd\_entropy\_atomic\_mass, entropy\_fie,  
 wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius,  
 wtd\_std\_atomic\_radius, range\_ElectronAffinity, std\_ElectronAffinity, entropy\_Valence, wtd\_entropy\_Valence

- **wtd\_std\_ElectronAffinity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **mean\_FusionHeat** has positive correlation with wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity
- **mean\_FusionHeat** has negative correlation with wtd\_std\_fie
- **mean\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_mean\_FusionHeat** has positive correlation with mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_mean\_Valence, wtd\_gmean\_Valence
- **wtd\_mean\_FusionHeat** has negative correlation with wtd\_std\_fie, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity
- **wtd\_mean\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity

- std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, mean\_Valence, gmean\_Valence,  
 entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence,  
 wtd\_std\_Valence, critical\_temp
- **gmean\_FusionHeat** has positive correlation with gmean\_Density, wtd\_gmean\_Density,  
 mean\_FusionHeat, wtd\_mean\_FusionHeat, wtd\_gmean\_FusionHeat, wtd\_range\_FusionHeat,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
 gmean\_Valence, wtd\_gmean\_Valence
  - **gmean\_FusionHeat** has negative correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_std\_atomic\_radius, range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence
  - **gmean\_FusionHeat** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
 gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass,  
 std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie,  
 wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density,  
 wtd\_mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density,  
 std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,  
 wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 wtd\_range\_ThermalConductivity, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence,  
 std\_Valence, wtd\_std\_Valence, critical\_temp
  - **wtd\_gmean\_FusionHeat** has positive correlation with gmean\_Density, wtd\_gmean\_Density,  
 mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence,  
 gmean\_Valence, wtd\_gmean\_Valence
  - **wtd\_gmean\_FusionHeat** has negative correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_entropy\_FusionHeat, range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
  - **wtd\_gmean\_FusionHeat** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass,  
 gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass,  
 std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie,  
 wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_gmean\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius,  
 mean\_Density, wtd\_mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density,  
 wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity,  
 gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity,  
 range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity,  
 entropy\_FusionHeat, range\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity,  
 wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence,  
 critical\_temp
  - **entropy\_FusionHeat** has positive correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, range\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie,  
 wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius,  
 wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity,  
 wtd\_entropy\_ElectronAffinity, wtd\_entropy\_FusionHeat, entropy\_ThermalConductivity, range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence,  
 critical\_temp

- **entropy\_FusionHeat** has negative correlation with wtd\_mean\_Valence, wtd\_gmean\_Valence
- **entropy\_FusionHeat** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, mean\_Valence, gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_entropy\_FusionHeat** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **wtd\_entropy\_FusionHeat** has negative correlation with gmean\_Density, wtd\_gmean\_Density, wtd\_gmean\_FusionHeat, wtd\_range\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
- **wtd\_entropy\_FusionHeat** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
- **range\_FusionHeat** has positive correlation with mean\_FusionHeat, wtd\_mean\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat
- **range\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence

- wtd\_std\_Valence, critical\_temp
- **wtd\_range\_FusionHeat** has positive correlation with mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat
- **wtd\_range\_FusionHeat** has negative correlation with wtd\_entropy\_FusionHeat
- **wtd\_range\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **std\_FusionHeat** has positive correlation with mean\_FusionHeat, wtd\_mean\_FusionHeat, wtd\_gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, wtd\_std\_FusionHeat
- **std\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_std\_FusionHeat** has positive correlation with mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat
- **wtd\_std\_FusionHeat** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,

wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

- **mean\_ThermalConductivity** has positive correlation with wtd\_mean\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity
- **mean\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_mean\_ThermalConductivity** has positive correlation with mean\_ThermalConductivity, wtd\_range\_ThermalConductivity, wtd\_std\_ThermalConductivity
- **wtd\_mean\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **gmean\_ThermalConductivity** has positive correlation with gmean\_Density, wtd\_gmean\_Density, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, wtd\_gmean\_ThermalConductivity

- **gmean\_ThermalConductivity** has negative correlation with wtd\_entropy\_atomic\_mass, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Valence, wtd\_entropy\_Valence
- **gmean\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **wtd\_gmean\_ThermalConductivity** has positive correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity
- **wtd\_gmean\_ThermalConductivity** has negative correlation with wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, range\_fie, std\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_std\_atomic\_radius
- **wtd\_gmean\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **entropy\_ThermalConductivity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, entropy\_fie, entropy\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_FusionHeat, wtd\_entropy\_ThermalConductivity
- **entropy\_ThermalConductivity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat,

wtd\_gmean\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp

- **wtd\_entropy\_ThermalConductivity** has positive correlation with entropy\_ThermalConductivity
- **wtd\_entropy\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **range\_ThermalConductivity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **range\_ThermalConductivity** has negative correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **range\_ThermalConductivity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_range\_ThermalConductivity** has positive correlation with mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity
- **wtd\_range\_ThermalConductivity** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass,

- wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie,  
 wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius,  
 wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius,  
 wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density,  
 entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density,  
 wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity,  
 wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat,  
 wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat,  
 wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence,  
 wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, range\_Valence, wtd\_range\_Valence,  
 std\_Valence, wtd\_std\_Valence, critical\_temp
- **std\_ThermalConductivity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **std\_ThermalConductivity** has negative correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
  - **std\_ThermalConductivity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_std\_ThermalConductivity** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **wtd\_std\_ThermalConductivity** has negative correlation with wtd\_gmean\_atomic\_radius, gmean\_Density, wtd\_gmean\_Density, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_std\_ThermalConductivity** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, wtd\_mean\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat

- std\_FusionHeat, wtd\_std\_FusionHeat, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity,  
 entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_Valence, std\_Valence,  
 wtd\_std\_Valence
- **mean\_Valence** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass,  
 wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, gmean\_ElectronAffinity, gmean\_FusionHeat, wtd\_gmean\_FusionHeat,  
 wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **mean\_Valence** has negative correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, en-  
 tropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity,  
 wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **mean\_Valence** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass, range\_atomic\_mass,  
 wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie,  
 wtd\_gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius,  
 wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density,  
 std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity,  
 entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity,  
 std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, en-  
 tropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat,  
 mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity,  
 wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity,  
 wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **wtd\_mean\_Valence** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass,  
 wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density,  
 gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, gmean\_ElectronAffinity, wtd\_mean\_FusionHeat,  
 gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence,  
 wtd\_range\_Valence
  - **wtd\_mean\_Valence** has negative correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, en-  
 tropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat,  
 range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, en-  
 tropy\_Valence, wtd\_entropy\_Valence, critical\_temp
  - **wtd\_mean\_Valence** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass,  
 range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass,  
 mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius,  
 gmean\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density,  
 range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity,  
 wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity,  
 std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat,  
 std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity,  
 gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity,  
 wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence,  
 wtd\_std\_Valence
  - **gmean\_Valence** has positive correlation with wtd\_mean\_atomic\_mass, gmean\_atomic\_mass,  
 wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density,  
 wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat,  
 mean\_Valence, wtd\_mean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **gmean\_Valence** has negative correlation with number\_of\_elements, entropy\_atomic\_mass,  
 wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, en-  
 tropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius,  
 wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, wtd\_entropy\_FusionHeat, range\_ThermalConductivity,  
 std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence,

critical\_temp

- **gmean\_Valence** has no correlation with mean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_gmean\_Valence** has positive correlation with wtd\_mean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_mean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_range\_Valence
- **wtd\_gmean\_Valence** has negative correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, wtd\_mean\_fie, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence, critical\_temp
- **wtd\_gmean\_Valence** has no correlation with mean\_atomic\_mass, gmean\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_entropy\_fie, wtd\_range\_fie, mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
- **entropy\_Valence** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, wtd\_entropy\_Valence, critical\_temp
- **entropy\_Valence** has negative correlation with wtd\_gmean\_atomic\_radius, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
- **entropy\_Valence** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_range\_atomic\_radius, mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, wtd\_range\_Valence, std\_Valence, wtd\_std\_Valence
- **wtd\_entropy\_Valence** has positive correlation with number\_of\_elements, entropy\_atomic\_mass,

- wtd\_entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, entropy\_fie, wtd\_entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_Density, wtd\_entropy\_Density, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_std\_ElectronAffinity, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, critical\_temp
- **wtd\_entropy\_Valence** has negative correlation with wtd\_range\_atomic\_radius, gmean\_Density, wtd\_gmean\_Density, wtd\_gmean\_FusionHeat, gmean\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, wtd\_range\_Valence
  - **wtd\_entropy\_Valence** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, wtd\_range\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, wtd\_range\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, mean\_Density, wtd\_mean\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_range\_ThermalConductivity, range\_Valence, std\_Valence, wtd\_std\_Valence
  - **range\_Valence** has positive correlation with std\_Valence, wtd\_std\_Valence
  - **range\_Valence** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, wtd\_range\_Valence, critical\_temp
  - **wtd\_range\_Valence** has positive correlation with wtd\_range\_atomic\_mass, wtd\_range\_atomic\_radius, gmean\_Density, wtd\_gmean\_Density, wtd\_range\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
  - **wtd\_range\_Valence** has negative correlation with wtd\_entropy\_atomic\_mass, range\_fie, wtd\_std\_fie, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_std\_atomic\_radius, wtd\_entropy\_FusionHeat, wtd\_std\_ThermalConductivity, wtd\_entropy\_Valence
  - **wtd\_range\_Valence** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, wtd\_range\_fie, std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity,

- mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, entropy\_Valence, range\_Valence, std\_Valence, wtd\_std\_Valence, critical\_temp
- **std\_Valence** has positive correlation with range\_Valence, wtd\_std\_Valence
  - **std\_Valence** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, wtd\_range\_Valence, critical\_temp
  - **wtd\_std\_Valence** has positive correlation with range\_Valence, std\_Valence
  - **wtd\_std\_Valence** has no correlation with number\_of\_elements, mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass, wtd\_gmean\_atomic\_mass, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, range\_atomic\_mass, wtd\_range\_atomic\_mass, std\_atomic\_mass, wtd\_std\_atomic\_mass, mean\_fie, wtd\_mean\_fie, gmean\_fie, wtd\_gmean\_fie, entropy\_fie, wtd\_entropy\_fie, range\_fie, wtd\_range\_fie, std\_fie, wtd\_std\_fie, mean\_atomic\_radius, wtd\_mean\_atomic\_radius, gmean\_atomic\_radius, wtd\_gmean\_atomic\_radius, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, wtd\_range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, mean\_Density, wtd\_mean\_Density, gmean\_Density, wtd\_gmean\_Density, entropy\_Density, wtd\_entropy\_Density, range\_Density, wtd\_range\_Density, std\_Density, wtd\_std\_Density, mean\_ElectronAffinity, wtd\_mean\_ElectronAffinity, gmean\_ElectronAffinity, wtd\_gmean\_ElectronAffinity, entropy\_ElectronAffinity, wtd\_entropy\_ElectronAffinity, range\_ElectronAffinity, wtd\_range\_ElectronAffinity, std\_ElectronAffinity, wtd\_std\_ElectronAffinity, mean\_FusionHeat, wtd\_mean\_FusionHeat, gmean\_FusionHeat, wtd\_gmean\_FusionHeat, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_FusionHeat, wtd\_range\_FusionHeat, std\_FusionHeat, wtd\_std\_FusionHeat, mean\_ThermalConductivity, wtd\_mean\_ThermalConductivity, gmean\_ThermalConductivity, wtd\_gmean\_ThermalConductivity, entropy\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, range\_ThermalConductivity, wtd\_range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence, entropy\_Valence, wtd\_entropy\_Valence, wtd\_range\_Valence, critical\_temp
  - **critical\_temp** has positive correlation with number\_of\_elements, entropy\_atomic\_mass, wtd\_entropy\_atomic\_mass, entropy\_fie, range\_fie, std\_fie, wtd\_std\_fie, entropy\_atomic\_radius, wtd\_entropy\_atomic\_radius, range\_atomic\_radius, std\_atomic\_radius, wtd\_std\_atomic\_radius, entropy\_FusionHeat, wtd\_entropy\_FusionHeat, range\_ThermalConductivity, std\_ThermalConductivity, wtd\_std\_ThermalConductivity, entropy\_Valence, wtd\_entropy\_Valence
  - **critical\_temp** has negative correlation with gmean\_Density, wtd\_gmean\_Density, mean\_Valence, wtd\_mean\_Valence, gmean\_Valence, wtd\_gmean\_Valence
  - **critical\_temp** has no correlation with mean\_atomic\_mass, wtd\_mean\_atomic\_mass, gmean\_atomic\_mass,

```
wtd_gmean_atomic_mass, range_atomic_mass, wtd_range_atomic_mass, std_atomic_mass,
wtd_std_atomic_mass, mean_fie, wtd_mean_fie, gmean_fie, wtd_gmean_fie, wtd_entropy_fie,
wtd_range_fie, mean_atomic_radius, wtd_mean_atomic_radius, gmean_atomic_radius,
wtd_gmean_atomic_radius, wtd_range_atomic_radius, mean_Density, wtd_mean_Density,
entropy_Density, wtd_entropy_Density, range_Density, wtd_range_Density, std_Density,
wtd_std_Density, mean_ElectronAffinity, wtd_mean_ElectronAffinity, gmean_ElectronAffinity,
wtd_gmean_ElectronAffinity, entropy_ElectronAffinity, wtd_entropy_ElectronAffinity, range_ElectronAffinity,
wtd_range_ElectronAffinity, std_ElectronAffinity, wtd_std_ElectronAffinity, mean_FusionHeat,
wtd_mean_FusionHeat, gmean_FusionHeat, wtd_gmean_FusionHeat, range_FusionHeat,
wtd_range_FusionHeat, std_FusionHeat, wtd_std_FusionHeat, mean_ThermalConductivity,
wtd_mean_ThermalConductivity, gmean_ThermalConductivity, wtd_gmean_ThermalConductivity,
entropy_ThermalConductivity, wtd_entropy_ThermalConductivity, wtd_range_ThermalConductivity,
range_Valence, wtd_range_Valence, std_Valence, wtd_std_Valence
```

However, based on the 0.001 significant level, we can see that some features has been crossed out, we will exclude these columns in one of the model development scenarios, therefore, for now we will store it in a list.

```
# Store the less correlated features
less_correlated <- c("gmean_fie", "mean_atomic_radius", "mean_ElectronAffinity",
                     "wtd_gmean_ElectronAffinity", "range_FusionHeat", "std_FusionHeat",
                     "wtd_std_FusionHeat", "wtd_entropy_ThermalConductivity",
                     "range_Valence", "std_Valence", "wtd_std_Valence")
```

Next, we will plot the distribution of critical temperature based on the number of elements of the materials.

### Number of Elements

```
# Visualize the Distribution of Critical Temperature on Number of Elements
ggplot(aes(x=critical_temp), data =train.data) +
  geom_density(aes(fill = number_of_elements)) +
  facet_wrap(~number_of_elements)
```

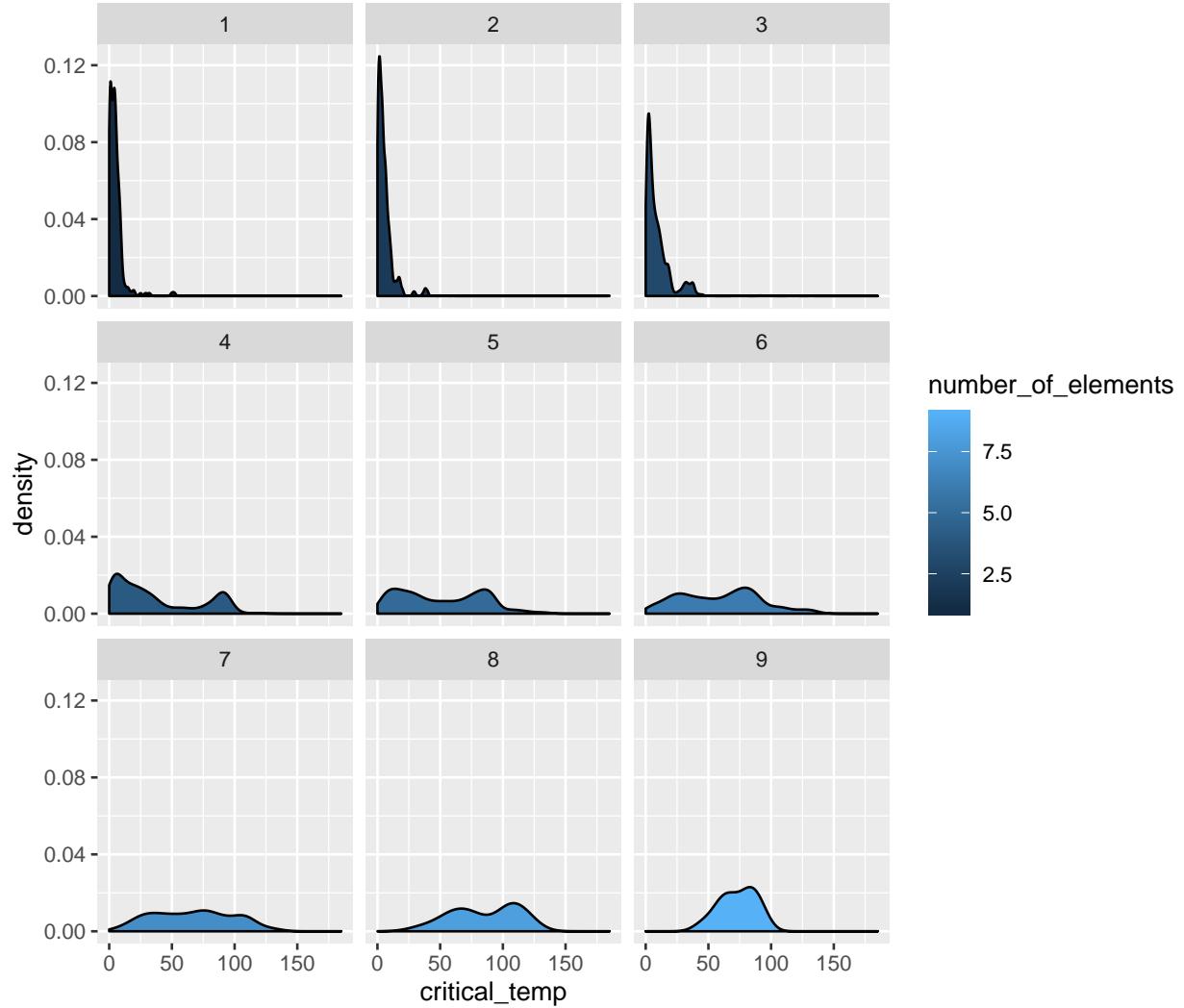


Figure 12: Critical Temperature Distribution on Number of Elements

From Figure 12 we can see that the different number of elements have different distribution of critical temperature. Materials with less than equal to three elements have a Right Skewed distribution of critical temperature, whereas materials with 4,5,6, and 8 elements have bimodal distribution. Meanwhile, the rests tend to have normal distribution.

#### Atomic Mass, First Ionization Energy, Atomic Radius, Density, Electron Affinity, Fusion Heat, Thermal Conductivity, and Valence

```
# Visualise the atomic mass on critical temperature
for (item in data_index[2:9]){
  print(train.data[,append(item,82)] %>%
    gather(-critical_temp, key = "var", value = "value") %>%
    ggplot(aes(x = critical_temp, y = value)) +
    geom_point(shape=18, color="#56B4E9") +
    facet_wrap(~ var, scales = "free", ncol = 3) +
    geom_smooth(method=lm, se=FALSE, color="red"))
  cat('\n\n')
}
```

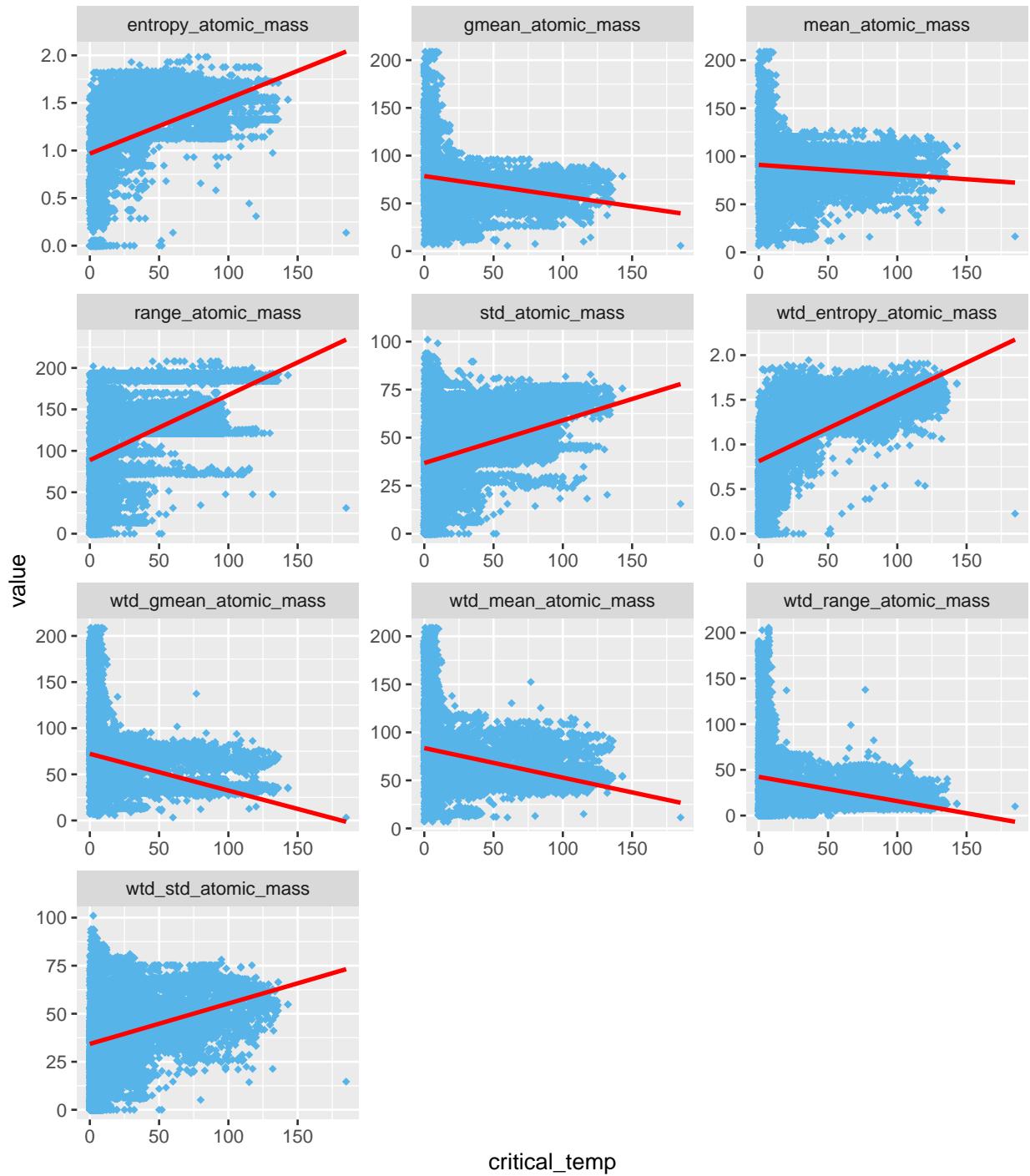


Figure 13: Atomic Mass Property on Critical Temperature

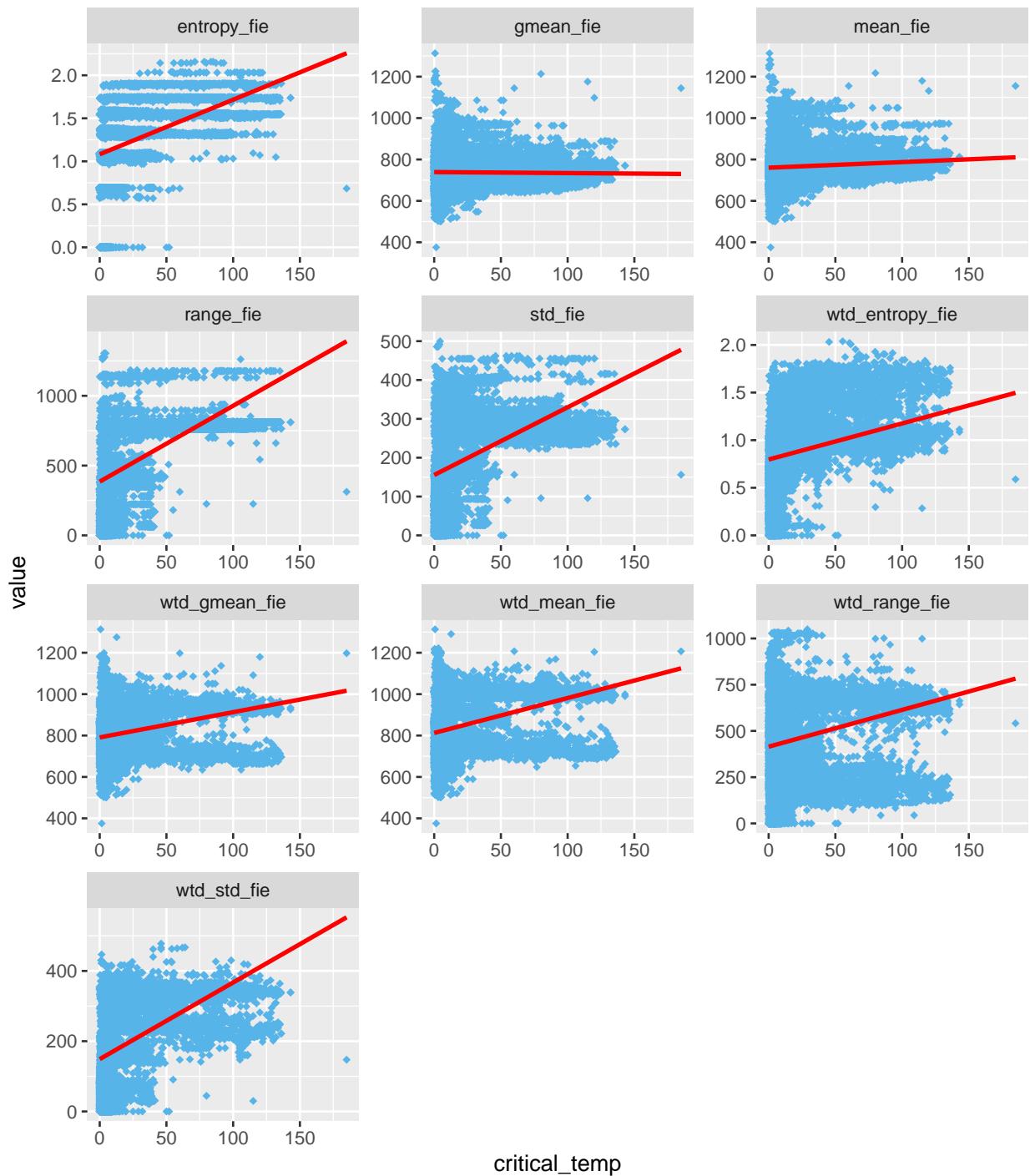


Figure 14: First Ionization Energy Property on Critical Temperature

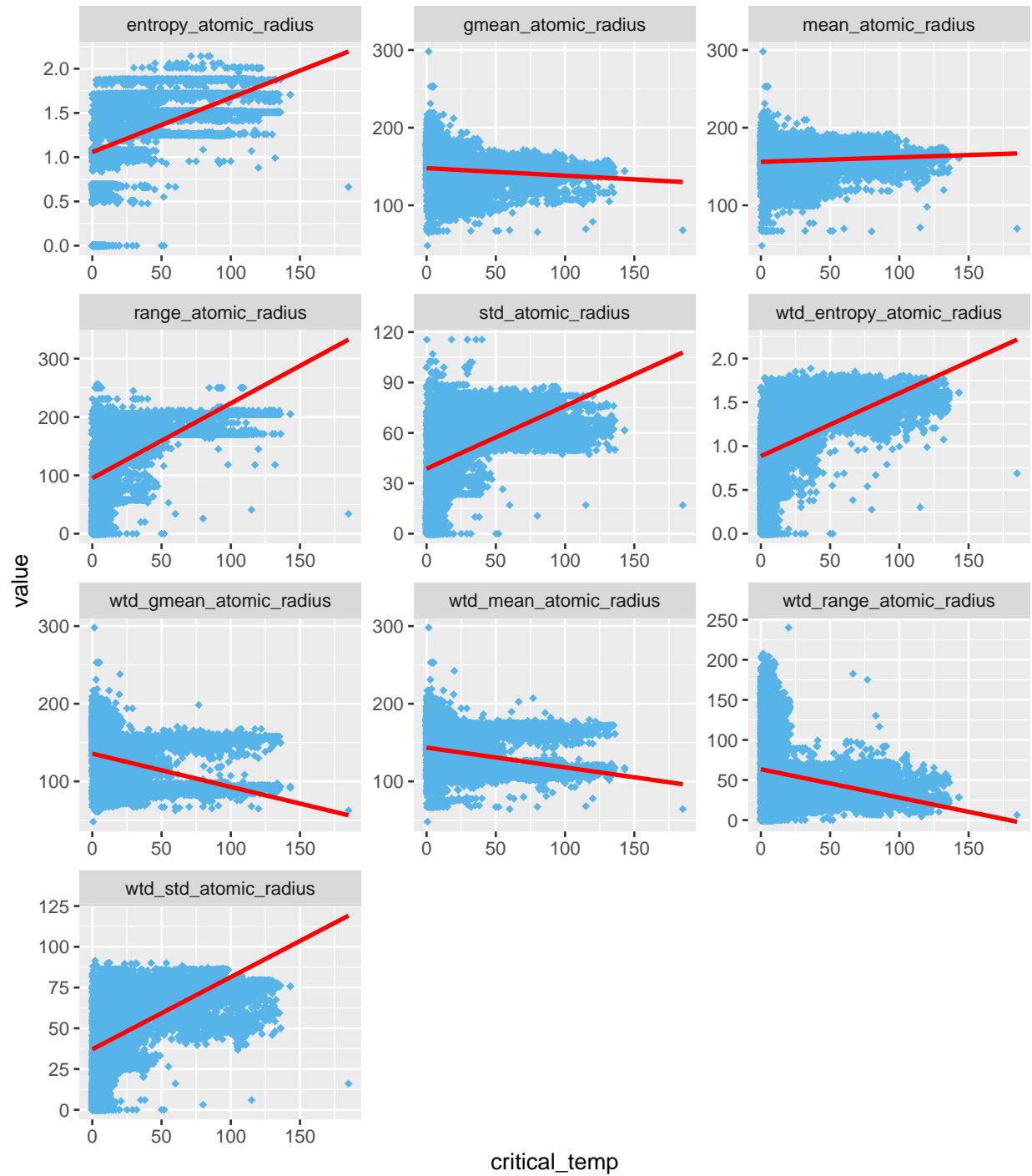


Figure 15: Atomic Radius Property on Critical Temperature

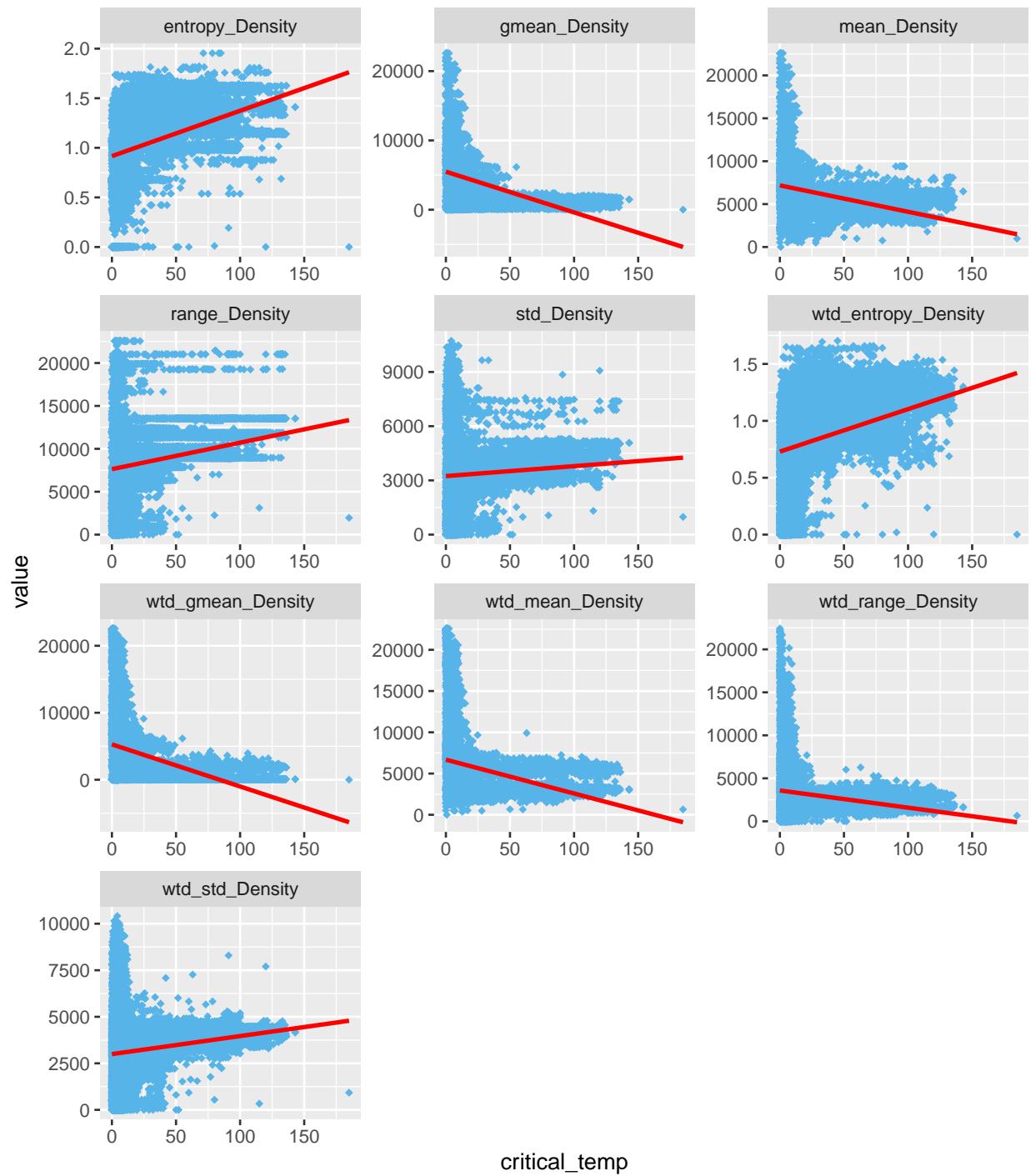


Figure 16: Density Property on Critical Temperature

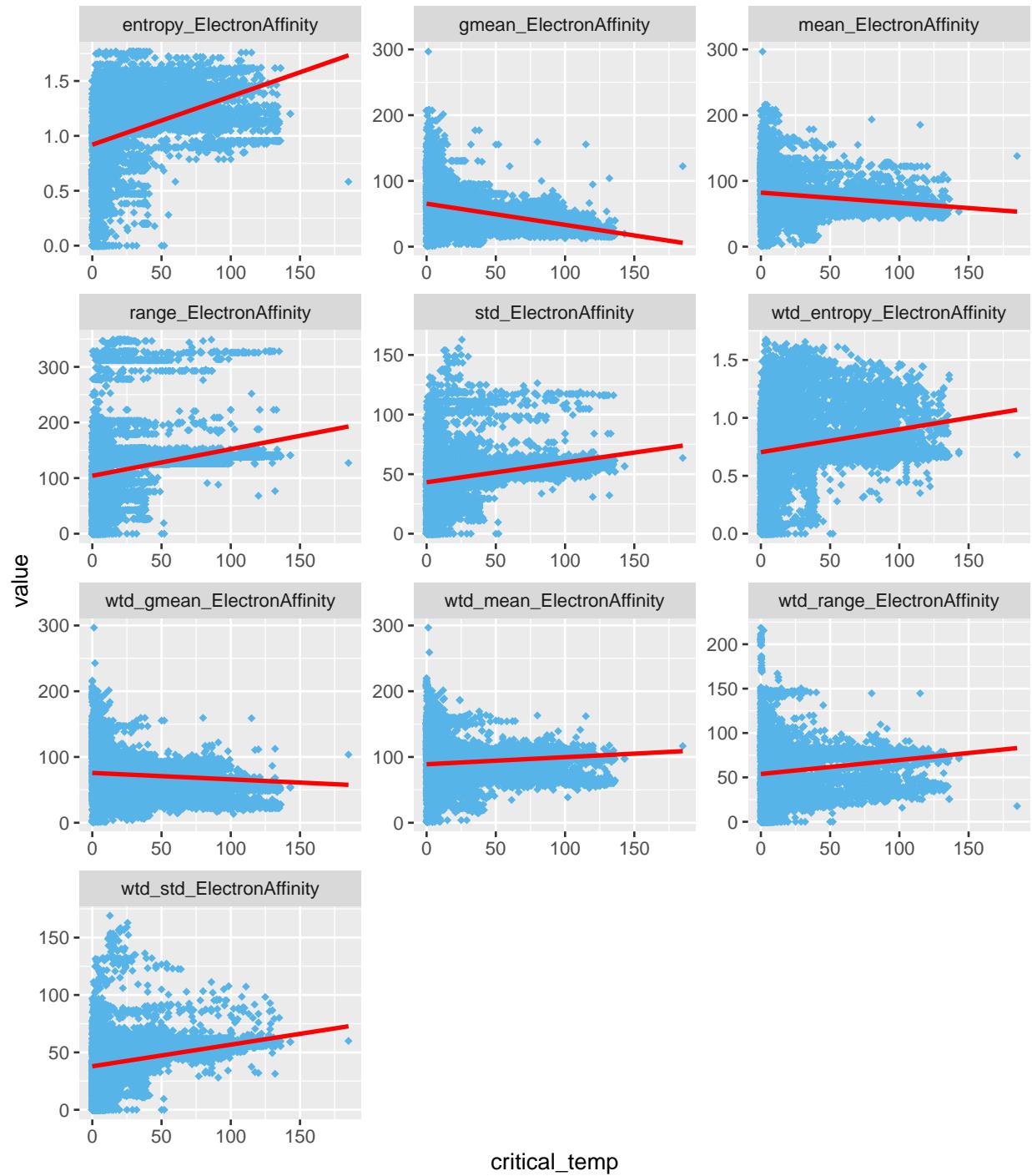


Figure 17: Electron Affinity Property on Critical Temperature

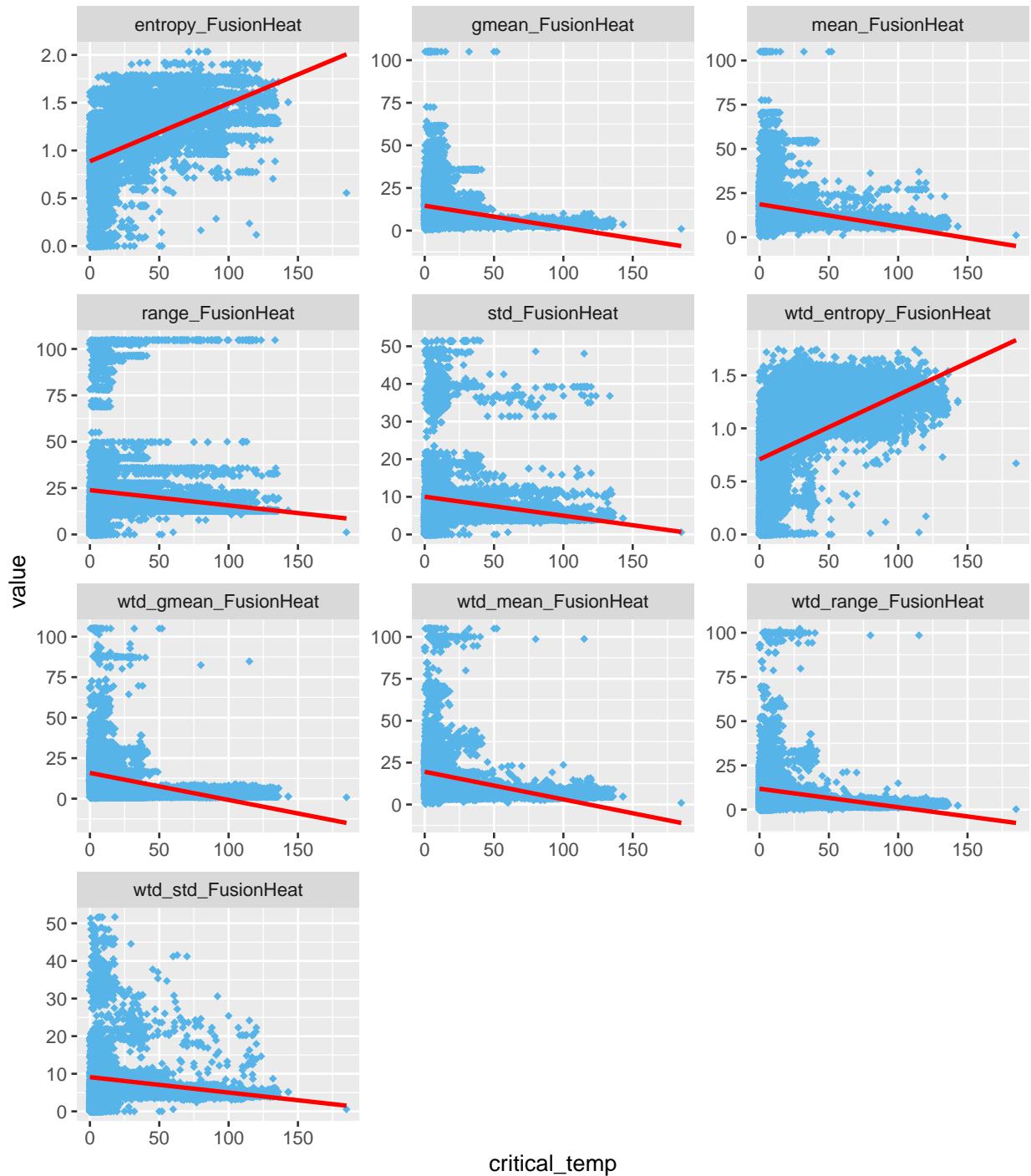


Figure 18: Fusion Heat Property on Critical Temperature

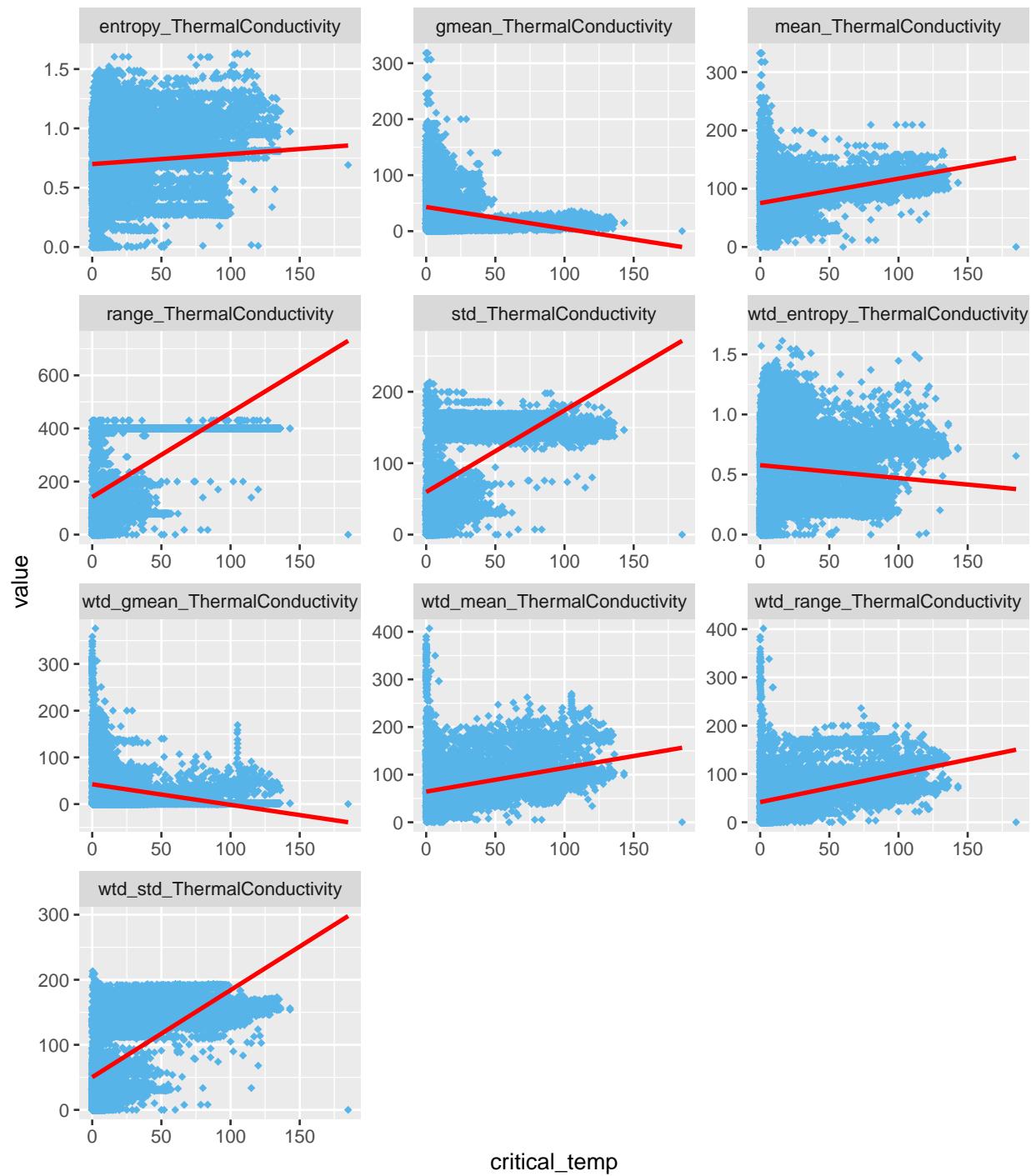


Figure 19: Thermal Conductivity Property on Critical Temperature

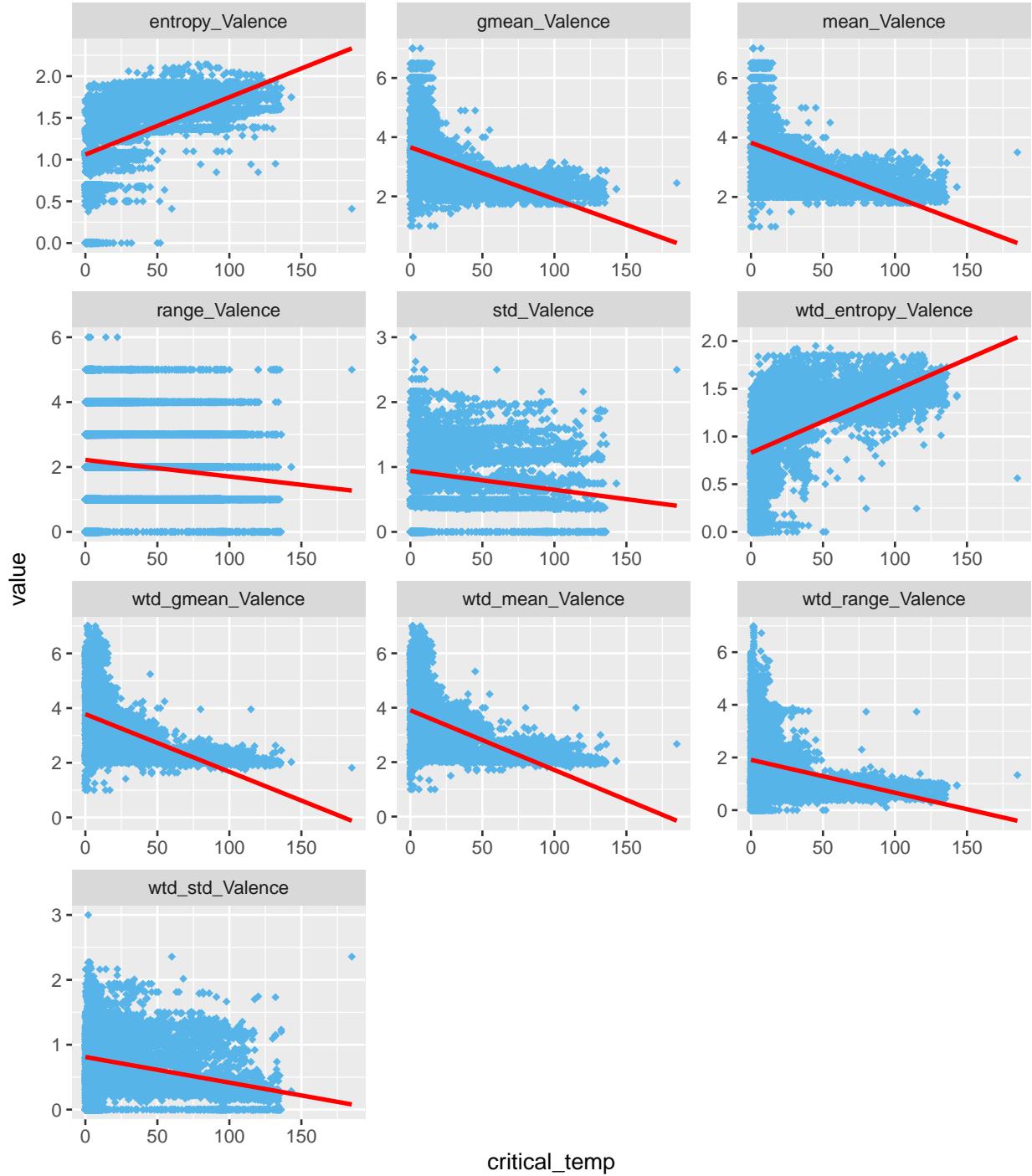


Figure 20: Valence Property on Critical Temperature

From the above figures, we can see that most of the trendlines are (almost) flat which means they have no correlation, and this supports the previous analysis of the correlation matrix. Some data transformation technique might change the correlation level. Therefore, the next step is data transformation.

## 2.3 Data Transformation

In this subsection, we will do data transformation. First, we will create a new dataframe to store the transformation results, so that in the future step we can compare the result between using original data and transformed data.

```
# Create a duplicate dataset
train.data.trans <- train.data
test.data.trans <- test.data
```

Number of Element

```
hist(train.data$number_of_elements, main = "", xlab = "")
```

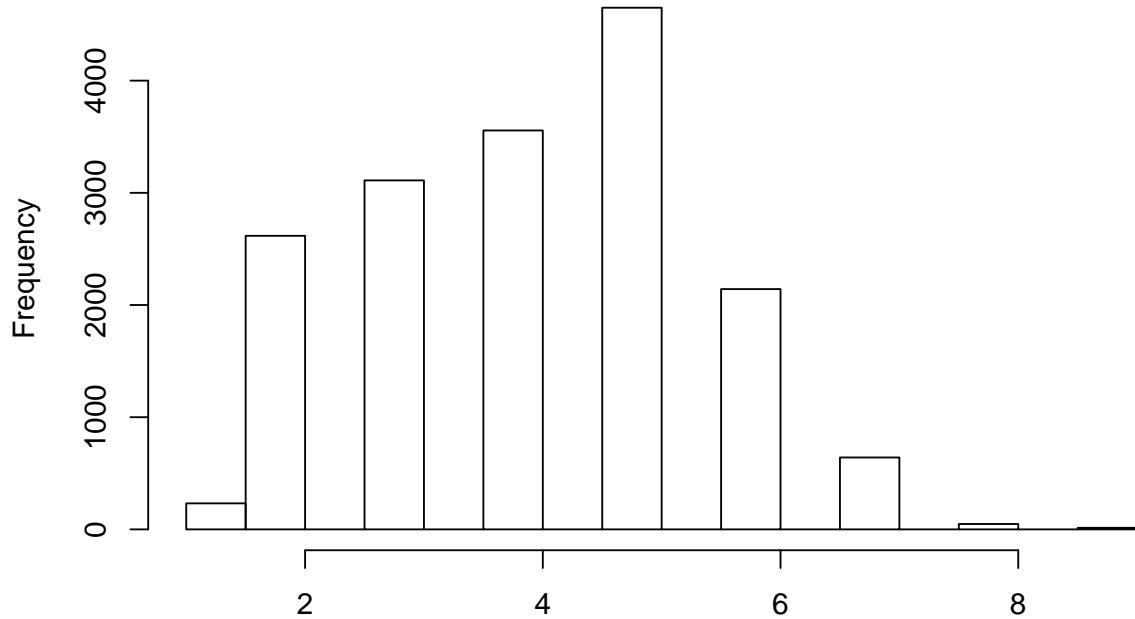


Figure 21: Number of Elements Histogram

We will not transform the number\_of\_elements variable, because it is a discrete variable.

**Atomic Mass, First Ionization Energy, Atomic Radius, Density, Electron Affinity, Fusion Heat, Thermal Conductivity, and Valence**

```
# Boxplot visualisation for the eight main properties
for(col in data_index[2:9]){
  par(mfrow = c(5,2))
```

```
for (each in col){  
  hist(train.data[,each], main = colnames(train.data)[each], xlab = "")  
}  
cat('\n\n')  
}
```

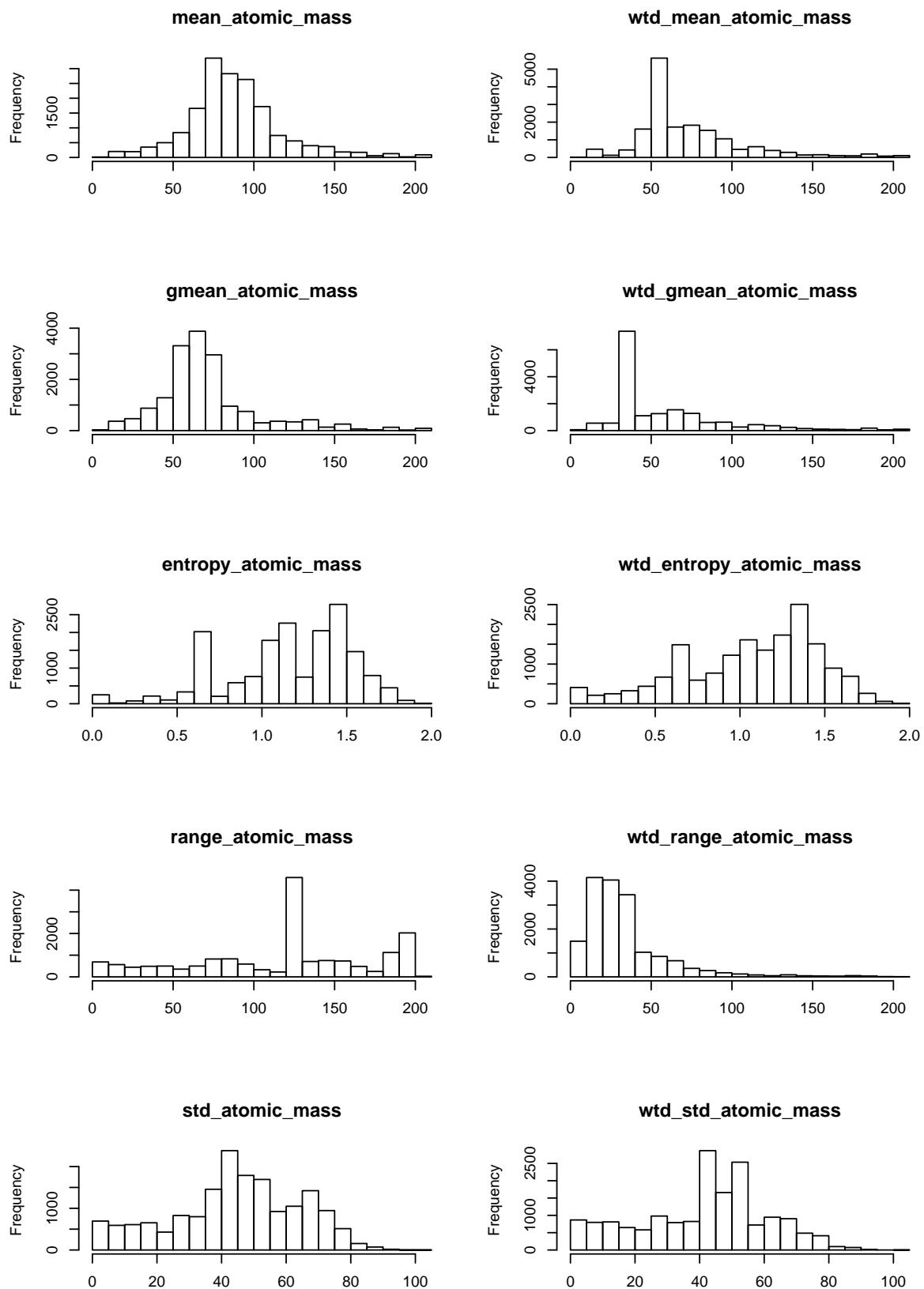


Figure 22: Atomic Mass Histogram

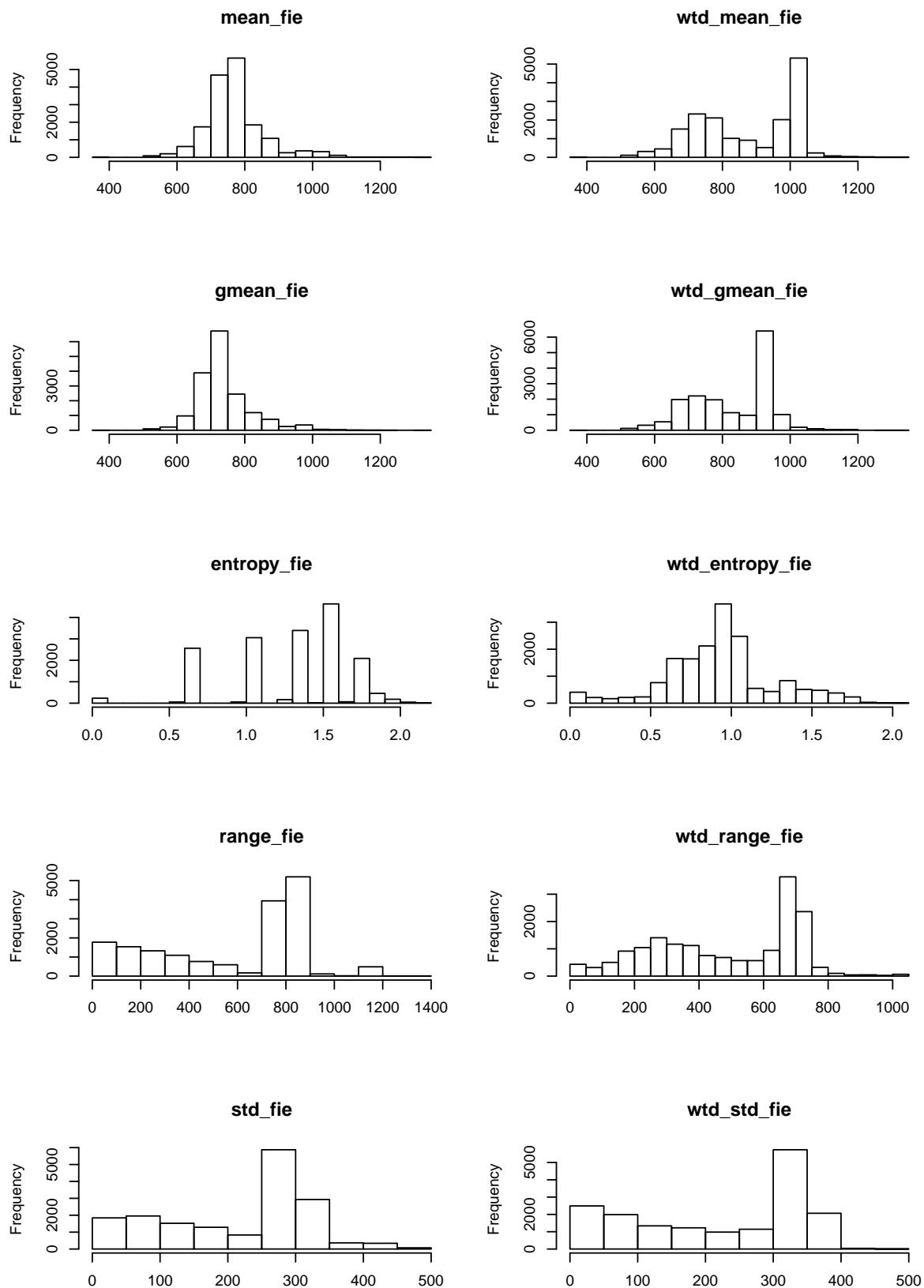


Figure 23: First Ionization Energy Histogram

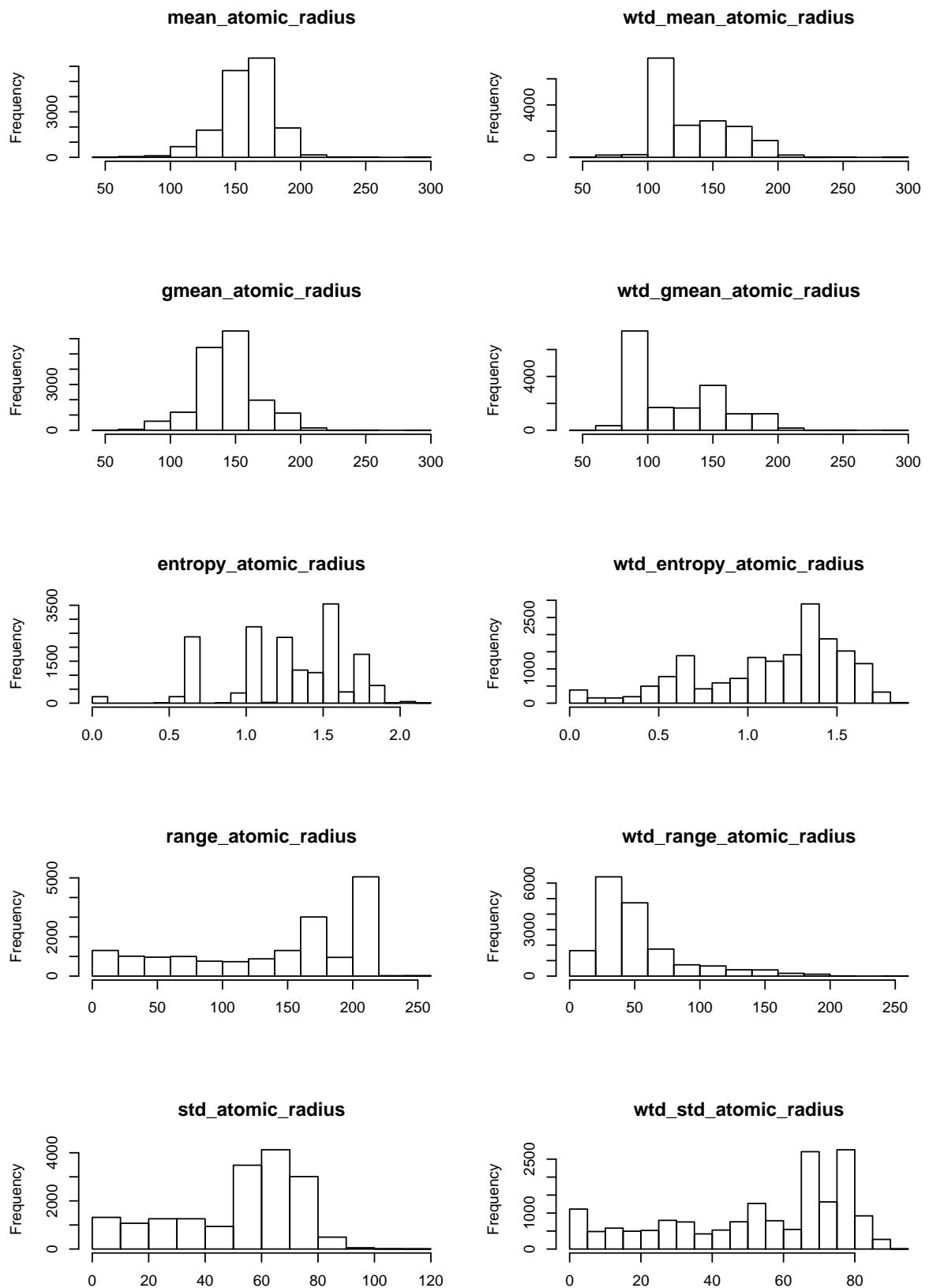


Figure 24: Atomic Radius Histogram

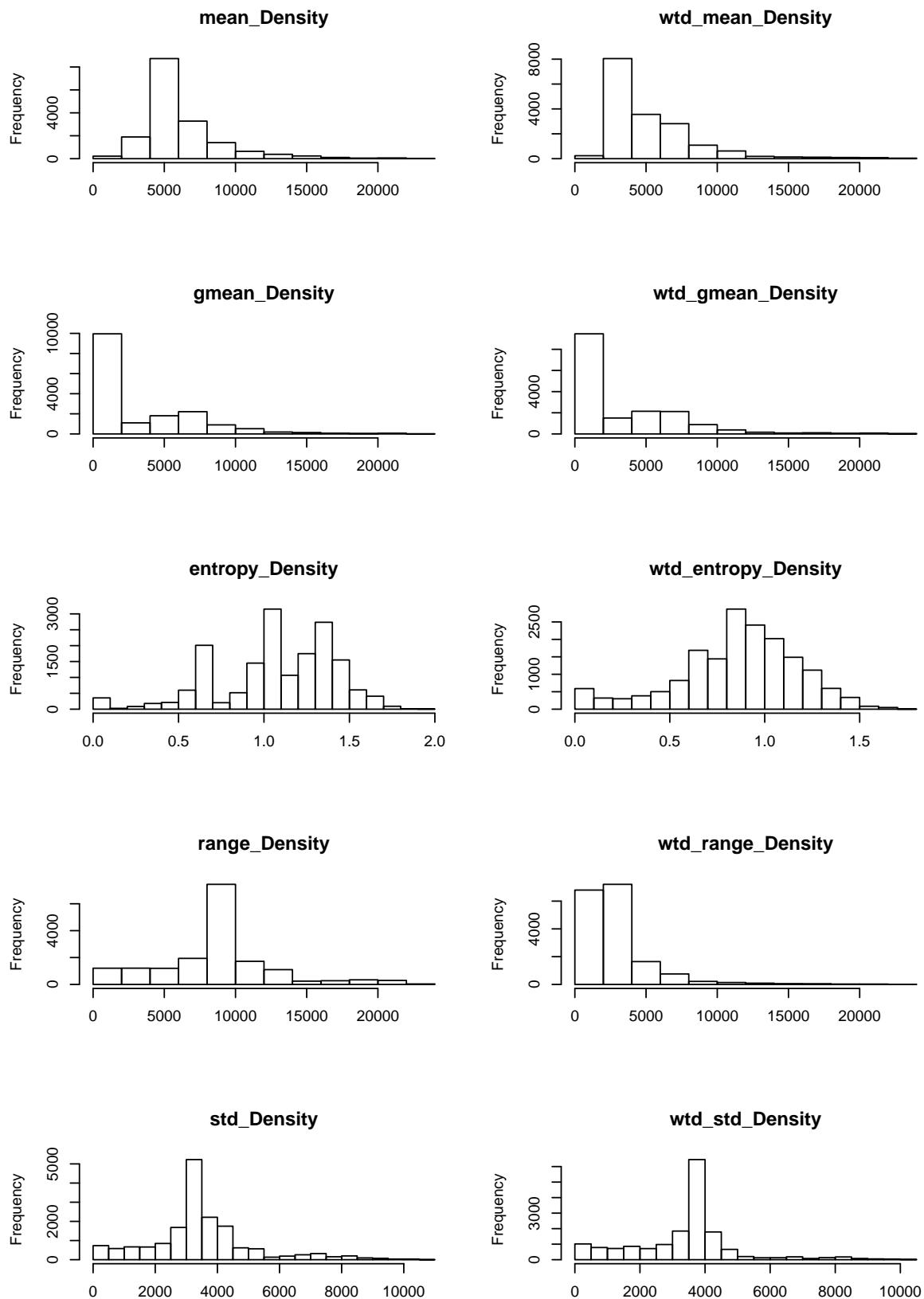


Figure 25: Density Histogram

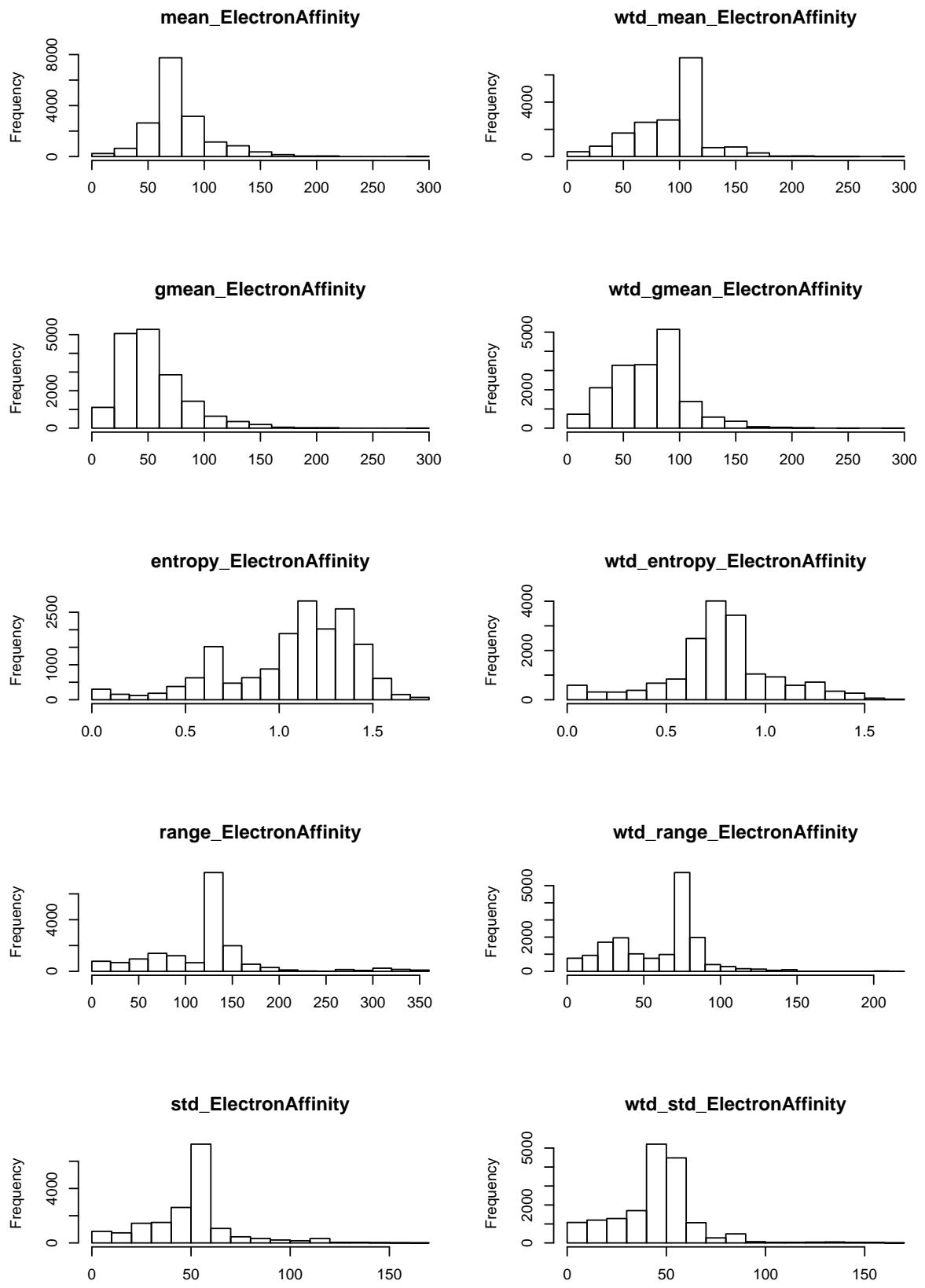


Figure 26: Electron Affinity Histogram

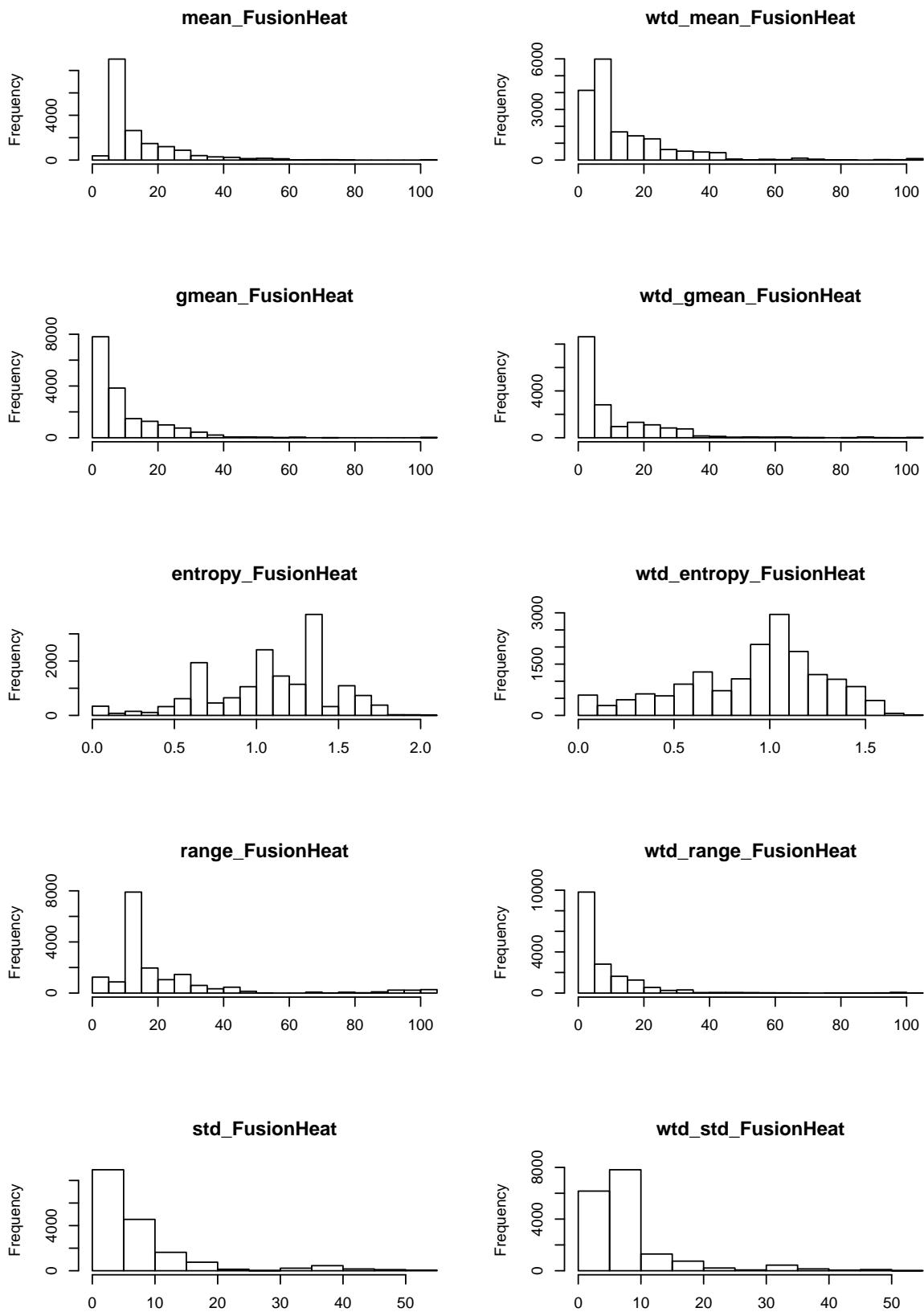


Figure 27: Fusion Heat Histogram

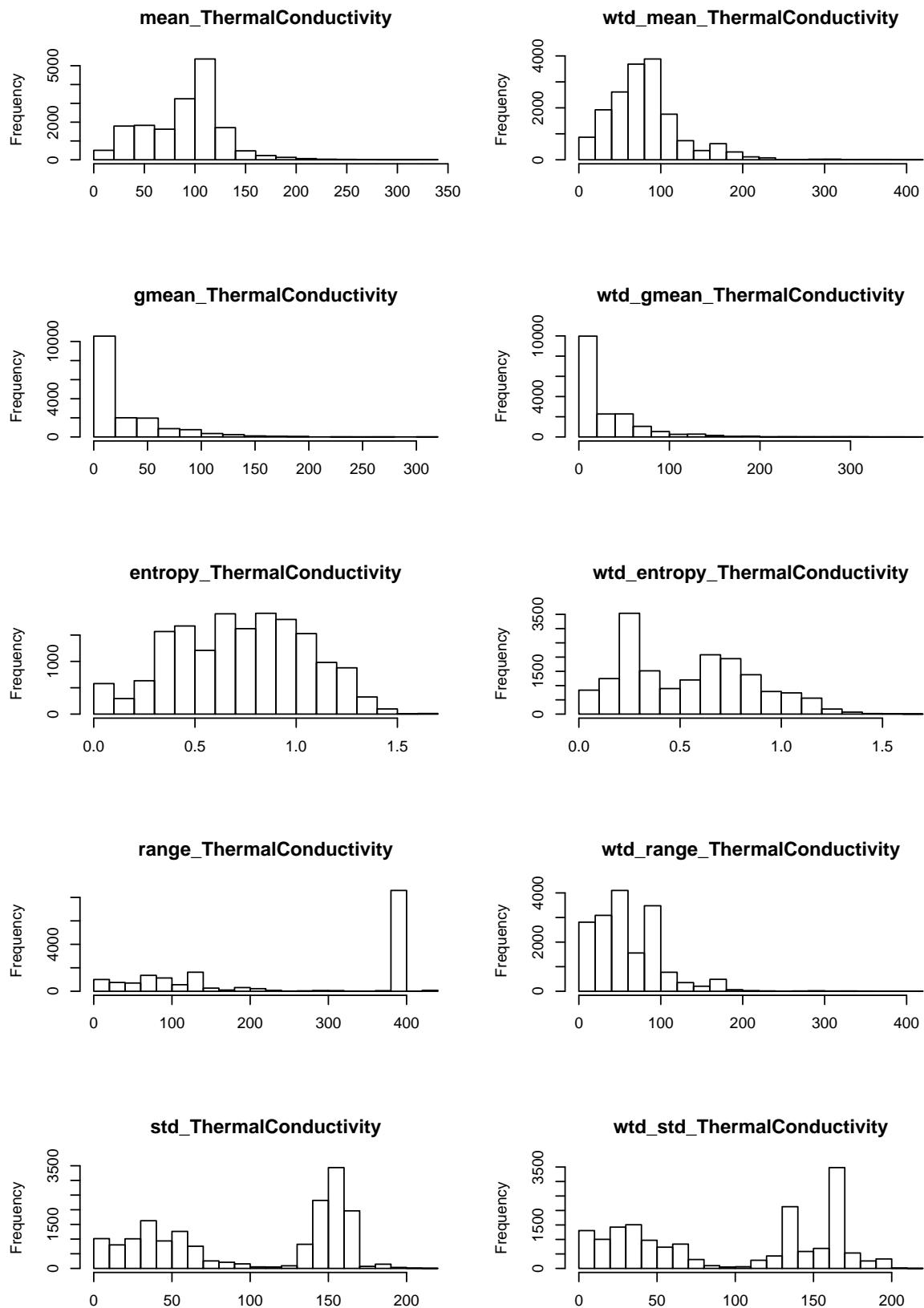


Figure 28: Thermal Conductivity Histogram  
89

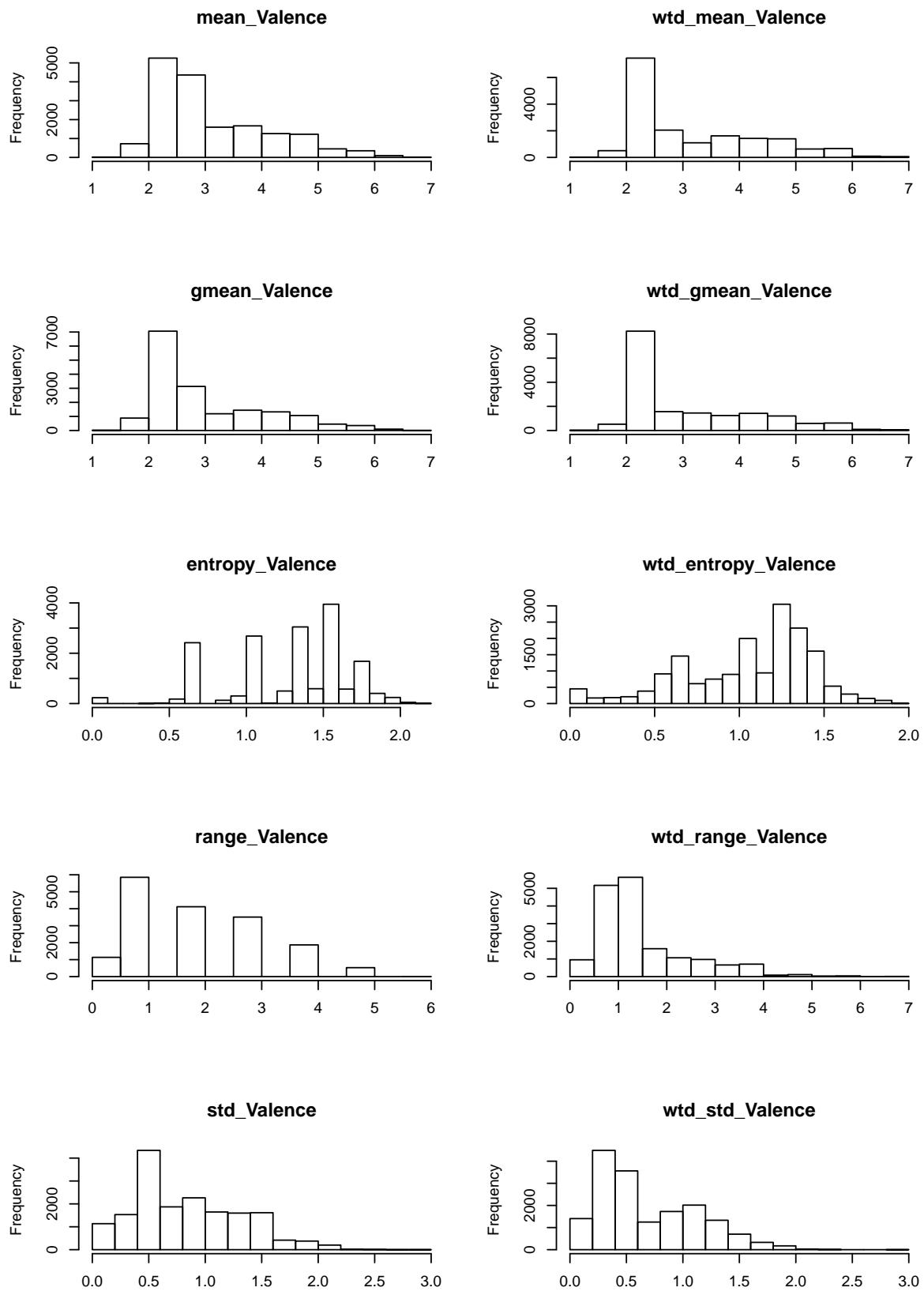


Figure 29: Valence Histogram

From the above figures, we can see that most of the variables have skewed distribution, therefore, we will apply the data transformation step to them, since the number of features is too many, therefore, we will use a function to perform a Box Cox Tranformation to the feature that has skewness greater than 0.75. Box Cox transformation is a way to transform non-normal dependent variables into a normal shape. More about Box Cox Tranformation at [Box](#)

```
# Skewness Calculation
skewed_feats <- sapply(names(train.data[,c(2:81)]), function(x) {
  skewness(train.data[[x]])
})

# Features skewness greater than the threshold (0.75)
skewed_feats <- skewed_feats[abs(skewed_feats) > 0.75]

## Transform skewed features with boxcox transformation
for (x in names(train.data[,c(2:81)])) {
  if(x %in% names(skewed_feats)){
    bc = BoxCoxTrans(train.data[[x]])
    train.data.trans[[x]] <- predict(bc, train.data[[x]])
    test.data.trans[[x]] <- predict(bc, test.data[[x]])
  }
}

# Boxplot visualisation for the eight main properties
for(col in data_index[2:9]){
  par(mfrow = c(5,2))
  for (each in col){
    hist(train.data.trans[,each], main = colnames(train.data.trans)[each], xlab = "")
  }
  cat('\n\n')
}
```

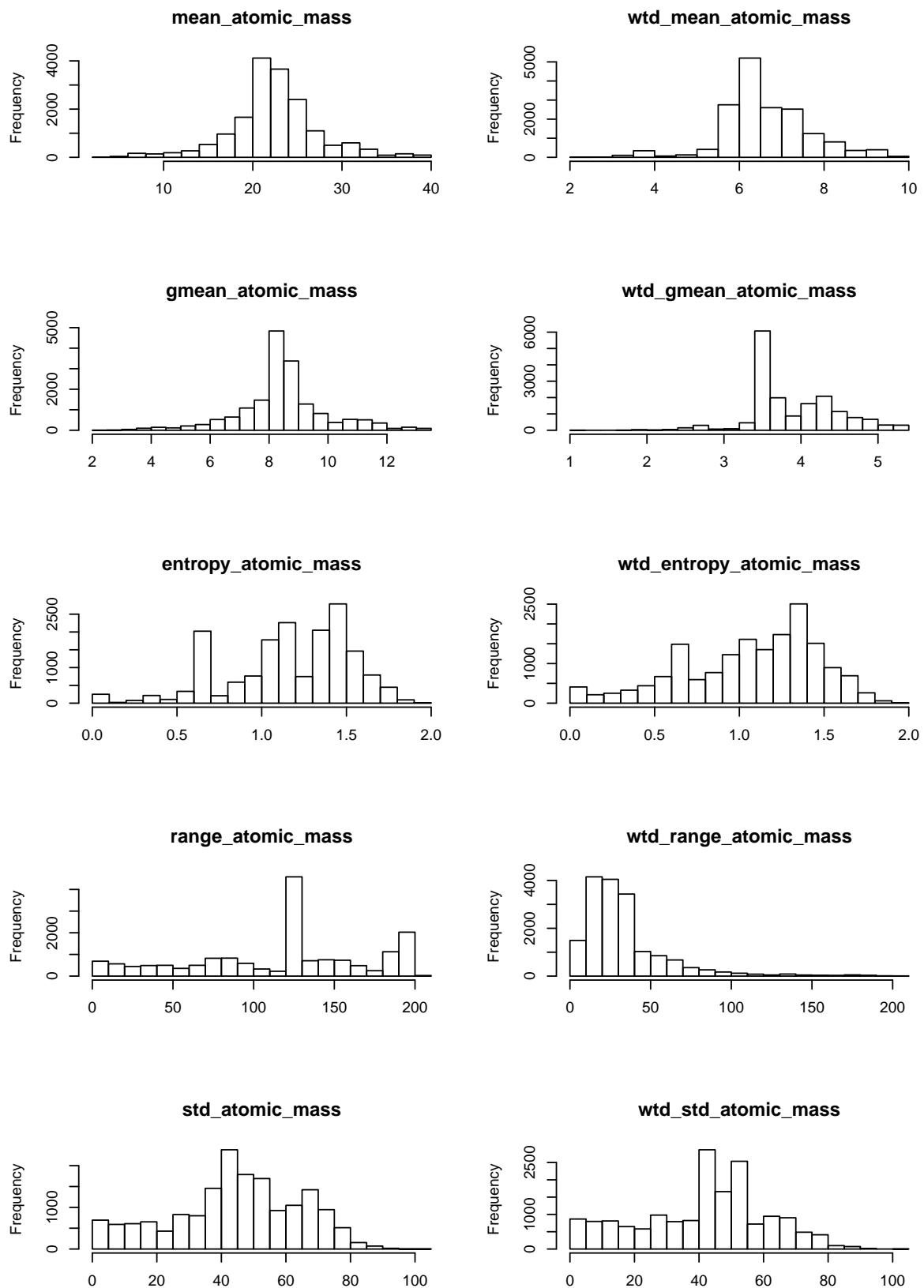


Figure 30: Atomic Mass Histogram After Transformation

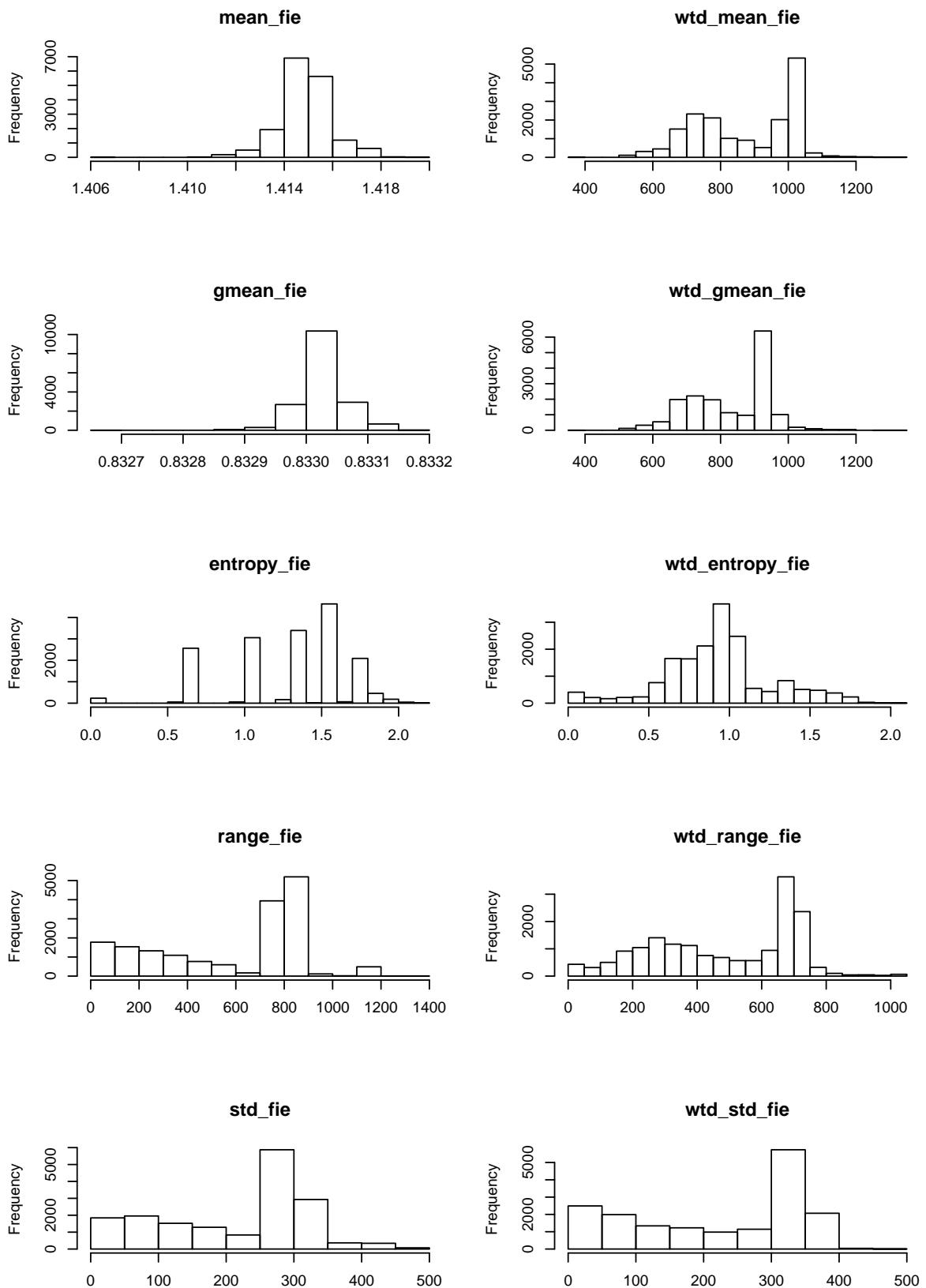


Figure 31: First Ionization Energy Histogram After Transformation

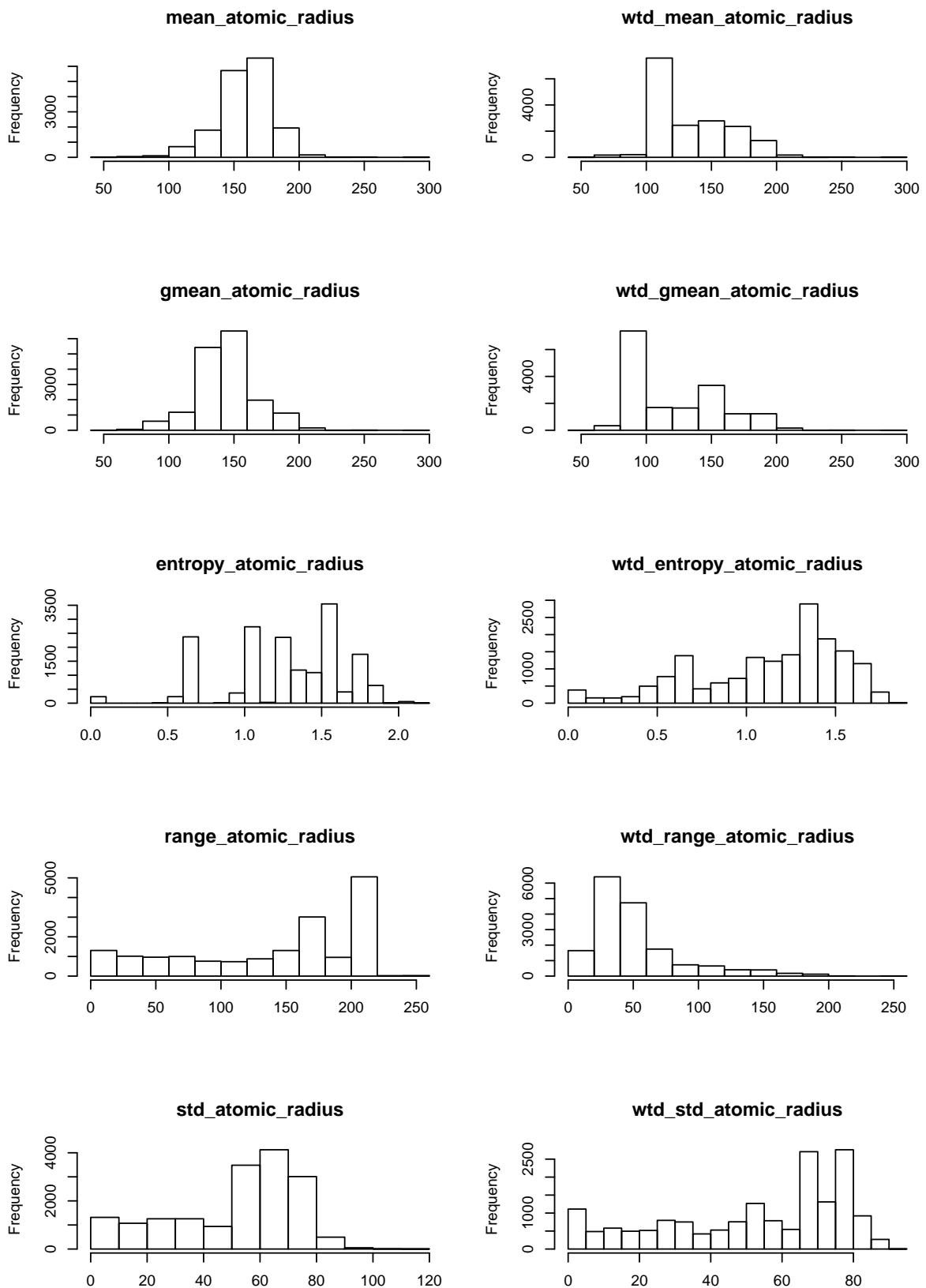


Figure 32: Atomic Radius Histogram After Transformation

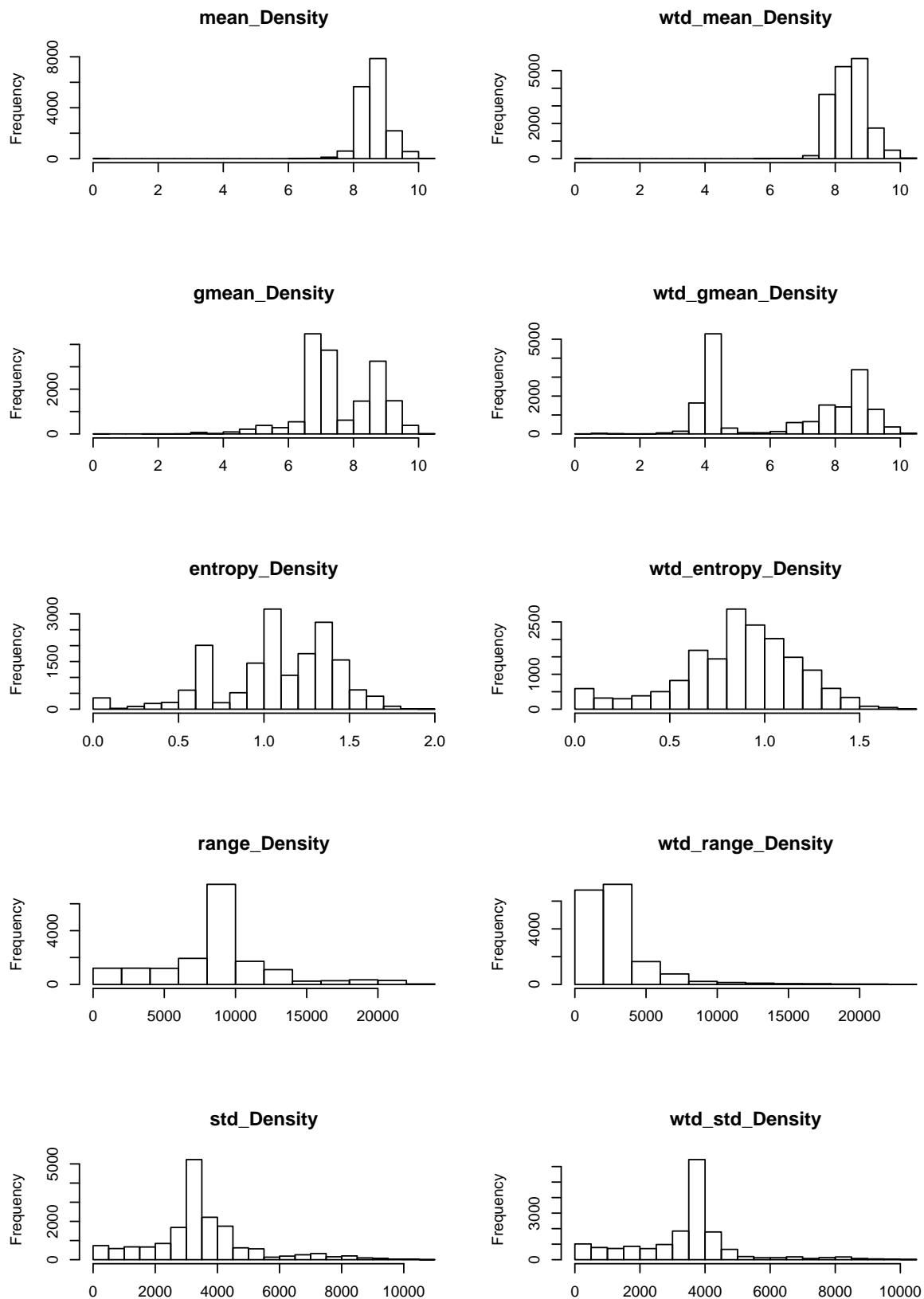


Figure 33: Density Histogram After Transformation

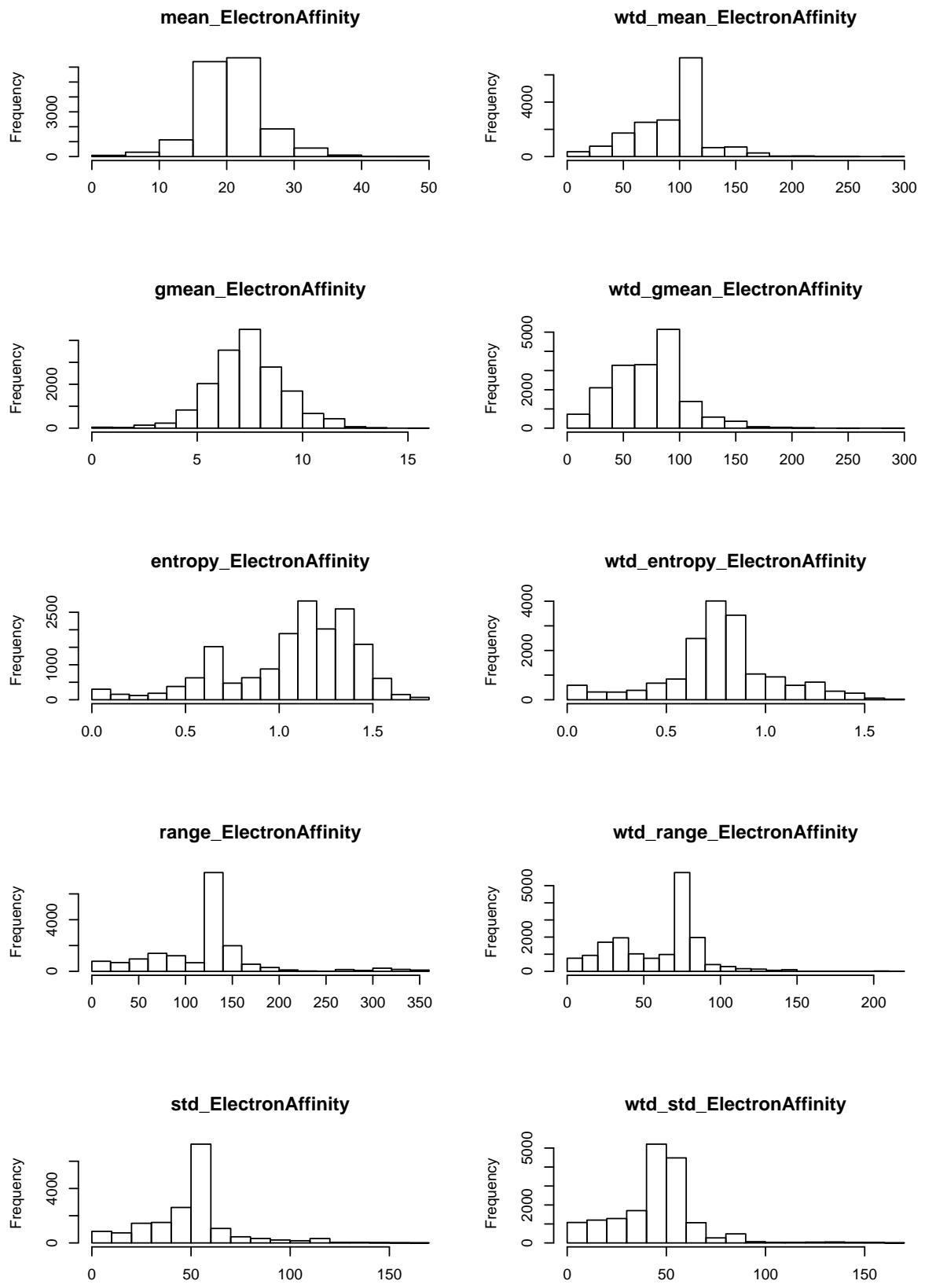


Figure 34: Electron Affinity Histogram After Transformation  
96

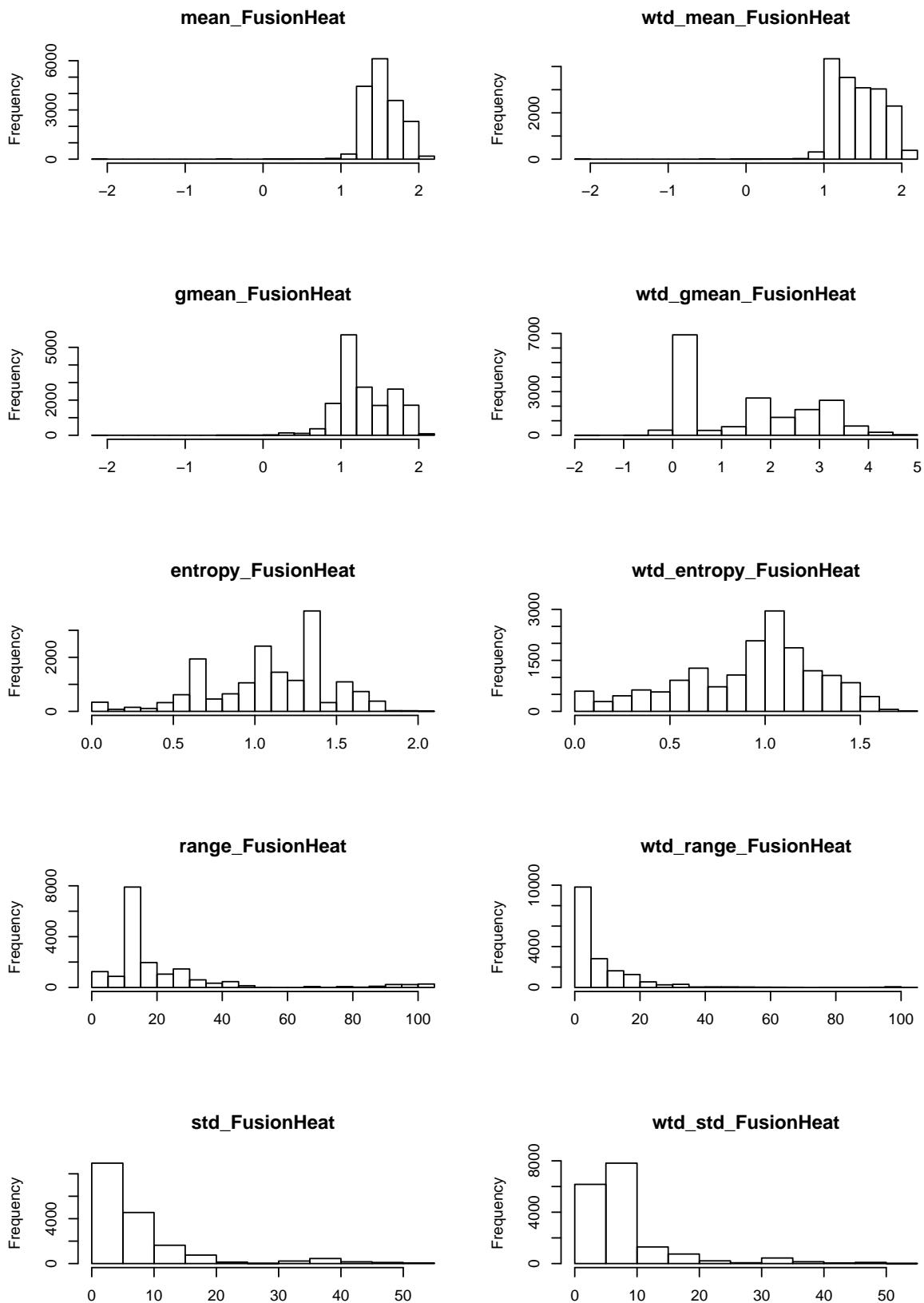


Figure 35: Fusion Heat Histogram After Transformation

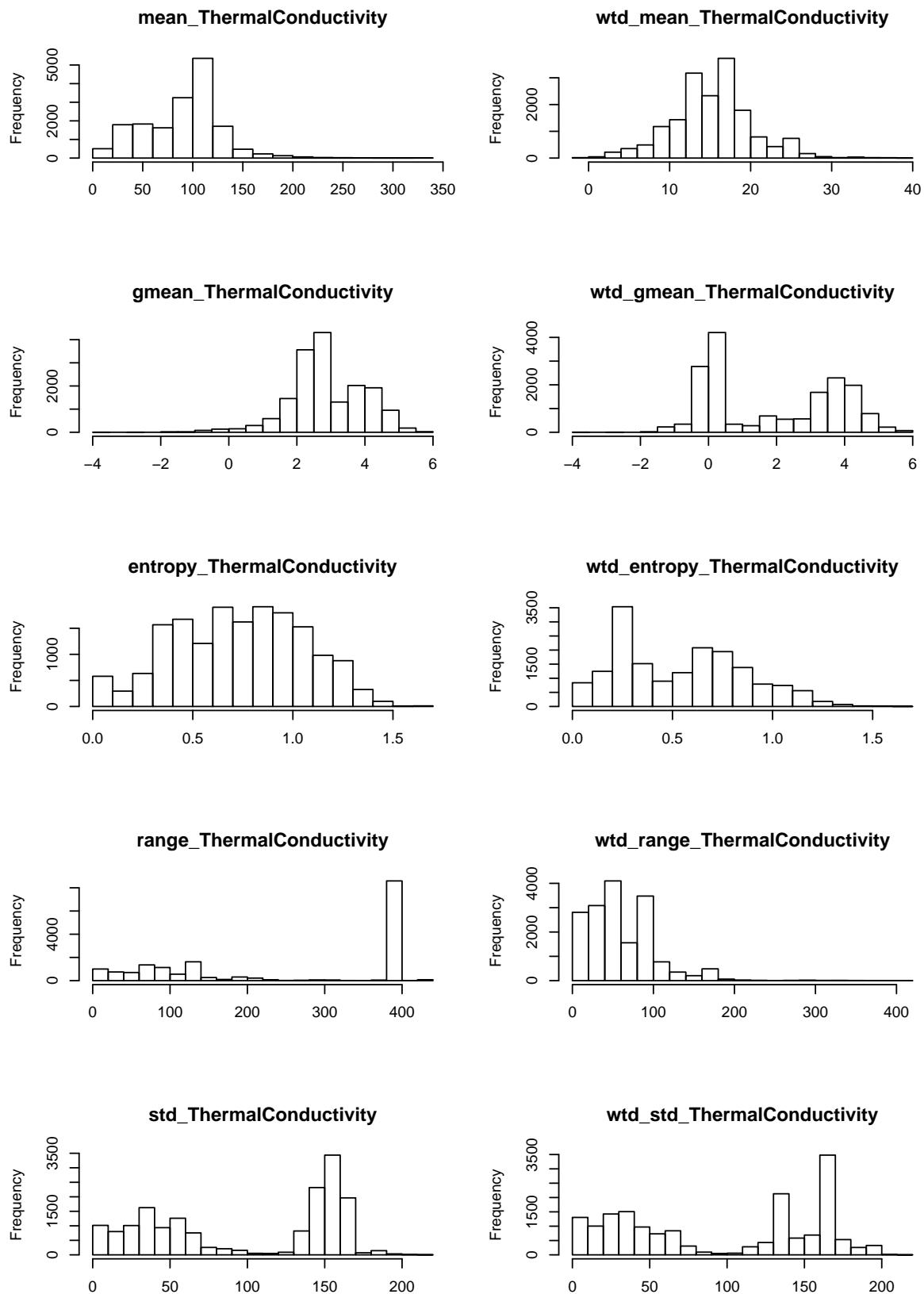


Figure 36: Thermal Conductivity Histogram After Transformation

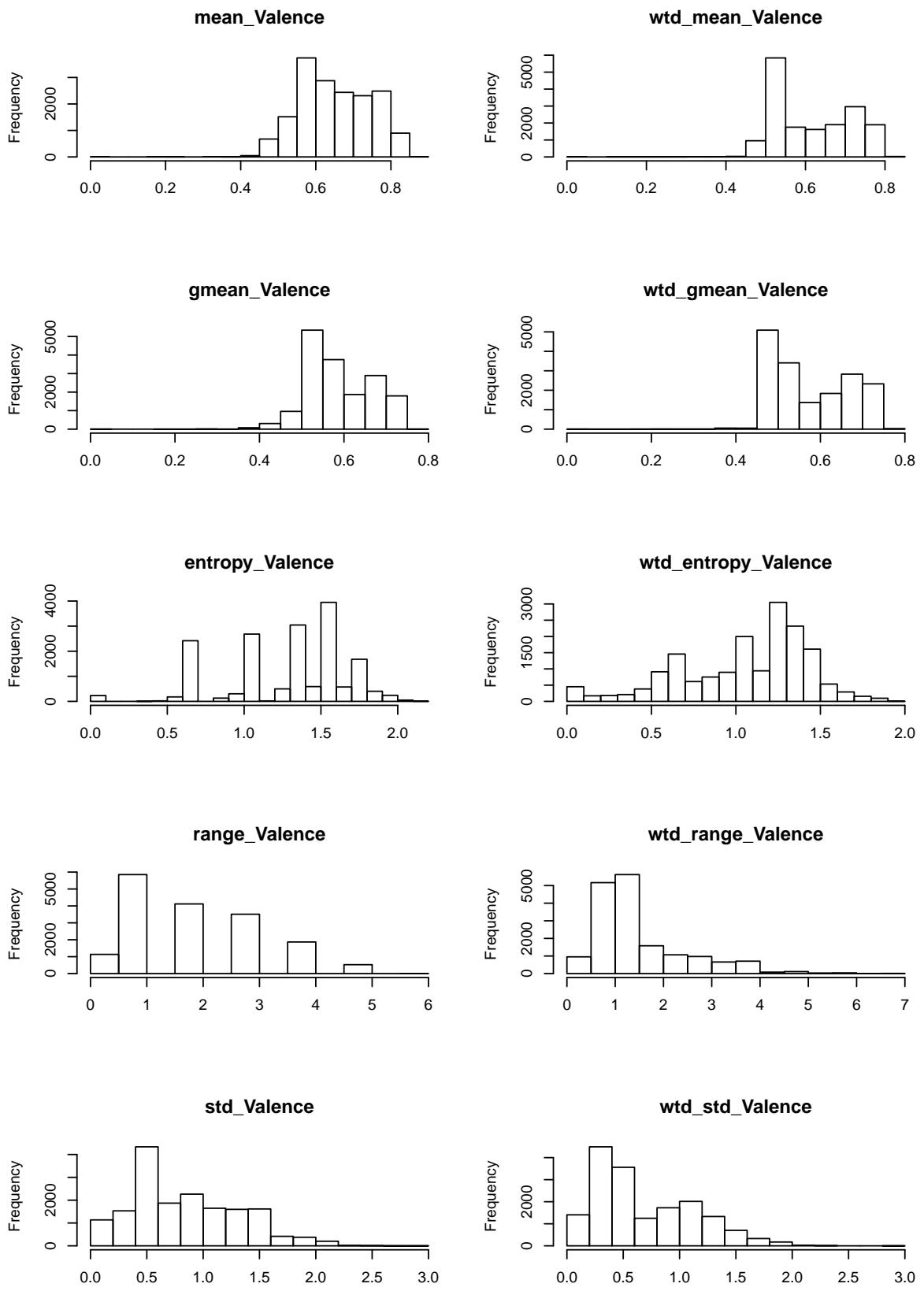


Figure 37: Valence Histogram After Transformation

From the above figures, we can see the distribution after transformation which tend to more normal compared to the previous result.

### Critical Temperature

```
# Check skewness for critical temperature  
skewness(train.data$critical_temp)
```

```
## [1] 0.8570089
```

From the result, it can be seen that the skewness of critical temperature is quite high, therefore, we need to perform the Box Cox transformation. We can also check it with QQ Plot and Histogram Plot.

```
# QQ Plot for Critical Temperature  
qqnorm(train.data[,82], main = ""); qqline(train.data[,82], col = 2,lwd=2,lty=2, main = "")
```

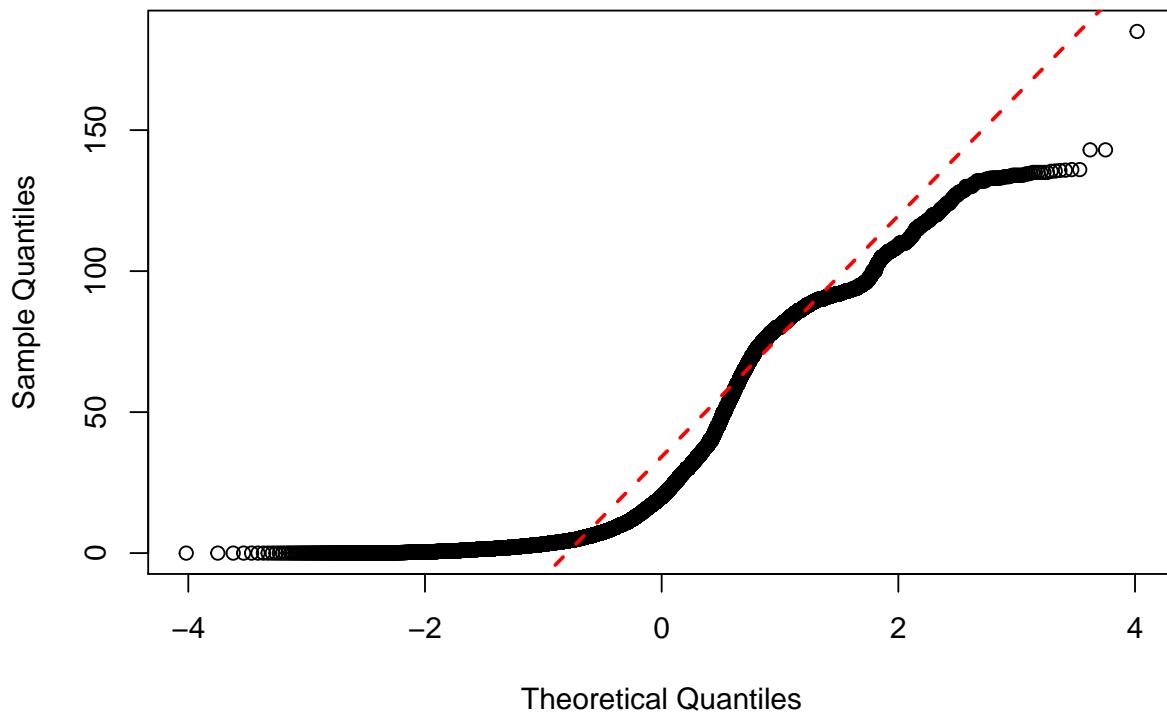


Figure 38: Critical Temperature QQ Plot

```
# Visualise the critical temperature distribution  
hist(train.data$critical_temp,  
      xlab="Critical Temperature", main = "")
```

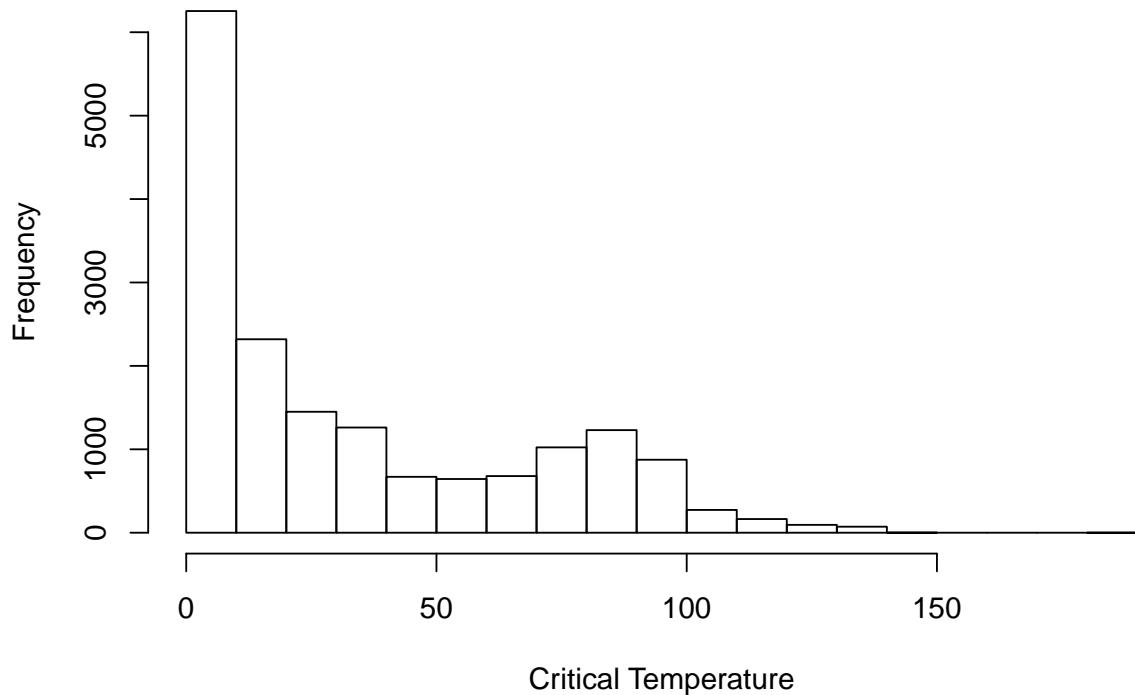


Figure 39: Critical Temperature Histogram

From Figure 38 and 39, critical temperature variable has a Right Skewed Distribution. Next, we will apply the transformation.

```
bc_temp <- BoxCoxTrans(train.data$critical_temp)
train.data.trans$critical_temp <- predict(bc_temp, train.data$critical_temp)
```

```
qqnorm(train.data.trans$critical_temp, main = "");
qqline(train.data.trans$critical_temp, col = 2, lwd=2,lty=2)
```

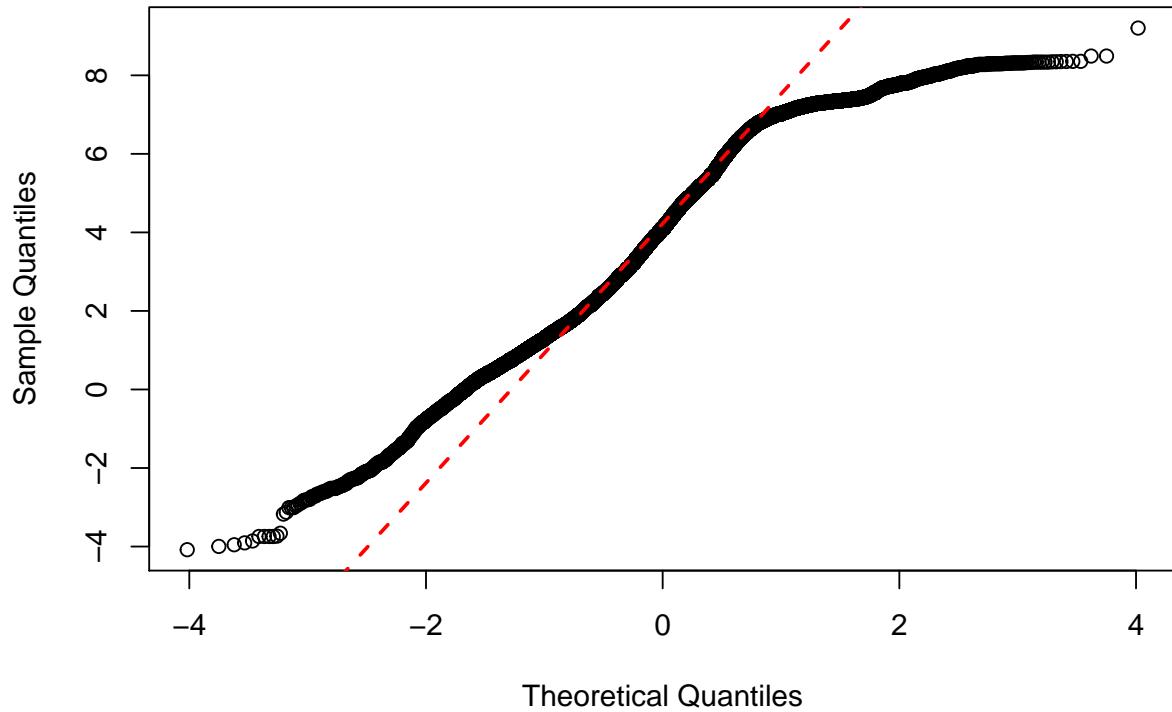


Figure 40: Critical Temperature QQ Plot After Transformation

```
hist(train.data.trans$critical_temp, xlab="Critical Temperature", main = "")
```

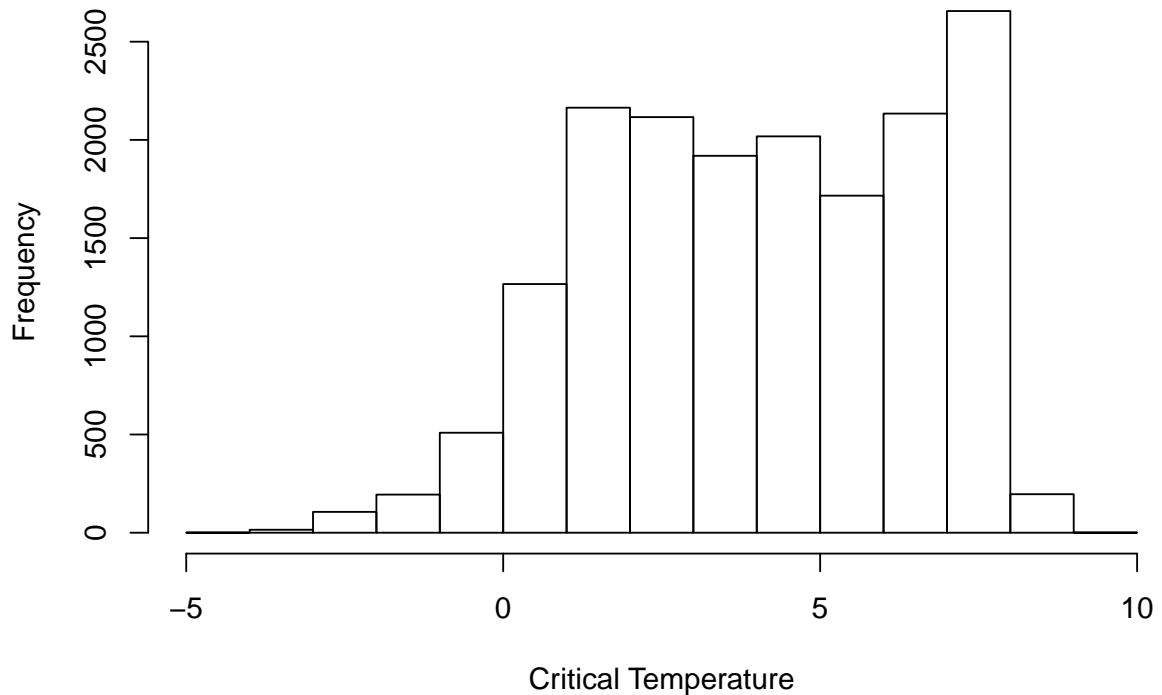


Figure 41: Critical Temperature Histogram After Transformation

Figure 40 and 41 show the QQ Plot and Histogram after transformation, which is more normal than before.

Now, we have done the data exploration section. Some of the major findings during this process are as follows.

- Most of the variables have skewed distribution, therefore, we might try a scenario with transformed data.
- Most of the variables has no strong correlation to either response variable or other independent variables. This is because the originally the dataset only have eight main properties + 1 variable number of elements, whereas the rest of the variables are derived from them.
- Entropy-related variables have very small range compared to other variables, therefore, we need to scale the data.

### 3 Model Development

In this section, we will develop some models for this assessment. In general, we will develop 14 models by using regression, regularization, instance-based, tree-based, dimensionality reduction, and ensemble algorithms. Notice that we will transform the dataset, therefore in total we will have 28 models. In order to support this, we will use a package called caret. The caret package (short for Classification And REgression Training) is a set of functions that attempt to streamline the process for creating predictive models. The package contains tools for data splitting, pre-processing, feature selection, model tuning using resampling, and variable importance estimation. More about caret can be found here [The]

In this section, we will not explain the advantages and disadvantages of each algorithm too deep, this is because we want this section only focus on the model development and fitting. Later in the model evaluation section, we will evaluate and elaborate the advantages and disadvantages of each algorithm deeply.

In the first subsection, we will develop the models for the original dataset and in the second subsection, we will develop the models for the transformed dataset.

### 3.1 Original Dataset

#### 3.1.1 Linear Regression with All Variables (81)

Linear regression is a linear approach to model the relationship between a scalar response (or dependent variable) and one or more explanatory variables (or independent variables). First, we will create a model with all the features (81 features), later we will improve the model with the finding from the previous section, stepwise techniques, and regularization techniques.

```
set.seed(seed)

# this is our control setting for all models, we perform 10-folds cross validation to all models
control <- trainControl(method = "cv", number = 10)

# Linear Model
linear_model1 <- train(critical_temp ~.,
                        data = train.data,
                        method = "lm",
                        preProc = c("range"),
                        trControl = control
                      )

summary(linear_model1)

## 
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -86.025  -9.357   0.550  11.011 167.595
##
## Coefficients:
##                               Estimate Std. Error t value Pr(>|t|)    
## (Intercept)                 -11.553    3.436  -3.362 0.000775 ***
## number_of_elements           -29.348    6.662  -4.405 1.06e-05 ***
## mean_atomic_mass              183.839   18.661   9.851 < 2e-16 ***
## wtd_mean_atomic_mass        -205.162   23.447  -8.750 < 2e-16 ***
## gmean_atomic_mass            -115.114   18.594  -6.191 6.11e-10 ***
## wtd_gmean_atomic_mass        155.386   22.592   6.878 6.28e-12 ***
## entropy_atomic_mass          -74.659   10.201  -7.319 2.62e-13 ***
## wtd_entropy_atomic_mass       5.508     7.980   0.690 0.490043  
## range_atomic_mass             45.027    3.861  11.663 < 2e-16 ***
## wtd_range_atomic_mass         5.354     5.068   1.056 0.290816  
## std_atomic_mass               -61.073   7.121  -8.576 < 2e-16 ***
## wtd_std_atomic_mass            13.359   6.222   2.147 0.031797 *
```

## mean_fie	133.260	67.224	1.982	0.047457	*
## wtd_mean_fie	-99.998	81.559	-1.226	0.220185	
## gmean_fie	-131.975	66.452	-1.986	0.047047	*
## wtd_gmean_fie	123.133	80.521	1.529	0.126232	
## entropy_fie	-198.926	49.090	-4.052	5.10e-05	***
## wtd_entropy_fie	95.376	10.952	8.708	< 2e-16	***
## range_fie	81.768	9.408	8.691	< 2e-16	***
## wtd_range_fie	22.561	4.306	5.240	1.63e-07	***
## std_fie	-85.790	12.535	-6.844	7.97e-12	***
## wtd_std_fie	-17.803	11.022	-1.615	0.106280	
## mean_atomic_radius	-173.026	50.821	-3.405	0.000664	***
## wtd_mean_atomic_radius	825.059	67.491	12.225	< 2e-16	***
## gmean_atomic_radius	93.933	50.923	1.845	0.065109	.
## wtd_gmean_atomic_radius	-733.337	66.043	-11.104	< 2e-16	***
## entropy_atomic_radius	122.181	42.407	2.881	0.003967	**
## wtd_entropy_atomic_radius	83.736	11.323	7.395	1.48e-13	***
## range_atomic_radius	52.681	6.406	8.224	< 2e-16	***
## wtd_range_atomic_radius	-20.607	4.312	-4.779	1.78e-06	***
## std_atomic_radius	-43.270	12.743	-3.396	0.000686	***
## wtd_std_atomic_radius	-32.350	9.006	-3.592	0.000329	***
## mean_Density	-111.751	12.737	-8.774	< 2e-16	***
## wtd_mean_Density	7.936	15.690	0.506	0.613012	
## gmean_Density	28.655	12.009	2.386	0.017036	*
## wtd_gmean_Density	41.915	14.946	2.804	0.005046	**
## entropy_Density	36.348	7.692	4.726	2.31e-06	***
## wtd_entropy_Density	-32.253	5.159	-6.252	4.16e-10	***
## range_Density	-36.029	5.438	-6.625	3.58e-11	***
## wtd_range_Density	-2.176	6.535	-0.333	0.739214	
## std_Density	67.663	8.385	8.070	7.52e-16	***
## wtd_std_Density	-17.926	6.034	-2.971	0.002973	**
## mean_ElectronAffinity	-31.868	15.596	-2.043	0.041038	*
## wtd_mean_ElectronAffinity	160.647	16.974	9.464	< 2e-16	***
## gmean_ElectronAffinity	51.789	13.459	3.848	0.000120	***
## wtd_gmean_ElectronAffinity	-175.502	14.992	-11.706	< 2e-16	***
## entropy_ElectronAffinity	10.601	5.190	2.042	0.041124	*
## wtd_entropy_ElectronAffinity	-36.048	4.183	-8.618	< 2e-16	***
## range_ElectronAffinity	-130.363	6.849	-19.033	< 2e-16	***
## wtd_range_ElectronAffinity	-32.072	5.175	-6.198	5.87e-10	***
## std_ElectronAffinity	206.799	10.712	19.305	< 2e-16	***
## wtd_std_ElectronAffinity	-94.812	7.415	-12.786	< 2e-16	***
## mean_FusionHeat	178.427	22.519	7.923	2.46e-15	***
## wtd_mean_FusionHeat	-212.731	22.946	-9.271	< 2e-16	***
## gmean_FusionHeat	-160.005	20.641	-7.752	9.58e-15	***
## wtd_gmean_FusionHeat	179.276	21.247	8.438	< 2e-16	***
## entropy_FusionHeat	-39.281	6.153	-6.384	1.77e-10	***
## wtd_entropy_FusionHeat	43.921	3.785	11.605	< 2e-16	***
## range_FusionHeat	-35.540	7.893	-4.503	6.75e-06	***
## wtd_range_FusionHeat	61.142	7.773	7.866	3.88e-15	***
## std_FusionHeat	-34.805	15.294	-2.276	0.022878	*
## wtd_std_FusionHeat	44.132	9.195	4.799	1.60e-06	***
## mean_ThermalConductivity	-33.171	9.354	-3.546	0.000392	***
## wtd_mean_ThermalConductivity	234.634	13.094	17.919	< 2e-16	***
## gmean_ThermalConductivity	-10.753	8.450	-1.272	0.203222	
## wtd_gmean_ThermalConductivity	-141.655	11.731	-12.075	< 2e-16	***

```

## entropy_ThermalConductivity      21.450    3.689    5.814 6.21e-09 ***
## wtd_entropy_ThermalConductivity  3.123     2.895    1.079 0.280710
## range_ThermalConductivity       -38.598    6.436   -5.998 2.04e-09 ***
## wtd_range_ThermalConductivity   -90.176    7.315   -12.328 < 2e-16 ***
## std_ThermalConductivity        66.987     9.989    6.706 2.06e-11 ***
## wtd_std_ThermalConductivity    -8.090     5.711   -1.416 0.156679
## mean_Valence                  -101.244   42.283   -2.394 0.016657 *
## wtd_mean_Valence                153.455   49.245    3.116 0.001835 **
## gmean_Valence                  126.782    39.974    3.172 0.001519 **
## wtd_gmean_Valence              -176.547   46.161   -3.825 0.000131 ***
## entropy_Valence                 142.964   30.018    4.763 1.93e-06 ***
## wtd_entropy_Valence             -140.273   12.250   -11.451 < 2e-16 ***
## range_Valence                  25.367     4.948    5.127 2.98e-07 ***
## wtd_range_Valence               -6.701     4.934   -1.358 0.174457
## std_Valence                     23.880     8.314    2.872 0.004082 **
## wtd_std_Valence                 -75.454    6.476   -11.651 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 17.68 on 16929 degrees of freedom
## Multiple R-squared:  0.7348, Adjusted R-squared:  0.7335
## F-statistic: 579.1 on 81 and 16929 DF,  p-value: < 2.2e-16

cat("MSE : ",linear_model1$results$RMSE^2)

```

```
## MSE : 313.6732
```

From above, we can see that the R-squared for the model is 0.7348 with Adjusted R-squared is 0.7335.

Notice that from the summary, we have some information, residuals, estimate, standard error, t-value and Pr(>t). Residuals are essentially the difference between the actual observed response values and the response values. Standard Error measures the average amount that the coefficient estimates vary from the actual average value of the response variable. The coefficient t-value is a measure of how many standard deviations our coefficient estimate is far away from 0. We want it to be far away from zero as this would indicate we could reject the null hypothesis. In general, t-values are also used to compute p-values. The Pr(>t) acronym found in the model output relates to the probability of observing any value equal or larger than t. A small p-value for the intercept and the slope indicates that we can reject the null hypothesis which allows us to conclude that there is a relationship between the predictor and response variable.

Therefore, the summary tells us about the features which are not important such as wtd\_entropy\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, wtd\_std\_fie, wtd\_mean\_Density, wtd\_range\_Density, gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_std\_ThermalConductivity, and wtd\_range\_Valence.

The Train MSE for this model is 313.6732

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(linear_model1, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

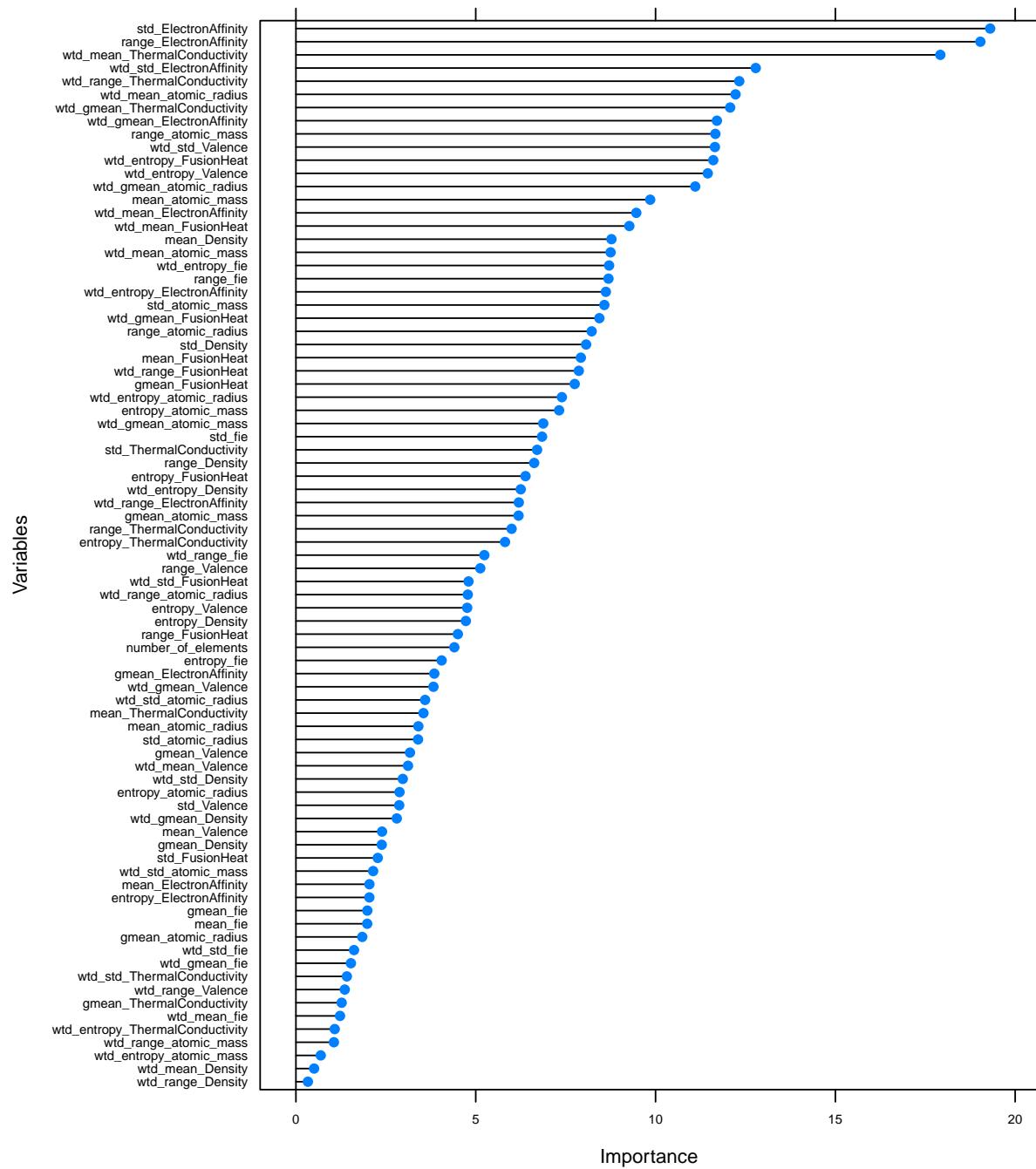


Figure 42: Variable Importance for Linear Regression Model 1

From above, it can be seen that std\_ElectronAffinity is the most important variable for this model, whereas wtd\_range\_Density is the least important variable for this model.

### 3.1.2 Linear Regression with Significant Variables

```

set.seed(seed)

# Store the less important variables
less_important <- c("wtd_entropy_atomic_mass", "wtd_range_atomic_mass", "wtd_mean_fie",
                     "wtd_gmean_fie", "wtd_std_fie", "wtd_mean_Density", "wtd_range_Density",
                     "gmean_ThermalConductivity", "wtd_entropy_ThermalConductivity",
                     "wtd_std_ThermalConductivity", "wtd_range_Valence")

# Linear Model
linear_model2 <- train(critical_temp ~.,
                        data = train.data[, -which(names(train.data) %in% less_important)],
                        method = "lm",
                        preProc = c("range"),
                        trControl = control
                       )

summary(linear_model2)

## 
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -85.172  -9.341   0.655  10.938 168.073
##
## Coefficients:
##                               Estimate Std. Error t value Pr(>|t|)    
## (Intercept)                 -10.092    3.348  -3.014 0.002582 **  
## number_of_elements          -29.141    6.477  -4.499 6.87e-06 *** 
## mean_atomic_mass            177.146   17.211  10.293 < 2e-16 *** 
## wtd_mean_atomic_mass       -181.742   19.798  -9.180 < 2e-16 *** 
## gmean_atomic_mass           -110.773   17.884  -6.194 6.00e-10 *** 
## wtd_gmean_atomic_mass      136.696   20.584   6.641 3.22e-11 *** 
## entropy_atomic_mass         -68.845    9.205  -7.479 7.85e-14 *** 
## range_atomic_mass            45.316    3.827  11.842 < 2e-16 *** 
## std_atomic_mass              -56.039    6.876  -8.150 3.90e-16 *** 
## wtd_std_atomic_mass          5.576     5.872   0.949 0.342385  
## mean_fie                      110.185   45.265   2.434 0.014934 *   
## gmean_fie                     -88.096   45.052  -1.955 0.050549 .  
## entropy_fie                  -167.360   44.474  -3.763 0.000168 *** 
## wtd_entropy_fie                90.447    9.872   9.162 < 2e-16 *** 
## range_fie                      77.325    9.345   8.275 < 2e-16 *** 
## wtd_range_fie                  24.008    3.759   6.387 1.73e-10 *** 
## std_fie                         -98.606   9.098  -10.838 < 2e-16 *** 
## mean_atomic_radius              -50.820   46.065  -1.103 0.269949  
## wtd_mean_atomic_radius          632.548   57.450  11.010 < 2e-16 *** 
## gmean_atomic_radius             -21.825   46.177  -0.473 0.636472  
## wtd_gmean_atomic_radius        -550.937   56.001  -9.838 < 2e-16 *** 
## entropy_atomic_radius            113.950   38.896   2.930 0.003398 **  
## wtd_entropy_atomic_radius       84.090    8.205  10.249 < 2e-16 ***

```

```

## range_atomic_radius      61.085    6.274   9.736 < 2e-16 ***
## wtd_range_atomic_radius -21.100    3.431  -6.150 7.92e-10 ***
## std_atomic_radius        -58.532   12.399  -4.721 2.37e-06 ***
## wtd_std_atomic_radius   -24.474    8.644  -2.831 0.004642 **
## mean_Density             -112.692   8.842  -12.746 < 2e-16 ***
## gmean_Density            24.667    8.743   2.821 0.004787 **
## wtd_gmean_Density        53.079    6.436   8.247 < 2e-16 ***
## entropy_Density          31.658    7.092   4.464 8.10e-06 ***
## wtd_entropy_Density      -27.048    3.994  -6.773 1.31e-11 ***
## range_Density            -35.994    5.416  -6.646 3.10e-11 ***
## std_Density              63.403    7.798   8.130 4.58e-16 ***
## wtd_std_Density          -11.671    4.734  -2.465 0.013703 *
## mean_ElectronAffinity   -53.949    14.820  -3.640 0.000273 ***
## wtd_mean_ElectronAffinity 188.625   16.344  11.541 < 2e-16 ***
## gmean_ElectronAffinity  71.419    12.682   5.631 1.81e-08 ***
## wtd_gmean_ElectronAffinity -202.524   14.116  -14.347 < 2e-16 ***
## entropy_ElectronAffinity 9.702     5.102   1.902 0.057232 .
## wtd_entropy_ElectronAffinity -33.570   4.096  -8.195 2.67e-16 ***
## range_ElectronAffinity  -130.097   6.758  -19.251 < 2e-16 ***
## wtd_range_ElectronAffinity -30.791   4.875  -6.316 2.75e-10 ***
## std_ElectronAffinity     214.855   10.411  20.637 < 2e-16 ***
## wtd_std_ElectronAffinity -105.798   6.748  -15.679 < 2e-16 ***
## mean_FusionHeat          163.432   22.113   7.391 1.53e-13 ***
## wtd_mean_FusionHeat      -190.011   21.966  -8.650 < 2e-16 ***
## gmean_FusionHeat         -155.200   20.294  -7.648 2.16e-14 ***
## wtd_gmean_FusionHeat    169.896   20.580   8.256 < 2e-16 ***
## entropy_FusionHeat       -37.225   5.994  -6.211 5.40e-10 ***
## wtd_entropy_FusionHeat   38.891    3.595  10.818 < 2e-16 ***
## range_FusionHeat         -37.564   7.690  -4.885 1.04e-06 ***
## wtd_range_FusionHeat     49.785    7.297   6.822 9.26e-12 ***
## std_FusionHeat           -26.532   14.886  -1.782 0.074703 .
## wtd_std_FusionHeat       39.077    8.786   4.448 8.74e-06 ***
## mean_ThermalConductivity -41.651    5.789  -7.195 6.53e-13 ***
## wtd_mean_ThermalConductivity 226.291   8.891  25.452 < 2e-16 ***
## wtd_gmean_ThermalConductivity -138.038   5.388  -25.618 < 2e-16 ***
## entropy_ThermalConductivity 26.125    2.654   9.842 < 2e-16 ***
## range_ThermalConductivity -44.449    6.143  -7.236 4.83e-13 ***
## wtd_range_ThermalConductivity -91.063   6.240  -14.593 < 2e-16 ***
## std_ThermalConductivity  73.551    7.895   9.316 < 2e-16 ***
## mean_Valence              -70.093   40.733  -1.721 0.085309 .
## wtd_mean_Valence         90.573    46.500   1.948 0.051453 .
## gmean_Valence             98.696   38.654   2.553 0.010678 *
## wtd_gmean_Valence        -116.400   43.875  -2.653 0.007986 **
## entropy_Valence           113.447   28.415   3.992 6.57e-05 ***
## wtd_entropy_Valence      -133.536   10.272  -13.001 < 2e-16 ***
## range_Valence             24.825    4.921   5.045 4.59e-07 ***
## std_Valence               17.983    8.055   2.233 0.025587 *
## wtd_std_Valence          -67.817    6.171  -10.990 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 17.7 on 16940 degrees of freedom
## Multiple R-squared:  0.7339, Adjusted R-squared:  0.7328
## F-statistic: 667.5 on 70 and 16940 DF,  p-value: < 2.2e-16

```

```
cat("MSE : ",linear_model2$results$RMSE^2)
```

```
## MSE : 314.3748
```

From above, we can see that the R-squared for the model is 0.7339 with Adjusted R-squared is 0.7328 Those 2 parameters are slightly worse than the previous model. For the R-Squared, the difference is only 0.0009, whereas the different for the Adjusted R-squared is 0.0007. However, we decrease the number of variables from 81 variables to 70 variables, which is better in term of complexity.

The Train MSE for this model is 314.3748

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(linear_model2, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

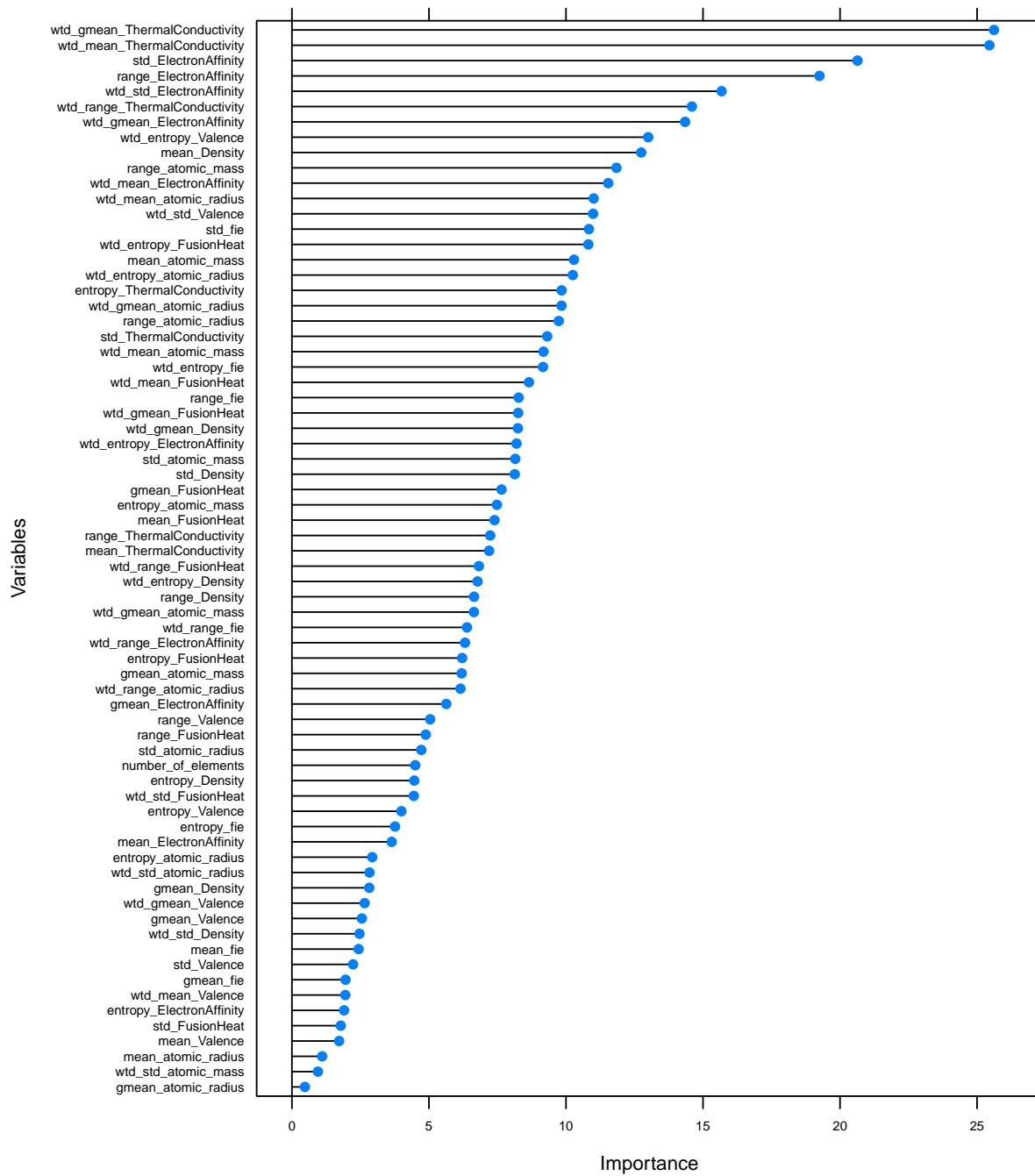


Figure 43: Variable Importance for Linear Regression Model 2

From above, it can be seen that `wtd_gmean_ThermalConductivity` is the most important variable for this model, whereas `gmean_atomic_radius` is the least important variable for this model.

### 3.1.3 Linear Regression with Strong Correlated Variables

```

set.seed(seed)

# Linear Model
linear_model3 <- train(critical_temp ~.,
                        data = train.data[, -which(names(train.data) %in% less_correlated)],
                        method = "lm",
                        preProc = c("range"),
                        trControl = control
                      )

summary(linear_model3)

##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##    Min      1Q  Median      3Q     Max
## -83.421 -9.756   0.382  10.925 154.100
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -16.4348   3.3642 -4.885 1.04e-06 ***
## number_of_elements -20.2007   6.6117 -3.055 0.002252 **
## mean_atomic_mass 126.8841  18.1224  7.001 2.63e-12 ***
## wtd_mean_atomic_mass -162.2372  22.7782 -7.122 1.10e-12 ***
## gmean_atomic_mass -62.5872  18.1163 -3.455 0.000552 ***
## wtd_gmean_atomic_mass 113.5021  21.8029  5.206 1.95e-07 ***
## entropy_atomic_mass -73.6373  9.9911 -7.370 1.78e-13 ***
## wtd_entropy_atomic_mass 15.2720  7.8499  1.946 0.051730 .
## range_atomic_mass 51.6815  3.8322 13.486 < 2e-16 ***
## wtd_range_atomic_mass 8.2795  5.0791  1.630 0.103094
## std_atomic_mass -46.5271  6.9440 -6.700 2.15e-11 ***
## wtd_std_atomic_mass -7.4362  5.9318 -1.254 0.210003
## mean_fie 20.1233  7.3019  2.756 0.005859 **
## wtd_mean_fie 62.3228  54.2622  1.149 0.250759
## wtd_gmean_fie -45.6024  53.6134 -0.851 0.395015
## entropy_fie -180.9149  47.6179 -3.799 0.000146 ***
## wtd_entropy_fie 131.6362  10.6019 12.416 < 2e-16 ***
## range_fie 80.4827  9.3159  8.639 < 2e-16 ***
## wtd_range_fie 25.2135  4.2333  5.956 2.64e-09 ***
## std_fie -77.6947  9.5046 -8.174 3.18e-16 ***
## wtd_std_fie -28.1083  7.9119 -3.553 0.000382 ***
## wtd_mean_atomic_radius 758.4448 42.2408 17.955 < 2e-16 ***
## gmean_atomic_radius -78.5072  8.0973 -9.695 < 2e-16 ***
## wtd_gmean_atomic_radius -656.4581 40.7024 -16.128 < 2e-16 ***
## entropy_atomic_radius 158.1214 41.4390  3.816 0.000136 ***
## wtd_entropy_atomic_radius 112.0102 10.8011 10.370 < 2e-16 ***
## range_atomic_radius 54.8804  6.2744  8.747 < 2e-16 ***
## wtd_range_atomic_radius -15.9813  4.3141 -3.704 0.000213 ***
## std_atomic_radius -71.9754  8.9931 -8.003 1.29e-15 ***

```

```

## wtd_std_atomic_radius      -18.2360    6.4089  -2.845 0.004441 **
## mean_Density               -87.3226   12.4848  -6.994 2.77e-12 ***
## wtd_mean_Density           -13.1687   15.3230  -0.859 0.390127
## gmean_Density              9.4050   11.8218   0.796 0.426293
## wtd_gmean_Density          52.8859   14.3075   3.696 0.000219 ***
## entropy_Density             7.1627    7.3900   0.969 0.332434
## wtd_entropy_Density         -24.2075   5.0697  -4.775 1.81e-06 ***
## range_Density               -30.4015   5.3768  -5.654 1.59e-08 ***
## wtd_range_Density           8.2908    6.4924   1.277 0.201621
## std_Density                46.0574   8.2960   5.552 2.87e-08 ***
## wtd_std_Density             -8.9124   5.9286  -1.503 0.132781
## wtd_mean_ElectronAffinity  6.7858    6.3366   1.071 0.284234
## gmean_ElectronAffinity     -2.0008   5.4504  -0.367 0.713559
## entropy_ElectronAffinity   14.1034   5.1746   2.725 0.006427 **
## wtd_entropy_ElectronAffinity -56.5313  3.9831 -14.193 < 2e-16 ***
## range_ElectronAffinity     -114.4798  6.7464 -16.969 < 2e-16 ***
## wtd_range_ElectronAffinity -46.2844   5.0971 -9.081 < 2e-16 ***
## std_ElectronAffinity       174.3103  9.6750  18.017 < 2e-16 ***
## wtd_std_ElectronAffinity   -40.7484   5.1299 -7.943 2.09e-15 ***
## mean_FusionHeat             27.7030  11.3510   2.441 0.014674 *
## wtd_mean_FusionHeat         -128.2403  13.3547 -9.603 < 2e-16 ***
## gmean_FusionHeat            -49.0395  12.7771 -3.838 0.000124 ***
## wtd_gmean_FusionHeat        115.3766  11.8859  9.707 < 2e-16 ***
## entropy_FusionHeat          -3.8999   4.8642 -0.802 0.422699
## wtd_entropy_FusionHeat      42.4018   3.4209  12.395 < 2e-16 ***
## wtd_range_FusionHeat        46.7646   6.6219  7.062 1.70e-12 ***
## mean_ThermalConductivity   -32.2796  8.7635 -3.683 0.000231 ***
## wtd_mean_ThermalConductivity 271.9926  12.2274  22.245 < 2e-16 ***
## gmean_ThermalConductivity  0.4779   7.9829  0.060 0.952260
## wtd_gmean_ThermalConductivity -175.8765  11.0496 -15.917 < 2e-16 ***
## entropy_ThermalConductivity 16.6772   2.8349  5.883 4.11e-09 ***
## range_ThermalConductivity  -39.4057   6.3144 -6.241 4.46e-10 ***
## wtd_range_ThermalConductivity -98.9132  6.6586 -14.855 < 2e-16 ***
## std_ThermalConductivity    73.2037   8.8643  8.258 < 2e-16 ***
## wtd_std_ThermalConductivity -25.9449   5.1352 -5.052 4.41e-07 ***
## mean_Valence                144.2086  29.1993  4.939 7.94e-07 ***
## wtd_mean_Valence            -337.0064  26.7845 -12.582 < 2e-16 ***
## gmean_Valence               -92.5297  27.6520 -3.346 0.000821 ***
## wtd_gmean_Valence           288.4305  24.0124  12.012 < 2e-16 ***
## entropy_Valence              58.7048  27.3152  2.149 0.031636 *
## wtd_entropy_Valence         -188.3078  11.7421 -16.037 < 2e-16 ***
## wtd_range_Valence            -0.8496   4.7840 -0.178 0.859053
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 17.95 on 16940 degrees of freedom
## Multiple R-squared:  0.7265, Adjusted R-squared:  0.7254
## F-statistic:  643 on 70 and 16940 DF,  p-value: < 2.2e-16

cat("MSE :",linear_model3$results$RMSE^2)

```

```
## MSE : 323.0719
```

From above, we can see that the R-squared for the model is 0.7265 with Adjusted R-squared is 0.7254.

Those 2 parameters are slightly worse than the first model. For the R-Squared, the difference is only 0.0083, whereas the difference for the Adjusted R-squared is 0.0081. However, we decrease the number of variables from 81 variables to 70 variables, which is better in term of complexity.

The Train MSE for this model is 323.0719

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(linear_model3, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

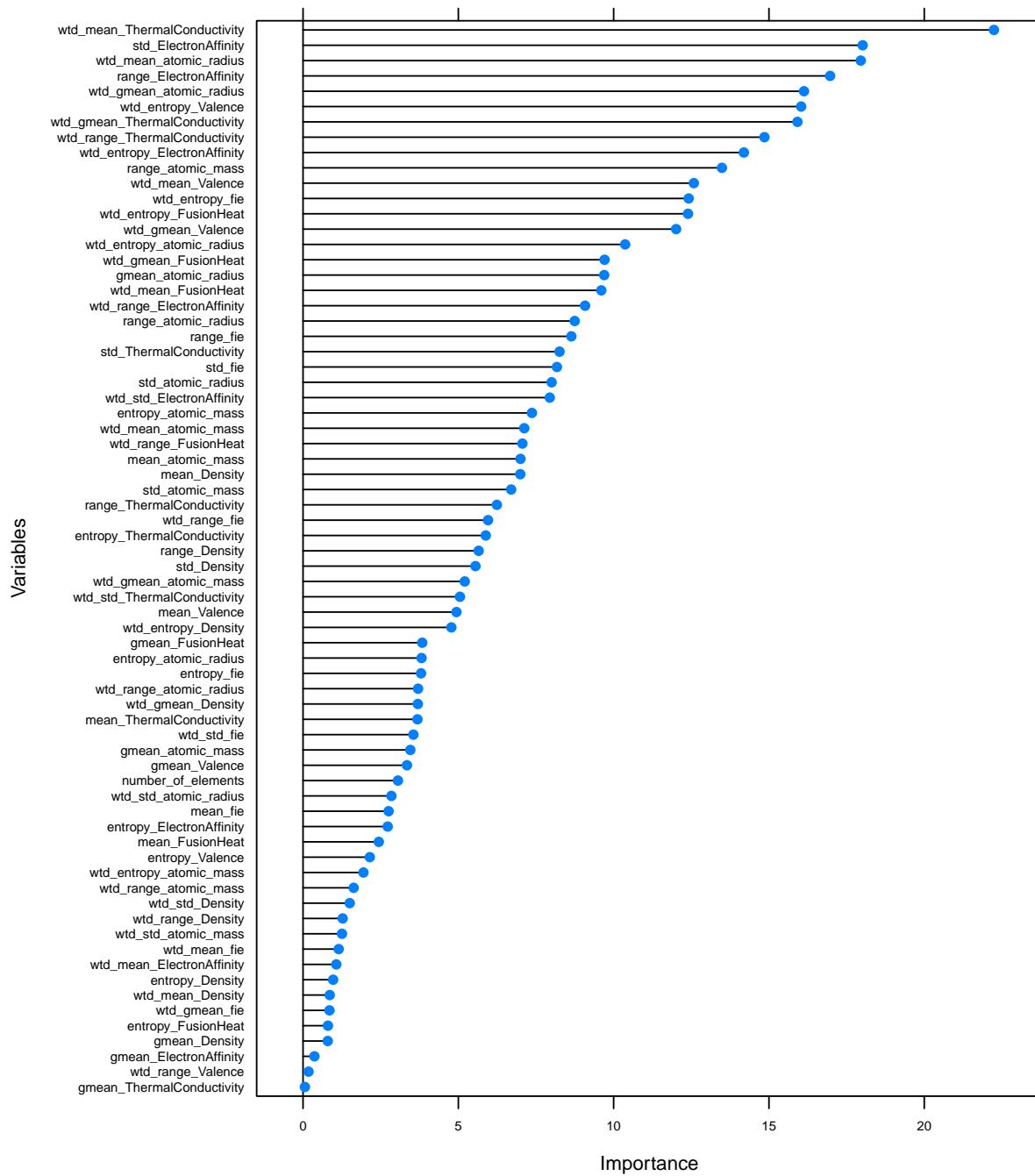


Figure 44: Variable Importance for Linear Regression Model 3

From above, it can be seen that `wtd_mean_ThermalConductivity` is the most important variable for this model, whereas `gmean_ThermalConductivity` is the least important variable for this model.

### 3.1.4 Linear Regression with Backwards Selection

The stepwise regression (or stepwise selection) consists of iteratively adding and removing predictors, in the predictive model, in order to find the subset of variables in the data set resulting in the best performing model, that is a model that lowers prediction error.

There are three strategies of stepwise regression [Bruce and Bruce, 2017]

- Backward selection (or backward elimination), which starts with all predictors in the model (full model), iteratively removes the least contributive predictors, and stops when you have a model where all predictors are statistically significant.
- Forward selection, which starts with no predictors in the model, iteratively adds the most contributive predictors, and stops when the improvement is no longer statistically significant.
- Stepwise selection (or sequential replacement), which is a combination of forward and backward selections. You start with no predictors, then sequentially add the most contributive predictors (like forward selection). After adding each new variable, remove any variables that no longer provide an improvement in the model fit (like backward selection).

In this sub section, we will perform the backward selection and in the next subsections, we will perform forward and stepwise selection.

```
# Helper Function for Plotting Metrics
plot_metrics <- function(model, x_axis, x_label) {
  par(mfrow = c(2, 2))
  plot(y = model$results$Rsquared, x = x_axis, xlab = x_label,
    ylab = "R-Squared", type = "l")
  points(x_axis[max(which(model$results$Rsquared == max(model$results$Rsquared)))],
    max(model$results$Rsquared),
    col = "red", cex = 2, pch = 20)
  plot(model$results$RMSE^2, x = x_axis, xlab = x_label, ylab = "MSE", type = "l")
  points(x_axis[max(which(model$results$RMSE == min(model$results$RMSE)))],
    min(model$results$RMSE)^2,
    col = "red", cex = 2, pch = 20)
  plot(model$results$MAE, x = x_axis, xlab = x_label, ylab = "MAE", type = "l")
  points(x_axis[max(which(model$results$MAE == min(model$results$MAE)))],
    min(model$results$MAE),
    col = "red", cex = 2, pch = 20)
}
```

```
set.seed(seed)

# Linear Regression with Backward Selection
linear_backward <- train(critical_temp ~., data = train.data,
  method = "leapBackward",
  tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
  trControl = control,
  preProc = c("range")
)
summary(linear_backward)
```

```
## Subset selection object
## 81 Variables (and intercept)
```

	Forced in	Forced out
##		
## number_of_elements	FALSE	FALSE
## mean_atomic_mass	FALSE	FALSE
## wtd_mean_atomic_mass	FALSE	FALSE
## gmean_atomic_mass	FALSE	FALSE
## wtd_gmean_atomic_mass	FALSE	FALSE
## entropy_atomic_mass	FALSE	FALSE
## wtd_entropy_atomic_mass	FALSE	FALSE
## range_atomic_mass	FALSE	FALSE
## wtd_range_atomic_mass	FALSE	FALSE
## std_atomic_mass	FALSE	FALSE
## wtd_std_atomic_mass	FALSE	FALSE
## mean_fie	FALSE	FALSE
## wtd_mean_fie	FALSE	FALSE
## gmean_fie	FALSE	FALSE
## wtd_gmean_fie	FALSE	FALSE
## entropy_fie	FALSE	FALSE
## wtd_entropy_fie	FALSE	FALSE
## range_fie	FALSE	FALSE
## wtd_range_fie	FALSE	FALSE
## std_fie	FALSE	FALSE
## wtd_std_fie	FALSE	FALSE
## mean_atomic_radius	FALSE	FALSE
## wtd_mean_atomic_radius	FALSE	FALSE
## gmean_atomic_radius	FALSE	FALSE
## wtd_gmean_atomic_radius	FALSE	FALSE
## entropy_atomic_radius	FALSE	FALSE
## wtd_entropy_atomic_radius	FALSE	FALSE
## range_atomic_radius	FALSE	FALSE
## wtd_range_atomic_radius	FALSE	FALSE
## std_atomic_radius	FALSE	FALSE
## wtd_std_atomic_radius	FALSE	FALSE
## mean_Density	FALSE	FALSE
## wtd_mean_Density	FALSE	FALSE
## gmean_Density	FALSE	FALSE
## wtd_gmean_Density	FALSE	FALSE
## entropy_Density	FALSE	FALSE
## wtd_entropy_Density	FALSE	FALSE
## range_Density	FALSE	FALSE
## wtd_range_Density	FALSE	FALSE
## std_Density	FALSE	FALSE
## wtd_std_Density	FALSE	FALSE
## mean_ElectronAffinity	FALSE	FALSE
## wtd_mean_ElectronAffinity	FALSE	FALSE
## gmean_ElectronAffinity	FALSE	FALSE
## wtd_gmean_ElectronAffinity	FALSE	FALSE
## entropy_ElectronAffinity	FALSE	FALSE
## wtd_entropy_ElectronAffinity	FALSE	FALSE
## range_ElectronAffinity	FALSE	FALSE
## wtd_range_ElectronAffinity	FALSE	FALSE
## std_ElectronAffinity	FALSE	FALSE
## wtd_std_ElectronAffinity	FALSE	FALSE
## mean_FusionHeat	FALSE	FALSE
## wtd_mean_FusionHeat	FALSE	FALSE

```

## gmean_FusionHeat           FALSE  FALSE
## wtd_gmean_FusionHeat      FALSE  FALSE
## entropy_FusionHeat        FALSE  FALSE
## wtd_entropy_FusionHeat    FALSE  FALSE
## range_FusionHeat          FALSE  FALSE
## wtd_range_FusionHeat      FALSE  FALSE
## std_FusionHeat            FALSE  FALSE
## wtd_std_FusionHeat        FALSE  FALSE
## mean_ThermalConductivity FALSE  FALSE
## wtd_mean_ThermalConductivity FALSE FALSE
## gmean_ThermalConductivity FALSE  FALSE
## wtd_gmean_ThermalConductivity FALSE FALSE
## entropy_ThermalConductivity FALSE FALSE
## wtd_entropy_ThermalConductivity FALSE FALSE
## range_ThermalConductivity FALSE  FALSE
## wtd_range_ThermalConductivity FALSE FALSE
## std_ThermalConductivity   FALSE  FALSE
## wtd_std_ThermalConductivity FALSE FALSE
## mean_Valence               FALSE  FALSE
## wtd_mean_Valence          FALSE  FALSE
## gmean_Valence              FALSE  FALSE
## wtd_gmean_Valence          FALSE  FALSE
## entropy_Valence            FALSE  FALSE
## wtd_entropy_Valence        FALSE  FALSE
## range_Valence              FALSE  FALSE
## wtd_range_Valence          FALSE  FALSE
## std_Valence                FALSE  FALSE
## wtd_std_Valence            FALSE  FALSE

## 1 subsets of each size up to 78
## Selection Algorithm: backward
##             number_of_elements mean_atomic_mass wtd_mean_atomic_mass
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##           gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
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##                      std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie
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##          gmean_fie wtd_gmean_fie entropy_fie wtd_entropy_fie range_fie
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##          wtd_range_fie std_fie wtd_std_fie mean_atomic_radius
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## 2 ( 1 ) " " " " " "
## 3 ( 1 ) " " " " " "
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## 5 ( 1 ) " " " " " "
## 6 ( 1 ) " " " " " "

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## 19 ( 1 )   " "
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## 23 ( 1 )   " "
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## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
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## 78  ( 1 ) "*"      "*"      "*"      "*"
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## 3  ( 1 ) " "           " "
## 4  ( 1 ) " "           " "
## 5  ( 1 ) " "           " "
## 6  ( 1 ) " "           " "
## 7  ( 1 ) " "           " "
## 8  ( 1 ) " "           " "
## 9  ( 1 ) " "           " "
## 10 ( 1 ) " "           " "
## 11 ( 1 ) " "           " "
## 12 ( 1 ) " "           " "
## 13 ( 1 ) " "           " "
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## 17 ( 1 ) "*"          " "
## 18 ( 1 ) "*"          " "
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## 20 ( 1 ) "*"          " "
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## 8  ( 1 ) " "             ""
## 9  ( 1 ) " "             ""
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## 9  ( 1 ) " "           " "           " "
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## 14 ( 1 ) " "           " "           " "

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## 68 ( 1 ) "*"

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## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
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## 18 ( 1 ) " "      " "      " "

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## 72  ( 1 ) "*"

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## 77  ( 1 ) " "      "*"      "*"
## 78  ( 1 ) " "      "*"      "*"
##          mean_ElectronAffinity wtd_mean_ElectronAffinity
## 1  ( 1 ) " "           " "
## 2  ( 1 ) " "           " "
## 3  ( 1 ) " "           " "
## 4  ( 1 ) " "           " "
## 5  ( 1 ) " "           " "
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## 7  ( 1 ) " "           "*"
## 8  ( 1 ) " "           "*"
## 9  ( 1 ) " "           "*"
## 10 ( 1 ) " "           "*"
## 11 ( 1 ) " "           "*"
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## 18 ( 1 ) " "           "*"
## 19 ( 1 ) " "           "*"
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## 22 ( 1 ) " "           "*"

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## 77  ( 1 ) "*"          "*"
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## 5  ( 1 ) " "          "*"
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## 7  ( 1 ) " "          "*"
## 8  ( 1 ) " "          "*"
## 9  ( 1 ) " "          "*"
## 10 ( 1 ) " "          "*"
## 11 ( 1 ) " "          "*"
## 12 ( 1 ) " "          "*"
## 13 ( 1 ) " "          "*"
## 14 ( 1 ) " "          "*"
## 15 ( 1 ) " "          "*"
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## 17 ( 1 ) " "          "*"
## 18 ( 1 ) " "          "*"
## 19 ( 1 ) " "          "*"
## 20 ( 1 ) " "          "*"
## 21 ( 1 ) " "          "*"
## 22 ( 1 ) " "          "*"
## 23 ( 1 ) " "          "*"
## 24 ( 1 ) " "          "*"
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## 26 ( 1 ) " "          "*"
## 27 ( 1 ) " "          "*"
## 28 ( 1 ) " "          "*"
## 29 ( 1 ) " "          "*"
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## 32 ( 1 ) " "          "*"
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## 39 ( 1 ) "*"          "*"
## 40 ( 1 ) "*"          "*"
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## 42 ( 1 ) "*"          "*"
## 43 ( 1 ) "*"          "*"
## 44 ( 1 ) "*"          "*"
## 45 ( 1 ) "*"          "*"
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## 48 ( 1 ) "*"          "*"
## 49 ( 1 ) "*"          "*"
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## 51 ( 1 ) "*"          "*"

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## 62  ( 1 ) "*"          "*"
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## 65  ( 1 ) "*"          "*"
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## 69  ( 1 ) "*"          "*"
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## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
## 78  ( 1 ) "*"          "*"
##           entropy_ElectronAffinity wtd_entropy_ElectronAffinity
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "
## 11 ( 1 ) " "          " "
## 12 ( 1 ) " "          " "
## 13 ( 1 ) " "          " "
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## 16 ( 1 ) " "          " "
## 17 ( 1 ) " "          " "
## 18 ( 1 ) " "          " "
## 19 ( 1 ) " "          " "
## 20 ( 1 ) " "          " "
## 21 ( 1 ) " "          " "
## 22 ( 1 ) " "          " "
## 23 ( 1 ) " "          " "
## 24 ( 1 ) " "          " "
## 25 ( 1 ) " "          " "
## 26 ( 1 ) " "          " "

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## 73  ( 1 ) "*"
## 74  ( 1 ) "*"
## 75  ( 1 ) "*"
## 76  ( 1 ) "*"
## 77  ( 1 ) "*"
## 78  ( 1 ) "*"
##          range_ElectronAffinity wtd_range_ElectronAffinity
## 1  ( 1 ) " "

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## 9  ( 1 )   "*" 
## 10 ( 1 )   "*" 
## 11 ( 1 )   "*" 
## 12 ( 1 )   "*" 
## 13 ( 1 )   "*" 
## 14 ( 1 )   "*" 
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## 22 ( 1 )   "*" 
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## 27 ( 1 )   "*" 
## 28 ( 1 )   "*" 
## 29 ( 1 )   "*" 
## 30 ( 1 )   "*" 
## 31 ( 1 )   "*" 
## 32 ( 1 )   "*" 
## 33 ( 1 )   "*" 
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## 42 ( 1 )   "*" 
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## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   "*" 
## 48 ( 1 )   "*" 
## 49 ( 1 )   "*"
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## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"

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## 60  ( 1 ) "*"      "*"
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## 62  ( 1 ) "*"      "*"
## 63  ( 1 ) "*"      "*"
## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
## 67  ( 1 ) "*"      "*"
## 68  ( 1 ) "*"      "*"
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## 70  ( 1 ) "*"      "*"
## 71  ( 1 ) "*"      "*"
## 72  ( 1 ) "*"      "*"
## 73  ( 1 ) "*"      "*"
## 74  ( 1 ) "*"      "*"
## 75  ( 1 ) "*"      "*"
## 76  ( 1 ) "*"      "*"
## 77  ( 1 ) "*"      "*"
## 78  ( 1 ) "*"      "*"
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## 2  ( 1 ) " "        " "        " "
## 3  ( 1 ) " "        " "        " "
## 4  ( 1 ) " "        " "        " "
## 5  ( 1 ) " "        " "        " "
## 6  ( 1 ) " "        " "        " "
## 7  ( 1 ) " "        " "        " "
## 8  ( 1 ) " "        " "        " "
## 9  ( 1 ) "*"      "*"      ""
## 10 ( 1 ) "*"      "*"      ""
## 11 ( 1 ) "*"      "*"      ""
## 12 ( 1 ) "*"      "*"      ""
## 13 ( 1 ) "*"      "*"      ""
## 14 ( 1 ) "*"      "*"      ""
## 15 ( 1 ) "*"      "*"      ""
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## 18 ( 1 ) "*"      "*"      ""
## 19 ( 1 ) "*"      "*"      ""
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## 22 ( 1 ) "*"      "*"      ""
## 23 ( 1 ) "*"      "*"      ""
## 24 ( 1 ) "*"      "*"      ""
## 25 ( 1 ) "*"      "*"      ""
## 26 ( 1 ) "*"      "*"      ""
## 27 ( 1 ) "*"      "*"      ""
## 28 ( 1 ) "*"      "*"      ""
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## 30 ( 1 ) "*"      "*"      ""

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## 42  ( 1 ) "*"          "*"
## 43  ( 1 ) "*"          "*"
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## 45  ( 1 ) "*"          "*"
## 46  ( 1 ) "*"          "*"
## 47  ( 1 ) "*"          "*"
## 48  ( 1 ) "*"          "*"
## 49  ( 1 ) "*"          "*"
## 50  ( 1 ) "*"          "*"
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## 59  ( 1 ) "*"          "*"
## 60  ( 1 ) "*"          "*"
## 61  ( 1 ) "*"          "*"
## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
## 66  ( 1 ) "*"          "*"
## 67  ( 1 ) "*"          "*"
## 68  ( 1 ) "*"          "*"
## 69  ( 1 ) "*"          "*"
## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"
## 72  ( 1 ) "*"          "*"
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## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
## 78  ( 1 ) "*"          "*"
##                               wtd_mean_FusionHeat gmean_FusionHeat wtd_gmean_FusionHeat
## 1  ( 1 ) " "           " "           " "
## 2  ( 1 ) " "           " "           " "
## 3  ( 1 ) " "           " "           " "
## 4  ( 1 ) " "           " "           " "
## 5  ( 1 ) " "           " "           " "

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## 22 ( 1 )   " "
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## 29 ( 1 )   " "
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## 34 ( 1 )   " "
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## 55 ( 1 )   "*"
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## 57 ( 1 )   "*"
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## 59 ( 1 )   "*"

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##          entropy_FusionHeat wtd_entropy_FusionHeat range_FusionHeat
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## 4  ( 1 ) " "      " "      " "
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## 7  ( 1 ) " "      " "      " "
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## 29 ( 1 ) " "      "*"      "*"
## 30 ( 1 ) " "      "*"      "*"
## 31 ( 1 ) " "      "*"      "*"
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## 34 ( 1 ) " "      "*"      "*"

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## 42 ( 1 ) " "      "*"      "*"
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## 77 ( 1 ) "*"      "*"      "*"
## 78 ( 1 ) "*"      "*"      "*"
##          wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
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## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "
## 6 ( 1 ) " "      " "      " "
## 7 ( 1 ) " "      " "      " "
## 8 ( 1 ) " "      " "      " "
## 9 ( 1 ) " "      " "      " "

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## 59  ( 1 ) "*"
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## 61  ( 1 ) "*"
## 62  ( 1 ) "*"
## 63  ( 1 ) "*"

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## 71  ( 1 ) "*"          " *"         "*"
## 72  ( 1 ) "*"          " *"         "*"
## 73  ( 1 ) "*"          " *"         "*"
## 74  ( 1 ) "*"          " *"         "*"
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## 77  ( 1 ) "*"          " *"         "*"
## 78  ( 1 ) "*"          " *"         "*"
##               mean_ThermalConductivity wtd_mean_ThermalConductivity
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## 2   ( 1 ) " "          "*"          "*"
## 3   ( 1 ) " "          "*"          "*"
## 4   ( 1 ) " "          "*"          "*"
## 5   ( 1 ) " "          "*"          "*"
## 6   ( 1 ) " "          "*"          "*"
## 7   ( 1 ) " "          "*"          "*"
## 8   ( 1 ) " "          "*"          "*"
## 9   ( 1 ) " "          "*"          "*"
## 10  ( 1 ) " "          "*"          "*"
## 11  ( 1 ) " "          "*"          "*"
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## 14  ( 1 ) " "          "*"          "*"
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## 18  ( 1 ) " "          "*"          "*"
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## 21  ( 1 ) " "          "*"          "*"
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## 23  ( 1 ) " "          "*"          "*"
## 24  ( 1 ) " "          "*"          "*"
## 25  ( 1 ) " "          "*"          "*"
## 26  ( 1 ) " "          "*"          "*"
## 27  ( 1 ) "*"          "*"          "*"
## 28  ( 1 ) "*"          "*"          "*"
## 29  ( 1 ) "*"          "*"          "*"
## 30  ( 1 ) "*"          "*"          "*"
## 31  ( 1 ) "*"          "*"          "*"
## 32  ( 1 ) "*"          "*"          "*"
## 33  ( 1 ) "*"          "*"          "*"
## 34  ( 1 ) "*"          "*"          "*"
## 35  ( 1 ) "*"          "*"          "*"
## 36  ( 1 ) "*"          "*"          "*"
## 37  ( 1 ) "*"          "*"          "*"
## 38  ( 1 ) "*"          "*"          "*"

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## 39  ( 1 ) "*"      "*"
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## 48  ( 1 ) "*"      "*"
## 49  ( 1 ) "*"      "*"
## 50  ( 1 ) "*"      "*"
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## 53  ( 1 ) "*"      "*"
## 54  ( 1 ) "*"      "*"
## 55  ( 1 ) "*"      "*"
## 56  ( 1 ) "*"      "*"
## 57  ( 1 ) "*"      "*"
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## 61  ( 1 ) "*"      "*"
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## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
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## 68  ( 1 ) "*"      "*"
## 69  ( 1 ) "*"      "*"
## 70  ( 1 ) "*"      "*"
## 71  ( 1 ) "*"      "*"
## 72  ( 1 ) "*"      "*"
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## 75  ( 1 ) "*"      "*"
## 76  ( 1 ) "*"      "*"
## 77  ( 1 ) "*"      "*"
## 78  ( 1 ) "*"      "*"
##          gmean_ThermalConductivity wtd_gmean_ThermalConductivity
## 1  ( 1 ) " "        " "
## 2  ( 1 ) " "        "*"
## 3  ( 1 ) " "        "*"
## 4  ( 1 ) " "        "*"
## 5  ( 1 ) " "        "*"
## 6  ( 1 ) " "        "*"
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## 13 ( 1 ) " "        "*"

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## 24  ( 1 ) " "      "*"
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## 28  ( 1 ) " "      "*"
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## 30  ( 1 ) " "      "*"
## 31  ( 1 ) " "      "*"
## 32  ( 1 ) " "      "*"
## 33  ( 1 ) " "      "*"
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## 36  ( 1 ) " "      "*"
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## 49  ( 1 ) " "      "*"
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## 51  ( 1 ) " "      "*"
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## 53  ( 1 ) " "      "*"
## 54  ( 1 ) " "      "*"
## 55  ( 1 ) " "      "*"
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## 62  ( 1 ) " "      "*"
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## 77  ( 1 ) "*"          "*"
## 78  ( 1 ) "*"          "*"
##           entropy_ThermalConductivity wtd_entropy_ThermalConductivity
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## 3  ( 1 ) " "          " "
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## 37 ( 1 ) "*"          " "
## 38 ( 1 ) "*"          " "
## 39 ( 1 ) "*"          " "
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## 42 ( 1 ) "*"          " "

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## 56  ( 1 ) "*"          " "
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## 59  ( 1 ) "*"          " "
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## 74  ( 1 ) "*"          " "
## 75  ( 1 ) "*"          " "
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##           range_ThermalConductivity wtd_range_ThermalConductivity
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## 3  ( 1 ) " "                  " "
## 4  ( 1 ) " "                  " "
## 5  ( 1 ) " "                  " "
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## 17 ( 1 ) " "                  " "

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## 70 ( 1 ) "*"
## 71 ( 1 ) "*"

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## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
## 78  ( 1 ) "*"          "*"
##           std_ThermalConductivity wtd_std_ThermalConductivity mean_Valence
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## 3  ( 1 ) " "          " "          " "
## 4  ( 1 ) " "          " "          " "
## 5  ( 1 ) " "          " "          " "
## 6  ( 1 ) " "          " "          " "
## 7  ( 1 ) " "          " "          " "
## 8  ( 1 ) " "          " "          " "
## 9  ( 1 ) " "          " "          " "
## 10 ( 1 ) " "          " "          " "
## 11 ( 1 ) " "          " "          " "
## 12 ( 1 ) " "          " "          " "
## 13 ( 1 ) " "          " "          " "
## 14 ( 1 ) " "          " "          " "
## 15 ( 1 ) " "          " "          " "
## 16 ( 1 ) " "          " "          " "
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## 20 ( 1 ) " "          " "          " "
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## 22 ( 1 ) " "          " "          " "
## 23 ( 1 ) " "          " "          " "
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## 27 ( 1 ) " "          " "          " "
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## 32 ( 1 ) "*"          " "          " "
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## 34 ( 1 ) "*"          " "          " "
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## 42 ( 1 ) "*"          " "          " "
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## 45 ( 1 ) "*"          " "          " "
## 46 ( 1 ) "*"          " "          " "

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## 74  ( 1 ) "*"
## 75  ( 1 ) "*"
## 76  ( 1 ) "*"
## 77  ( 1 ) "*"
## 78  ( 1 ) "*"
##          wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
## 1  ( 1 ) " "           " "           " "           " "
## 2  ( 1 ) " "           " "           " "           " "
## 3  ( 1 ) " "           " "           " "           " "
## 4  ( 1 ) " "           " "           " "           " "
## 5  ( 1 ) " "           " "           " "           " "
## 6  ( 1 ) " "           " "           " "           " "
## 7  ( 1 ) " "           " "           " "           " "
## 8  ( 1 ) " "           " "           " "           " "
## 9  ( 1 ) " "           " "           " "           " "
## 10 ( 1 ) " "           " "           " "           " "
## 11 ( 1 ) " "           " "           " "           " "
## 12 ( 1 ) " "           " "           " "           " "
## 13 ( 1 ) " "           " "           " "           " "
## 14 ( 1 ) " "           " "           " "           " "
## 15 ( 1 ) " "           " "           " "           " "
## 16 ( 1 ) " "           " "           " "           " "
## 17 ( 1 ) " "           " "           " "           " "
## 18 ( 1 ) " "           " "           " "           " "
## 19 ( 1 ) " "           " "           " "           " "
## 20 ( 1 ) " "           " "           " "           " "
## 21 ( 1 ) " "           " "           " "           " "

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## 74 ( 1 ) "*"
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## 77  ( 1 ) "*"      "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"      "*"
##          wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
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## 2  ( 1 ) " "       " "       " "       " "
## 3  ( 1 ) " "       " "       " "       " "
## 4  ( 1 ) " "       " "       " "       " "
## 5  ( 1 ) " "       " "       " "       " "
## 6  ( 1 ) " "       " "       " "       " "
## 7  ( 1 ) " "       " "       " "       " "
## 8  ( 1 ) " "       " "       " "       " "
## 9  ( 1 ) " "       " "       " "       " "
## 10 ( 1 ) " "       " "       " "       " "
## 11 ( 1 ) " "       " "       " "       " "
## 12 ( 1 ) " "       " "       " "       " "
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## 14 ( 1 ) "*"      "*"      "*"      "*"
## 15 ( 1 ) "*"      "*"      "*"      "*"
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## 18 ( 1 ) "*"      "*"      "*"      "*"
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## 24 ( 1 ) "*"      "*"      "*"      "*"
## 25 ( 1 ) "*"      "*"      "*"      "*"
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## 27 ( 1 ) "*"      "*"      "*"      "*"
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## 29 ( 1 ) "*"      "*"      "*"      "*"
## 30 ( 1 ) "*"      "*"      "*"      "*"
## 31 ( 1 ) "*"      "*"      "*"      "*"
## 32 ( 1 ) "*"      "*"      "*"      "*"
## 33 ( 1 ) "*"      "*"      "*"      "*"
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## 47 ( 1 ) "*"      "*"      "*"      "*"
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## 72  ( 1 ) "*"      "*"      " "      "*"
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## 77  ( 1 ) "*"      "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"      "*"
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## 72 ( 1 ) "*"
## 73 ( 1 ) "*"
## 74 ( 1 ) "*"
## 75 ( 1 ) "*"
## 76 ( 1 ) "*"
## 77 ( 1 ) "*"
## 78 ( 1 ) "*"
```

```
linear_backward$results
```

```
##      nvmax      RMSE   Rsquared      MAE     RMSESD   RsquaredSD     MAESD
## 1      1 32.04370 0.1259774 26.23693 0.5293090 0.015268471 0.6209199
## 2      2 22.84632 0.5550393 17.11527 0.3812094 0.012850961 0.3062085
## 3      3 22.25954 0.5776231 16.95775 0.3518940 0.012114431 0.4069670
## 4      4 21.63083 0.6012075 16.57540 0.2284447 0.008563008 0.3041260
## 5      5 21.04027 0.6227036 16.15896 0.2104071 0.008755214 0.2297206
## 6      6 20.70922 0.6345370 15.98279 0.2303307 0.009607904 0.2184908
## 7      7 20.54310 0.6403451 15.82721 0.2719419 0.010075414 0.3034487
## 8      8 20.18288 0.6528629 15.49568 0.2833591 0.010745900 0.2693101
## 9      9 19.93726 0.6612568 15.23782 0.2750239 0.010253651 0.2555308
## 10    10 19.67328 0.6701779 15.05168 0.3359860 0.010908778 0.3400943
## 11    11 19.64001 0.6712413 15.02792 0.3225616 0.011151653 0.3395429
## 12    12 19.49529 0.6760820 14.96450 0.3242160 0.010890476 0.2974578
## 13    13 19.42091 0.6785249 14.90735 0.3085360 0.011480592 0.2813762
## 14    14 19.28507 0.6830167 14.78380 0.2681633 0.009889528 0.2560837
## 15    15 19.20766 0.6855418 14.69870 0.2626109 0.010607768 0.2398646
## 16    16 19.10888 0.6888044 14.59119 0.2457582 0.009322300 0.2206972
## 17    17 19.02699 0.6914326 14.54186 0.2380386 0.009429725 0.2117208
## 18    18 18.90740 0.6953130 14.42028 0.2298510 0.008249558 0.2059086
## 19    19 18.79063 0.6990816 14.29769 0.2578635 0.008502639 0.2484904
## 20    20 18.70297 0.7018859 14.25558 0.2721153 0.008684165 0.2145287
## 21    21 18.64387 0.7037528 14.18880 0.2689917 0.008553147 0.2167572
## 22    22 18.59110 0.7054433 14.16208 0.2684564 0.008458939 0.2333003
## 23    23 18.53664 0.7071837 14.10565 0.2691800 0.008210746 0.2272632
## 24    24 18.47279 0.7091843 14.03604 0.2716846 0.008321046 0.2250023
## 25    25 18.40924 0.7111753 13.96552 0.2730312 0.008152767 0.2428288
## 26    26 18.37433 0.7122687 13.91444 0.2674058 0.008237241 0.2459362
## 27    27 18.34188 0.7132921 13.91976 0.2746972 0.008260699 0.2328116
## 28    28 18.30845 0.7143250 13.89630 0.2799699 0.008866682 0.2172049
## 29    29 18.28064 0.7151940 13.90180 0.2744790 0.008968860 0.2232293
## 30    30 18.25919 0.7158646 13.86344 0.2734955 0.009228300 0.2283895
## 31    31 18.21975 0.7170880 13.82704 0.2773012 0.009371472 0.2476062
## 32    32 18.19227 0.7179276 13.80069 0.2834154 0.010001255 0.2338019
## 33    33 18.16462 0.7187800 13.77775 0.2648390 0.009601664 0.2259876
## 34    34 18.12900 0.7198844 13.75282 0.2850531 0.009916318 0.2368309
## 35    35 18.08792 0.7211439 13.73005 0.2779006 0.009625977 0.2358588
## 36    36 18.04099 0.7225809 13.67242 0.2830633 0.009622474 0.2192928
## 37    37 18.01046 0.7235063 13.63895 0.2968948 0.010000245 0.2107823
## 38    38 18.00143 0.7237812 13.62136 0.3027572 0.010143568 0.2296614
## 39    39 17.96221 0.7249849 13.59648 0.3024769 0.009975409 0.2204579
## 40    40 17.94219 0.7256007 13.58345 0.3084305 0.009938407 0.2271195
## 41    41 17.91672 0.7263807 13.56194 0.3048014 0.009943000 0.2234136
## 42    42 17.91219 0.7265143 13.55827 0.3033487 0.009892143 0.2256655
## 43    43 17.89342 0.7270822 13.54212 0.3070081 0.010122759 0.2241666
## 44    44 17.88765 0.7272569 13.53427 0.3077516 0.010143914 0.2205088
## 45    45 17.88111 0.7274592 13.52510 0.3036997 0.010056057 0.2088512
## 46    46 17.86952 0.7278153 13.51434 0.2990745 0.009926464 0.2127944
## 47    47 17.84207 0.7286522 13.49119 0.2985625 0.010052282 0.2135798
## 48    48 17.83220 0.7289562 13.49197 0.3012703 0.009950001 0.2041783
## 49    49 17.81818 0.7293768 13.47349 0.3100333 0.010198648 0.2111786
## 50    50 17.80429 0.7298013 13.46092 0.3110479 0.010188873 0.2082153
```

```

## 51 51 17.79889 0.7299713 13.46132 0.3125565 0.010226526 0.2132501
## 52 52 17.79630 0.7300516 13.45438 0.3043909 0.009976777 0.2125147
## 53 53 17.78537 0.7303801 13.43682 0.3107237 0.010052924 0.2209418
## 54 54 17.78125 0.7305099 13.43706 0.3077205 0.010014043 0.2255542
## 55 55 17.77895 0.7305794 13.43762 0.3157974 0.010171922 0.2272520
## 56 56 17.76579 0.7309744 13.43115 0.3147431 0.010149165 0.2231316
## 57 57 17.76086 0.7311232 13.43153 0.3201159 0.010219043 0.2246484
## 58 58 17.74606 0.7315732 13.42362 0.3154200 0.010216968 0.2210837
## 59 59 17.73961 0.7317685 13.41792 0.3182204 0.010259831 0.2253550
## 60 60 17.74265 0.7316806 13.41612 0.3189908 0.010253665 0.2271744
## 61 61 17.73900 0.7317903 13.40641 0.3187515 0.010199545 0.2289514
## 62 62 17.73386 0.7319472 13.40056 0.3177765 0.010171357 0.2293579
## 63 63 17.73004 0.7320637 13.39269 0.3127838 0.010046913 0.2266843
## 64 64 17.72654 0.7321666 13.39183 0.3114044 0.009971024 0.2256489
## 65 65 17.72540 0.7322007 13.39279 0.3132001 0.010064323 0.2220137
## 66 66 17.72612 0.7321821 13.39471 0.3134649 0.010026958 0.2212111
## 67 67 17.72490 0.7322217 13.39840 0.3110997 0.010009508 0.2192199
## 68 68 17.72364 0.7322584 13.40135 0.3121553 0.010045983 0.2185761
## 69 69 17.72106 0.7323354 13.40284 0.3099024 0.009965874 0.2195442
## 70 70 17.72079 0.7323431 13.40456 0.3085339 0.009920888 0.2190536
## 71 71 17.72111 0.7323369 13.40535 0.3089338 0.009917466 0.2206867
## 72 72 17.71934 0.7323897 13.40732 0.3085702 0.009925944 0.2184024
## 73 73 17.71436 0.7325388 13.40433 0.3125969 0.010013715 0.2197020
## 74 74 17.71252 0.7325947 13.40236 0.3122025 0.010003304 0.2240391
## 75 75 17.71121 0.7326352 13.40159 0.3120241 0.009999614 0.2238718
## 76 76 17.71124 0.7326353 13.40111 0.3104409 0.009949036 0.2220569
## 77 77 17.71062 0.7326550 13.40286 0.3110048 0.009960783 0.2216944
## 78 78 17.71047 0.7326597 13.40466 0.3108979 0.009931172 0.2222802
## 79 79 17.71093 0.7326458 13.40426 0.3124002 0.009950355 0.2239246
## 80 80 17.71097 0.7326450 13.40313 0.3117693 0.009931926 0.2223707
## 81 81 17.71082 0.7326498 13.40288 0.3121764 0.009942553 0.2221992

```

From the above results, we can see how backward selection works and the corresponding errors to the number of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_backward, linear_backward$results$nvmax, "Number of Variables")
```

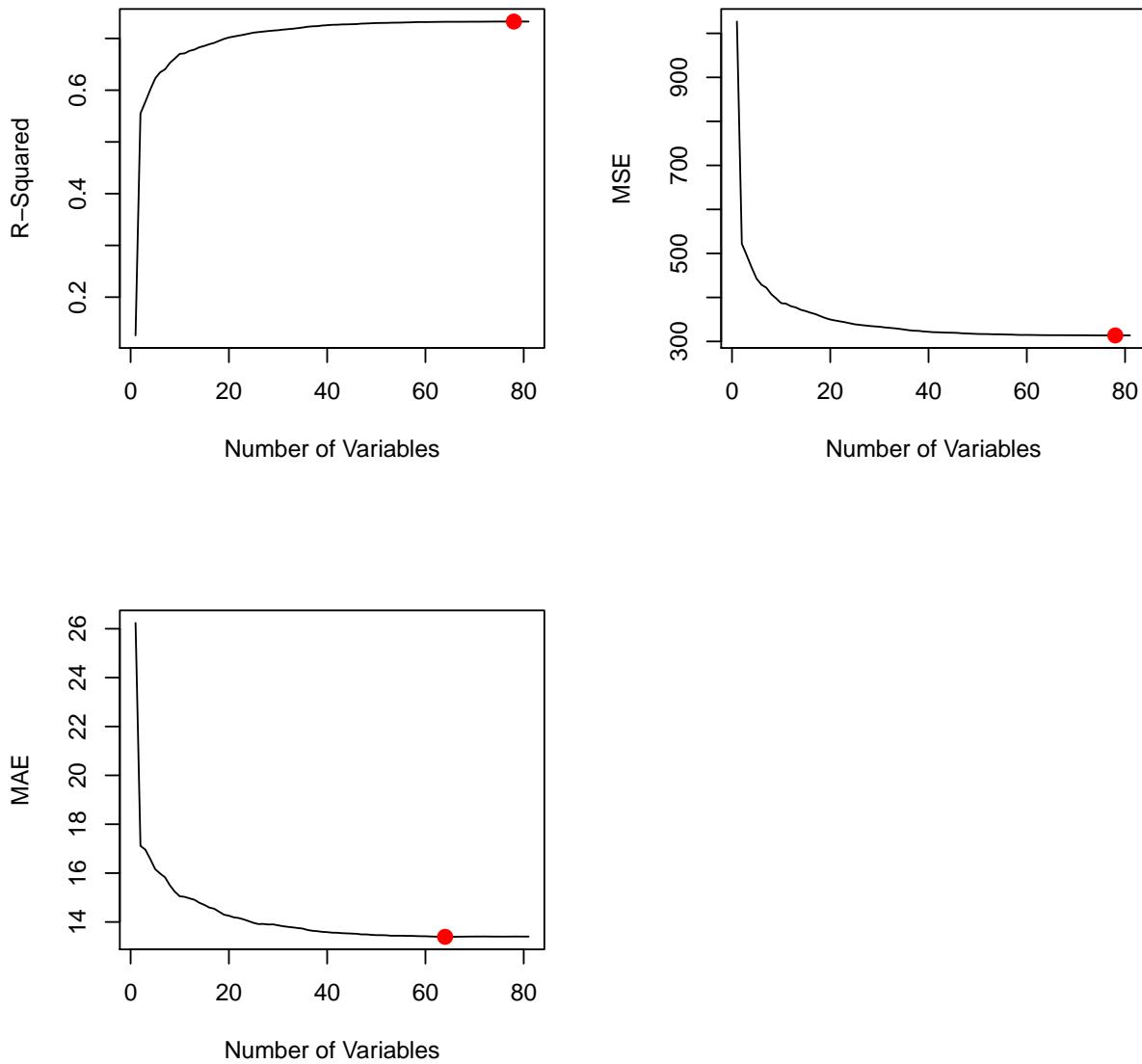


Figure 45: R-Squared, MSE, and MAE for Backward Selection

```
linear_backward$bestTune
```

```
##      nvmax
## 78      78
```

```
coef(linear_backward$finalModel, linear_backward$bestTune$nvmax)
```

```
##                               (Intercept)          number_of_elements
##                               -11.573639                  -28.994327
## mean_atomic_mass           wtd_mean_atomic_mass
```

```

##          184.472235          -205.004368
##      gmean_atomic_mass          156.258740
##          -115.910930          range_atomic_mass
##      entropy_atomic_mass          -71.933596          44.836116
##          -71.933596          std_atomic_mass
##      wtd_range_atomic_mass          3.393727          -59.756620
##          3.393727          mean_fie
##      wtd_std_atomic_mass          12.227349          129.879147
##          12.227349          gmean_fie
##      wtd_mean_fie          -102.078981          -128.906865
##          -102.078981          entropy_fie
##      wtd_gmean_fie          125.673527          -200.848897
##          125.673527          range_fie
##      wtd_entropy_fie          95.674944          81.782496
##          95.674944          std_fie
##      wtd_range_fie          22.448945          -86.111803
##          22.448945          mean_atomic_radius
##      wtd_std_fie          -17.112311          -173.402087
##          -17.112311          gmean_atomic_radius
##      wtd_mean_atomic_radius          830.126939          94.136062
##          830.126939          entropy_atomic_radius
##      wtd_gmean_atomic_radius          -738.395644          119.182515
##          -738.395644          range_atomic_radius
##      wtd_entropy_atomic_radius          88.132979          52.648872
##          88.132979          std_atomic_radius
##      wtd_range_atomic_radius          -19.957122          -42.884823
##          -19.957122          mean_Density
##      wtd_std_atomic_radius          -33.051235          -107.697319
##          -33.051235          wtd_gmean_Density
##          gmean_Density          25.837185          47.361322
##          25.837185          wtd_entropy_Density
##          entropy_Density          34.858855          -30.384036
##          34.858855          std_Density
##          range_Density          -35.881233          65.554275
##          -35.881233          mean_ElectronAffinity
##          wtd_std_Density          -15.820461          -32.255578
##          -15.820461          gmean_ElectronAffinity
##          wtd_mean_ElectronAffinity          160.886379          52.338272
##          160.886379          entropy_ElectronAffinity
##          wtd_gmean_ElectronAffinity          -175.911012          10.325925
##          -175.911012          range_ElectronAffinity
##          wtd_entropy_ElectronAffinity          -35.935453          -129.921412
##          -35.935453          std_ElectronAffinity
##          wtd_range_ElectronAffinity          -32.401748          206.826315
##          -32.401748          mean_FusionHeat
##          wtd_std_ElectronAffinity          -95.196041          177.580572
##          -95.196041          gmean_FusionHeat
##          wtd_mean_FusionHeat          -210.000808          -160.078416
##          -210.000808          entropy_FusionHeat
##          wtd_gmean_FusionHeat          177.505527          -38.923036
##          177.505527          range_FusionHeat
##          wtd_entropy_FusionHeat          43.226668          -35.872753
##          43.226668          std_FusionHeat

```

```

##                               60.480150          -33.446042
##             wtd_std_FusionHeat      mean_ThermalConductivity
##                               42.543723          -33.957300
##     wtd_mean_ThermalConductivity gmean_ThermalConductivity
##                               236.187912          -9.714436
##     wtd_gmean_ThermalConductivity entropy_ThermalConductivity
##                               -143.251700          21.701053
## wtd_entropy_ThermalConductivity range_ThermalConductivity
##                               2.923127          -38.885095
##     wtd_range_ThermalConductivity std_ThermalConductivity
##                               -89.846540          67.466499
##     wtd_std_ThermalConductivity   mean_Valence
##                               -8.419764          -96.602062
##             wtd_mean_Valence      gmean_Valence
##                               149.205486          122.345524
##             wtd_gmean_Valence      entropy_Valence
##                               -172.387557          146.008439
##     wtd_entropy_Valence        range_Valence
##                               -140.787489          25.402219
##     wtd_range_Valence         std_Valence
##                               -6.655578          23.555227
##     wtd_std_Valence
##                               -75.103338

```

```
getTrainPerf(linear_backward)
```

```

##   TrainRMSE TrainRsquared TrainMAE      method
## 1  17.71047    0.7326597 13.40466 leapBackward

```

From the above metrics, it can be seen that based on R-Squared and MSE, the best model is the model with 78 variables, however, MAE choose a model with less variables. By using the feature from caret package, we can decide that the best model is the model with 78 variables. The list of 78 variables is provided above. The R-Squared for this model is 0.7326597 with Train MSE is 313.66.

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_backward, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

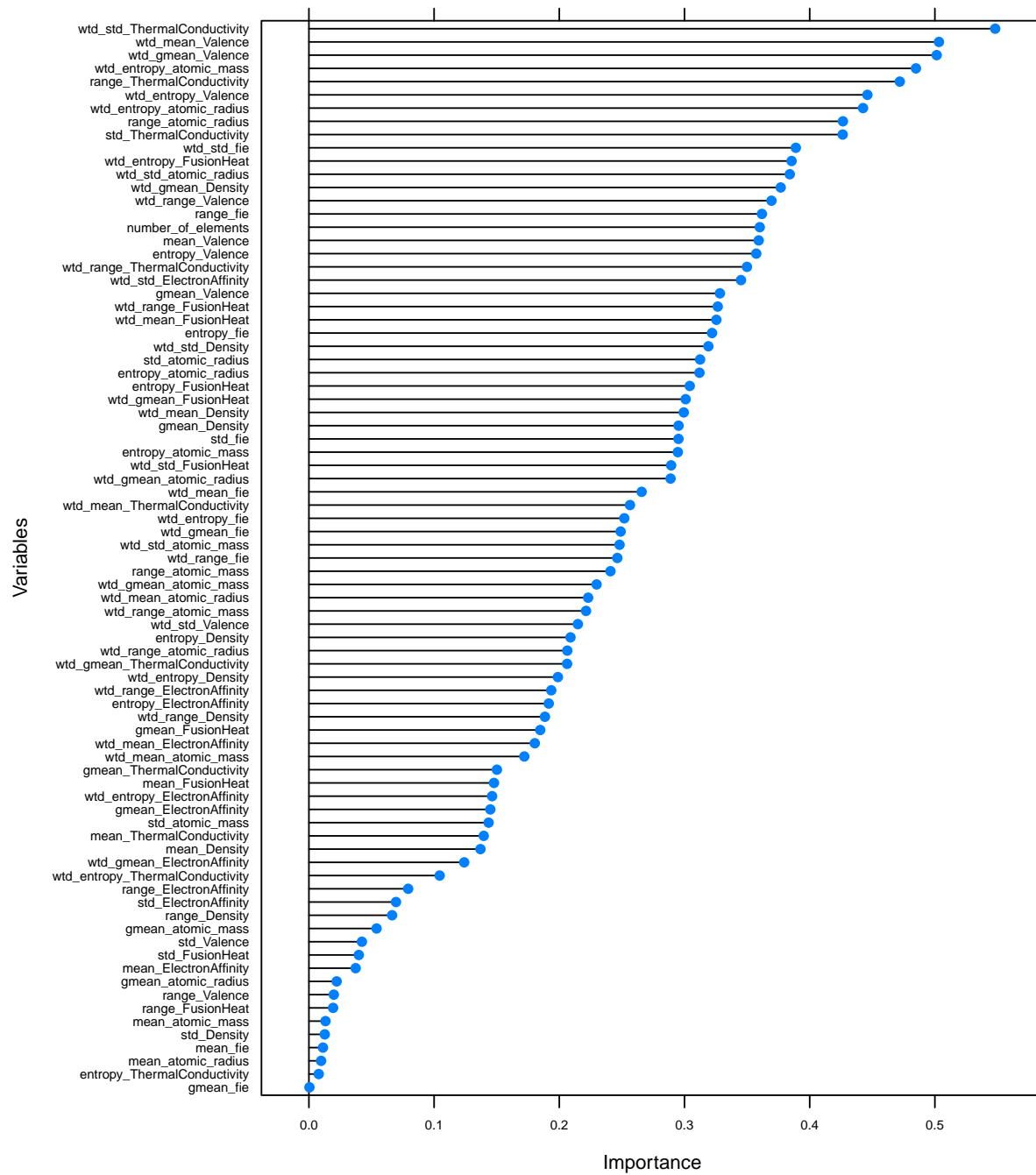


Figure 46: Variable Importance for Backward Selection

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.1.5 Linear Regression with Forward Selection

In this sub section, we will perform the forward selection and in the next subsection, we will perform stepwise selection.

```
set.seed(seed)

# Linear Regression with Forward Selection
linear_forward <- train(critical_temp ~., data = train.data,
                        method = "leapForward",
                        tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
                        trControl = control,
                        preProc = c("range")
)
summary(linear_forward)

## Subset selection object
## 81 Variables  (and intercept)
##                                     Forced in    Forced out
## number_of_elements                 FALSE      FALSE
## mean_atomic_mass                  FALSE      FALSE
## wtd_mean_atomic_mass              FALSE      FALSE
## gmean_atomic_mass                FALSE      FALSE
## wtd_gmean_atomic_mass             FALSE      FALSE
## entropy_atomic_mass               FALSE      FALSE
## wtd_entropy_atomic_mass           FALSE      FALSE
## range_atomic_mass                 FALSE      FALSE
## wtd_range_atomic_mass              FALSE      FALSE
## std_atomic_mass                  FALSE      FALSE
## wtd_std_atomic_mass               FALSE      FALSE
## mean_fie                         FALSE      FALSE
## wtd_mean_fie                     FALSE      FALSE
## gmean_fie                        FALSE      FALSE
## wtd_gmean_fie                    FALSE      FALSE
## entropy_fie                      FALSE      FALSE
## wtd_entropy_fie                  FALSE      FALSE
## range_fie                        FALSE      FALSE
## wtd_range_fie                    FALSE      FALSE
## std_fie                          FALSE      FALSE
## wtd_std_fie                      FALSE      FALSE
## mean_atomic_radius                FALSE      FALSE
## wtd_mean_atomic_radius            FALSE      FALSE
## gmean_atomic_radius               FALSE      FALSE
## wtd_gmean_atomic_radius           FALSE      FALSE
## entropy_atomic_radius             FALSE      FALSE
## wtd_entropy_atomic_radius         FALSE      FALSE
## range_atomic_radius               FALSE      FALSE
## wtd_range_atomic_radius           FALSE      FALSE
## std_atomic_radius                 FALSE      FALSE
## wtd_std_atomic_radius             FALSE      FALSE
## mean_Density                      FALSE      FALSE
## wtd_mean_Density                  FALSE      FALSE
## gmean_Density                     FALSE      FALSE
## wtd_gmean_Density                 FALSE      FALSE
```

```

## entropy_Density           FALSE  FALSE
## wtd_entropy_Density       FALSE  FALSE
## range_Density             FALSE  FALSE
## wtd_range_Density         FALSE  FALSE
## std_Density               FALSE  FALSE
## wtd_std_Density           FALSE  FALSE
## mean_ElectronAffinity    FALSE  FALSE
## wtd_mean_ElectronAffinity FALSE  FALSE
## gmean_ElectronAffinity   FALSE  FALSE
## wtd_gmean_ElectronAffinity FALSE  FALSE
## entropy_ElectronAffinity FALSE  FALSE
## wtd_entropy_ElectronAffinity FALSE  FALSE
## range_ElectronAffinity   FALSE  FALSE
## wtd_range_ElectronAffinity FALSE  FALSE
## std_ElectronAffinity     FALSE  FALSE
## wtd_std_ElectronAffinity  FALSE  FALSE
## mean_FusionHeat           FALSE  FALSE
## wtd_mean_FusionHeat        FALSE  FALSE
## gmean_FusionHeat          FALSE  FALSE
## wtd_gmean_FusionHeat      FALSE  FALSE
## entropy_FusionHeat        FALSE  FALSE
## wtd_entropy_FusionHeat    FALSE  FALSE
## range_FusionHeat          FALSE  FALSE
## wtd_range_FusionHeat       FALSE  FALSE
## std_FusionHeat             FALSE  FALSE
## wtd_std_FusionHeat         FALSE  FALSE
## mean_ThermalConductivity  FALSE  FALSE
## wtd_mean_ThermalConductivity FALSE  FALSE
## gmean_ThermalConductivity FALSE  FALSE
## wtd_gmean_ThermalConductivity FALSE  FALSE
## entropy_ThermalConductivity FALSE  FALSE
## wtd_entropy_ThermalConductivity FALSE  FALSE
## range_ThermalConductivity FALSE  FALSE
## wtd_range_ThermalConductivity FALSE  FALSE
## std_ThermalConductivity   FALSE  FALSE
## wtd_std_ThermalConductivity FALSE  FALSE
## mean_Valence               FALSE  FALSE
## wtd_mean_Valence           FALSE  FALSE
## gmean_Valence              FALSE  FALSE
## wtd_gmean_Valence          FALSE  FALSE
## entropy_Valence            FALSE  FALSE
## wtd_entropy_Valence        FALSE  FALSE
## range_Valence              FALSE  FALSE
## wtd_range_Valence          FALSE  FALSE
## std_Valence                FALSE  FALSE
## wtd_std_Valence            FALSE  FALSE
## 1 subsets of each size up to 77
## Selection Algorithm: forward
##          number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1  ( 1 )    " "           " "           " "
## 2  ( 1 )    " "           " "           " "
## 3  ( 1 )    " "           " "           " "
## 4  ( 1 )    " "           " "           " "
## 5  ( 1 )    " "           " "           " "

```



```

## 60  ( 1 ) " "      " "
## 61  ( 1 ) " "      "*" "
## 62  ( 1 ) " "      "*" "
## 63  ( 1 ) " "      "*" "
## 64  ( 1 ) " "      "*" "
## 65  ( 1 ) " "      "*" "
## 66  ( 1 ) " "      "*" "
## 67  ( 1 ) " "      "*" "
## 68  ( 1 ) "*" "
## 69  ( 1 ) "*" "
## 70  ( 1 ) "*" "
## 71  ( 1 ) "*" "
## 72  ( 1 ) "*" "
## 73  ( 1 ) "*" "
## 74  ( 1 ) "*" "
## 75  ( 1 ) "*" "
## 76  ( 1 ) "*" "
## 77  ( 1 ) "*" "
##          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1  ( 1 ) " "      " "      " "
## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      " "
## 20 ( 1 ) " "      " "      " "
## 21 ( 1 ) " "      " "      " "
## 22 ( 1 ) " "      " "      " "
## 23 ( 1 ) " "      " "      " "
## 24 ( 1 ) " "      " "      "*"
## 25 ( 1 ) " "      " "      "*"
## 26 ( 1 ) " "      " "      "*"
## 27 ( 1 ) " "      " "      "*"
## 28 ( 1 ) " "      " "      "*"
## 29 ( 1 ) " "      " "      "*"
## 30 ( 1 ) " "      " "      "*"
## 31 ( 1 ) " "      " "      "*"
## 32 ( 1 ) " "      " "      "*"
## 33 ( 1 ) " "      " "      "*"
## 34 ( 1 ) " "      " "      "*"
## 35 ( 1 ) " "      " "      "*"

```

```

## 36 ( 1 ) " "      " "      "*"
## 37 ( 1 ) " "      " "      "*"
## 38 ( 1 ) " "      " "      "*"
## 39 ( 1 ) " "      " "      "*"
## 40 ( 1 ) " "      " "      "*"
## 41 ( 1 ) " "      " "      "*"
## 42 ( 1 ) " "      " "      "*"
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## 44 ( 1 ) " "      " "      "*"
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## 48 ( 1 ) " "      " "      "*"
## 49 ( 1 ) " "      " "      "*"
## 50 ( 1 ) " "      " "      "*"
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## 52 ( 1 ) " "      " "      "*"
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## 54 ( 1 ) " "      " "      "*"
## 55 ( 1 ) " "      " "      "*"
## 56 ( 1 ) " "      " "      "*"
## 57 ( 1 ) "*"     " "      "*"
## 58 ( 1 ) "*"     " "      "*"
## 59 ( 1 ) "*"     " "      "*"
## 60 ( 1 ) "*"     " "      "*"
## 61 ( 1 ) "*"     " "      "*"
## 62 ( 1 ) "*"     "*"     "*"
## 63 ( 1 ) "*"     "*"     "*"
## 64 ( 1 ) "*"     "*"     "*"
## 65 ( 1 ) "*"     "*"     "*"
## 66 ( 1 ) "*"     "*"     "*"
## 67 ( 1 ) "*"     "*"     "*"
## 68 ( 1 ) "*"     "*"     "*"
## 69 ( 1 ) "*"     "*"     "*"
## 70 ( 1 ) "*"     "*"     "*"
## 71 ( 1 ) "*"     "*"     "*"
## 72 ( 1 ) "*"     "*"     "*"
## 73 ( 1 ) "*"     "*"     "*"
## 74 ( 1 ) "*"     "*"     "*"
## 75 ( 1 ) "*"     "*"     "*"
## 76 ( 1 ) "*"     "*"     "*"
## 77 ( 1 ) "*"     "*"     "*"
##          wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1 ( 1 ) " "      " "      " "
## 2 ( 1 ) " "      " "      " "
## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "
## 6 ( 1 ) " "      " "      " "
## 7 ( 1 ) " "      " "      " "
## 8 ( 1 ) " "      " "      " "
## 9 ( 1 ) " "      " "      " "
## 10 ( 1 ) " "     " "      " "
## 11 ( 1 ) " "     " "      " "

```

```

## 12 ( 1 ) " "
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## 17 ( 1 ) " "
## 18 ( 1 ) " "
## 19 ( 1 ) "*"
## 20 ( 1 ) "*"
## 21 ( 1 ) "*"
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## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 60  ( 1 ) "*"      "*"      "*"
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## 70  ( 1 ) "*"      "*"      "*"
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## 76  ( 1 ) "*"      "*"      "*"
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##          mean_Density wtd_mean_Density gmean_Density wtd_gmean_Density
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## 3  ( 1 ) " "      " "      " "      " "
## 4  ( 1 ) " "      " "      " "      " "
## 5  ( 1 ) " "      " "      " "      " "
## 6  ( 1 ) " "      " "      " "      " "
## 7  ( 1 ) " "      " "      " "      " "
## 8  ( 1 ) " "      " "      " "      " "
## 9  ( 1 ) " "      " "      " "      " "
## 10 ( 1 ) " "      " "      " "      " "
## 11 ( 1 ) " "      " "      " "      " "
## 12 ( 1 ) " "      " "      " "      " "
## 13 ( 1 ) " "      " "      " "      " "
## 14 ( 1 ) " "      " "      " "      " "
## 15 ( 1 ) " "      " "      " "      " "
## 16 ( 1 ) " "      " "      " "      " "
## 17 ( 1 ) " "      " "      " "      " "
## 18 ( 1 ) " "      " "      " "      " "
## 19 ( 1 ) " "      " "      " "      " "
## 20 ( 1 ) " "      " "      " "      " "
## 21 ( 1 ) " "      " "      " "      " "
## 22 ( 1 ) " "      " "      " "      " "
## 23 ( 1 ) " "      " "      " "      " "
## 24 ( 1 ) " "      " "      " "      " "
## 25 ( 1 ) " "      " "      " "      " "
## 26 ( 1 ) " "      " "      " "      " "
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## 32 ( 1 ) " "      " "      " "      " "
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## 3 ( 1 ) " " " " "
## 4 ( 1 ) " " " " "
## 5 ( 1 ) " " " " "
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## 10 ( 1 ) " " " " "
## 11 ( 1 ) " " " " "

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## 65 ( 1 ) "*"

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## 6  ( 1 ) " "      " "      " "
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## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
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## 20 ( 1 ) " "      " "      " "
## 21 ( 1 ) " "      " "      " "
## 22 ( 1 ) " "      " "      " "
## 23 ( 1 ) " "      " "      " "
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## 32 ( 1 ) " "      " "      " "
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## 34 ( 1 ) " "      " "      " "
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## 37 ( 1 ) " "      " "      " "
## 38 ( 1 ) " "      " "      " "
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## 40 ( 1 ) " "      " "      " "
## 41 ( 1 ) " "      " "      " "

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## 74  ( 1 ) " "
## 75  ( 1 ) " "
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## 77  ( 1 ) " "
##               mean_ElectronAffinity wtd_mean_ElectronAffinity
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## 3  ( 1 ) " "           " "
## 4  ( 1 ) " "           " "
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## 6  ( 1 ) " "           " "
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## 9  ( 1 ) " "           "*"
## 10 ( 1 ) " "           "*"
## 11 ( 1 ) " "           "*"
## 12 ( 1 ) " "           "*"
## 13 ( 1 ) " "           "*"
## 14 ( 1 ) " "           "*"
## 15 ( 1 ) " "           "*"
## 16 ( 1 ) " "           "*"
## 17 ( 1 ) " "           "*"

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## 63 ( 1 ) "*"
## 64 ( 1 ) "*"
## 65 ( 1 ) "*"
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## 67 ( 1 ) "*"
## 68 ( 1 ) "*"
## 69 ( 1 ) "*"
## 70 ( 1 ) "*"
## 71 ( 1 ) "*"

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## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
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## 2  ( 1 ) "*"          " "
## 3  ( 1 ) "*"          " "
## 4  ( 1 ) "*"          " "
## 5  ( 1 ) "*"          " "
## 6  ( 1 ) "*"          "*"
## 7  ( 1 ) "*"          "*"
## 8  ( 1 ) "*"          "*"
## 9  ( 1 ) "*"          "*"
## 10 ( 1 ) "*"          "*"
## 11 ( 1 ) "*"          "*"
## 12 ( 1 ) "*"          "*"
## 13 ( 1 ) "*"          "*"
## 14 ( 1 ) "*"          "*"
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## 17 ( 1 ) "*"          "*"
## 18 ( 1 ) "*"          "*"
## 19 ( 1 ) "*"          "*"
## 20 ( 1 ) "*"          "*"
## 21 ( 1 ) "*"          "*"
## 22 ( 1 ) "*"          "*"
## 23 ( 1 ) "*"          "*"
## 24 ( 1 ) "*"          "*"
## 25 ( 1 ) "*"          "*"
## 26 ( 1 ) "*"          "*"
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## 35 ( 1 ) "*"          "*"
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## 38 ( 1 ) "*"          "*"
## 39 ( 1 ) "*"          "*"
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## 41 ( 1 ) "*"          "*"
## 42 ( 1 ) "*"          "*"
## 43 ( 1 ) "*"          "*"
## 44 ( 1 ) "*"          "*"
## 45 ( 1 ) "*"          "*"
## 46 ( 1 ) "*"          "*"
## 47 ( 1 ) "*"          "*"

```

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## 50  ( 1 ) "*"          "*"
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## 59  ( 1 ) "*"          "*"
## 60  ( 1 ) "*"          "*"
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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
## 66  ( 1 ) "*"          "*"
## 67  ( 1 ) "*"          "*"
## 68  ( 1 ) "*"          "*"
## 69  ( 1 ) "*"          "*"
## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"
## 72  ( 1 ) "*"          "*"
## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
##           entropy_ElectronAffinity wtd_entropy_ElectronAffinity
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) "*"          " "
## 6  ( 1 ) "*"          " "
## 7  ( 1 ) "*"          " "
## 8  ( 1 ) "*"          " "
## 9  ( 1 ) "*"          " "
## 10 ( 1 ) "*"          " "
## 11 ( 1 ) "*"          " "
## 12 ( 1 ) "*"          " "
## 13 ( 1 ) "*"          " "
## 14 ( 1 ) "*"          " "
## 15 ( 1 ) "*"          " "
## 16 ( 1 ) "*"          " "
## 17 ( 1 ) "*"          " "
## 18 ( 1 ) "*"          " "
## 19 ( 1 ) "*"          " "
## 20 ( 1 ) "*"          " "
## 21 ( 1 ) "*"          " "
## 22 ( 1 ) "*"          " "
## 23 ( 1 ) "*"          " "

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## 29  ( 1 ) "*"          ""
## 30  ( 1 ) "*"          ""
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## 34  ( 1 ) "*"          ""
## 35  ( 1 ) "*"          ""
## 36  ( 1 ) "*"          ""
## 37  ( 1 ) "*"          ""
## 38  ( 1 ) "*"          ""
## 39  ( 1 ) "*"          ""
## 40  ( 1 ) "*"          ""
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## 42  ( 1 ) "*"          "*"
## 43  ( 1 ) "*"          "*"
## 44  ( 1 ) "*"          "*"
## 45  ( 1 ) "*"          "*"
## 46  ( 1 ) "*"          "*"
## 47  ( 1 ) "*"          "*"
## 48  ( 1 ) "*"          "*"
## 49  ( 1 ) "*"          "*"
## 50  ( 1 ) "*"          "*"
## 51  ( 1 ) "*"          "*"
## 52  ( 1 ) "*"          "*"
## 53  ( 1 ) "*"          "*"
## 54  ( 1 ) "*"          "*"
## 55  ( 1 ) "*"          "*"
## 56  ( 1 ) "*"          "*"
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## 58  ( 1 ) "*"          "*"
## 59  ( 1 ) "*"          "*"
## 60  ( 1 ) "*"          "*"
## 61  ( 1 ) "*"          "*"
## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
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## 68  ( 1 ) "*"          "*"
## 69  ( 1 ) "*"          "*"
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## 71  ( 1 ) "*"          "*"
## 72  ( 1 ) "*"          "*"
## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
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## 77  ( 1 ) "*"          "*"

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##          range_ElectronAffinity wtd_range_ElectronAffinity
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## 26 ( 1 ) "*"
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## 49 ( 1 ) "*"
## 50 ( 1 ) "*"
## 51 ( 1 ) "*"
## 52 ( 1 ) "*"
## 53 ( 1 ) "*"

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## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
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## 68  ( 1 ) "*"      "*"
## 69  ( 1 ) "*"      "*"
## 70  ( 1 ) "*"      "*"
## 71  ( 1 ) "*"      "*"
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##          std_ElectronAffinity wtd_std_ElectronAffinity mean_FusionHeat
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## 4  ( 1 ) " "           " "           " "
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## 6  ( 1 ) " "           " "           " "
## 7  ( 1 ) " "           " "           " "
## 8  ( 1 ) " "           " "           " "
## 9  ( 1 ) " "           "*"          " "
## 10 ( 1 ) " "           "*"          " "
## 11 ( 1 ) " "           "*"          " "
## 12 ( 1 ) " "           "*"          " "
## 13 ( 1 ) " "           "*"          " "
## 14 ( 1 ) " "           "*"          " "
## 15 ( 1 ) " "           "*"          " "
## 16 ( 1 ) " "           "*"          " "
## 17 ( 1 ) " "           "*"          " "
## 18 ( 1 ) " "           "*"          " "
## 19 ( 1 ) " "           "*"          " "
## 20 ( 1 ) " "           "*"          " "
## 21 ( 1 ) " "           "*"          " "
## 22 ( 1 ) " "           "*"          " "
## 23 ( 1 ) " "           "*"          " "
## 24 ( 1 ) " "           "*"          " "
## 25 ( 1 ) "*"          "*"          " "
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## 27 ( 1 ) "*"          "*"          " "
## 28 ( 1 ) "*"          "*"          " "
## 29 ( 1 ) "*"          "*"          " "

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## 42  ( 1 ) "*"          "*"
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## 47  ( 1 ) "*"          "*"
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## 49  ( 1 ) "*"          "*"
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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
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## 67  ( 1 ) "*"          "*"
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## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"
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## 74  ( 1 ) "*"          "*"
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## 77  ( 1 ) "*"          "*"
##                               wtd_mean_FusionHeat gmean_FusionHeat wtd_gmean_FusionHeat
## 1  ( 1 ) " "           " "           " "
## 2  ( 1 ) " "           " "           " "
## 3  ( 1 ) " "           " "           " "
## 4  ( 1 ) " "           " "           " "
## 5  ( 1 ) " "           " "           " "

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## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   " "
## 32 ( 1 )   " "
## 33 ( 1 )   " "
## 34 ( 1 )   " "
## 35 ( 1 )   " "
## 36 ( 1 )   " "
## 37 ( 1 )   " "
## 38 ( 1 )   " "
## 39 ( 1 )   " "
## 40 ( 1 )   " "
## 41 ( 1 )   " "
## 42 ( 1 )   " "
## 43 ( 1 )   " "
## 44 ( 1 )   " "
## 45 ( 1 )   " "
## 46 ( 1 )   " "
## 47 ( 1 )   " "
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 60  ( 1 ) "*"      " "      "*"
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## 70  ( 1 ) "*"      " "      "*"
## 71  ( 1 ) "*"      " "      "*"
## 72  ( 1 ) "*"      "*"      "*"
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## 75  ( 1 ) "*"      "*"      "*"
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## 77  ( 1 ) "*"      "*"      "*"
##
##          entropy_FusionHeat wtd_entropy_FusionHeat range_FusionHeat
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## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
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## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
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## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      " "
## 20 ( 1 ) " "      " "      " "
## 21 ( 1 ) " "      " "      " "
## 22 ( 1 ) " "      " "      " "
## 23 ( 1 ) " "      "*"      " "
## 24 ( 1 ) " "      "*"      " "
## 25 ( 1 ) " "      "*"      " "
## 26 ( 1 ) " "      "*"      " "
## 27 ( 1 ) " "      "*"      " "
## 28 ( 1 ) " "      "*"      " "
## 29 ( 1 ) " "      "*"      " "
## 30 ( 1 ) " "      "*"      " "
## 31 ( 1 ) " "      "*"      " "
## 32 ( 1 ) " "      "*"      " "
## 33 ( 1 ) " "      "*"      " "
## 34 ( 1 ) " "      "*"      " "
## 35 ( 1 ) " "      "*"      " "

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## 45  ( 1 ) " "
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## 65  ( 1 ) "*"
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## 68  ( 1 ) "*"
## 69  ( 1 ) "*"
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## 72  ( 1 ) "*"
## 73  ( 1 ) "*"
## 74  ( 1 ) "*"
## 75  ( 1 ) "*"
## 76  ( 1 ) "*"
## 77  ( 1 ) "*"
##          wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
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## 2  ( 1 ) " "           " "           " "
## 3  ( 1 ) " "           " "           " "
## 4  ( 1 ) " "           " "           " "
## 5  ( 1 ) " "           " "           " "
## 6  ( 1 ) " "           " "           " "
## 7  ( 1 ) " "           " "           " "
## 8  ( 1 ) " "           " "           " "
## 9  ( 1 ) " "           " "           " "
## 10 ( 1 ) " "           " "           " "
## 11 ( 1 ) " "           " "           " "

```

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## 21  ( 1 ) " "
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## 24  ( 1 ) " "
## 25  ( 1 ) " "
## 26  ( 1 ) " "
## 27  ( 1 ) " "
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## 57  ( 1 ) "*"
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## 62  ( 1 ) "*"
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## 64  ( 1 ) "*"
## 65  ( 1 ) "*"

```

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## 66 ( 1 ) "*"      "*"      "*"
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## 69 ( 1 ) "*"      "*"      "*"
## 70 ( 1 ) "*"      "*"      "*"
## 71 ( 1 ) "*"      "*"      "*"
## 72 ( 1 ) "*"      "*"      "*"
## 73 ( 1 ) "*"      "*"      "*"
## 74 ( 1 ) "*"      "*"      "*"
## 75 ( 1 ) "*"      "*"      "*"
## 76 ( 1 ) "*"      "*"      "*"
## 77 ( 1 ) "*"      "*"      "*"
##
##          mean_ThermalConductivity wtd_mean_ThermalConductivity
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## 2 ( 1 ) " "      " "      "
## 3 ( 1 ) " "      " "      "
## 4 ( 1 ) " "      " "      "
## 5 ( 1 ) " "      " "      "
## 6 ( 1 ) " "      " "      "
## 7 ( 1 ) " "      " "      "
## 8 ( 1 ) " "      " "      "
## 9 ( 1 ) " "      " "      "
## 10 ( 1 ) " "     " "      "
## 11 ( 1 ) " "     " "      "
## 12 ( 1 ) " "     " "      "
## 13 ( 1 ) " "     " "      "
## 14 ( 1 ) " "     " "      "
## 15 ( 1 ) " "     " "      "
## 16 ( 1 ) " "     " "      "
## 17 ( 1 ) " "     " "      "
## 18 ( 1 ) " "     " "      "
## 19 ( 1 ) " "     " "      "
## 20 ( 1 ) " "     " "      "
## 21 ( 1 ) " "     "*"      "
## 22 ( 1 ) " "     "*"      "
## 23 ( 1 ) " "     "*"      "
## 24 ( 1 ) " "     "*"      "
## 25 ( 1 ) " "     "*"      "
## 26 ( 1 ) " "     "*"      "
## 27 ( 1 ) " "     "*"      "
## 28 ( 1 ) " "     "*"      "
## 29 ( 1 ) " "     "*"      "
## 30 ( 1 ) " "     "*"      "
## 31 ( 1 ) " "     "*"      "
## 32 ( 1 ) " "     "*"      "
## 33 ( 1 ) " "     "*"      "
## 34 ( 1 ) " "     "*"      "
## 35 ( 1 ) " "     "*"      "
## 36 ( 1 ) " "     "*"      "
## 37 ( 1 ) " "     "*"      "
## 38 ( 1 ) " "     "*"      "
## 39 ( 1 ) " "     "*"      "
## 40 ( 1 ) " "     "*"      "
## 41 ( 1 ) " "     "*"      "

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## 42  ( 1 ) " "          "*"
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## 46  ( 1 ) " "          "*"
## 47  ( 1 ) " "          "*"
## 48  ( 1 ) " "          "*"
## 49  ( 1 ) " "          "*"
## 50  ( 1 ) " "          "*"
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## 52  ( 1 ) " "          "*"
## 53  ( 1 ) " "          "*"
## 54  ( 1 ) " "          "*"
## 55  ( 1 ) " "          "*"
## 56  ( 1 ) " "          "*"
## 57  ( 1 ) " "          "*"
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## 59  ( 1 ) " "          "*"
## 60  ( 1 ) " "          "*"
## 61  ( 1 ) " "          "*"
## 62  ( 1 ) " "          "*"
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## 64  ( 1 ) "*"          "*"
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## 68  ( 1 ) "*"          "*"
## 69  ( 1 ) "*"          "*"
## 70  ( 1 ) "*"          "*"
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## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
##               gmean_ThermalConductivity wtd_gmean_ThermalConductivity
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "
## 11 ( 1 ) " "          " "
## 12 ( 1 ) " "          " "
## 13 ( 1 ) " "          " "
## 14 ( 1 ) " "          " "
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## 17 ( 1 ) "*"          " "

```

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## 25  ( 1 ) "*"          "*"
## 26  ( 1 ) "*"          "*"
## 27  ( 1 ) "*"          "*"
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## 29  ( 1 ) "*"          "*"
## 30  ( 1 ) "*"          "*"
## 31  ( 1 ) "*"          "*"
## 32  ( 1 ) "*"          "*"
## 33  ( 1 ) "*"          "*"
## 34  ( 1 ) "*"          "*"
## 35  ( 1 ) "*"          "*"
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## 37  ( 1 ) "*"          "*"
## 38  ( 1 ) "*"          "*"
## 39  ( 1 ) "*"          "*"
## 40  ( 1 ) "*"          "*"
## 41  ( 1 ) "*"          "*"
## 42  ( 1 ) "*"          "*"
## 43  ( 1 ) "*"          "*"
## 44  ( 1 ) "*"          "*"
## 45  ( 1 ) "*"          "*"
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## 47  ( 1 ) "*"          "*"
## 48  ( 1 ) "*"          "*"
## 49  ( 1 ) "*"          "*"
## 50  ( 1 ) "*"          "*"
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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
## 66  ( 1 ) "*"          "*"
## 67  ( 1 ) "*"          "*"
## 68  ( 1 ) "*"          "*"
## 69  ( 1 ) "*"          "*"
## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"

```

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## 72  ( 1 ) "*"          "*"
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## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
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##           entropy_ThermalConductivity wtd_entropy_ThermalConductivity
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
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## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "
## 11 ( 1 ) " "          "*"
## 12 ( 1 ) " "          "*"
## 13 ( 1 ) " "          "*"
## 14 ( 1 ) " "          "*"
## 15 ( 1 ) " "          "*"
## 16 ( 1 ) " "          "*"
## 17 ( 1 ) " "          "*"
## 18 ( 1 ) " "          "*"
## 19 ( 1 ) " "          "*"
## 20 ( 1 ) " "          "*"
## 21 ( 1 ) " "          "*"
## 22 ( 1 ) " "          "*"
## 23 ( 1 ) " "          "*"
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## 30 ( 1 ) " "          "*"
## 31 ( 1 ) " "          "*"
## 32 ( 1 ) " "          "*"
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## 40 ( 1 ) " "          "*"
## 41 ( 1 ) " "          "*"
## 42 ( 1 ) " "          "*"
## 43 ( 1 ) " "          "*"
## 44 ( 1 ) " "          "*"
## 45 ( 1 ) " "          "*"
## 46 ( 1 ) " "          "*"
## 47 ( 1 ) " "          "*"

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## 59  ( 1 ) " "          "*"
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
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## 5  ( 1 ) " "          " "
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## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) "*"          " "
## 11 ( 1 ) "*"          " "
## 12 ( 1 ) "*"          " "
## 13 ( 1 ) "*"          " "
## 14 ( 1 ) "*"          " "
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## 16 ( 1 ) "*"          " "
## 17 ( 1 ) "*"          " "
## 18 ( 1 ) "*"          " "
## 19 ( 1 ) "*"          " "
## 20 ( 1 ) "*"          " "
## 21 ( 1 ) "*"          " "
## 22 ( 1 ) "*"          " "
## 23 ( 1 ) "*"          " "

```

```

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## 32  ( 1 ) "*"          "*"
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## 34  ( 1 ) "*"          "*"
## 35  ( 1 ) "*"          "*"
## 36  ( 1 ) "*"          "*"
## 37  ( 1 ) "*"          "*"
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## 40  ( 1 ) "*"          "*"
## 41  ( 1 ) "*"          "*"
## 42  ( 1 ) "*"          "*"
## 43  ( 1 ) "*"          "*"
## 44  ( 1 ) "*"          "*"
## 45  ( 1 ) "*"          "*"
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## 47  ( 1 ) "*"          "*"
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## 49  ( 1 ) "*"          "*"
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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
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## 68  ( 1 ) "*"          "*"
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## 71  ( 1 ) "*"          "*"
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## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
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## 77  ( 1 ) "*"          "*"

```

```

##          std_ThermalConductivity wtd_std_ThermalConductivity mean_Valence
## 1      ( 1 ) " "             "*"                  " "
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## 4      ( 1 ) " "             "*"                  " "
## 5      ( 1 ) " "             "*"                  " "
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## 7      ( 1 ) " "             "*"                  " "
## 8      ( 1 ) " "             "*"                  " "
## 9      ( 1 ) " "             "*"                  " "
## 10     ( 1 ) " "             "*"                  " "
## 11     ( 1 ) " "             "*"                  " "
## 12     ( 1 ) " "             "*"                  " "
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## 14     ( 1 ) " "             "*"                  " "
## 15     ( 1 ) " "             "*"                  " "
## 16     ( 1 ) " "             "*"                  " "
## 17     ( 1 ) " "             "*"                  " "
## 18     ( 1 ) " "             "*"                  " "
## 19     ( 1 ) " "             "*"                  " "
## 20     ( 1 ) " "             "*"                  " "
## 21     ( 1 ) " "             "*"                  " "
## 22     ( 1 ) " "             "*"                  " "
## 23     ( 1 ) " "             "*"                  " "
## 24     ( 1 ) " "             "*"                  " "
## 25     ( 1 ) " "             "*"                  " "
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## 27     ( 1 ) " "             "*"                  " "
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## 29     ( 1 ) " "             "*"                  " "
## 30     ( 1 ) " "             "*"                  " "
## 31     ( 1 ) " "             "*"                  "*"
## 32     ( 1 ) "*"             "*"                  "*"
## 33     ( 1 ) "*"             "*"                  "*"
## 34     ( 1 ) "*"             "*"                  "*"
## 35     ( 1 ) "*"             "*"                  "*"
## 36     ( 1 ) "*"             "*"                  "*"
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## 39     ( 1 ) "*"             "*"                  "*"
## 40     ( 1 ) "*"             "*"                  "*"
## 41     ( 1 ) "*"             "*"                  "*"
## 42     ( 1 ) "*"             "*"                  "*"
## 43     ( 1 ) "*"             "*"                  "*"
## 44     ( 1 ) "*"             "*"                  "*"
## 45     ( 1 ) "*"             "*"                  "*"
## 46     ( 1 ) "*"             "*"                  "*"
## 47     ( 1 ) "*"             "*"                  "*"
## 48     ( 1 ) "*"             "*"                  "*"
## 49     ( 1 ) "*"             "*"                  "*"
## 50     ( 1 ) "*"             "*"                  "*"
## 51     ( 1 ) "*"             "*"                  "*"
## 52     ( 1 ) "*"             "*"                  "*"
## 53     ( 1 ) "*"             "*"                  "*"

```

```

## 54  ( 1 ) "*"      "*"      "*"
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## 57  ( 1 ) "*"      "*"      "*"
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## 62  ( 1 ) "*"      "*"      "*"
## 63  ( 1 ) "*"      "*"      "*"
## 64  ( 1 ) "*"      "*"      "*"
## 65  ( 1 ) "*"      "*"      "*"
## 66  ( 1 ) "*"      "*"      "*"
## 67  ( 1 ) "*"      "*"      "*"
## 68  ( 1 ) "*"      "*"      "*"
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## 71  ( 1 ) "*"      "*"      "*"
## 72  ( 1 ) "*"      "*"      "*"
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## 75  ( 1 ) "*"      "*"      "*"
## 76  ( 1 ) "*"      "*"      "*"
## 77  ( 1 ) "*"      "*"      "*"
##
##          wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
## 1  ( 1 ) " "        " "        " "        " "
## 2  ( 1 ) " "        " "        " "        " "
## 3  ( 1 ) " "        " "        " "        " "
## 4  ( 1 ) " "        " "        " "        " "
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## 16 ( 1 ) " "        " "        " "        " "
## 17 ( 1 ) " "        " "        " "        " "
## 18 ( 1 ) " "        " "        " "        " "
## 19 ( 1 ) " "        " "        " "        " "
## 20 ( 1 ) " "        " "        " "        " "
## 21 ( 1 ) " "        " "        " "        " "
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## 26 ( 1 ) " "        " "        " "        " "
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##          wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
## 1  ( 1 ) " "           " "           " "           " "
## 2  ( 1 ) " "           " "           " "           " "
## 3  ( 1 ) " "           " "           " "           " "
## 4  ( 1 ) " "           " "           " "           " "
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##          wtd_std_Valence
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## 77  ( 1 ) "*"

linear_forward$results

##      nvmax      RMSE   Rsquared       MAE     RMSESD   RsquaredSD     MAESD
## 1      1 23.73833 0.5198107 18.24597 0.2467303 0.008466076 0.2298375
## 2      2 22.81227 0.5565342 17.65525 0.2210382 0.008908434 0.2063558
## 3      3 22.05517 0.5854512 17.25921 0.2957349 0.012466668 0.2425789
## 4      4 21.72173 0.5978175 16.90860 0.3374081 0.014453997 0.1857944
## 5      5 21.29542 0.6134370 16.61848 0.3778655 0.016185903 0.1983296
## 6      6 20.90255 0.6275990 16.37802 0.3264582 0.014053826 0.2648299
## 7      7 20.65973 0.6361913 16.04096 0.2920101 0.012308641 0.2814510
## 8      8 20.44840 0.6436264 15.84942 0.2362018 0.010759199 0.3458239

```

```

## 9   9 20.21726 0.6516605 15.66839 0.1591493 0.008700021 0.2365919
## 10 10 20.01897 0.6584743 15.50320 0.1629440 0.008574226 0.1621404
## 11 11 19.87848 0.6632557 15.38467 0.1739788 0.008533073 0.1505681
## 12 12 19.72196 0.6685431 15.26423 0.1996169 0.009561488 0.1401573
## 13 13 19.60739 0.6723732 15.10559 0.2327685 0.010567219 0.1760852
## 14 14 19.51013 0.6755885 15.05251 0.2745805 0.011979349 0.2556974
## 15 15 19.34159 0.6811493 14.88909 0.2708535 0.011700876 0.2214814
## 16 16 19.23319 0.6847187 14.82679 0.2362953 0.010432044 0.1992795
## 17 17 19.15821 0.6871807 14.76190 0.2478722 0.010461981 0.2323833
## 18 18 19.07000 0.6900599 14.66550 0.2688695 0.010929484 0.2232983
## 19 19 18.99702 0.6924211 14.60502 0.2911516 0.011780956 0.2307324
## 20 20 18.94330 0.6941455 14.54334 0.2627523 0.010782708 0.2237316
## 21 21 18.86583 0.6966181 14.45771 0.2807253 0.011302579 0.1984940
## 22 22 18.77679 0.6994896 14.35312 0.2738715 0.010698343 0.1942594
## 23 23 18.72343 0.7012073 14.31925 0.2721300 0.010466391 0.1663548
## 24 24 18.67789 0.7026510 14.29976 0.2893890 0.010841539 0.2103072
## 25 25 18.61694 0.7045756 14.24552 0.3060343 0.011267914 0.2214945
## 26 26 18.56449 0.7062326 14.21372 0.3009003 0.011372001 0.1905650
## 27 27 18.53142 0.7072845 14.18273 0.2927245 0.011046489 0.1898480
## 28 28 18.47796 0.7089521 14.14517 0.3189204 0.011662484 0.2099341
## 29 29 18.43708 0.7102567 14.10283 0.3246690 0.011588977 0.1985040
## 30 30 18.39213 0.7116566 14.05925 0.3541031 0.012177285 0.2436569
## 31 31 18.35621 0.7127859 14.02666 0.3531056 0.011979207 0.2615678
## 32 32 18.30659 0.7143200 13.98883 0.3722808 0.012457228 0.2749419
## 33 33 18.26260 0.7156886 13.95322 0.3632201 0.012284031 0.2517629
## 34 34 18.24893 0.7161088 13.93252 0.3550896 0.012103865 0.2460239
## 35 35 18.21883 0.7170549 13.90062 0.3383907 0.011582065 0.2297450
## 36 36 18.20316 0.7175487 13.87544 0.3387244 0.011440999 0.2358838
## 37 37 18.18346 0.7181653 13.85715 0.3292188 0.011400439 0.2396760
## 38 38 18.17970 0.7182878 13.85202 0.3288243 0.011275741 0.2347118
## 39 39 18.16147 0.7188615 13.83527 0.3290270 0.011134941 0.2424228
## 40 40 18.14772 0.7192925 13.83436 0.3230107 0.010754953 0.2362127
## 41 41 18.12385 0.7200392 13.80058 0.3279972 0.010719222 0.2398850
## 42 42 18.10396 0.7206512 13.78353 0.3312226 0.010742229 0.2440994
## 43 43 18.08427 0.7212645 13.76549 0.3390495 0.011006730 0.2436726
## 44 44 18.07143 0.7216497 13.74303 0.3389884 0.010979027 0.2529285
## 45 45 18.04869 0.7223525 13.71084 0.3432128 0.010815015 0.2556653
## 46 46 18.04295 0.7225231 13.70509 0.3385765 0.010893194 0.2465662
## 47 47 18.03132 0.7228830 13.68760 0.3441187 0.011043538 0.2553348
## 48 48 18.01165 0.7234934 13.65850 0.3441356 0.010937448 0.2608298
## 49 49 17.98643 0.7242658 13.63506 0.3280247 0.010372263 0.2416579
## 50 50 17.96737 0.7248479 13.61804 0.3282897 0.010358095 0.2509953
## 51 51 17.95393 0.7252581 13.60049 0.3341766 0.010397884 0.2621126
## 52 52 17.94138 0.7256434 13.57946 0.3265825 0.010113092 0.2573829
## 53 53 17.92342 0.7261957 13.56464 0.3191117 0.009934734 0.2496826
## 54 54 17.89831 0.7269674 13.53968 0.3015028 0.009633552 0.2399810
## 55 55 17.88544 0.7273584 13.53199 0.3064983 0.009642969 0.2376841
## 56 56 17.87558 0.7276569 13.52475 0.3144243 0.009771791 0.2414646
## 57 57 17.86500 0.7279818 13.51946 0.3074627 0.009585689 0.2388151
## 58 58 17.85799 0.7281942 13.51212 0.3034718 0.009594191 0.2313942
## 59 59 17.84398 0.7286229 13.49914 0.2999975 0.009543701 0.2179494
## 60 60 17.83006 0.7290450 13.49174 0.3048548 0.009609353 0.2256842
## 61 61 17.81383 0.7295404 13.47444 0.2932016 0.009417662 0.2150176
## 62 62 17.80000 0.7299518 13.46292 0.2909553 0.009461976 0.2145968

```

```

## 63 63 17.78679 0.7303513 13.45134 0.2963763 0.009597557 0.2117412
## 64 64 17.77825 0.7306111 13.44536 0.2924122 0.009651199 0.2115119
## 65 65 17.76661 0.7309610 13.43695 0.2964247 0.009703778 0.2170407
## 66 66 17.76052 0.7311440 13.43176 0.3008094 0.009734558 0.2131872
## 67 67 17.75861 0.7312058 13.42544 0.2988624 0.009666614 0.2129381
## 68 68 17.75414 0.7313399 13.42260 0.2995263 0.009662565 0.2156213
## 69 69 17.74020 0.7317568 13.40788 0.2978271 0.009643074 0.2110090
## 70 70 17.73378 0.7319583 13.40246 0.3012223 0.009654543 0.2120376
## 71 71 17.72485 0.7322290 13.39341 0.3032956 0.009635701 0.2190654
## 72 72 17.71740 0.7324501 13.38481 0.3092984 0.009866048 0.2198417
## 73 73 17.71604 0.7324943 13.38500 0.3074836 0.009800274 0.2201505
## 74 74 17.71617 0.7324909 13.38877 0.3081321 0.009805760 0.2167691
## 75 75 17.71721 0.7324571 13.39293 0.3122232 0.009940941 0.2221894
## 76 76 17.71157 0.7326270 13.39664 0.3139614 0.009996603 0.2225069
## 77 77 17.71018 0.7326693 13.39815 0.3148735 0.010001909 0.2246336
## 78 78 17.71248 0.7325999 13.40047 0.3141119 0.009981937 0.2217926
## 79 79 17.71332 0.7325729 13.40138 0.3131849 0.009990205 0.2227423
## 80 80 17.71153 0.7326274 13.40254 0.3129975 0.009965694 0.2220446
## 81 81 17.71082 0.7326498 13.40288 0.3121764 0.009942553 0.2221992

```

From the above results, we can see how forward selection works and the corresponding errors to the number of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_forward, linear_forward$results$nvmax, "Number of Variables")
```

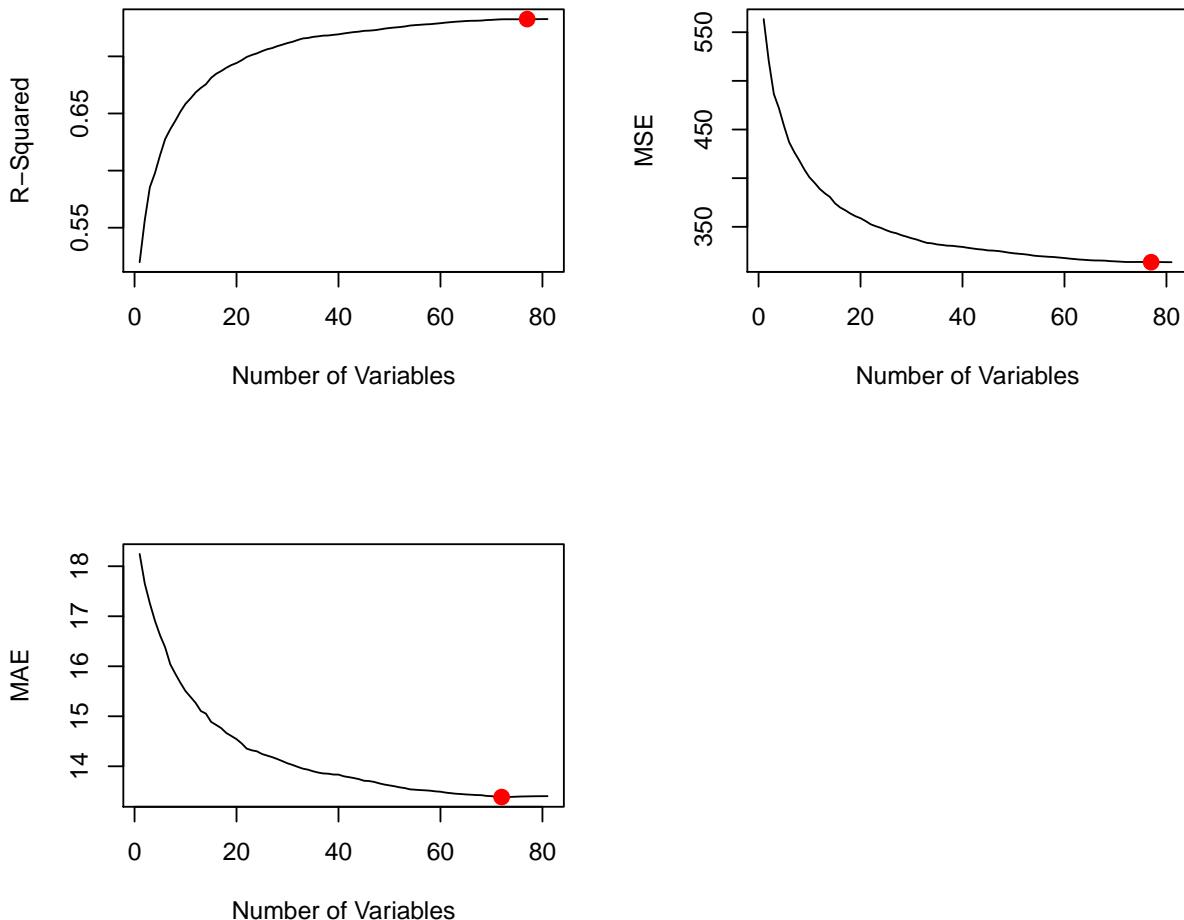


Figure 47: R-Squared, MSE, and MAE for Forward Selection

```
linear_forward$bestTune
```

```
##      nvmax
## 77    77

coef(linear_forward$finalModel, linear_forward$bestTune$nvmax)

##              (Intercept)          number_of_elements
##                  -12.399314           -27.631871
##      mean_atomic_mass        wtd_mean_atomic_mass
##                  182.288259           -203.375196
##      gmean_atomic_mass       wtd_gmean_atomic_mass
##                 -114.807531            155.634827
##      entropy_atomic_mass     wtd_entropy_atomic_mass
##                  -72.874578             4.487481
##      range_atomic_mass       wtd_range_atomic_mass
```

```

##          44.831363          4.099148
##      std_atomic_mass      wtd_std_atomic_mass
##          -60.238623          13.035743
##      wtd_mean_fie      entropy_fie
##          25.033850          -182.601772
##      wtd_entropy_fie      range_fie
##          98.606081          82.468504
##      wtd_range_fie      std_fie
##          23.067433          -69.568168
##      wtd_std_fie      mean_atomic_radius
##          -33.044540          -147.124571
##      wtd_mean_atomic_radius      gmean_atomic_radius
##          793.204259          68.580948
##      wtd_gmean_atomic_radius      entropy_atomic_radius
##          -700.891704          104.971111
##      wtd_entropy_atomic_radius      range_atomic_radius
##          84.309992          52.594109
##      wtd_range_atomic_radius      std_atomic_radius
##          -20.024369          -46.260766
##      wtd_std_atomic_radius      mean_Density
##          -30.131009          -112.443175
##      wtd_mean_Density      gmean_Density
##          6.520147          32.571275
##      wtd_gmean_Density      entropy_Density
##          38.629716          35.707075
##      wtd_entropy_Density      range_Density
##          -31.672503          -35.046025
##      std_Density      wtd_std_Density
##          66.422190          -17.822688
##      mean_ElectronAffinity      wtd_mean_ElectronAffinity
##          -32.647295          162.157019
##      gmean_ElectronAffinity      wtd_gmean_ElectronAffinity
##          53.037189          -177.747945
##      entropy_ElectronAffinity      wtd_entropy_ElectronAffinity
##          10.472984          -35.737511
##      range_ElectronAffinity      wtd_range_ElectronAffinity
##          -130.102278          -31.879974
##      std_ElectronAffinity      wtd_std_ElectronAffinity
##          206.479637          -94.874368
##      mean_FusionHeat      wtd_mean_FusionHeat
##          173.417245          -207.614934
##      gmean_FusionHeat      wtd_gmean_FusionHeat
##          -157.280247          176.918559
##      entropy_FusionHeat      wtd_entropy_FusionHeat
##          -41.313057          44.103962
##      range_FusionHeat      wtd_range_FusionHeat
##          -37.265271          59.454701
##      std_FusionHeat      wtd_std_FusionHeat
##          -32.630266          43.995621
##      mean_ThermalConductivity      wtd_mean_ThermalConductivity
##          -35.186503          236.748634
##      gmean_ThermalConductivity      wtd_gmean_ThermalConductivity
##          -9.473831          -142.972585
##      entropy_ThermalConductivity      wtd_entropy_ThermalConductivity

```

```

##          22.225903      2.972715
## range_ThermalConductivity    wtd_range_ThermalConductivity
##          -38.888090     -90.308482
## std_ThermalConductivity     wtd_std_ThermalConductivity
##          67.984965      -8.187868
## mean_Valence                wtd_mean_Valence
##          -95.132880     150.766156
## gmean_Valence               wtd_gmean_Valence
##          120.369625     -172.973657
## entropy_Valence             wtd_entropy_Valence
##          140.944728     -142.371904
## range_Valence               wtd_range_Valence
##          25.770202      -7.623901
## std_Valence                 wtd_std_Valence
##          22.291184      -74.602313

```

```
getTrainPerf(linear_forward)
```

```

##   TrainRMSE TrainRsquared TrainMAE      method
## 1  17.71018     0.7326693 13.39815 leapForward

```

From the above metrics, it can be seen that based on R-Squared and MSE, the best model is the model with 77 variables, however, MAE choose a model with less variables. By using the feature from caret package, we can decide that the best model is the model with 77 variables. The list of 77 variables is provided above. The R-Squared for this model is 0.7326 with Train MSE is 313.64

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_forward, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

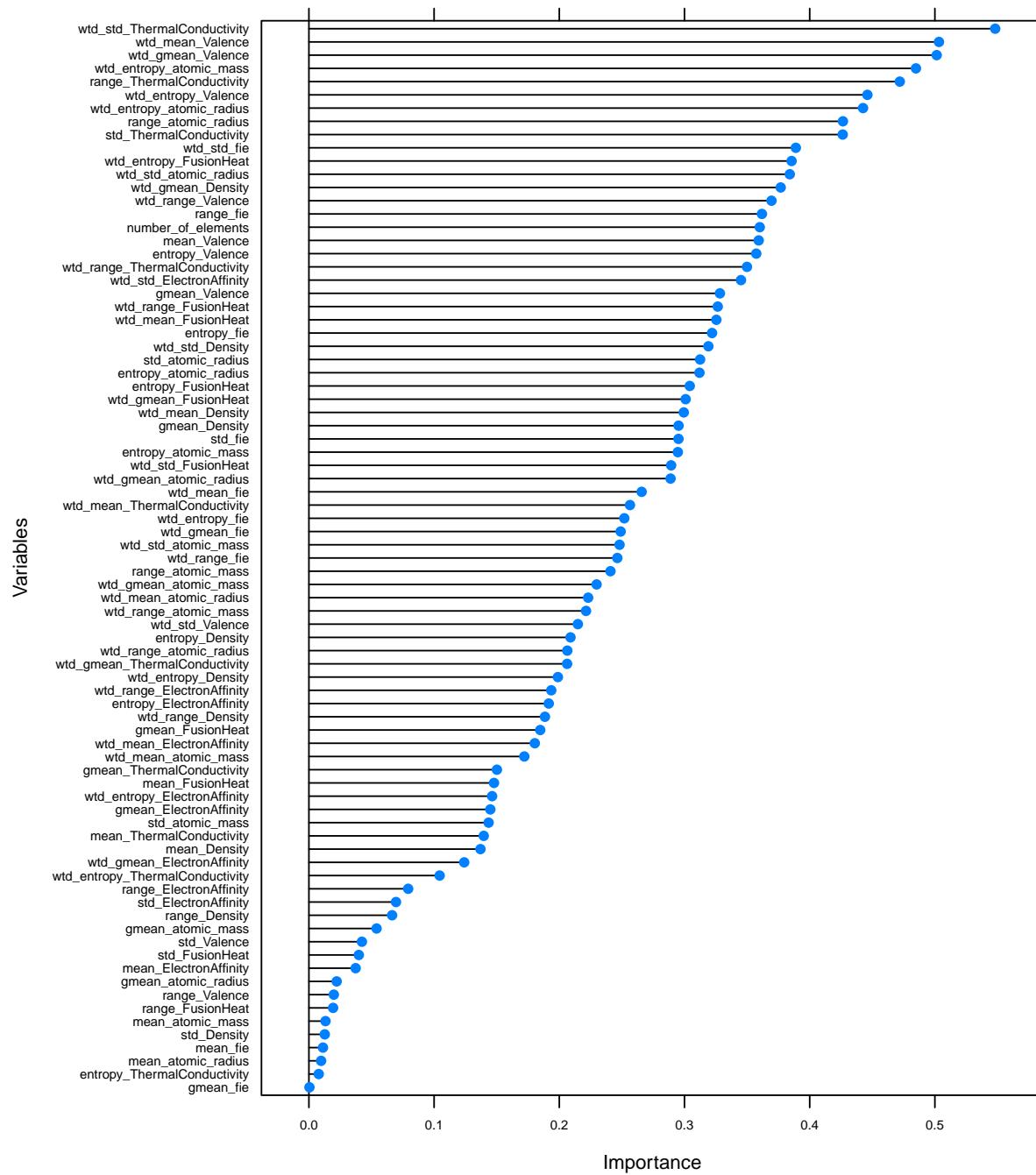


Figure 48: Variables Importance for Forward Selection

From above, it can be seen that wtd\_std\_ThermalConductivity is the most important variable for this model, whereas gmean\_fie is the least important variable for this model.

### 3.1.6 Linear Regression with Stepwise Selection

In this sub section, we will perform the stepwise selection which is the combination of forward and backward selections.

```
set.seed(seed)

# Linear Regression with Stepwise Selection
linear_stepwise <- train(critical_temp ~., data = train.data,
                         method = "leapSeq",
                         tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
                         trControl = control,
                         preProc = c("range")
                        )

summary(linear_stepwise)

## Subset selection object
## 81 Variables  (and intercept)
##                                     Forced in    Forced out
## number_of_elements           FALSE      FALSE
## mean_atomic_mass             FALSE      FALSE
## wtd_mean_atomic_mass        FALSE      FALSE
## gmean_atomic_mass           FALSE      FALSE
## wtd_gmean_atomic_mass       FALSE      FALSE
## entropy_atomic_mass         FALSE      FALSE
## wtd_entropy_atomic_mass     FALSE      FALSE
## range_atomic_mass           FALSE      FALSE
## wtd_range_atomic_mass       FALSE      FALSE
## std_atomic_mass              FALSE      FALSE
## wtd_std_atomic_mass         FALSE      FALSE
## mean_fie                     FALSE      FALSE
## wtd_mean_fie                 FALSE      FALSE
## gmean_fie                    FALSE      FALSE
## wtd_gmean_fie                FALSE      FALSE
## entropy_fie                  FALSE      FALSE
## wtd_entropy_fie              FALSE      FALSE
## range_fie                    FALSE      FALSE
## wtd_range_fie                FALSE      FALSE
## std_fie                      FALSE      FALSE
## wtd_std_fie                  FALSE      FALSE
## mean_atomic_radius           FALSE      FALSE
## wtd_mean_atomic_radius       FALSE      FALSE
## gmean_atomic_radius          FALSE      FALSE
## wtd_gmean_atomic_radius     FALSE      FALSE
## entropy_atomic_radius        FALSE      FALSE
## wtd_entropy_atomic_radius   FALSE      FALSE
## range_atomic_radius          FALSE      FALSE
## wtd_range_atomic_radius     FALSE      FALSE
## std_atomic_radius            FALSE      FALSE
## wtd_std_atomic_radius        FALSE      FALSE
## mean_Density                  FALSE      FALSE
## wtd_mean_Density              FALSE      FALSE
## gmean_Density                 FALSE      FALSE
```

```

## wtd_gmean_Density           FALSE  FALSE
## entropy_Density             FALSE  FALSE
## wtd_entropy_Density         FALSE  FALSE
## range_Density               FALSE  FALSE
## wtd_range_Density           FALSE  FALSE
## std_Density                 FALSE  FALSE
## wtd_std_Density              FALSE  FALSE
## mean_ElectronAffinity       FALSE  FALSE
## wtd_mean_ElectronAffinity   FALSE  FALSE
## gmean_ElectronAffinity      FALSE  FALSE
## wtd_gmean_ElectronAffinity  FALSE  FALSE
## entropy_ElectronAffinity    FALSE  FALSE
## wtd_entropy_ElectronAffinity FALSE  FALSE
## range_ElectronAffinity      FALSE  FALSE
## wtd_range_ElectronAffinity  FALSE  FALSE
## std_ElectronAffinity        FALSE  FALSE
## wtd_std_ElectronAffinity    FALSE  FALSE
## mean_FusionHeat              FALSE  FALSE
## wtd_mean_FusionHeat          FALSE  FALSE
## gmean_FusionHeat             FALSE  FALSE
## wtd_gmean_FusionHeat         FALSE  FALSE
## entropy_FusionHeat           FALSE  FALSE
## wtd_entropy_FusionHeat        FALSE  FALSE
## range_FusionHeat              FALSE  FALSE
## wtd_range_FusionHeat          FALSE  FALSE
## std_FusionHeat                FALSE  FALSE
## wtd_std_FusionHeat            FALSE  FALSE
## mean_ThermalConductivity    FALSE  FALSE
## wtd_mean_ThermalConductivity FALSE  FALSE
## gmean_ThermalConductivity   FALSE  FALSE
## wtd_gmean_ThermalConductivity FALSE  FALSE
## entropy_ThermalConductivity FALSE  FALSE
## wtd_entropy_ThermalConductivity FALSE  FALSE
## range_ThermalConductivity   FALSE  FALSE
## wtd_range_ThermalConductivity FALSE  FALSE
## std_ThermalConductivity     FALSE  FALSE
## wtd_std_ThermalConductivity  FALSE  FALSE
## mean_Valence                 FALSE  FALSE
## wtd_mean_Valence             FALSE  FALSE
## gmean_Valence                FALSE  FALSE
## wtd_gmean_Valence            FALSE  FALSE
## entropy_Valence              FALSE  FALSE
## wtd_entropy_Valence          FALSE  FALSE
## range_Valence                FALSE  FALSE
## wtd_range_Valence            FALSE  FALSE
## std_Valence                  FALSE  FALSE
## wtd_std_Valence              FALSE  FALSE
## 1 subsets of each size up to 81
## Selection Algorithm: 'sequential replacement'
##          number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1  ( 1 )    " "           " "           " "
## 2  ( 1 )    " "           " "           " "
## 3  ( 1 )    " "           " "           " "
## 4  ( 1 )    " "           " "           " "

```

```

## 5  ( 1 )   " "
## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   "*" "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   "*" "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   "*" "
## 32 ( 1 )   " "
## 33 ( 1 )   " "
## 34 ( 1 )   " "
## 35 ( 1 )   " "
## 36 ( 1 )   " "
## 37 ( 1 )   " "
## 38 ( 1 )   " "
## 39 ( 1 )   " "
## 40 ( 1 )   " "
## 41 ( 1 )   "*" "
## 42 ( 1 )   "*" "
## 43 ( 1 )   "*" "
## 44 ( 1 )   "*" "
## 45 ( 1 )   "*" "
## 46 ( 1 )   "*" "
## 47 ( 1 )   "*" "
## 48 ( 1 )   "*" "
## 49 ( 1 )   "*" "
## 50 ( 1 )   "*" "
## 51 ( 1 )   "*" "
## 52 ( 1 )   "*" "
## 53 ( 1 )   "*" "
## 54 ( 1 )   "*" "
## 55 ( 1 )   "*" "
## 56 ( 1 )   "*" "
## 57 ( 1 )   "*" "
## 58 ( 1 )   "*" "

```

```

## 59  ( 1 ) "*"      "*"      "*"
## 60  ( 1 ) "*"      "*"      "*"
## 61  ( 1 ) "*"      "*"      "*"
## 62  ( 1 ) "*"      "*"      "*"
## 63  ( 1 ) "*"      "*"      "*"
## 64  ( 1 ) "*"      "*"      "*"
## 65  ( 1 ) "*"      "*"      "*"
## 66  ( 1 ) "*"      "*"      "*"
## 67  ( 1 ) "*"      "*"      "*"
## 68  ( 1 ) "*"      "*"      "*"
## 69  ( 1 ) "*"      "*"      "*"
## 70  ( 1 ) "*"      "*"      "*"
## 71  ( 1 ) "*"      "*"      "*"
## 72  ( 1 ) "*"      "*"      "*"
## 73  ( 1 ) "*"      "*"      "*"
## 74  ( 1 ) "*"      "*"      "*"
## 75  ( 1 ) "*"      "*"      "*"
## 76  ( 1 ) "*"      "*"      "*"
## 77  ( 1 ) "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"
## 79  ( 1 ) "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"
## 81  ( 1 ) "*"      "*"      "*"
##          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1  ( 1 ) " "        " "        " "
## 2  ( 1 ) " "        " "        " "
## 3  ( 1 ) " "        " "        " "
## 4  ( 1 ) " "        " "        " "
## 5  ( 1 ) " "        " "        " "
## 6  ( 1 ) " "        " "        " "
## 7  ( 1 ) " "        " "        " "
## 8  ( 1 ) " "        " "        " "
## 9  ( 1 ) " "        " "        " "
## 10 ( 1 ) " "        " "        " "
## 11 ( 1 ) " "        " "        " "
## 12 ( 1 ) " "        " "        " "
## 13 ( 1 ) " "        " "        " "
## 14 ( 1 ) "*"      "*"      "*"
## 15 ( 1 ) " "        " "        " "
## 16 ( 1 ) " "        " "        " "
## 17 ( 1 ) " "        " "        " "
## 18 ( 1 ) " "        " "        " "
## 19 ( 1 ) " "        " "        " "
## 20 ( 1 ) " "        " "        "*"
## 21 ( 1 ) " "        " "        "*"
## 22 ( 1 ) " "        " "        "*"
## 23 ( 1 ) " "        " "        "*"
## 24 ( 1 ) " "        " "        "*"
## 25 ( 1 ) "*"      "*"      "*"
## 26 ( 1 ) " "        " "        " "
## 27 ( 1 ) " "        " "        " "
## 28 ( 1 ) " "        " "        " "
## 29 ( 1 ) " "        " "        " "
## 30 ( 1 ) " "        " "        " "

```

```

## 31  ( 1 ) "*"          "*"          "*"
## 32  ( 1 ) " "          " "          "*"
## 33  ( 1 ) " "          " "          "*"
## 34  ( 1 ) " "          " "          "*"
## 35  ( 1 ) " "          " "          "*"
## 36  ( 1 ) " "          " "          "*"
## 37  ( 1 ) " "          " "          "*"
## 38  ( 1 ) " "          " "          "*"
## 39  ( 1 ) " "          " "          "*"
## 40  ( 1 ) " "          " "          "*"
## 41  ( 1 ) " "          " "          "*"
## 42  ( 1 ) " "          " "          "*"
## 43  ( 1 ) " "          " "          "*"
## 44  ( 1 ) " "          " "          "*"
## 45  ( 1 ) " "          " "          "*"
## 46  ( 1 ) "*"          "*"          "*"
## 47  ( 1 ) " "          " "          "*"
## 48  ( 1 ) "*"          "*"          "*"
## 49  ( 1 ) "*"          "*"          "*"
## 50  ( 1 ) " "          " "          "*"
## 51  ( 1 ) " "          " "          "*"
## 52  ( 1 ) " "          " "          "*"
## 53  ( 1 ) " "          " "          "*"
## 54  ( 1 ) "*"          "*"          "*"
## 55  ( 1 ) " "          " "          "*"
## 56  ( 1 ) " "          " "          "*"
## 57  ( 1 ) " "          " "          "*"
## 58  ( 1 ) " "          " "          "*"
## 59  ( 1 ) " "          " "          "*"
## 60  ( 1 ) "*"          "*"          "*"
## 61  ( 1 ) "*"          "*"          "*"
## 62  ( 1 ) "*"          "*"          "*"
## 63  ( 1 ) "*"          "*"          "*"
## 64  ( 1 ) "*"          "*"          "*"
## 65  ( 1 ) "*"          "*"          "*"
## 66  ( 1 ) "*"          "*"          "*"
## 67  ( 1 ) "*"          "*"          "*"
## 68  ( 1 ) "*"          "*"          "*"
## 69  ( 1 ) "*"          "*"          "*"
## 70  ( 1 ) "*"          "*"          "*"
## 71  ( 1 ) "*"          "*"          "*"
## 72  ( 1 ) "*"          "*"          "*"
## 73  ( 1 ) "*"          "*"          "*"
## 74  ( 1 ) "*"          "*"          "*"
## 75  ( 1 ) "*"          "*"          "*"
## 76  ( 1 ) "*"          "*"          "*"
## 77  ( 1 ) "*"          "*"          "*"
## 78  ( 1 ) "*"          "*"          "*"
## 79  ( 1 ) "*"          "*"          "*"
## 80  ( 1 ) "*"          "*"          "*"
## 81  ( 1 ) "*"          "*"          "*"
##                  wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1  ( 1 ) " "          " "          " "
## 2  ( 1 ) " "          " "          " "

```

```

## 3 ( 1 ) " "
## 4 ( 1 ) " "
## 5 ( 1 ) " "
## 6 ( 1 ) " "
## 7 ( 1 ) " "
## 8 ( 1 ) " "
## 9 ( 1 ) " "
## 10 ( 1 ) " "
## 11 ( 1 ) " "
## 12 ( 1 ) " "
## 13 ( 1 ) " "
## 14 ( 1 ) "*"
## 15 ( 1 ) "*"
## 16 ( 1 ) "*"
## 17 ( 1 ) "*"
## 18 ( 1 ) "*"
## 19 ( 1 ) "*"
## 20 ( 1 ) "*"
## 21 ( 1 ) "*"
## 22 ( 1 ) "*"
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## 24 ( 1 ) "*"
## 25 ( 1 ) "*"
## 26 ( 1 ) "*"
## 27 ( 1 ) "*"
## 28 ( 1 ) "*"
## 29 ( 1 ) "*"
## 30 ( 1 ) "*"
## 31 ( 1 ) "*"
## 32 ( 1 ) "*"
## 33 ( 1 ) "*"
## 34 ( 1 ) "*"
## 35 ( 1 ) "*"
## 36 ( 1 ) "*"
## 37 ( 1 ) "*"
## 38 ( 1 ) "*"
## 39 ( 1 ) "*"
## 40 ( 1 ) "*"
## 41 ( 1 ) " "
## 42 ( 1 ) " "
## 43 ( 1 ) " "
## 44 ( 1 ) " "
## 45 ( 1 ) " "
## 46 ( 1 ) "*"
## 47 ( 1 ) "*"
## 48 ( 1 ) "*"
## 49 ( 1 ) "*"
## 50 ( 1 ) "*"
## 51 ( 1 ) "*"
## 52 ( 1 ) "*"
## 53 ( 1 ) "*"
## 54 ( 1 ) "*"
## 55 ( 1 ) "*"
## 56 ( 1 ) "*"

```

```

## 57 ( 1 ) " "
## 58 ( 1 ) " "
## 59 ( 1 ) " "
## 60 ( 1 ) " "
## 61 ( 1 ) " "
## 62 ( 1 ) " "
## 63 ( 1 ) " "
## 64 ( 1 ) " "
## 65 ( 1 ) " "
## 66 ( 1 ) " "
## 67 ( 1 ) " "
## 68 ( 1 ) " "
## 69 ( 1 ) " "
## 70 ( 1 ) "*"
## 71 ( 1 ) "*"
## 72 ( 1 ) "*"
## 73 ( 1 ) " "
## 74 ( 1 ) " "
## 75 ( 1 ) " "
## 76 ( 1 ) "*"
## 77 ( 1 ) "*"
## 78 ( 1 ) "*"
## 79 ( 1 ) "*"
## 80 ( 1 ) "*"
## 81 ( 1 ) "*"

##          std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie
## 1 ( 1 ) " "           " "           " "           " "
## 2 ( 1 ) " "           " "           " "           " "
## 3 ( 1 ) " "           " "           " "           " "
## 4 ( 1 ) " "           " "           " "           " "
## 5 ( 1 ) " "           " "           " "           " "
## 6 ( 1 ) " "           " "           " "           " "
## 7 ( 1 ) " "           " "           " "           " "
## 8 ( 1 ) " "           " "           " "           " "
## 9 ( 1 ) " "           " "           " "           " "
## 10 ( 1 ) " "          " "           " "           " "
## 11 ( 1 ) " "          " "           " "           " "
## 12 ( 1 ) " "          " "           " "           " "
## 13 ( 1 ) " "          "*"          " "           " "
## 14 ( 1 ) "*"          "*"          "*"          "*"
## 15 ( 1 ) " "          "*"          "*"          " "
## 16 ( 1 ) " "          "*"          "*"          " "
## 17 ( 1 ) " "          "*"          "*"          " "
## 18 ( 1 ) " "          "*"          "*"          " "
## 19 ( 1 ) " "          "*"          "*"          " "
## 20 ( 1 ) " "          "*"          "*"          " "
## 21 ( 1 ) " "          "*"          "*"          " "
## 22 ( 1 ) " "          "*"          "*"          " "
## 23 ( 1 ) " "          "*"          "*"          " "
## 24 ( 1 ) " "          "*"          "*"          " "
## 25 ( 1 ) "*"          "*"          "*"          "*"
## 26 ( 1 ) " "          "*"          "*"          " "
## 27 ( 1 ) " "          "*"          "*"          " "
## 28 ( 1 ) " "          "*"          "*"          " "

```

```

## 29  ( 1 ) " "
## 30  ( 1 ) " "
## 31  ( 1 ) "*"
## 32  ( 1 ) " "
## 33  ( 1 ) " "
## 34  ( 1 ) " "
## 35  ( 1 ) " "
## 36  ( 1 ) " "
## 37  ( 1 ) " "
## 38  ( 1 ) " "
## 39  ( 1 ) " "
## 40  ( 1 ) " "
## 41  ( 1 ) " "
## 42  ( 1 ) " "
## 43  ( 1 ) " "
## 44  ( 1 ) " "
## 45  ( 1 ) " "
## 46  ( 1 ) "*"
## 47  ( 1 ) " "
## 48  ( 1 ) "*"
## 49  ( 1 ) "*"
## 50  ( 1 ) " "
## 51  ( 1 ) "*"
## 52  ( 1 ) "*"
## 53  ( 1 ) "*"
## 54  ( 1 ) "*"
## 55  ( 1 ) "*"
## 56  ( 1 ) "*"
## 57  ( 1 ) "*"
## 58  ( 1 ) "*"
## 59  ( 1 ) "*"
## 60  ( 1 ) "*"
## 61  ( 1 ) "*"
## 62  ( 1 ) "*"
## 63  ( 1 ) "*"
## 64  ( 1 ) "*"
## 65  ( 1 ) "*"
## 66  ( 1 ) "*"
## 67  ( 1 ) "*"
## 68  ( 1 ) "*"
## 69  ( 1 ) "*"
## 70  ( 1 ) "*"
## 71  ( 1 ) "*"
## 72  ( 1 ) "*"
## 73  ( 1 ) "*"
## 74  ( 1 ) "*"
## 75  ( 1 ) "*"
## 76  ( 1 ) "*"
## 77  ( 1 ) "*"
## 78  ( 1 ) "*"
## 79  ( 1 ) "*"
## 80  ( 1 ) "*"
## 81  ( 1 ) "*"
##               gmean_fie wtd_gmean_fie entropy_fie wtd_entropy_fie range_fie

```

```

## 1 ( 1 ) " "
## 2 ( 1 ) " "
## 3 ( 1 ) " "
## 4 ( 1 ) " "
## 5 ( 1 ) " "
## 6 ( 1 ) " "
## 7 ( 1 ) " "
## 8 ( 1 ) " "
## 9 ( 1 ) " "
## 10 ( 1 ) " "
## 11 ( 1 ) " "
## 12 ( 1 ) " "
## 13 ( 1 ) " "
## 14 ( 1 ) "*"
## 15 ( 1 ) " "
## 16 ( 1 ) " "
## 17 ( 1 ) " "
## 18 ( 1 ) " "
## 19 ( 1 ) " "
## 20 ( 1 ) " "
## 21 ( 1 ) " "
## 22 ( 1 ) " "
## 23 ( 1 ) " "
## 24 ( 1 ) " "
## 25 ( 1 ) "*"
## 26 ( 1 ) " "
## 27 ( 1 ) " "
## 28 ( 1 ) " "
## 29 ( 1 ) " "
## 30 ( 1 ) " "
## 31 ( 1 ) "*"
## 32 ( 1 ) " "
## 33 ( 1 ) " "
## 34 ( 1 ) " "
## 35 ( 1 ) " "
## 36 ( 1 ) " "
## 37 ( 1 ) " "
## 38 ( 1 ) " "
## 39 ( 1 ) " "
## 40 ( 1 ) " "
## 41 ( 1 ) " "
## 42 ( 1 ) " "
## 43 ( 1 ) " "
## 44 ( 1 ) " "
## 45 ( 1 ) " "
## 46 ( 1 ) "*"
## 47 ( 1 ) " "
## 48 ( 1 ) "*"
## 49 ( 1 ) "*"
## 50 ( 1 ) " "
## 51 ( 1 ) " "
## 52 ( 1 ) " "
## 53 ( 1 ) " "
## 54 ( 1 ) "*"

```

```

## 55 ( 1 ) " "      " "      "*"      "*"      "*"
## 56 ( 1 ) " "      " "      "*"      "*"      "*"
## 57 ( 1 ) " "      " "      "*"      "*"      "*"
## 58 ( 1 ) " "      " "      "*"      "*"      "*"
## 59 ( 1 ) " "      " "      "*"      "*"      "*"
## 60 ( 1 ) " "      " "      "*"      "*"      "*"
## 61 ( 1 ) " "      " "      "*"      "*"      "*"
## 62 ( 1 ) " "      " "      "*"      "*"      "*"
## 63 ( 1 ) " "      " "      "*"      "*"      "*"
## 64 ( 1 ) " "      " "      "*"      "*"      "*"
## 65 ( 1 ) " "      " "      "*"      "*"      "*"
## 66 ( 1 ) " "      " "      "*"      "*"      "*"
## 67 ( 1 ) " "      " "      "*"      "*"      "*"
## 68 ( 1 ) " "      " "      "*"      "*"      "*"
## 69 ( 1 ) " "      " "      "*"      "*"      "*"
## 70 ( 1 ) "*"      "*"      "*"      "*"      "*"
## 71 ( 1 ) "*"      "*"      "*"      "*"      "*"
## 72 ( 1 ) "*"      "*"      "*"      "*"      "*"
## 73 ( 1 ) " "      " "      "*"      "*"      "*"
## 74 ( 1 ) " "      " "      "*"      "*"      "*"
## 75 ( 1 ) " "      " "      "*"      "*"      "*"
## 76 ( 1 ) " "      " "      "*"      "*"      "*"
## 77 ( 1 ) " "      " "      "*"      "*"      "*"
## 78 ( 1 ) " "      " "      "*"      "*"      "*"
## 79 ( 1 ) "*"      "*"      "*"      "*"      "*"
## 80 ( 1 ) "*"      "*"      "*"      "*"      "*"
## 81 ( 1 ) "*"      "*"      "*"      "*"      "*"
##          wtd_range_fie std_fie wtd_std_fie mean_atomic_radius
## 1 ( 1 ) " "      " "      " "      " "
## 2 ( 1 ) " "      " "      " "      " "
## 3 ( 1 ) " "      " "      " "      " "
## 4 ( 1 ) " "      " "      " "      " "
## 5 ( 1 ) " "      " "      " "      " "
## 6 ( 1 ) " "      " "      " "      " "
## 7 ( 1 ) " "      " "      " "      " "
## 8 ( 1 ) " "      " "      " "      " "
## 9 ( 1 ) " "      " "      " "      " "
## 10 ( 1 ) " "     " "      " "      " "
## 11 ( 1 ) " "     " "      " "      " "
## 12 ( 1 ) " "     " "      " "      " "
## 13 ( 1 ) " "     " "      " "      " "
## 14 ( 1 ) " "     " "      " "      " "
## 15 ( 1 ) " "     " "      " "      " "
## 16 ( 1 ) " "     " "      " "      " "
## 17 ( 1 ) " "     " "      " "      " "
## 18 ( 1 ) " "     " "      " "      " "
## 19 ( 1 ) " "     " "      " "      " "
## 20 ( 1 ) " "     " "      " "      " "
## 21 ( 1 ) " "     " "      " "      " "
## 22 ( 1 ) " "     " "      " "      " "
## 23 ( 1 ) " "     " "      " "      " "
## 24 ( 1 ) " "     " "      " "      " "
## 25 ( 1 ) "*"      "*"      "*"      "*"      " "
## 26 ( 1 ) " "     " "      " "      " "

```

```

## 27 ( 1 ) " "
## 28 ( 1 ) "*" "
## 29 ( 1 ) "*" "
## 30 ( 1 ) "*" "
## 31 ( 1 ) "*" "
## 32 ( 1 ) "*" "
## 33 ( 1 ) "*" "
## 34 ( 1 ) "*" "
## 35 ( 1 ) "*" "
## 36 ( 1 ) "*" "
## 37 ( 1 ) "*" "
## 38 ( 1 ) "*" "
## 39 ( 1 ) "*" "
## 40 ( 1 ) "*" "
## 41 ( 1 ) "*" "
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## 43 ( 1 ) "*" "
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## 46 ( 1 ) "*" "
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## 48 ( 1 ) "*" "
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## 50 ( 1 ) "*" "
## 51 ( 1 ) "*" "
## 52 ( 1 ) "*" "
## 53 ( 1 ) "*" "
## 54 ( 1 ) "*" "
## 55 ( 1 ) "*" "
## 56 ( 1 ) "*" "
## 57 ( 1 ) "*" "
## 58 ( 1 ) "*" "
## 59 ( 1 ) "*" "
## 60 ( 1 ) "*" "
## 61 ( 1 ) "*" "
## 62 ( 1 ) "*" "
## 63 ( 1 ) "*" "
## 64 ( 1 ) "*" "
## 65 ( 1 ) "*" "
## 66 ( 1 ) "*" "
## 67 ( 1 ) "*" "
## 68 ( 1 ) "*" "
## 69 ( 1 ) "*" "
## 70 ( 1 ) "*" "
## 71 ( 1 ) "*" "
## 72 ( 1 ) "*" "
## 73 ( 1 ) "*" "
## 74 ( 1 ) "*" "
## 75 ( 1 ) "*" "
## 76 ( 1 ) "*" "
## 77 ( 1 ) "*" "
## 78 ( 1 ) "*" "
## 79 ( 1 ) "*" "
## 80 ( 1 ) "*" "

```

```

## 81  ( 1 ) "*"          "*"      "*"      "*"
##           wtd_mean_atomic_radius gmean_atomic_radius
## 1  ( 1 ) " "           " "
## 2  ( 1 ) " "           " "
## 3  ( 1 ) " "           " "
## 4  ( 1 ) " "           " "
## 5  ( 1 ) " "           " "
## 6  ( 1 ) " "           " "
## 7  ( 1 ) " "           " "
## 8  ( 1 ) " "           " "
## 9  ( 1 ) " "           " "
## 10 ( 1 ) " "           " "
## 11 ( 1 ) " "           " "
## 12 ( 1 ) " "           " "
## 13 ( 1 ) " "           " "
## 14 ( 1 ) " "           " "
## 15 ( 1 ) " "           " "
## 16 ( 1 ) " "           " "
## 17 ( 1 ) " "           " "
## 18 ( 1 ) " "           " "
## 19 ( 1 ) " "           " "
## 20 ( 1 ) " "           " "
## 21 ( 1 ) " "           " "
## 22 ( 1 ) " "           " "
## 23 ( 1 ) " "           " "
## 24 ( 1 ) " "           " "
## 25 ( 1 ) "*"          "*"      "*"      "*"
## 26 ( 1 ) " "           " "
## 27 ( 1 ) " "           " "
## 28 ( 1 ) " "           " "
## 29 ( 1 ) " "           " "
## 30 ( 1 ) " "           " "
## 31 ( 1 ) "*"          "*"      "*"      "*"
## 32 ( 1 ) " "           " "
## 33 ( 1 ) " "           " "
## 34 ( 1 ) " "           " "
## 35 ( 1 ) " "           " "
## 36 ( 1 ) " "           " "
## 37 ( 1 ) " "           " "
## 38 ( 1 ) " "           " "
## 39 ( 1 ) "*"          "*"      "*"      "*"
## 40 ( 1 ) "*"          "*"      "*"      "*"
## 41 ( 1 ) "*"          "*"      "*"      "*"
## 42 ( 1 ) "*"          "*"      "*"      "*"
## 43 ( 1 ) "*"          "*"      "*"      "*"
## 44 ( 1 ) "*"          "*"      "*"      "*"
## 45 ( 1 ) "*"          "*"      "*"      "*"
## 46 ( 1 ) "*"          "*"      "*"      "*"
## 47 ( 1 ) "*"          "*"      "*"      "*"
## 48 ( 1 ) "*"          "*"      "*"      "*"
## 49 ( 1 ) "*"          "*"      "*"      "*"
## 50 ( 1 ) "*"          "*"      "*"      "*"
## 51 ( 1 ) "*"          "*"      "*"      "*"
## 52 ( 1 ) "*"          "*"      "*"      "*"

```

```

## 53  ( 1 ) "*"          "*"
## 54  ( 1 ) "*"          "*"
## 55  ( 1 ) "*"          "*"
## 56  ( 1 ) "*"          "*"
## 57  ( 1 ) "*"          "*"
## 58  ( 1 ) "*"          ""
## 59  ( 1 ) "*"          ""
## 60  ( 1 ) "*"          ""
## 61  ( 1 ) "*"          ""
## 62  ( 1 ) "*"          ""
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          ""
## 66  ( 1 ) "*"          ""
## 67  ( 1 ) "*"          ""
## 68  ( 1 ) "*"          ""
## 69  ( 1 ) "*"          ""
## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"
## 72  ( 1 ) "*"          "*"
## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
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## 78  ( 1 ) "*"          "*"
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##           wtd_gmean_atomic_radius entropy_atomic_radius
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
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## 9  ( 1 ) " "          " "
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## 11 ( 1 ) " "          " "
## 12 ( 1 ) " "          " "
## 13 ( 1 ) " "          " "
## 14 ( 1 ) " "          " "
## 15 ( 1 ) " "          " "
## 16 ( 1 ) " "          " "
## 17 ( 1 ) " "          " "
## 18 ( 1 ) " "          " "
## 19 ( 1 ) " "          " "
## 20 ( 1 ) " "          " "
## 21 ( 1 ) " "          " "
## 22 ( 1 ) " "          " "
## 23 ( 1 ) " "          " "
## 24 ( 1 ) " "          "*"

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## 37  ( 1 ) " "          "*"
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## 62  ( 1 ) "*"          " "
## 63  ( 1 ) "*"          " "
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
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## 72  ( 1 ) "*"          "*"
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## 74  ( 1 ) "*"          "*"
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## 78  ( 1 ) "*"          "*"

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## 9  ( 1 ) " "           "*"
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## 19 ( 1 ) " "           "*"
## 20 ( 1 ) " "           "*"
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## 23 ( 1 ) "*"          "*"
## 24 ( 1 ) "*"          "*"
## 25 ( 1 ) " "           " "
## 26 ( 1 ) "*"          "*"
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## 30 ( 1 ) "*"          "*"
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## 50 ( 1 ) "*"          "*"

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## 70  ( 1 ) "*"          "*"
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## 73  ( 1 ) "*"          "*"
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## 78  ( 1 ) "*"          "*"
## 79  ( 1 ) "*"          "*"
## 80  ( 1 ) "*"          "*"
## 81  ( 1 ) "*"          "*"
##           wtd_range_atomic_radius std_atomic_radius wtd_std_atomic_radius
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## 3  ( 1 ) " "          " "          " "
## 4  ( 1 ) " "          " "          " "
## 5  ( 1 ) " "          " "          " "
## 6  ( 1 ) " "          " "          " "
## 7  ( 1 ) " "          " "          " "
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## 9  ( 1 ) " "          "*"         " "
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## 11 ( 1 ) " "          "*"         " "
## 12 ( 1 ) " "          "*"         " "
## 13 ( 1 ) " "          "*"         " "
## 14 ( 1 ) " "          " "          " "
## 15 ( 1 ) " "          " "          " "
## 16 ( 1 ) " "          "*"         " "
## 17 ( 1 ) " "          " "          " "
## 18 ( 1 ) " "          "*"         " "
## 19 ( 1 ) " "          "*"         " "
## 20 ( 1 ) " "          "*"         " "
## 21 ( 1 ) " "          "*"         "*"
## 22 ( 1 ) " "          "*"         "*"

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## 37 ( 1 ) " "
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## 72 ( 1 ) "*"
## 73 ( 1 ) "*"
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## 75 ( 1 ) "*"
## 76 ( 1 ) "*"

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## 81 ( 1 ) "*"      "*"      "*"
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## 2 ( 1 ) " "       " "       " "       " "
## 3 ( 1 ) " "       " "       " "       " "
## 4 ( 1 ) " "       " "       " "       " "
## 5 ( 1 ) " "       " "       " "       " "
## 6 ( 1 ) " "       " "       " "       " "
## 7 ( 1 ) " "       " "       " "       " "
## 8 ( 1 ) " "       " "       " "       " "
## 9 ( 1 ) " "       " "       " "       " "
## 10 ( 1 ) " "      " "       " "       " "
## 11 ( 1 ) " "      " "       " "       " "
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## 15 ( 1 ) " "      " "       " "       " "
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## 47 ( 1 ) "*"      " "       " "       "*"
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## 55  ( 1 ) "*"      "*"      " "      "*"
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## 57  ( 1 ) "*"      "*"      " "      "*"
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## 77  ( 1 ) "*"      "*"      "*"      "*"
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## 79  ( 1 ) "*"      "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"      "*"
## 81  ( 1 ) "*"      "*"      "*"      "*"
##          entropy_Density wtd_entropy_Density range_Density
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## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      "*"
## 16 ( 1 ) " "      " "      "*"
## 17 ( 1 ) " "      " "      "*"
## 18 ( 1 ) "*"      " "      "*"
## 19 ( 1 ) "*"      " "      "*"
## 20 ( 1 ) " "      " "      "*"

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## 21 ( 1 ) " "      " "
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## 25 ( 1 ) " "      " "
## 26 ( 1 ) " "      " *"
## 27 ( 1 ) " "      " *"
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## 73 ( 1 ) "*"
## 74 ( 1 ) "*"

```

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## 81  ( 1 ) "*"      "*"      "*"
##          wtd_range_Density std_Density wtd_std_Density
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## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
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## 81  ( 1 ) "*"
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## 2  ( 1 ) " "
## 3  ( 1 ) " "
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## 9  ( 1 ) " "
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## 11 ( 1 ) " "
## 12 ( 1 ) "*"
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## 14 ( 1 ) " "
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## 18 ( 1 ) "*"

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## 27  ( 1 ) " "     "*"
## 28  ( 1 ) " "     "*"
## 29  ( 1 ) " "     "*"
## 30  ( 1 ) " "     "*"
## 31  ( 1 ) " "     " "
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## 34  ( 1 ) " "     "*"
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## 38  ( 1 ) " "     "*"
## 39  ( 1 ) " "     "*"
## 40  ( 1 ) " "     "*"
## 41  ( 1 ) " "     "*"
## 42  ( 1 ) " "     "*"
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## 62  ( 1 ) "*"      "*"
## 63  ( 1 ) "*"      "*"
## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
## 67  ( 1 ) "*"      "*"
## 68  ( 1 ) "*"      "*"
## 69  ( 1 ) "*"      "*"
## 70  ( 1 ) "*"      "*"
## 71  ( 1 ) "*"      "*"
## 72  ( 1 ) "*"      "*"

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## 78  ( 1 ) "*"          "*"
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## 80  ( 1 ) "*"          "*"
## 81  ( 1 ) "*"          "*"
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## 5  ( 1 ) " "           "*"
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## 7  ( 1 ) " "           "*"
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## 9  ( 1 ) " "           "*"
## 10 ( 1 ) " "           "*"
## 11 ( 1 ) "*"          "*"
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## 14 ( 1 ) " "           " "
## 15 ( 1 ) " "           "*"
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## 17 ( 1 ) "*"          "*"
## 18 ( 1 ) "*"          "*"
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## 23 ( 1 ) "*"          "*"
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## 28 ( 1 ) "*"          "*"
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## 6  ( 1 ) " "      " "
## 7  ( 1 ) " "      " "
## 8  ( 1 ) " "      " "
## 9  ( 1 ) " "      " "
## 10 ( 1 ) " "      " "
## 11 ( 1 ) " "      " "
## 12 ( 1 ) " "      " "
## 13 ( 1 ) " "      " "
## 14 ( 1 ) " "      " "
## 15 ( 1 ) " "      " "
## 16 ( 1 ) " "      " "

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## 17 ( 1 ) "*"          " "
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## 24 ( 1 ) "*"          " "
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## 27 ( 1 ) "*"          " "
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## 42 ( 1 ) "*"          "*"

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## 55  ( 1 ) "*"          "*"
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## 59  ( 1 ) "*"          "*"
## 60  ( 1 ) "*"          "*"
## 61  ( 1 ) "*"          "*"
## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
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## 69  ( 1 ) "*"          "*"
## 70  ( 1 ) "*"          "*"
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## 72  ( 1 ) "*"          "*"
## 73  ( 1 ) "*"          "*"
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## 14 ( 1 ) " "          " "          " "

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## 27  ( 1 ) "*"      "*"
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## 62  ( 1 ) "*"      "*"
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## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
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## 68  ( 1 ) "*"      "*"

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## 40 ( 1 ) "*"      " "        "*"

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## 81  ( 1 ) "*" "
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## 10 ( 1 ) " "           " "           " "
## 11 ( 1 ) " "           " "           " "
## 12 ( 1 ) " "           " "           " "

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## 2  ( 1 ) " "      " "      " "
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## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "

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## 81  ( 1 ) "*"      "*"
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## 2  ( 1 ) " "           " "
## 3  ( 1 ) " "           " "
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## 5  ( 1 ) " "           " "
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## 8 ( 1 ) " "          " "

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## 62 ( 1 )   "*"

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##          range_ThermalConductivity wtd_range_ThermalConductivity
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## 3  ( 1 ) " "           ""
## 4  ( 1 ) " "           ""
## 5  ( 1 ) " "           ""
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## 21 ( 1 ) " "           ""
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## 3  ( 1 ) " "          "*"          " "
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## 5  ( 1 ) " "          "*"          " "
## 6  ( 1 ) " "          "*"          " "

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## 3  ( 1 ) " "           " "           " "           " "
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## 80 ( 1 ) "*"      " * "      " * "      " * "
## 81 ( 1 ) "*"      " * "      " * "      " * "
##          wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
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## 3 ( 1 ) " "          " "          " "          " "
## 4 ( 1 ) " "

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```

```
linear_stepwise$results
```

```

##      nvmax      RMSE   Rsquared       MAE     RMSESD   RsquaredSD     MAESD
## 1      1 23.73833 0.5198107 18.24597 0.2467303 0.008466076 0.2298375
## 2      2 22.81227 0.5565342 17.65525 0.2210382 0.008908434 0.2063558
## 3      3 22.05517 0.5854512 17.25921 0.2957349 0.012466668 0.2425789
## 4      4 21.44967 0.6079547 16.80859 0.1902049 0.009495616 0.1626152
## 5      5 20.94882 0.6260647 16.48752 0.1811812 0.009939315 0.1866227
## 6      6 20.65791 0.6363753 16.15813 0.1497790 0.008627713 0.1621507
## 7      7 20.42467 0.6444857 15.77413 0.1506396 0.007452758 0.1722256
## 8      8 20.19085 0.6525663 15.53950 0.1727360 0.008070484 0.2021921
## 9      9 20.08628 0.6561573 15.37467 0.1733370 0.008073159 0.2081623
## 10     10 19.95712 0.6605658 15.27684 0.2204478 0.009785714 0.2431182
## 11     11 19.84711 0.6642904 15.18689 0.2062608 0.009209924 0.2231133
## 12     12 19.47425 0.5624059 17.46256 2.9996511 0.116454434 2.6196366
## 13     13 19.49608 0.6760180 14.97198 0.2153065 0.009185978 0.2166335
## 14     14 21.01814 0.6189685 16.25351 2.6528841 0.095152665 2.2603950
## 15     15 19.23726 0.6845941 14.78316 0.2648730 0.010715295 0.2502442
## 16     16 19.15280 0.6873783 14.72849 0.2677283 0.010515987 0.2499363
## 17     17 19.37103 0.6783915 14.93678 1.4160226 0.054288170 1.2044688
## 18     18 18.81484 0.6983497 14.42151 0.2651940 0.010190725 0.2144369
## 19     19 19.24847 0.6826173 14.78607 1.7633286 0.058601855 1.5052031
## 20     20 18.71024 0.7016834 14.34049 0.2972580 0.010869079 0.2145273
## 21     21 18.57375 0.7059954 14.18874 0.2851093 0.010618735 0.1973841
## 22     22 19.53018 0.6715072 15.02221 2.0064124 0.075306826 1.7254898
## 23     23 19.54566 0.6719601 15.03494 2.0032314 0.067810768 1.7835990
## 24     24 18.85860 0.6955012 14.42263 1.2809648 0.046863222 0.9186043
## 25     25 20.23097 0.6481733 15.58316 1.9071366 0.067011522 1.5355338
## 26     26 19.63294 0.6687791 15.00885 1.7873368 0.062474142 1.3132910
## 27     27 18.68769 0.7011153 14.25856 1.1324197 0.042359089 0.8733350
## 28     28 18.31912 0.7139229 13.97156 0.3554812 0.012755330 0.2240875
## 29     29 18.29218 0.7147791 13.95479 0.3497483 0.012631397 0.2216918
## 30     30 18.27532 0.7152976 13.92564 0.3594464 0.012492489 0.2283411
## 31     31 18.70541 0.7005624 14.27269 1.1384730 0.040664946 0.8571907
## 32     32 18.46368 0.7086652 14.09605 0.8759586 0.032392815 0.7719977
## 33     33 18.44803 0.7093946 14.07016 0.9122316 0.029594942 0.7735902
## 34     34 18.75347 0.6994644 14.29068 1.2978527 0.039221282 1.0553353
## 35     35 18.14593 0.7193157 13.80553 0.3435066 0.011951093 0.2562691
## 36     36 18.55734 0.7056099 14.16643 0.9022816 0.032906938 0.7005858
## 37     37 18.07839 0.7214137 13.74413 0.3203197 0.011216062 0.2344987
## 38     38 18.50986 0.7074288 14.08119 1.0233810 0.031989186 0.8898199
## 39     39 18.02162 0.7231893 13.67634 0.3152629 0.010759998 0.2443067
## 40     40 18.00471 0.7237114 13.66772 0.3214395 0.010944748 0.2446574
## 41     41 18.50465 0.7077961 14.04686 1.0730459 0.029874587 0.8919080
## 42     42 18.36398 0.7119089 13.94287 0.8316131 0.028875809 0.6307944
## 43     43 18.13738 0.7191311 13.77210 0.8354926 0.027321640 0.6653856
## 44     44 18.59135 0.7044549 14.18683 0.9664592 0.035015001 0.8069281
## 45     45 18.34733 0.7125916 13.94022 0.9775478 0.030177907 0.8602860
## 46     46 18.48173 0.7084421 14.04869 0.7705166 0.024518900 0.6976773
## 47     47 18.52803 0.7065902 14.06751 1.0062096 0.034029719 0.8118066
## 48     48 17.88492 0.7273658 13.53908 0.3058756 0.010350026 0.2211942
## 49     49 17.99885 0.7235895 13.65373 0.5319870 0.019064230 0.4261569
## 50     50 18.00994 0.7231980 13.67502 0.5907482 0.021645727 0.5345946
## 51     51 17.94229 0.7253934 13.58997 0.4644628 0.016581216 0.3269786
## 52     52 17.81933 0.7293657 13.48636 0.2888482 0.009769506 0.2167636
## 53     53 17.80715 0.7297347 13.47225 0.2864604 0.009676574 0.2060466

```

```

## 54 54 17.92455 0.7259632 13.56802 0.6008896 0.019115922 0.4795112
## 55 55 17.94827 0.7253246 13.57351 0.6939688 0.018940710 0.5166638
## 56 56 18.01152 0.7231940 13.65481 0.6192455 0.020160598 0.5215576
## 57 57 17.77178 0.7308104 13.43654 0.2808082 0.009305431 0.2057986
## 58 58 17.76091 0.7311324 13.42743 0.2814998 0.009496839 0.2015860
## 59 59 17.86921 0.7276803 13.52470 0.5600936 0.017818067 0.4400633
## 60 60 17.75192 0.7314054 13.41864 0.2944774 0.009710834 0.2082803
## 61 61 17.74611 0.7315868 13.41198 0.2890453 0.009532863 0.2080024
## 62 62 17.99532 0.7237217 13.67669 0.4827916 0.017857607 0.3927361
## 63 63 18.01902 0.7232938 13.67457 0.4291906 0.011433986 0.4980903
## 64 64 17.72303 0.7322774 13.38482 0.3074985 0.009862481 0.2194202
## 65 65 17.72189 0.7323136 13.38828 0.3083437 0.009887866 0.2156790
## 66 66 17.71662 0.7324726 13.38655 0.3079031 0.009886833 0.2176267
## 67 67 17.80086 0.7298371 13.45741 0.3471107 0.012673949 0.2347961
## 68 68 17.81645 0.7293525 13.45360 0.3803426 0.013596563 0.2534678
## 69 69 17.71652 0.7324757 13.39406 0.3113975 0.009922334 0.2213003
## 70 70 17.78133 0.7305335 13.44979 0.2578971 0.008106677 0.2087535
## 71 71 17.83950 0.7287479 13.48007 0.2560245 0.009048804 0.1713487
## 72 72 17.82745 0.7290878 13.47383 0.4253165 0.012396125 0.2942630
## 73 73 17.77802 0.7306418 13.43337 0.2778794 0.008613770 0.2228334
## 74 74 17.78626 0.7303950 13.44844 0.2735603 0.008349011 0.2269027
## 75 75 17.80639 0.7297426 13.46333 0.3562727 0.011006008 0.2228424
## 76 76 17.71128 0.7326348 13.39889 0.3138844 0.009949738 0.2261672
## 77 77 17.73192 0.7320052 13.40324 0.3138033 0.010007702 0.2243926
## 78 78 17.76619 0.7309957 13.42684 0.2677058 0.008617195 0.2094641
## 79 79 17.77662 0.7306697 13.42074 0.2663622 0.008812767 0.1928822
## 80 80 17.74447 0.7316210 13.38998 0.3222360 0.010100445 0.2126880
## 81 81 17.71082 0.7326498 13.40288 0.3121764 0.009942553 0.2221992

```

From the above results, we can see how stepwise selection works and the corresponding errors to the number of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_stepwise, linear_stepwise$results$nvmax, "Number of Variables")
```

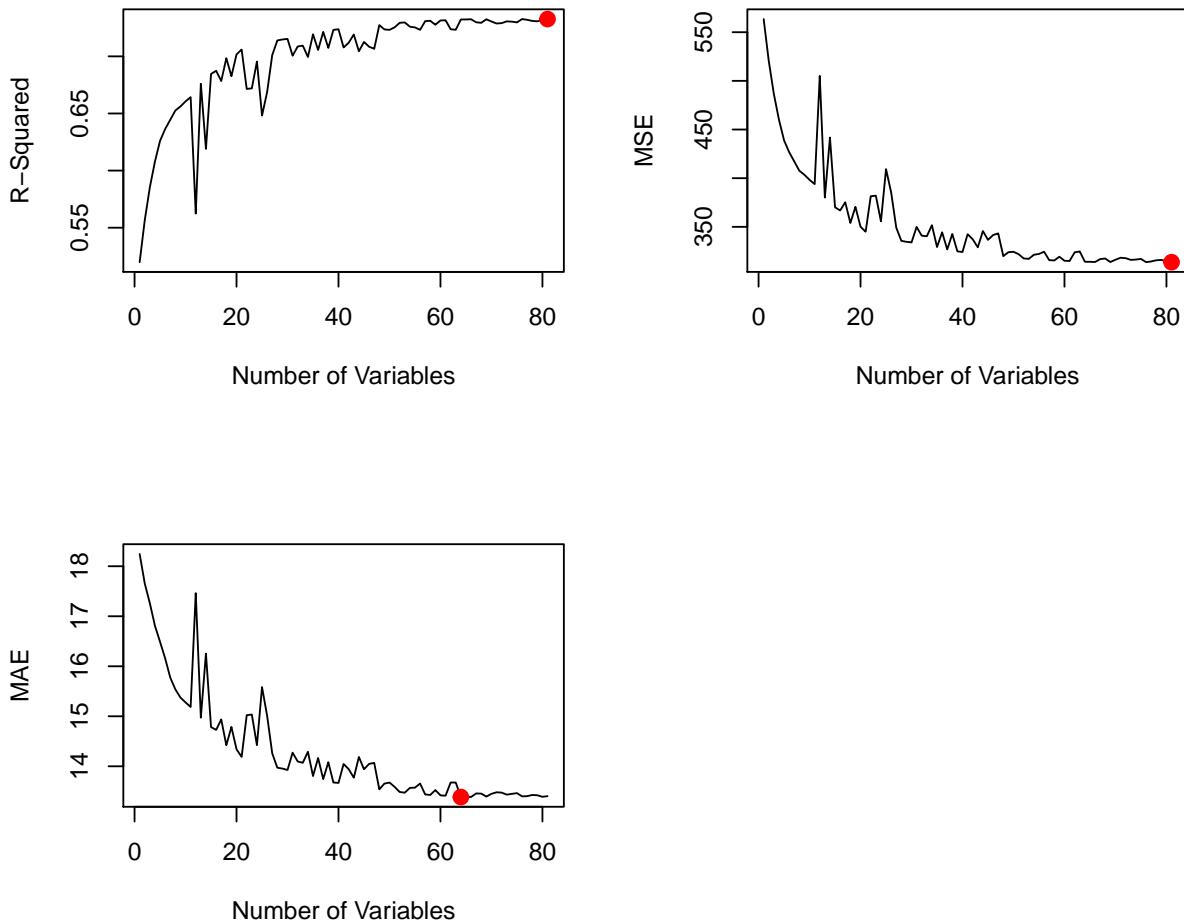


Figure 49: R-Squared, MSE, and MAE for Stepwise Selection

```
linear_stepwise$bestTune

##      nvmax
## 81     81

coef(linear_stepwise$finalModel, linear_stepwise$bestTune$nvmax)

##              (Intercept)          number_of_elements
##                 -11.552623           -29.347923
##      mean_atomic_mass        wtd_mean_atomic_mass
##                183.838528           -205.162353
##      gmean_atomic_mass       wtd_gmean_atomic_mass
##                -115.114215            155.385680
##      entropy_atomic_mass     wtd_entropy_atomic_mass
##                  -74.658643             5.507998
##      range_atomic_mass       wtd_range_atomic_mass
```

```

##          45.027497      5.353503
## std_atomic_mass      wtd_std_atomic_mass
##          -61.072593     13.358930
## mean_fie            wtd_mean_fie
##          133.260300    -99.998268
## gmean_fie           wtd_gmean_fie
##          -131.975004    123.132676
## entropy_fie         wtd_entropy_fie
##          -198.925646    95.376297
## range_fie           wtd_range_fie
##          81.767787    22.560872
## std_fie             wtd_std_fie
##          -85.789985   -17.803468
## mean_atomic_radius  wtd_mean_atomic_radius
##          -173.026262    825.059330
## gmean_atomic_radius wtd_gmean_atomic_radius
##          93.933277   -733.337195
## entropy_atomic_radius wtd_entropy_atomic_radius
##          122.181241    83.736432
## range_atomic_radius wtd_range_atomic_radius
##          52.681325   -20.607446
## std_atomic_radius   wtd_std_atomic_radius
##          -43.269724   -32.350249
## mean_Density         wtd_mean_Density
##          -111.750928    7.935565
## gmean_Density        wtd_gmean_Density
##          28.655192    41.914717
## entropy_Density      wtd_entropy_Density
##          36.347583   -32.252993
## range_Density        wtd_range_Density
##          -36.029088   -2.175651
## std_Density          wtd_std_Density
##          67.662583   -17.925956
## mean_ElectronAffinity wtd_mean_ElectronAffinity
##          -31.868396   160.646544
## gmean_ElectronAffinity wtd_gmean_ElectronAffinity
##          51.789208   -175.501782
## entropy_ElectronAffinity wtd_entropy_ElectronAffinity
##          10.600568   -36.048263
## range_ElectronAffinity wtd_range_ElectronAffinity
##          -130.362783   -32.072054
## std_ElectronAffinity wtd_std_ElectronAffinity
##          206.799330   -94.812042
## mean_FusionHeat       wtd_mean_FusionHeat
##          178.426834   -212.730936
## gmean_FusionHeat      wtd_gmean_FusionHeat
##          -160.004844   179.276311
## entropy_FusionHeat    wtd_entropy_FusionHeat
##          -39.280702   43.920705
## range_FusionHeat       wtd_range_FusionHeat
##          -35.540265   61.141726
## std_FusionHeat         wtd_std_FusionHeat
##          -34.804605   44.132412
## mean_ThermalConductivity wtd_mean_ThermalConductivity

```

```

##          -33.171094           234.634308
## gmean_ThermalConductivity   wtd_gmean_ThermalConductivity
##          -10.752832           -141.654674
## entropy_ThermalConductivity wtd_entropy_ThermalConductivity
##          21.449701            3.123154
## range_ThermalConductivity  wtd_range_ThermalConductivity
##          -38.598450           -90.175670
## std_ThermalConductivity    wtd_std_ThermalConductivity
##          66.986580            -8.089653
## mean_Valence                wtd_mean_Valence
##          -101.243994          153.454682
## gmean_Valence               wtd_gmean_Valence
##          126.782416           -176.546638
## entropy_Valence             wtd_entropy_Valence
##          142.964275           -140.272893
## range_Valence               wtd_range_Valence
##          25.367238            -6.700735
## std_Valence                 wtd_std_Valence
##          23.880257            -75.454151

```

```
getTrainPerf(linear_stepwise)
```

```

##   TrainRMSE TrainRsquared TrainMAE   method
## 1  17.71082     0.7326498 13.40288  leapSeq

```

From the above metrics, it can be seen that based on R-Squared and MSE, the best model is the model with 81 variables, however, MAE choose a model with less variables. By using the feature from caret package, we can decide that the best model is the model with 81 variables. The list of 81 variables is provided above. The R-Squared for this model is 0.7326498 with Train MSE is 313.6441

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_stepwise, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

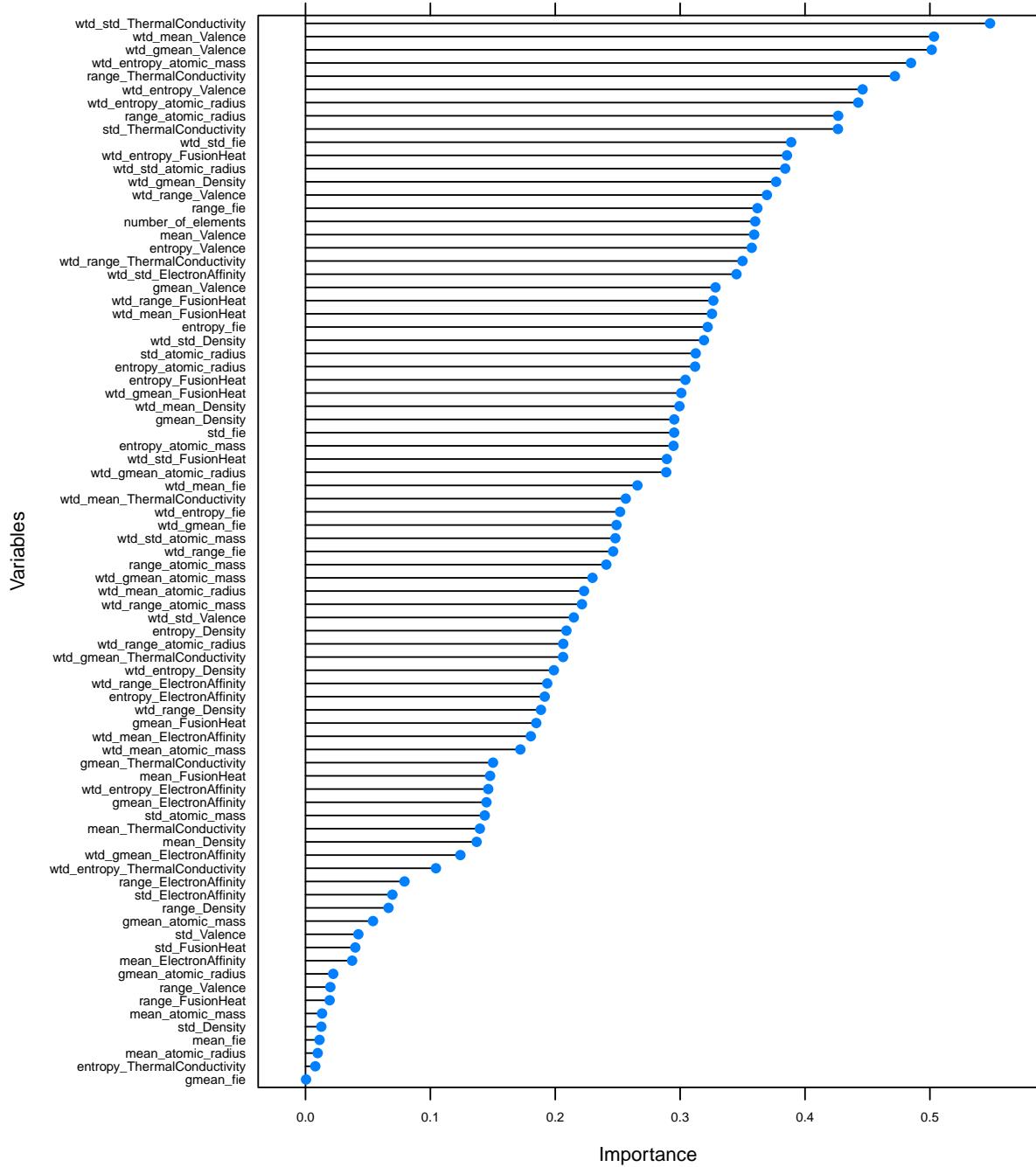


Figure 50: Variables Importance for Stepwise Selection

From above, it can be seen that wtd\_std\_ThermalConductivity is the most important variable for this model, whereas gmean\_fie is the least important variable for this model.

From above, we can see that both backward, forward and stepwise selection have almost the same train R-Squared and MSE. However, backward selection produces the least complexity model with 77 variables, whereas forward selection and stepwise selection have 78 and 81 variables consecutively. Therefore, we can

conclude that backward selection gives a better result among them

### 3.1.7 Ridge Regression

The standard linear model performs poorly in a situation, where you have a large multivariate data set containing a number of variables superior to the number of samples.

A better alternative is the penalized regression allowing to create a linear regression model that is penalized, for having too many variables in the model, by adding a constraint in the equation [Bruce and Bruce, 2017]. This is also known as shrinkage or regularization methods.

The consequence of imposing this penalty, is to reduce the coefficient values towards zero. This allows the less contributive variables to have a coefficient close to zero or equal zero.

Note that, the shrinkage requires the selection of a tuning parameter (lambda) that determines the amount of shrinkage.

In this sub section, we will perform Ridge regression. Ridge regression shrinks the regression coefficients, so that variables, with minor contribution to the outcome, have their coefficients close to zero.

The shrinkage of the coefficients is achieved by penalizing the regression model with a penalty term called L2-norm, which is the sum of the squared coefficients.

The amount of the penalty can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

lambda_seq <- seq(0.01, 1, length = 15)

# Ridge Regression
ridge_model <- train(
  critical_temp ~., data = train.data, method = "ridge",
  trControl = control,
  tuneGrid = expand.grid(lambda = lambda_seq),
  preProc = c("range")
)

ridge_model$results

##          lambda      RMSE   Rsquared      MAE     RMSESD  RsquaredSD      MAESD
## 1  0.01000000 18.27208  0.7154740 13.92682  0.2585789  0.009453411  0.1900263
## 2  0.08071429 19.10376  0.6899108 14.79484  0.1934721  0.008349144  0.1562966
## 3  0.15142857 19.62604  0.6776089 15.38499  0.1792526  0.008076491  0.1508664
## 4  0.22214286 20.18715  0.6682202 15.97571  0.1854141  0.008025315  0.1581446
## 5  0.29285714 20.81810  0.6606085 16.59218  0.2024658  0.008044932  0.1758759
## 6  0.36357143 21.52478  0.6542523 17.23866  0.2250152  0.008084767  0.1986669
## 7  0.43428571 22.30535  0.6488297 17.92435  0.2500045  0.008126895  0.2196425
## 8  0.50500000 23.15479  0.6441232 18.65398  0.2757610  0.008165132  0.2440978
## 9  0.57571429 24.06672  0.6399791 19.43174  0.3013918  0.008197738  0.2735716
## 10 0.64642857 25.03440  0.6362856 20.25308  0.3264392  0.008224674  0.3011943
## 11 0.71714286 26.05119  0.6329595 21.11216  0.3506905  0.008246512  0.3259465
## 12 0.78785714 27.11091  0.6299373 22.00531  0.3740718  0.008263993  0.3492660
## 13 0.85857143 28.20788  0.6271698 22.92486  0.3965867  0.008277851  0.3698251
## 14 0.92928571 29.33702  0.6246182 23.87059  0.4182809  0.008288747  0.3868058
## 15 1.00000000 30.49380  0.6222516 24.84195  0.4392204  0.008297248  0.4051341
```

From the above results, we can see the corresponding errors to the lambda values. Here, we will plot and see the optimal lambda.

```
plot_metrics(ridge_model, ridge_model$results$lambda, "Lambda")
```

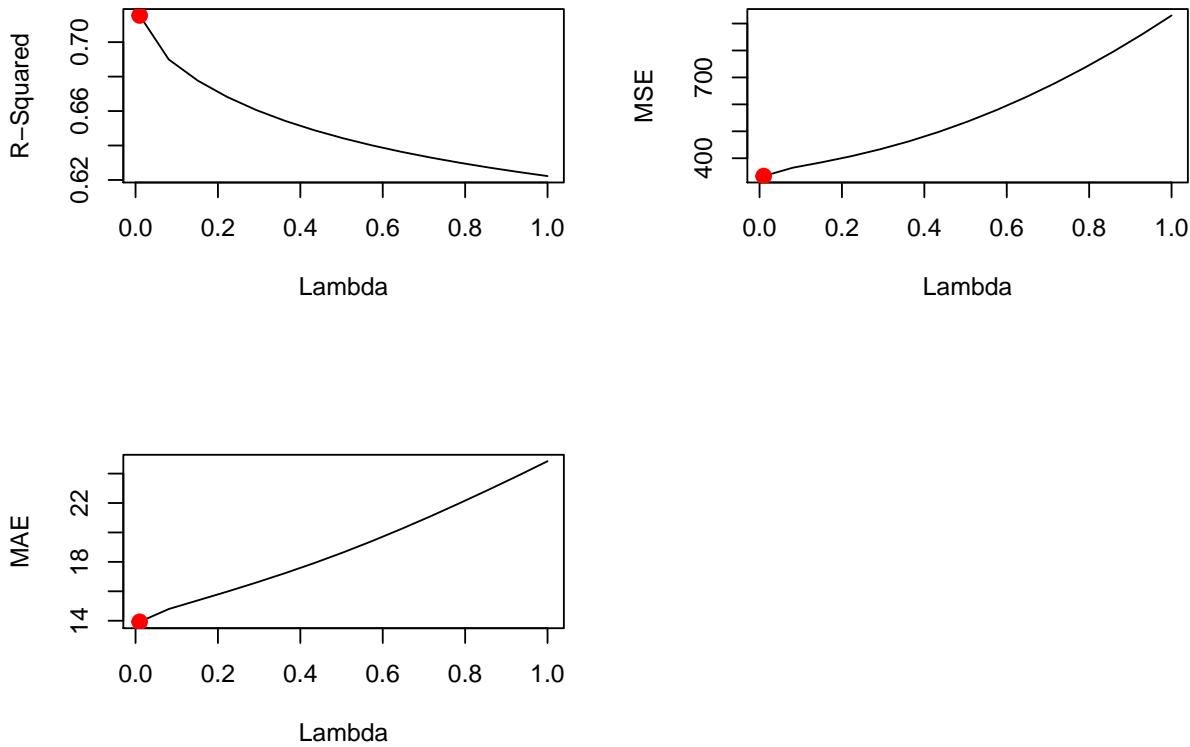


Figure 51: R-Squared, MSE, and MAE for Ridge Regression

```
ridge_model$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next we will show the coefficient after regularization.

```
varImp(ridge_model)$importance
```

```
##                                     Overall
## number_of_elements                65.666830
## mean_atomic_mass                  2.340670
## wtd_mean_atomic_mass              31.332214
## gmean_atomic_mass                 9.789289
## wtd_gmean_atomic_mass             41.873592
## entropy_atomic_mass               53.717397
```

```

## wtd_entropy_atomic_mass          88.439537
## range_atomic_mass               43.896261
## wtd_range_atomic_mass          40.332190
## std_atomic_mass                26.126408
## wtd_std_atomic_mass            45.220901
## mean_fie                       1.969445
## wtd_mean_fie                  48.444039
## gmean_fie                      0.000000
## wtd_gmean_fie                 45.381919
## entropy_fie                   58.711572
## wtd_entropy_fie                45.914068
## range_fie                      65.983263
## wtd_range_fie                 44.894401
## std_fie                        53.815465
## wtd_std_fie                   70.925237
## mean_atomic_radius             1.702301
## wtd_mean_atomic_radius        40.639964
## gmean_atomic_radius            3.970195
## wtd_gmean_atomic_radius       52.658746
## entropy_atomic_radius         56.874572
## wtd_entropy_atomic_radius     80.723038
## range_atomic_radius           77.791891
## wtd_range_atomic_radius       37.603038
## std_atomic_radius              56.967153
## wtd_std_atomic_radius         70.044923
## mean_Density                  24.938698
## wtd_mean_Density              54.589447
## gmean_Density                 53.827694
## wtd_gmean_Density             68.720521
## entropy_Density               38.066656
## wtd_entropy_Density           36.228805
## range_Density                 12.054532
## wtd_range_Density             34.339177
## std_Density                   2.232043
## wtd_std_Density               58.173311
## mean_ElectronAffinity         6.736804
## wtd_mean_ElectronAffinity    32.860649
## gmean_ElectronAffinity        26.375327
## wtd_gmean_ElectronAffinity   22.565659
## entropy_ElectronAffinity     34.896012
## wtd_entropy_ElectronAffinity  26.634459
## range_ElectronAffinity        14.392845
## wtd_range_ElectronAffinity   35.260218
## std_ElectronAffinity          12.620594
## wtd_std_ElectronAffinity      62.926880
## mean_FusionHeat               26.907726
## wtd_mean_FusionHeat           59.338381
## gmean_FusionHeat              33.655417
## wtd_gmean_FusionHeat          54.858189
## entropy_FusionHeat            55.457733
## wtd_entropy_FusionHeat         70.307323
## range_FusionHeat              3.449967
## wtd_range_FusionHeat          59.540820
## std_FusionHeat                7.198470

```

```

## wtd_std_FusionHeat           52.743087
## mean_ThermalConductivity   25.413098
## wtd_mean_ThermalConductivity 46.740051
## gmean_ThermalConductivity  27.335587
## wtd_gmean_ThermalConductivity 37.572795
## entropy_ThermalConductivity 1.354467
## wtd_entropy_ThermalConductivity 18.985751
## range_ThermalConductivity  86.084589
## wtd_range_ThermalConductivity 63.805474
## std_ThermalConductivity    77.761604
## wtd_std_ThermalConductivity 100.000000
## mean_Valence                65.510304
## wtd_mean_Valence            91.800565
## gmean_Valence               59.856849
## wtd_gmean_Valence           91.469039
## entropy_Valence             65.156151
## wtd_entropy_Valence         81.364893
## range_Valence                3.552174
## wtd_range_Valence           67.378506
## std_Valence                  7.647729
## wtd_std_Valence              39.144031

```

```
getTrainPerf(ridge_model)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 18.27208      0.715474 13.92682 ridge

```

From the above metrics, the R-Squared for this model is 0.715474 with Train MSE is 333.868

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(ridge_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

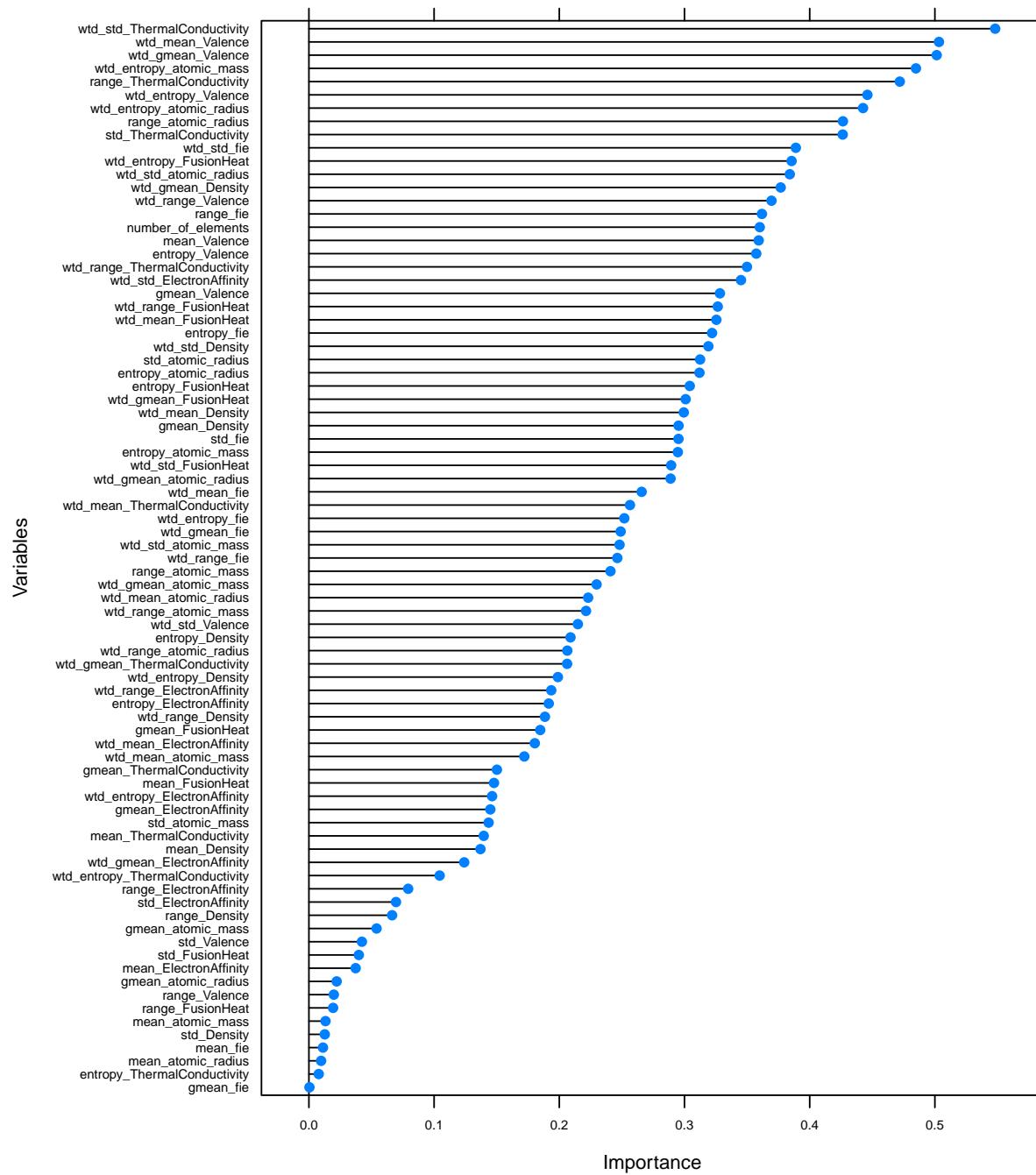


Figure 52: Variables Importance for Ridge Regression

From above, it can be seen that wtd\_std\_ThermalConductivity is the most important variable for this model, whereas gmean\_fie is the least important variable for this model.

### 3.1.8 Lasso Regression

Lasso shrinks the regression coefficients toward zero by penalizing the regression model with a penalty term called L1-norm, which is the sum of the absolute coefficients.

In the case of lasso regression, the penalty has the effect of forcing some of the coefficient estimates, with a minor contribution to the model, to be exactly equal to zero. This means that, lasso can be also seen as an alternative to the subset selection methods for performing variable selection in order to reduce the complexity of the model.

The amount of the penalty for Lasso also can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

# Lasso Regression
lasso_model <- train(
  critical_temp ~., data = train.data, method = "glmnet",
  trControl = control,
  tuneGrid = expand.grid(alpha = 1, lambda = lambda_seq),
  preProc = c("range")
)

lasso_model$results

##     alpha    lambda      RMSE   Rsquared      MAE      RMSESD  RsquaredSD
## 1  0.01000000 17.84523 0.7285869 13.51040 0.2905034 0.009898130
## 2  0.08071429 18.44139 0.7103681 14.04472 0.2528200 0.009392143
## 3  0.15142857 18.87863 0.6965615 14.44823 0.2241348 0.008963708
## 4  0.22214286 19.07457 0.6904030 14.64189 0.2102880 0.009055703
## 5  0.29285714 19.22162 0.6858104 14.80283 0.1977354 0.009186995
## 6  0.36357143 19.37847 0.6808474 14.97865 0.1819227 0.009150279
## 7  0.43428571 19.50162 0.6769856 15.10199 0.1709654 0.008995864
## 8  0.50500000 19.59166 0.6742615 15.18468 0.1612679 0.008776663
## 9  0.57571429 19.67722 0.6716883 15.25997 0.1537835 0.008616586
## 10 0.64642857 19.76628 0.6689831 15.33701 0.1511898 0.008621574
## 11 0.71714286 19.86025 0.6660920 15.41643 0.1492294 0.008615916
## 12 0.78785714 19.96318 0.6628608 15.50323 0.1486597 0.008625183
## 13 0.85857143 20.07524 0.6592674 15.59753 0.1505789 0.008652214
## 14 0.92928571 20.19732 0.6552751 15.69841 0.1553790 0.008740919
## 15 1.00000000 20.31093 0.6515475 15.78933 0.1581347 0.008776455
##     MAESD
## 1  0.2122962
## 2  0.1762160
## 3  0.1490102
## 4  0.1398793
## 5  0.1293614
## 6  0.1209383
## 7  0.1225509
## 8  0.1200034
## 9  0.1189056
## 10 0.1171334
## 11 0.1173222
## 12 0.1191419
## 13 0.1224520
```

```

## 14 0.1252319
## 15 0.1262976

plot_metrics(lasso_model, lasso_model$results$lambda, "Lambda")

```

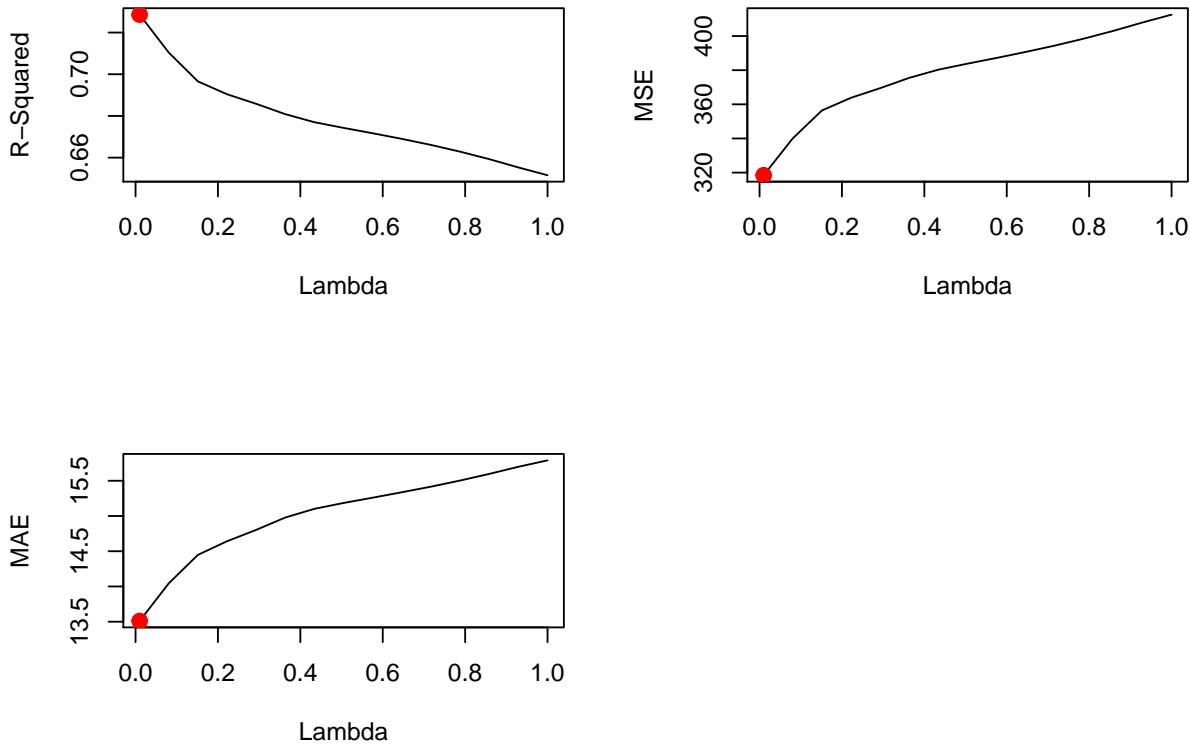


Figure 53: R-Squared, MSE, and MAE for Lasso Regression

```
lasso_model$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next, we will plot the list of coefficients for this model.

```
coef(lasso_model$finalModel, lasso_model$bestTune$lambda)
```

```

## 82 x 1 sparse Matrix of class "dgCMatrix"
##                                         1
## (Intercept)           -9.09482257
## number_of_elements   -28.29652898
## mean_atomic_mass     56.94068266
## wtd_mean_atomic_mass -39.81242081
## gmean_atomic_mass    -0.07301793

```

```

## wtd_gmean_atomic_mass          .
## entropy_atomic_mass           -68.22737180
## wtd_entropy_atomic_mass       19.93942776
## range_atomic_mass             37.62985025
## wtd_range_atomic_mass         0.73188248
## std_atomic_mass              -19.09921316
## wtd_std_atomic_mass          -24.12704788
## mean_fie                      6.27235597
## wtd_mean_fie                 13.59417716
## gmean_fie                     .
## wtd_gmean_fie                .
## entropy_fie                  .
## wtd_entropy_fie              62.48395566
## range_fie                     69.86507218
## wtd_range_fie                18.98326768
## std_fie                       -64.86309307
## wtd_std_fie                  -10.06968940
## mean_atomic_radius            150.43469014
## wtd_mean_atomic_radius        170.52250830
## gmean_atomic_radius           -204.90937972
## wtd_gmean_atomic_radius      -99.86720001
## entropy_atomic_radius         .
## wtd_entropy_atomic_radius    42.98173737
## range_atomic_radius           58.38552173
## wtd_range_atomic_radius      -21.44417238
## std_atomic_radius             -101.56147841
## wtd_std_atomic_radius        31.02490993
## mean_Density                  -73.20770430
## wtd_mean_Density              -2.67952116
## gmean_Density                 0.70566410
## wtd_gmean_Density             45.39854661
## entropy_Density               27.06067916
## wtd_entropy_Density           -29.99114219
## range_Density                 -26.97324800
## wtd_range_Density             0.66126778
## std_Density                   42.87093083
## wtd_std_Density               -10.11380680
## mean_ElectronAffinity         -23.53870337
## wtd_mean_ElectronAffinity    158.69878804
## gmean_ElectronAffinity        43.76693683
## wtd_gmean_ElectronAffinity   -171.44853806
## entropy_ElectronAffinity     5.83673233
## wtd_entropy_ElectronAffinity -33.60300763
## range_ElectronAffinity        -125.62963093
## wtd_range_ElectronAffinity   -36.20332842
## std_ElectronAffinity          196.07004823
## wtd_std_ElectronAffinity     -88.75212208
## mean_FusionHeat               9.42941077
## wtd_mean_FusionHeat           -25.76485128
## gmean_FusionHeat              -1.29104345
## wtd_gmean_FusionHeat          7.34068881
## entropy_FusionHeat            -17.68662902
## wtd_entropy_FusionHeat        36.95223100
## range_FusionHeat              -30.32686309

```

```

## wtd_range_FusionHeat          40.05255638
## std_FusionHeat                19.29621201
## wtd_std_FusionHeat            -13.06894205
## mean_ThermalConductivity     -9.83072854
## wtd_mean_ThermalConductivity 188.95344253
## gmean_ThermalConductivity    -26.02640536
## wtd_gmean_ThermalConductivity -109.84710093
## entropy_ThermalConductivity  7.95891765
## wtd_entropy_ThermalConductivity 12.58824750
## range_ThermalConductivity   -22.02415920
## wtd_range_ThermalConductivity -69.13887349
## std_ThermalConductivity      24.44146686
## wtd_std_ThermalConductivity   10.63866454
## mean_Valence                  .
## wtd_mean_Valence              .
## gmean_Valence                 13.37436061
## wtd_gmean_Valence             -15.97839597
## entropy_Valence               59.07175783
## wtd_entropy_Valence           -85.57613993
## range_Valence                 23.28131667
## wtd_range_Valence             9.27702212
## std_Valence                   .
## wtd_std_Valence               -54.61692191

```

```
getTrainPerf(lasso_model)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 17.84523      0.7285869 13.5104 glmnet

```

From the above metrics, the R-Squared for this model is 0.7285869 with Train MSE is 318.45

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(lasso_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables", cex=0.75))

```

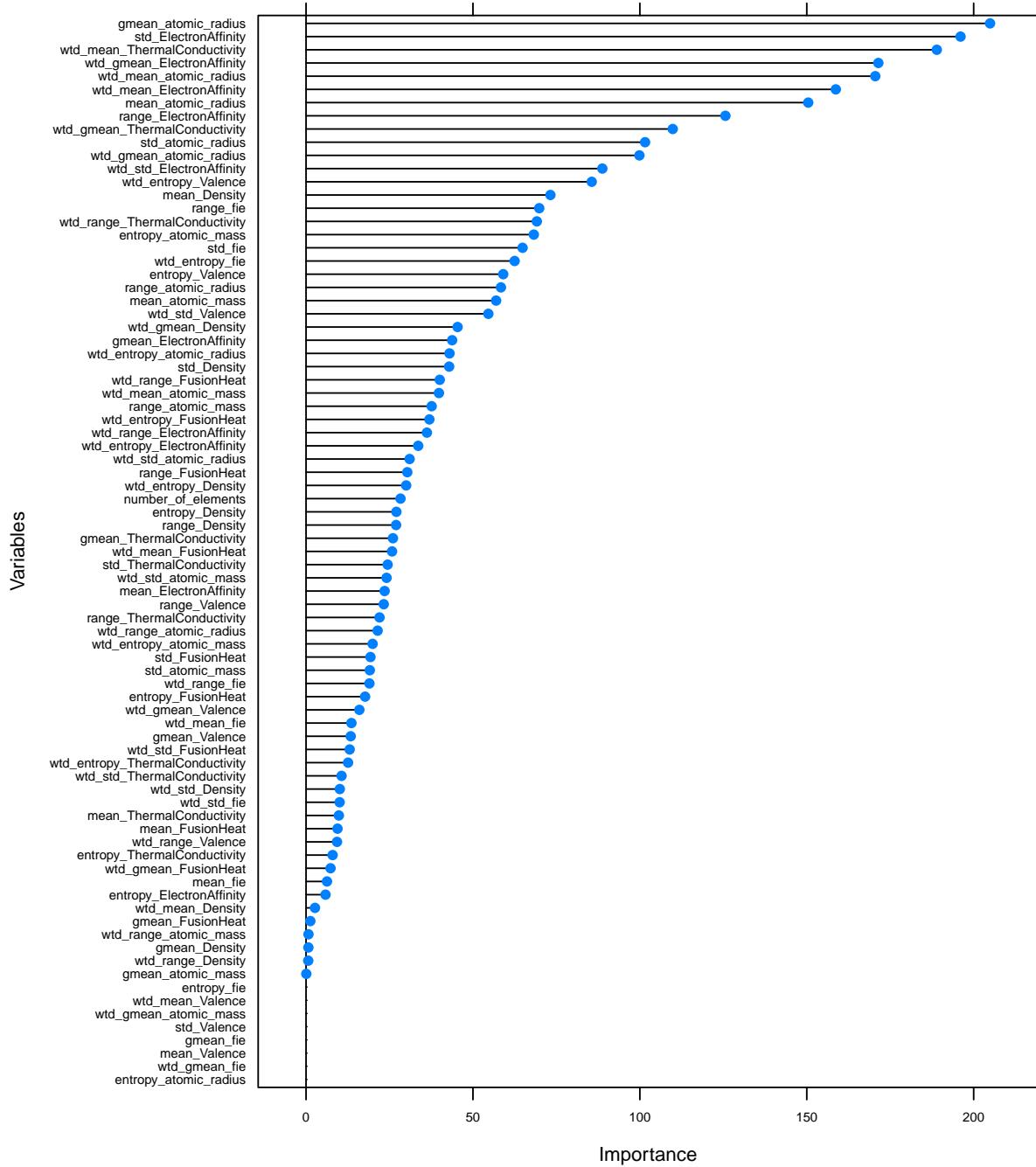


Figure 54: Variables Importance for Lasso Regression

From the plot, we can see that some variables have zero importance, this is because lasso some of the variables' coefficient to zero, which is different compared to ridge regression. In addition, the most important variable is `gmean_atomic_radius`.

### 3.1.9 Elastic Net

Elastic Net produces a regression model that is penalized with both the L1 and L2 regularizations. The consequence of this is to effectively shrink coefficients and to set some coefficients to zero.

The amount of the penalty for Elastic Net also can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

# Elastic Net Regression
elastic_net_model <- train(
  critical_temp ~., data = train.data, method = "glmnet",
  trControl = control,
  tuneGrid = expand.grid(alpha = 0.5, lambda = lambda_seq),
  preProc = c("range")
)

elastic_net_model$results

##   alpha     lambda      RMSE    Rsquared      MAE      RMSESD  RsquaredSD
## 1  0.5 0.01000000 17.81262 0.7295577 13.47831 0.2987725 0.010155559
## 2  0.5 0.08071429 18.23708 0.7166608 13.87199 0.2697910 0.009645171
## 3  0.5 0.15142857 18.47328 0.7094147 14.07223 0.2439207 0.009175505
## 4  0.5 0.22214286 18.71791 0.7017390 14.29339 0.2281976 0.008960148
## 5  0.5 0.29285714 18.91570 0.6954563 14.48525 0.2146152 0.008842833
## 6  0.5 0.36357143 19.03667 0.6916504 14.60954 0.2050775 0.008812648
## 7  0.5 0.43428571 19.10882 0.6894508 14.68794 0.1948648 0.008795384
## 8  0.5 0.50500000 19.18505 0.6871044 14.77058 0.1874702 0.008799075
## 9  0.5 0.57571429 19.26405 0.6846511 14.85815 0.1811771 0.008868520
## 10 0.5 0.64642857 19.34924 0.6819732 14.95087 0.1746145 0.008935911
## 11 0.5 0.71714286 19.43882 0.6791291 15.04668 0.1677958 0.008923672
## 12 0.5 0.78785714 19.51673 0.6766685 15.12558 0.1622321 0.008847200
## 13 0.5 0.85857143 19.58258 0.6746089 15.18893 0.1577121 0.008800901
## 14 0.5 0.92928571 19.64743 0.6725764 15.25174 0.1535228 0.008748413
## 15 0.5 1.00000000 19.70896 0.6706580 15.31031 0.1503419 0.008635636
##           MAESD
## 1  0.2205485
## 2  0.1915822
## 3  0.1710412
## 4  0.1547992
## 5  0.1470517
## 6  0.1387456
## 7  0.1304914
## 8  0.1248349
## 9  0.1200845
## 10 0.1159150
## 11 0.1145334
## 12 0.1165037
## 13 0.1168319
## 14 0.1158279
## 15 0.1155689
```

From the above results, we can see the corresponding errors to the lambda values. Here, we will plot and see the optimal lambda.

```
plot_metrics(elastic_net_model, elastic_net_model$results$lambda, "Lambda")
```

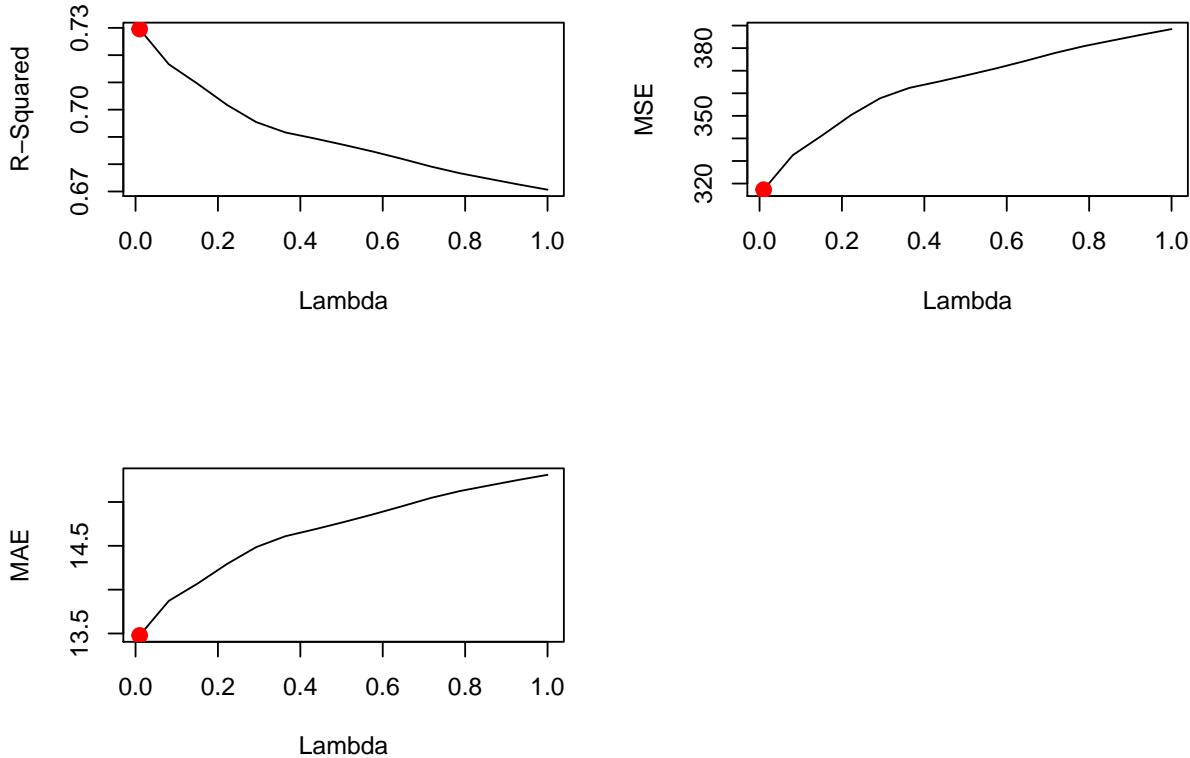


Figure 55: R-Squared, MSE, and MAE for Elastic Net Regression

```
elastic_net_model$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next, we will plot the list of coefficients for this model.

```
coef(elastic_net_model$finalModel, elastic_net_model$bestTune$lambda)
```

```
## 82 x 1 sparse Matrix of class "dgCMatrix"
##                                     1
## (Intercept)           -9.87772620
## number_of_elements   -29.71201506
## mean_atomic_mass     70.48964288
## wtd_mean_atomic_mass -46.43015077
## gmean_atomic_mass    -11.49854599
## wtd_gmean_atomic_mass  4.83799120
## entropy_atomic_mass   -73.68092670
## wtd_entropy_atomic_mass 21.06391889
```

```

## range_atomic_mass          40.12476748
## wtd_range_atomic_mass      2.28608571
## std_atomic_mass           -26.90780517
## wtd_std_atomic_mass        -21.60464480
## mean_fie                   7.26132788
## wtd_mean_fie               12.23495623
## gmean_fie                  .
## wtd_gmean_fie              1.24057929
## entropy_fie                -0.49479237
## wtd_entropy_fie            68.47156777
## range_fie                  72.81499688
## wtd_range_fie              18.88795757
## std_fie                    -69.01118657
## wtd_std_fie                -8.51151221
## mean_atomic_radius         180.10878360
## wtd_mean_atomic_radius     170.89145471
## gmean_atomic_radius        -236.13144701
## wtd_gmean_atomic_radius    -98.17556667
## entropy_atomic_radius      -0.14333043
## wtd_entropy_atomic_radius   46.66078270
## range_atomic_radius         59.99314218
## wtd_range_atomic_radius    -21.33675755
## std_atomic_radius          -110.66019721
## wtd_std_atomic_radius      34.13341473
## mean_Density                -79.35762514
## wtd_mean_Density            -10.56913872
## gmean_Density               2.15934733
## wtd_gmean_Density           56.13421632
## entropy_Density             31.09464138
## wtd_entropy_Density         -30.47764387
## range_Density               -30.30067417
## wtd_range_Density            0.02984101
## std_Density                 49.26119165
## wtd_std_Density              -9.57911752
## mean_ElectronAffinity       -35.79427144
## wtd_mean_ElectronAffinity   172.72737057
## gmean_ElectronAffinity      53.38944296
## wtd_gmean_ElectronAffinity  -183.35698661
## entropy_ElectronAffinity    6.34640972
## wtd_entropy_ElectronAffinity -33.31221565
## range_ElectronAffinity      -127.06906709
## wtd_range_ElectronAffinity   -36.50887051
## std_ElectronAffinity         202.43720318
## wtd_std_ElectronAffinity    -94.46205731
## mean_FusionHeat              27.37813389
## wtd_mean_FusionHeat          -45.91202369
## gmean_FusionHeat             -18.29070802
## wtd_gmean_FusionHeat         25.42436249
## entropy_FusionHeat           -21.16345841
## wtd_entropy_FusionHeat        37.04066328
## range_FusionHeat              -37.57769456
## wtd_range_FusionHeat          41.10323830
## std_FusionHeat                23.47537591
## wtd_std_FusionHeat            -10.20993960

```

```

## mean_ThermalConductivity      -14.56413361
## wtd_mean_ThermalConductivity 197.88035498
## gmean_ThermalConductivity    -23.99697088
## wtd_gmean_ThermalConductivity -114.57590794
## entropy_ThermalConductivity 10.88877992
## wtd_entropy_ThermalConductivity 10.72609601
## range_ThermalConductivity   -27.44480948
## wtd_range_ThermalConductivity -74.32575873
## std_ThermalConductivity      35.29886684
## wtd_std_ThermalConductivity   7.72826590
## mean_Valence                  .
## wtd_mean_Valence              .
## gmean_Valence                 18.09524348
## wtd_gmean_Valence             -19.20327938
## entropy_Valence               66.16206192
## wtd_entropy_Valence           -96.85399741
## range_Valence                 24.77503660
## wtd_range_Valence             7.49561555
## std_Valence                   -0.32280177
## wtd_std_Valence               -55.32095188

```

```
getTrainPerf(elastic_net_model)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 17.81262 0.7295577 13.47831 glmnet

```

From the above metrics, the R-Squared for this model is 0.7295577 with Train MSE is 317.28

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(elastic_net_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

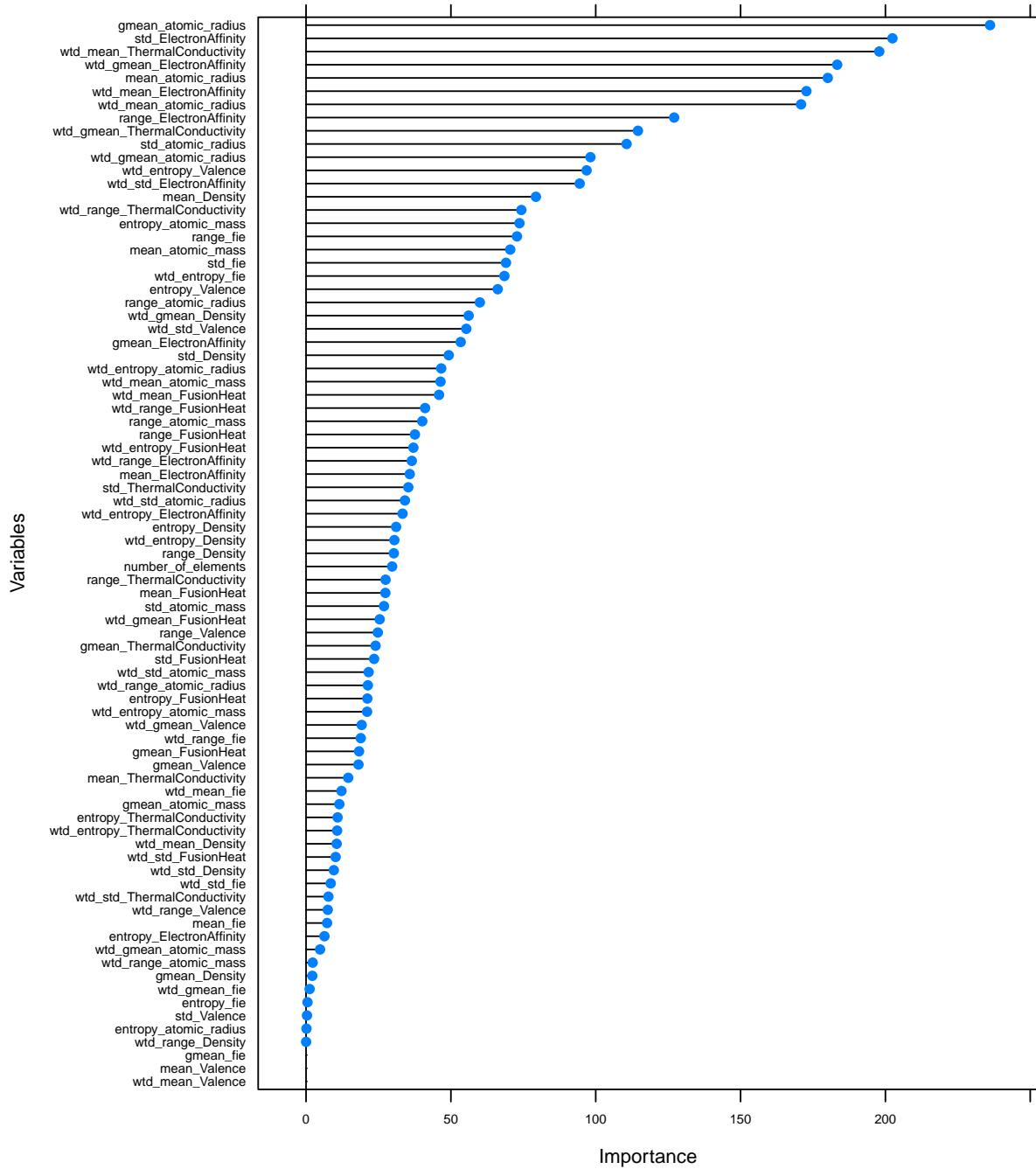


Figure 56: Variables Importance for Elastic Net Regression

From the plot, we can see that some variables have zero importance, however, compared to lasso regression, the number of zero importance is less. This is because elastic net is the combination between ridge and lasso regressions. In addition, the most important variable for this model is gmean\_atomic\_radius.

### 3.1.10 Principal Component Regression

The principal component regression (PCR) first applies Principal Component Analysis on the data set to summarize the original predictor variables into few new variables also known as principal components (PCs), which are a linear combination of the original data. Here we will try to force the model to only have maximum 40 number of components.

```

set.seed(seed)

# Principal Component Regression
pcr_model <- train(critical_temp ~ .,
                     data      = train.data,
                     method    = "pcr",
                     tuneGrid  = expand.grid(ncomp = seq(2,40,2)),
                     trControl = control,
                     preProc  = c("range"))
summary(pcr_model)

## Data: X dimension: 17011 81
## Y dimension: 17011 1
## Fit method: svdpc
## Number of components considered: 40
## TRAINING: % variance explained
##          1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X        49.47    60.01   68.04   74.08   78.34   81.49   84.31
## .outcome 47.06    49.27   52.15   53.27   54.21   55.93   55.96
##          8 comps  9 comps 10 comps 11 comps 12 comps 13 comps
## X        86.73    88.76   90.14   91.46   92.63   93.62
## .outcome 55.99    56.35   57.02   57.07   57.14   59.61
##          14 comps 15 comps 16 comps 17 comps 18 comps 19 comps
## X        94.48    95.16   95.81   96.31   96.74   97.12
## .outcome 59.62    59.99   60.79   60.80   62.29   62.40
##          20 comps 21 comps 22 comps 23 comps 24 comps 25 comps
## X        97.44    97.74   97.98   98.20   98.37   98.53
## .outcome 62.53    64.04   65.33   67.02   67.04   67.72
##          26 comps 27 comps 28 comps 29 comps 30 comps 31 comps
## X        98.67    98.8    98.91   99.01   99.10   99.18
## .outcome 67.72    67.9    67.92   67.98   68.39   68.62
##          32 comps 33 comps 34 comps 35 comps 36 comps 37 comps
## X        99.25    99.31   99.37   99.43   99.48   99.53
## .outcome 68.85    68.87   68.97   69.12   69.17   69.21
##          38 comps 39 comps 40 comps
## X        99.57    99.62   99.65
## .outcome 69.23    69.30   69.35

pcr_model$results

##   ncomp     RMSE  Rsquared       MAE     RMSESD  RsquaredSD     MAESD
## 1      2 24.40247 0.4925201 19.41498 0.3180709 0.009247166 0.2288239
## 2      4 23.39496 0.5335877 18.23649 0.2556745 0.008177744 0.1535284
## 3      6 22.73567 0.5595330 18.01104 0.2085836 0.008692367 0.1655058
## 4      8 22.71376 0.5603842 17.96420 0.2297706 0.009277577 0.1746421
## 5     10 22.45290 0.5704319 17.76857 0.2411792 0.010343726 0.1746315

```

```

## 6 12 22.40949 0.5720876 17.78944 0.2354649 0.010561857 0.1776203
## 7 14 21.78508 0.5955989 17.16058 0.2334546 0.011931839 0.2031259
## 8 16 21.46630 0.6072933 16.85921 0.2410273 0.011445841 0.1892886
## 9 18 21.05592 0.6221612 16.62824 0.2014742 0.010658905 0.1599906
## 10 20 20.97413 0.6251087 16.53842 0.2060061 0.010337178 0.1849974
## 11 22 20.16173 0.6535609 15.83423 0.2438315 0.010846988 0.1446445
## 12 24 19.67744 0.6699894 15.46676 0.2159067 0.009091393 0.1815952
## 13 26 19.47797 0.6766619 15.15211 0.2174018 0.009026766 0.1511762
## 14 28 19.42122 0.6785425 15.07414 0.2304719 0.009448635 0.1495935
## 15 30 19.27656 0.6832948 14.91450 0.2166738 0.009084859 0.1764577
## 16 32 19.13913 0.6878102 14.69017 0.2245577 0.009261464 0.1799668
## 17 34 19.10854 0.6888170 14.66208 0.2242055 0.009168008 0.1787153
## 18 36 19.04848 0.6907674 14.59287 0.2270335 0.008943400 0.1837082
## 19 38 19.02416 0.6915518 14.56679 0.2291379 0.009233026 0.1839595
## 20 40 18.99579 0.6924624 14.55011 0.2500166 0.009855617 0.1934809

```

```
plot_metrics(pcr_model, pcr_model$results$ncomp, "Number of Component")
```

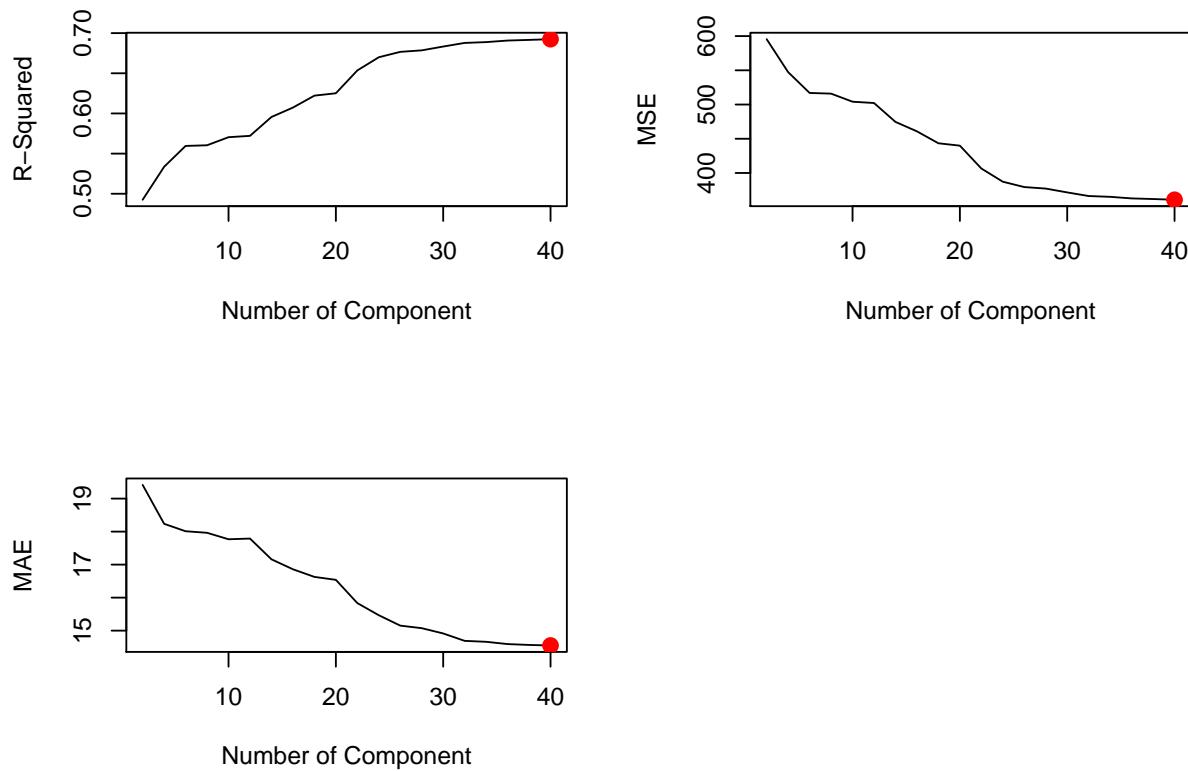


Figure 57: R-Squared, MSE, and MAE for Principal Component Regression

```
pcr_model$bestTune
```

```

##      ncomp
## 20     40

```

From the above results, we can see the corresponding errors to the number of principal components. Here, we will plot and see the optimal number of principal components.

```
getTrainPerf(pcr_model)

##   TrainRMSE TrainRsquared TrainMAE method
## 1  18.99579     0.6924624 14.55011    pcr

varImp(pcr_model)$importance

##                                     Overall
## number_of_elements                65.666830
## mean_atomic_mass                  2.340670
## wtd_mean_atomic_mass              31.332214
## gmean_atomic_mass                 9.789289
## wtd_gmean_atomic_mass             41.873592
## entropy_atomic_mass               53.717397
## wtd_entropy_atomic_mass           88.439537
## range_atomic_mass                 43.896261
## wtd_range_atomic_mass              40.332190
## std_atomic_mass                  26.126408
## wtd_std_atomic_mass               45.220901
## mean_fie                          1.969445
## wtd_mean_fie                      48.444039
## gmean_fie                         0.000000
## wtd_gmean_fie                     45.381919
## entropy_fie                        58.711572
## wtd_entropy_fie                   45.914068
## range_fie                          65.983263
## wtd_range_fie                      44.894401
## std_fie                            53.815465
## wtd_std_fie                        70.925237
## mean_atomic_radius                 1.702301
## wtd_mean_atomic_radius              40.639964
## gmean_atomic_radius                3.970195
## wtd_gmean_atomic_radius            52.658746
## entropy_atomic_radius              56.874572
## wtd_entropy_atomic_radius          80.723038
## range_atomic_radius                 77.791891
## wtd_range_atomic_radius             37.603038
## std_atomic_radius                  56.967153
## wtd_std_atomic_radius              70.044923
## mean_Density                        24.938698
## wtd_mean_Density                   54.589447
## gmean_Density                       53.827694
## wtd_gmean_Density                  68.720521
## entropy_Density                     38.066656
## wtd_entropy_Density                 36.228805
## range_Density                        12.054532
## wtd_range_Density                   34.339177
## std_Density                          2.232043
## wtd_std_Density                     58.173311
## mean_ElectronAffinity                6.736804
```

```

## wtd_mean_ElectronAffinity      32.860649
## gmean_ElectronAffinity        26.375327
## wtd_gmean_ElectronAffinity    22.565659
## entropy_ElectronAffinity     34.896012
## wtd_entropy_ElectronAffinity  26.634459
## range_ElectronAffinity       14.392845
## wtd_range_ElectronAffinity   35.260218
## std_ElectronAffinity         12.620594
## wtd_std_ElectronAffinity     62.926880
## mean_FusionHeat              26.907726
## wtd_mean_FusionHeat          59.338381
## gmean_FusionHeat             33.655417
## wtd_gmean_FusionHeat         54.858189
## entropy_FusionHeat           55.457733
## wtd_entropy_FusionHeat       70.307323
## range_FusionHeat              3.449967
## wtd_range_FusionHeat         59.540820
## std_FusionHeat                7.198470
## wtd_std_FusionHeat           52.743087
## mean_ThermalConductivity    25.413098
## wtd_mean_ThermalConductivity 46.740051
## gmean_ThermalConductivity   27.335587
## wtd_gmean_ThermalConductivity 37.572795
## entropy_ThermalConductivity 1.354467
## wtd_entropy_ThermalConductivity 18.985751
## range_ThermalConductivity   86.084589
## wtd_range_ThermalConductivity 63.805474
## std_ThermalConductivity     77.761604
## wtd_std_ThermalConductivity 100.000000
## mean_Valence                 65.510304
## wtd_mean_Valence             91.800565
## gmean_Valence                 59.856849
## wtd_gmean_Valence            91.469039
## entropy_Valence               65.156151
## wtd_entropy_Valence          81.364893
## range_Valence                  3.552174
## wtd_range_Valence            67.378506
## std_Valence                   7.647729
## wtd_std_Valence              39.144031

```

From the above metrics, the R-Squared for this model is 0.6924624 with Train MSE is 360.84. However, now the model only has 40 variables as the predictors which is far from the original model.

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(pcr_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

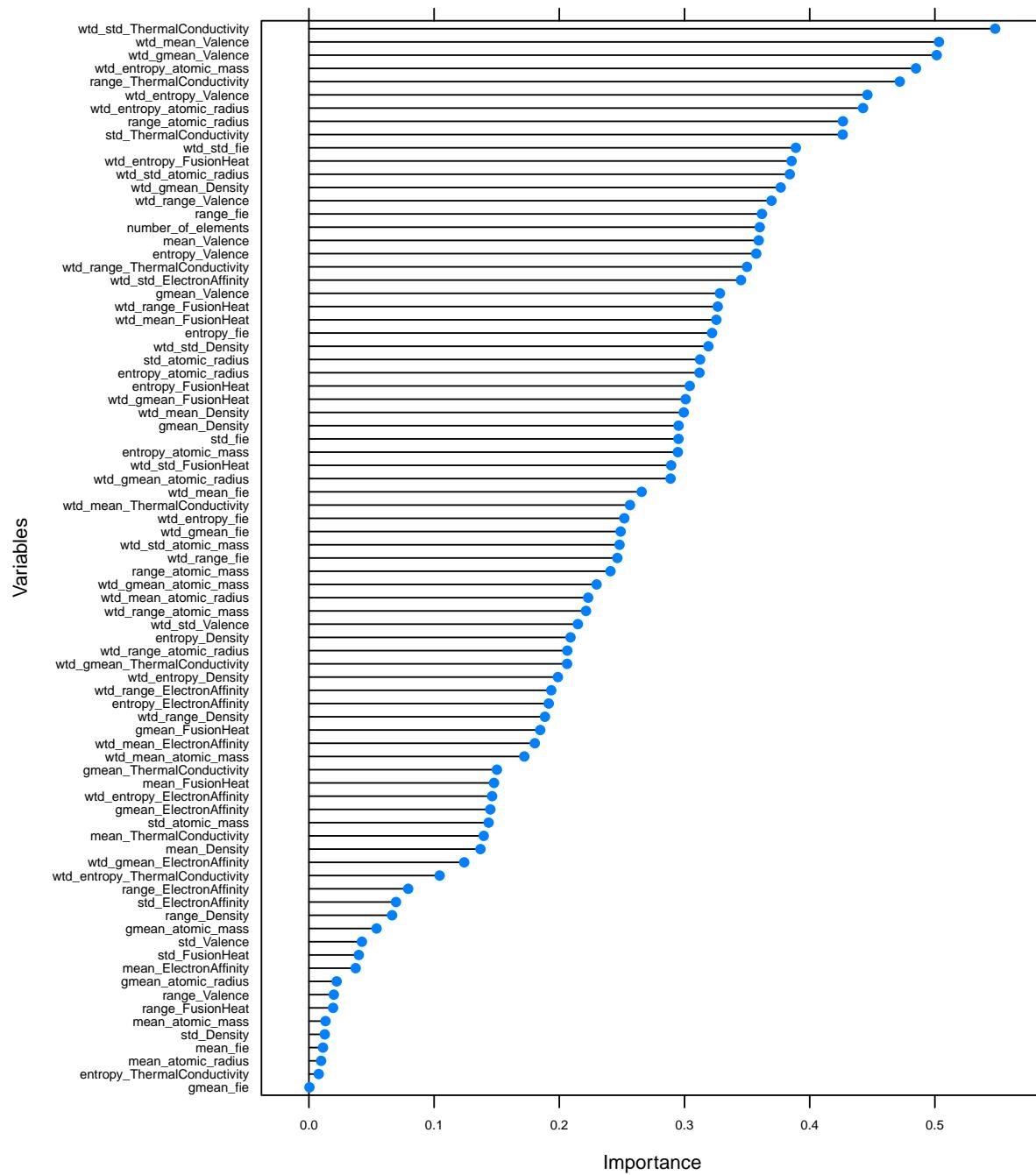


Figure 58: Variables Importance for Principal Component Regression

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.1.11 K-Nearest Neighbor Regression

K-Nearest Neighbor is a non-parametric method used for classification and regression. In both cases, the input consists of the k closest training examples in the feature space. For regression, the prediction is the average of the response variable of the closest neighbors. Here we will let the cross validation to choose number of k between 1 and 5.

```
set.seed(seed)

# K-Nearest Neighbor Regression
knn_model <- train(critical_temp ~ .,
                     method      = "knn",
                     tuneGrid    = expand.grid(k = c(1:5)),
                     trControl   = control,
                     data        = train.data,
                     preProc    = c("range"))

knn_model$results

##   k      RMSE  Rsquared       MAE     RMSESD  RsquaredSD     MAESD
## 1 1 10.91167 0.9006322 5.661060 0.4709377 0.008542947 0.1767043
## 2 2 10.56758 0.9057533 5.578382 0.3971130 0.007185562 0.1884706
## 3 3 10.61870 0.9044507 5.758037 0.3705649 0.006348395 0.2056233
## 4 4 10.83918 0.9002138 5.980812 0.4169344 0.007612337 0.2513110
## 5 5 11.04712 0.8962535 6.185279 0.3908263 0.007317765 0.2314490
```

From the above results, we can see the corresponding errors to the number of k. Here, we will plot and see the optimal number of k.

```
plot_metrics(knn_model, knn_model$results$k, "k")
```

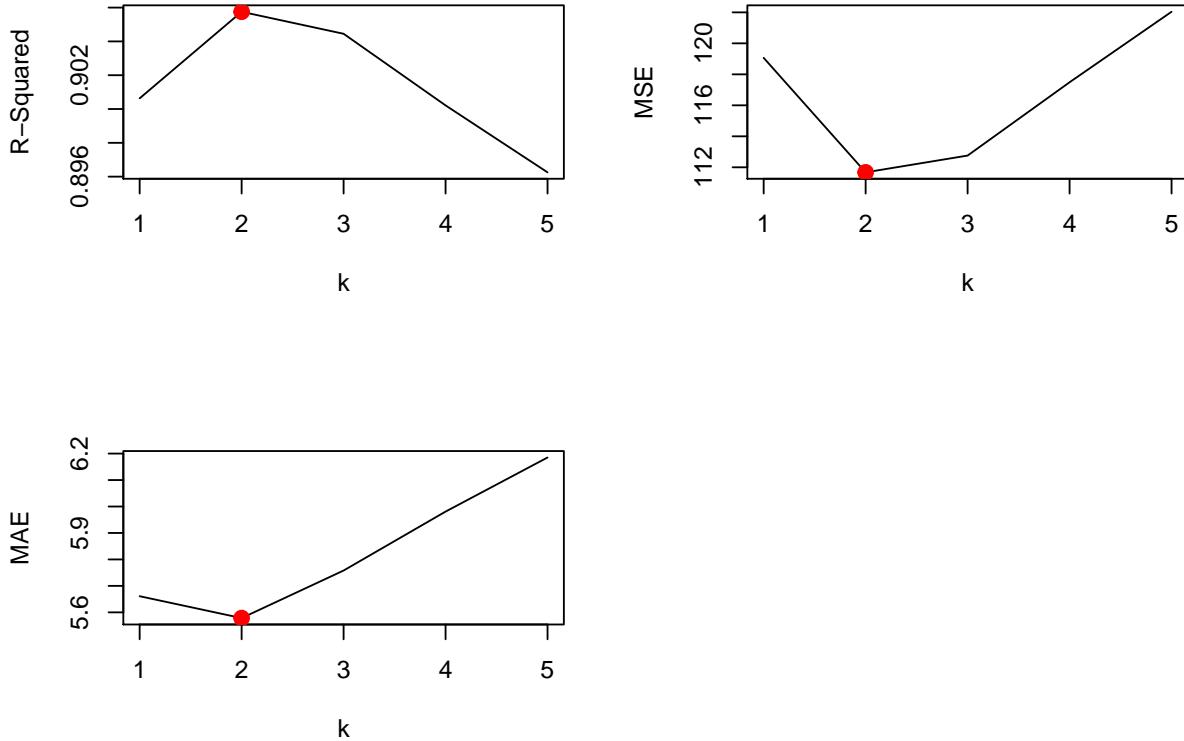


Figure 59: R-Squared, MSE, and MAE for KNN Regression

```
# Best tuning parameter k that minimize the RMSE
knn_model$bestTune
```

```
##      k
## 2 2
```

```
getTrainPerf(knn_model)
```

```
##      TrainRMSE TrainRsquared TrainMAE method
## 1 10.56758     0.9057533 5.578382 knn
```

From the result, we know that the best  $k$  is 2 with R-Squared 0.9057 and MSE 111.67. So far, this is the best model we have.

Here, we show the variable importance for this model.

```
varImp(knn_model, scale = FALSE)$importance
```

```
##                                              Overall
## number_of_elements                      0.3601224431
## mean_atomic_mass                       0.0132644523
```

```

## wtd_mean_atomic_mass          0.1720605759
## gmean_atomic_mass            0.0540629652
## wtd_gmean_atomic_mass        0.2297991342
## entropy_atomic_mass          0.2946715118
## wtd_entropy_atomic_mass      0.4848559723
## range_atomic_mass            0.2408779512
## wtd_range_atomic_mass        0.2213563770
## std_atomic_mass              0.1435466804
## wtd_std_atomic_mass          0.2481334360
## mean_fie                      0.0112311343
## wtd_mean_fie                 0.2657876103
## gmean_fie                     0.0004438412
## wtd_gmean_fie                0.2490153844
## entropy_fie                  0.3220262349
## wtd_entropy_fie               0.2519301375
## range_fie                     0.3618556522
## wtd_range_fie                0.2463450900
## std_fie                       0.2952086611
## wtd_std_fie                  0.3889244539
## mean_atomic_radius            0.0097678961
## wtd_mean_atomic_radius        0.2230421516
## gmean_atomic_radius           0.0221898933
## wtd_gmean_atomic_radius       0.2888729368
## entropy_atomic_radius         0.3119643880
## wtd_entropy_atomic_radius     0.4425901964
## range_atomic_radius           0.4265353533
## wtd_range_atomic_radius       0.2064079194
## std_atomic_radius             0.3124714830
## wtd_std_atomic_radius         0.3841026869
## mean_Density                  0.1370412057
## wtd_mean_Density              0.2994480102
## gmean_Density                 0.2952756440
## wtd_gmean_Density             0.3768485038
## entropy_Density               0.2089473062
## wtd_entropy_Density           0.1988808014
## range_Density                 0.0664704367
## wtd_range_Density             0.1885306934
## std_Density                   0.0126694694
## wtd_std_Density               0.3190780045
## mean_ElectronAffinity         0.0373435119
## wtd_mean_ElectronAffinity     0.1804323136
## gmean_ElectronAffinity        0.1449100944
## wtd_gmean_ElectronAffinity    0.1240433001
## entropy_ElectronAffinity      0.1915806587
## wtd_entropy_ElectronAffinity   0.1463294443
## range_ElectronAffinity        0.0792781409
## wtd_range_ElectronAffinity    0.1935755341
## std_ElectronAffinity          0.0695709452
## wtd_std_ElectronAffinity      0.3451148458
## mean_FusionHeat               0.1478262170
## wtd_mean_FusionHeat            0.3254594685
## gmean_FusionHeat               0.1847855168
## wtd_gmean_FusionHeat           0.3009200017
## entropy_FusionHeat             0.3042038971

```

```

## wtd_entropy_FusionHeat          0.3855399384
## range_FusionHeat               0.0193404344
## wtd_range_FusionHeat           0.3265682914
## std_FusionHeat                 0.0398722031
## wtd_std_FusionHeat              0.2893349003
## mean_ThermalConductivity      0.1396396530
## wtd_mean_ThermalConductivity   0.2564543149
## gmean_ThermalConductivity     0.1501697502
## wtd_gmean_ThermalConductivity  0.2062422695
## entropy_ThermalConductivity   0.0078626971
## wtd_entropy_ThermalConductivity 0.1044349818
## range_ThermalConductivity     0.4719571565
## wtd_range_ThermalConductivity  0.3499271935
## std_ThermalConductivity       0.4263694613
## wtd_std_ThermalConductivity    0.5481763933
## mean_Valence                  0.3592651026
## wtd_mean_Valence              0.5032654171
## gmean_Valence                 0.3282992890
## wtd_gmean_Valence             0.5014495452
## entropy_Valence               0.3573252876
## wtd_entropy_Valence            0.4461058445
## range_Valence                 0.0199002543
## wtd_range_Valence              0.3694978531
## std_Valence                   0.0423329431
## wtd_std_Valence                0.2148484399

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(knn_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

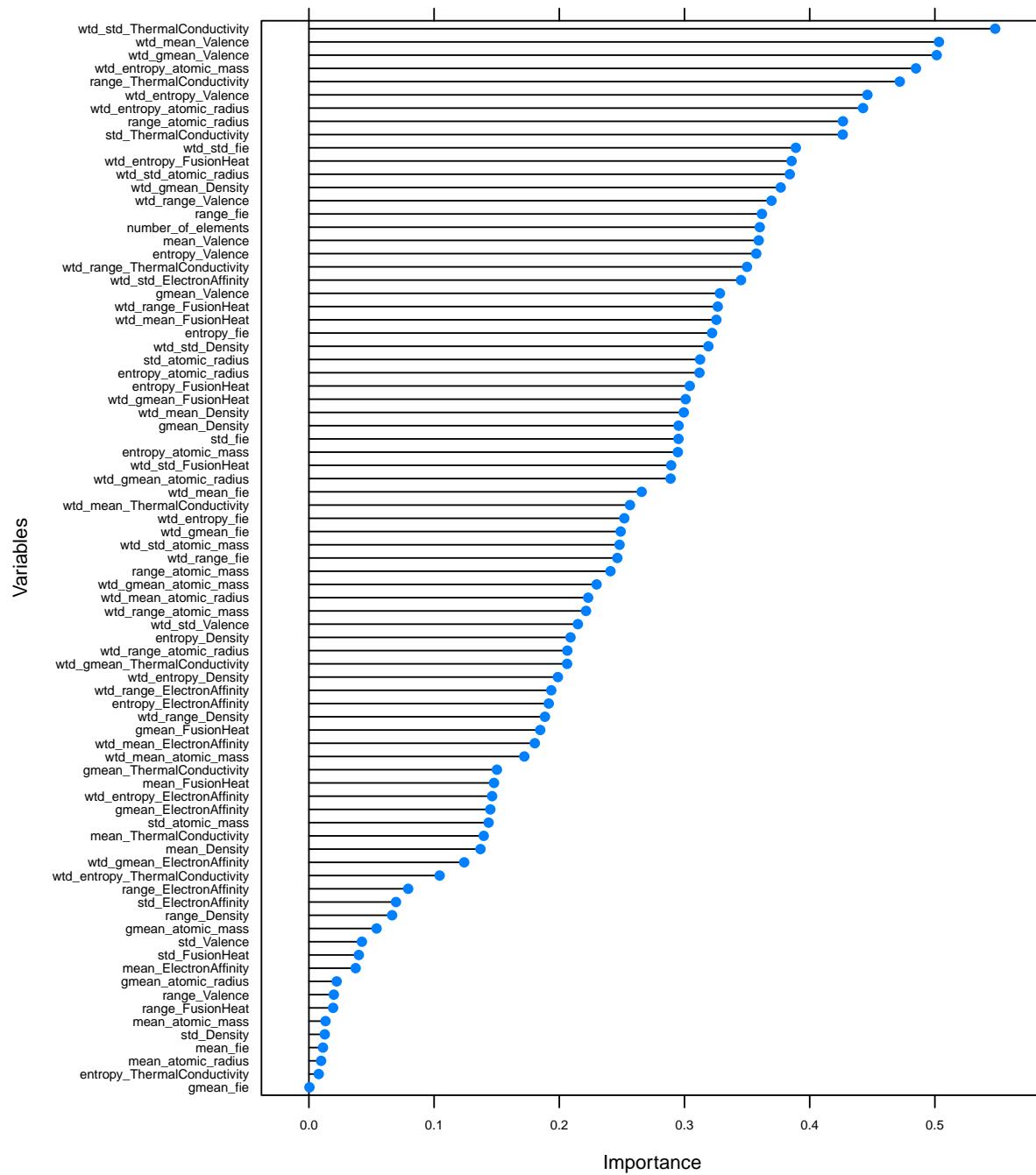


Figure 60: Variables Importance for KNN Regression

From above, it can be seen that wtd\_std\_ThermalConductivity is the most important variable for this model, whereas gmean\_fie is the least important variable for this model.

### 3.1.12 Random Forest

Random forest provides a strong improvement, which consists of applying bagging to the data and bootstrap sampling to the predictor variables at each split [Bruce and Bruce, 2017]. This means that at each splitting step of the tree algorithm, a random sample of n predictors is chosen as split candidates from the full set of the predictors.

Here, we will perform a random forest algorithm by using ranger library, there are three main parameter to be tuned which are mtry, splitrule and min.node.size. mtry is number of variables to possibly split at in each node. Default is the (rounded down) square root of the number variables.

```
set.seed(seed)

# Random Forest
random_forest_model <- train(
  critical_temp ~ ., data = train.data,
  trControl = trainControl( method = "cv", number = 10, search = "random"),
  tuneLength = 5,
  method = "ranger",
  importance = 'impurity',
  preProc = c("range")
)

## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 85%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 85%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.

random_forest_model$results

##   min.node.size mtry    splitrule      RMSE  Rsquared       MAE     RMSESD
## 1             13     1  extratrees 12.095359 0.8793231 7.809327 0.2551946
## 2             13    19  variance   9.543582 0.9226495 5.445220 0.2611817
## 5             18    42  variance   9.597827 0.9217681 5.492328 0.2448081
## 3             13    54  maxstat  9.999149 0.9154153 5.780137 0.3132500
## 4             13    57  maxstat 10.009954 0.9152356 5.793017 0.3082412
##   RsquaredSD     MAESD
```

```

## 1 0.005710353 0.1978485
## 2 0.005046475 0.1280939
## 5 0.004803360 0.1330127
## 3 0.005656953 0.1383970
## 4 0.005524426 0.1377434

```

From the above results, we can see the corresponding errors to the number of mtry, splitrule, and minimum node size. Here, we will plot and see the optimal number of those three parameters.

```

random_forest_model$bestTune

##   mtry splitrule min.node.size
## 2    19      variance        13

getTrainPerf(random_forest_model)

##   TrainRMSE TrainRsquared TrainMAE method
## 1  9.543582     0.9226495  5.44522 ranger

```

From above, we can see that the optimal model is the model with mtry = 19, splitrule = variance and min.node.size = 13 with R-Squared = 0.9226495 and MSE = 91.07

Here, we show the variable importance for this model.

```

varImp(random_forest_model, scale = FALSE)$importance

##                                     Overall
## number_of_elements            3370.912
## mean_atomic_mass              49252.025
## wtd_mean_atomic_mass         112798.575
## gmean_atomic_mass             40826.069
## wtd_gmean_atomic_mass        80466.792
## entropy_atomic_mass          51235.752
## wtd_entropy_atomic_mass     600720.134
## range_atomic_mass             69787.020
## wtd_range_atomic_mass        92415.769
## std_atomic_mass               311201.101
## wtd_std_atomic_mass          126772.770
## mean_fie                      35352.064
## wtd_mean_fie                  67228.404
## gmean_fie                     33698.960
## wtd_gmean_fie                 57744.647
## entropy_fie                   49340.296
## wtd_entropy_fie                189370.858
## range_fie                      296136.947
## wtd_range_fie                  149703.213
## std_fie                        112353.017
## wtd_std_fie                    79802.967
## mean_atomic_radius              39862.538
## wtd_mean_atomic_radius         75523.999
## gmean_atomic_radius             34555.079
## wtd_gmean_atomic_radius        80236.276

```

```

## entropy_atomic_radius           43087.270
## wtd_entropy_atomic_radius      169081.448
## range_atomic_radius            1569768.692
## wtd_range_atomic_radius        69257.174
## std_atomic_radius              68295.898
## wtd_std_atomic_radius          88889.255
## mean_Density                   72116.022
## wtd_mean_Density               70587.400
## gmean_Density                  281841.554
## wtd_gmean_Density              155560.537
## entropy_Density                76121.071
## wtd_entropy_Density             114340.872
## range_Density                  27588.321
## wtd_range_Density              64895.692
## std_Density                     118851.733
## wtd_std_Density                80458.053
## mean_ElectronAffinity          39800.487
## wtd_mean_ElectronAffinity       91623.719
## gmean_ElectronAffinity          133933.456
## wtd_gmean_ElectronAffinity      365207.123
## entropy_ElectronAffinity        35890.793
## wtd_entropy_ElectronAffinity    73185.679
## range_ElectronAffinity          60244.849
## wtd_range_ElectronAffinity      284180.427
## std_ElectronAffinity            137247.350
## wtd_std_ElectronAffinity         457015.216
## mean_FusionHeat                 33550.461
## wtd_mean_FusionHeat              60658.395
## gmean_FusionHeat                26059.260
## wtd_gmean_FusionHeat             118264.884
## entropy_FusionHeat              47790.220
## wtd_entropy_FusionHeat            135578.969
## range_FusionHeat                 14799.419
## wtd_range_FusionHeat              71945.970
## std_FusionHeat                  35628.268
## wtd_std_FusionHeat                77878.781
## mean_ThermalConductivity        112410.097
## wtd_mean_ThermalConductivity     427809.990
## gmean_ThermalConductivity        45882.033
## wtd_gmean_ThermalConductivity    483466.435
## entropy_ThermalConductivity     64610.582
## wtd_entropy_ThermalConductivity   208998.230
## range_ThermalConductivity        2604644.221
## wtd_range_ThermalConductivity     228001.742
## std_ThermalConductivity          1017119.454
## wtd_std_ThermalConductivity       2399536.072
## mean_Valence                     131505.487
## wtd_mean_Valence                 823341.748
## gmean_Valence                    166133.937
## wtd_gmean_Valence                 688858.019
## entropy_Valence                  294596.298
## wtd_entropy_Valence                1130611.574
## range_Valence                      10038.877
## wtd_range_Valence                  123637.676

```

```
## std_Valence          36987.362
## wtd_std_Valence     200239.735
```

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(random_forest_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

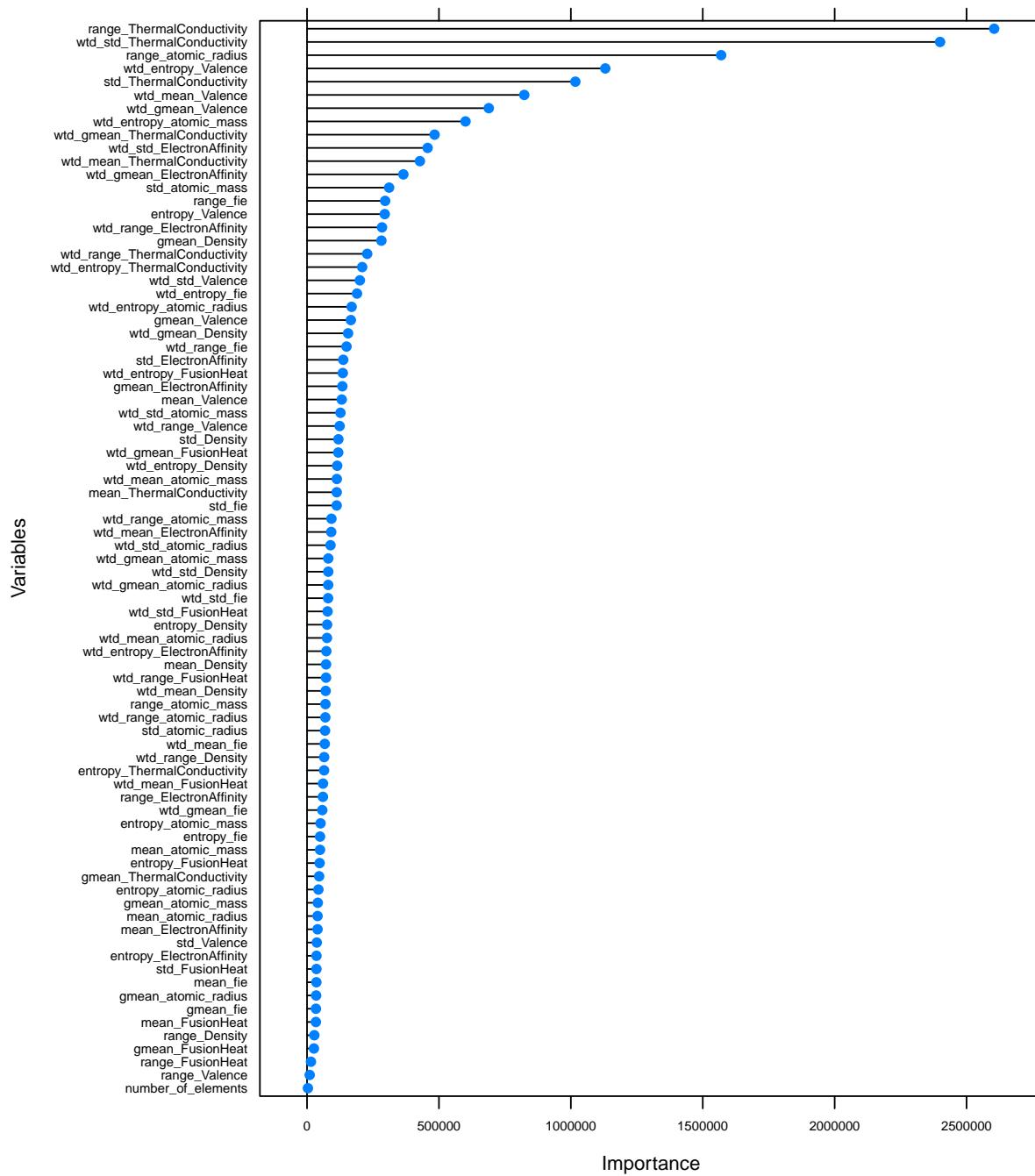


Figure 61: Variables Importance for Random Forest

From above, it can be seen that range\_ThermalConductivity is the most important variable for this model, whereas number\_of\_elements is the least important variable for this model.

### 3.1.13 Gradient Boosting Machine

Compared to random forests which build an ensemble of deep independent trees, GBMs build an ensemble of shallow and weak successive trees with each tree learning and improving on the previous. When combined, these many weak successive trees produce a powerful combination that are often hard to beat with other algorithms.

For a gradient boosting machine (GBM) model, there are four main tuning parameters, n.trees (number of iterations), interaction.depth (complexity of the tree), shrinkage (learning rate), and m.minobsinnode (the minimum number of training set samples in a node to commence splitting).

For the parameters tuning process, we can use apply manual grid search, random grid search or random search tuning. Grid search technique for some cases are more effective, however, it is very time consuming and need much computational cost. Therefore, for this assignment purpose, we will only apply random search tuning with tune length = 4.

```
set.seed(seed)

# Gradient Boosting Machine
gbm_model <- train(critical_temp ~ .,
                     data = train.data,
                     method = "gbm",
                     tuneLength = 4,
                     preProc = c("range"),
                     trControl = trainControl( method = "cv", number = 10, search = "random"),
                     verbose = FALSE
                    )

gbm_model$results

##   shrinkage interaction.depth n.minobsinnode n.trees      RMSE    Rsquared
## 4 0.4164612             1           11     3046 12.17026 0.8737658
## 2 0.3090364             7           24     3111 10.43280 0.9076958
## 3 0.3274399             3           22     3117 10.46041 0.9069501
## 1 0.1703574             7           11     4304 10.06240 0.9138527
##          MAE      RMSESD  RsquaredSD      MAESD
## 4 8.171220 0.2497181 0.005848432 0.1899617
## 2 6.224663 0.3175089 0.006273582 0.1539533
## 3 6.456195 0.2901703 0.006028570 0.1640039
## 1 5.900777 0.3439156 0.006584877 0.1374132

gbm_model$finalModel

## A gradient boosted model with gaussian loss function.
## 4304 iterations were performed.
## There were 81 predictors of which 80 had non-zero influence.

gbm_model$bestTune

##   n.trees interaction.depth shrinkage n.minobsinnode
## 1     4304                  7 0.1703574            11
```

```
getTrainPerf(gbm_model)
```

```
##   TrainRMSE TrainRsquared TrainMAE method
## 1    10.0624      0.9138527 5.900777    gbm
```

From above, we can see that the optimal model is the model with shrinkage = 0.06237055, n.trees = 3380, interaction.depth = 9, and m.minobsinnode = 13. The R-Squared and MSE are 0.9207168 and 92.91 consecutively.

Here, we show the variable importance for this model.

```
varImp(gbm_model, scale = FALSE)$importance
```

	Overall
## number_of_elements	0.000
## mean_atomic_mass	105184.722
## wtd_mean_atomic_mass	367908.076
## gmean_atomic_mass	211576.773
## wtd_gmean_atomic_mass	426703.361
## entropy_atomic_mass	94740.986
## wtd_entropy_atomic_mass	1068122.790
## range_atomic_mass	106881.257
## wtd_range_atomic_mass	303376.289
## std_atomic_mass	859460.567
## wtd_std_atomic_mass	438885.498
## mean_fie	128645.465
## wtd_mean_fie	224152.520
## gmean_fie	82018.938
## wtd_gmean_fie	253303.769
## entropy_fie	159992.846
## wtd_entropy_fie	273010.690
## range_fie	244930.562
## wtd_range_fie	313897.967
## std_fie	230866.201
## wtd_std_fie	641694.203
## mean_atomic_radius	358135.614
## wtd_mean_atomic_radius	672501.215
## gmean_atomic_radius	108535.099
## wtd_gmean_atomic_radius	201180.899
## entropy_atomic_radius	180122.229
## wtd_entropy_atomic_radius	326779.031
## range_atomic_radius	2549013.131
## wtd_range_atomic_radius	263281.241
## std_atomic_radius	230786.302
## wtd_std_atomic_radius	744943.377
## mean_Density	342686.636
## wtd_mean_Density	437455.893
## gmean_Density	350536.028
## wtd_gmean_Density	203102.500
## entropy_Density	165163.620
## wtd_entropy_Density	578598.583
## range_Density	7215.969
## wtd_range_Density	153067.365

```

## std_Density           91275.307
## wtd_std_Density      371806.290
## mean_ElectronAffinity 87814.934
## wtd_mean_ElectronAffinity 219060.718
## gmean_ElectronAffinity 756847.040
## wtd_gmean_ElectronAffinity 339470.176
## entropy_ElectronAffinity 93900.389
## wtd_entropy_ElectronAffinity 245251.037
## range_ElectronAffinity 96741.118
## wtd_range_ElectronAffinity 169175.577
## std_ElectronAffinity 135595.387
## wtd_std_ElectronAffinity 448790.976
## mean_FusionHeat       170344.320
## wtd_mean_FusionHeat   418139.812
## gmean_FusionHeat      192396.147
## wtd_gmean_FusionHeat  262138.332
## entropy_FusionHeat   102060.703
## wtd_entropy_FusionHeat 289772.548
## range_FusionHeat      36624.860
## wtd_range_FusionHeat  307597.241
## std_FusionHeat        112496.721
## wtd_std_FusionHeat    191129.219
## mean_ThermalConductivity 245168.543
## wtd_mean_ThermalConductivity 615671.459
## gmean_ThermalConductivity 86960.979
## wtd_gmean_ThermalConductivity 3512612.407
## entropy_ThermalConductivity 131030.807
## wtd_entropy_ThermalConductivity 686848.160
## range_ThermalConductivity 11525224.807
## wtd_range_ThermalConductivity 367479.571
## std_ThermalConductivity 248086.835
## wtd_std_ThermalConductivity 1882174.312
## mean_Valence          74003.477
## wtd_mean_Valence      658971.887
## gmean_Valence         214671.624
## wtd_gmean_Valence    939026.245
## entropy_Valence       43583.830
## wtd_entropy_Valence   2006408.737
## range_Valence         19534.028
## wtd_range_Valence    426626.299
## std_Valence           79137.435
## wtd_std_Valence       409514.403

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(gbm_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

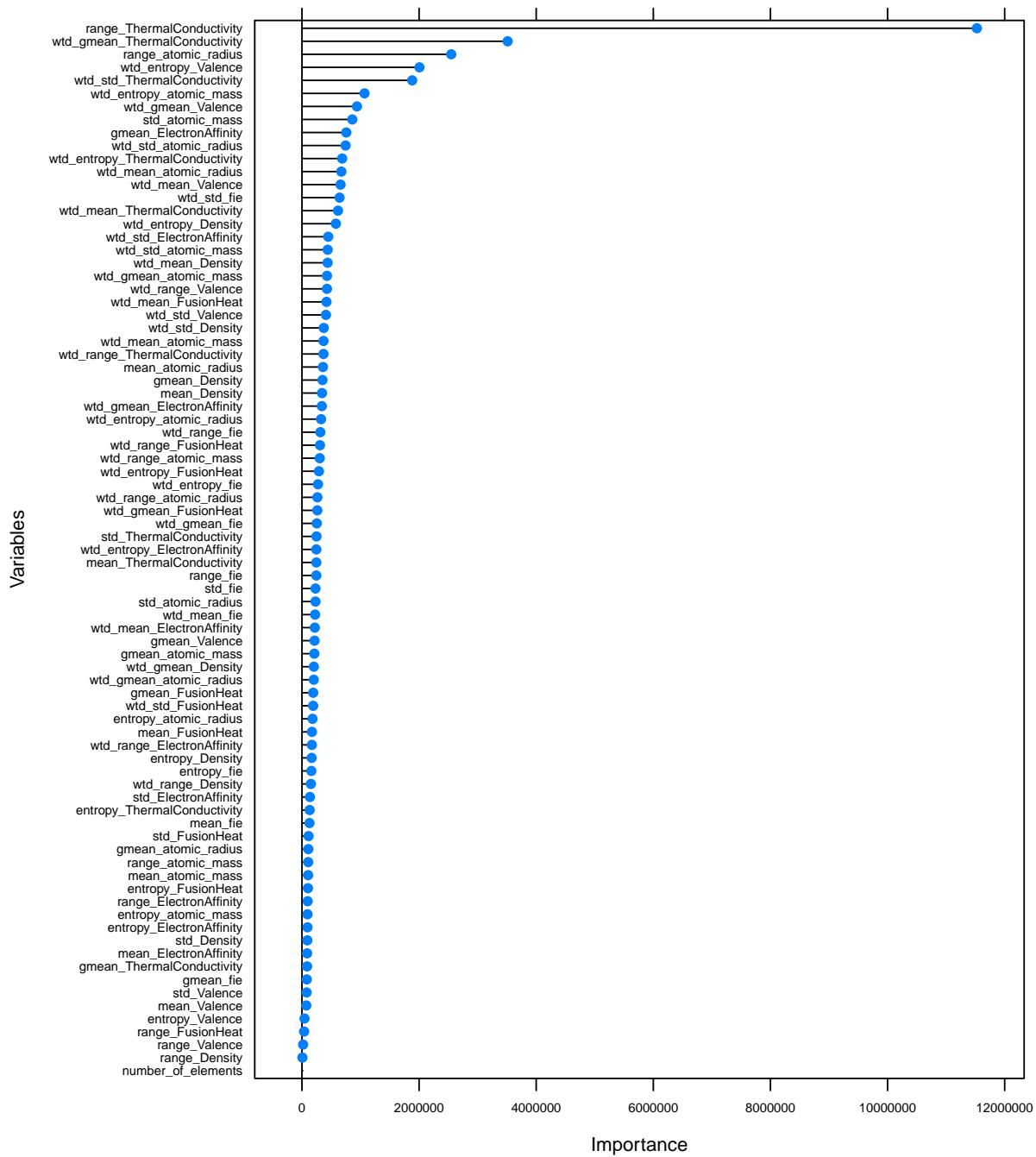


Figure 62: Variables Importance for Gradient Boosting Machine

From above, it can be seen that range\_ThermalConductivity is the most important variable for this model, whereas number\_of\_elements is the least important variable for this model which is same to random forest model.

### 3.1.14 XG-Boost Regression

XG-Boost is an optimized distributed gradient boosting library designed to be highly efficient, flexible and portable. It implements machine learning algorithms under the Gradient Boosting framework. However, xgboost used a more regularized model formalization to control over-fitting, which gives it better performance.

For this algorithm, the main parameters for tuning are nrounds, max\_depth, eta, gamma, colsample\_bytree, min\_child\_weight, and subsample. eta is the learning rate, gamma specifies the minimum loss reduction required to make a split, colsample\_bytree denotes the fraction of columns to be randomly samples for each tree, min\_child\_weight defines the minimum sum of weights of all observations required in a child and subsample denotes the fraction of observations to be randomly samples for each tree.

For the parameters tuning process, we can use apply manual grid search, random grid search or random search tuning. Grid search technique for some cases are more effective, however, it is very time consuming and need much computational cost. Therefore, for this assignment purpose, we will only apply random search tuning with tune length = 4

```
set.seed(seed)

# XG-Boost Regression
xgb_model <- train(
  critical_temp ~.,
  data = train.data,
  trControl = trainControl( method = "cv", number = 10, search = "random"),
  tuneLength = 4,
  method = "xgbTree",
  verbose = FALSE,
  preProc = c("range"),
  nthread = 1
)

xgb_model$results

##          eta max_depth     gamma colsample_bytree min_child_weight subsample
## 4 0.4164612         1 2.923158      0.3746891            3 0.6442732
## 2 0.3090364         7 9.234335      0.4067283            6 0.8579489
## 3 0.3274399         3 8.372956      0.3928904            0 0.9359936
## 1 0.1703574         7 2.862233      0.4266450            4 0.8735088
##   nrounds     RMSE    Rsquared      MAE     RMSESD   RsquaredSD      MAESD
## 4      610 13.38396 0.8473734 9.287666 0.3417019 0.007917328 0.25867940
## 2      623 10.12991 0.9126916 5.759949 0.3212580 0.006233656 0.08665987
## 3      624 10.40901 0.9076818 6.407887 0.2610009 0.005125411 0.14453055
## 1      861  9.80534 0.9180491 5.478948 0.3660403 0.006761859 0.13148534

xgb_model$finalModel

## ##### xgb.Booster
## raw: 3.1 Mb
## call:
##   xgboost::xgb.train(params = list(eta = param$eta, max_depth = param$max_depth,
##     gamma = param$gamma, colsample_bytree = param$colsample_bytree,
##     min_child_weight = param$min_child_weight, subsample = param$subsample),
##     data = x, nrounds = param$nrounds, verbose = FALSE, objective = "reg:linear",
##     nthread = 1)
## params (as set within xgb.train):
```

```

##   eta = "0.170357416570419", max_depth = "7", gamma = "2.86223284667358", colsample_bytree = "0.426645"
## xgb.attributes:
##   niter
## # of features: 81
## niter: 861
## nfeatures : 81
## xNames : number_of_elements mean_atomic_mass wtd_mean_atomic_mass gmean_atomic_mass wtd_gmean_atomic_
## problemType : Regression
## tuneValue :
##   nrounds max_depth      eta      gamma colsample_bytree min_child_weight
## 1     861          7 0.1703574 2.862233      0.426645          4
##   subsample
## 1 0.8735088
## obsLevels : NA
## param :
##   $verbose
## [1] FALSE
##
## $nthread
## [1] 1

```

```
xgb_model$bestTune
```

```

##   nrounds max_depth      eta      gamma colsample_bytree min_child_weight
## 1     861          7 0.1703574 2.862233      0.426645          4
##   subsample
## 1 0.8735088

```

```
getTrainPerf(xgb_model)
```

```

##   TrainRMSE TrainRsquared TrainMAE   method
## 1    9.80534      0.9180491 5.478948 xgbTree

```

From above, we can see that the optimal model is the model with nrounds = 861, max\_depth = 7, eta = 0.1703574, gamma = 2.862233, colsample\_bytree = 0.426645, min\_child\_weight = 4, and subsample = 0.8735088. The R-Squared and MSE are 0.9180491 and 96.04 consecutively.

Here, we show the variable importance for this model.

```
varImp(xgb_model, scale = FALSE)$importance
```

	Overall
## wtd_std_ThermalConductivity	0.1833985004
## range_atomic_radius	0.1516724931
## std_ThermalConductivity	0.1360941790
## wtd_range_ElectronAffinity	0.0599052433
## wtd_entropy_Valence	0.0397473131
## wtd_gmean_Valence	0.0311815385
## range_ThermalConductivity	0.0280936023
## wtd_gmean_ThermalConductivity	0.0252104518
## std_atomic_mass	0.0208547003
## wtd_mean_Valence	0.0167488525

```

## wtd_entropy_atomic_mass          0.0153435727
## wtd_range_ThermalConductivity  0.0126380898
## wtd_entropy_ThermalConductivity 0.0118670944
## std_fie                         0.0117395348
## wtd_entropy_Density              0.0097124498
## wtd_entropy_fie                 0.0094283580
## wtd_gmean_Density               0.0089330818
## wtd_std_atomic_radius           0.0088365793
## wtd_std_atomic_mass             0.0079036057
## mean_Density                     0.0079036018
## std_ElectronAffinity            0.0078769725
## gmean_atomic_radius              0.0077550568
## wtd_range_atomic_mass           0.0069576729
## gmean_ElectronAffinity          0.0067418122
## wtd_range_fie                   0.0064030743
## wtd_mean_atomic_mass            0.0062451135
## wtd_mean_ThermalConductivity   0.0060653258
## wtd_std_ElectronAffinity        0.0059817750
## wtd_gmean_atomic_mass           0.0057188644
## entropy_ThermalConductivity    0.0055986567
## gmean_Density                   0.0055103874
## wtd_entropy_atomic_radius       0.0054396420
## std_Density                      0.0053152478
## wtd_entropy_ElectronAffinity    0.0048158965
## mean_ThermalConductivity       0.0045968323
## wtd_std_Density                 0.0045635686
## wtd_gmean_ElectronAffinity     0.0045394619
## wtd_std_Valence                0.0045373845
## wtd_mean_atomic_radius          0.0045115038
## wtd_range_Density               0.0043803889
## entropy_Density                 0.0041364475
## wtd_mean_FusionHeat             0.0038470845
## wtd_mean_ElectronAffinity       0.0037904262
## wtd_entropy_FusionHeat           0.0037732809
## wtd_range_Valence               0.0037331735
## wtd_gmean_fie                  0.0034378450
## wtd_mean_Density                0.0033754767
## wtd_mean_fie                   0.0033555047
## range_fie                       0.0032799057
## entropy_atomic_radius           0.0030510928
## wtd_range_atomic_radius          0.0029413217
## wtd_gmean_FusionHeat            0.0028448838
## std_FusionHeat                  0.0027979493
## wtd_std_FusionHeat               0.0027774616
## wtd_std_fie                     0.0027205606
## range_ElectronAffinity          0.0026347004
## mean_atomic_radius               0.0026276110
## gmean_Valence                   0.0026089667
## wtd_gmean_atomic_radius          0.0024637524
## entropy_atomic_mass              0.0024526542
## range_atomic_mass                0.0022021521
## mean_Valence                    0.0021078295
## std_atomic_radius                0.0020018670
## mean_FusionHeat                  0.0019285303

```

```

## entropy_ElectronAffinity          0.0016626498
## gmean_atomic_mass                0.0015275952
## gmean_ThermalConductivity       0.0015224407
## entropy_FusionHeat              0.0014671974
## gmean_FusionHeat                 0.0014574101
## wtd_range_FusionHeat            0.0014557312
## mean_atomic_mass                0.0014314825
## mean_fie                         0.0011738577
## entropy_fie                      0.0011410209
## range_Density                    0.0010085751
## gmean_fie                        0.0010053327
## mean_ElectronAffinity           0.0008783310
## number_of_elements               0.0006269857
## range_FusionHeat                 0.0005783794
## range_Valence                   0.0005254303
## std_Valence                      0.0004746162
## entropy_Valence                  0.0004050058

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(xgb_model, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

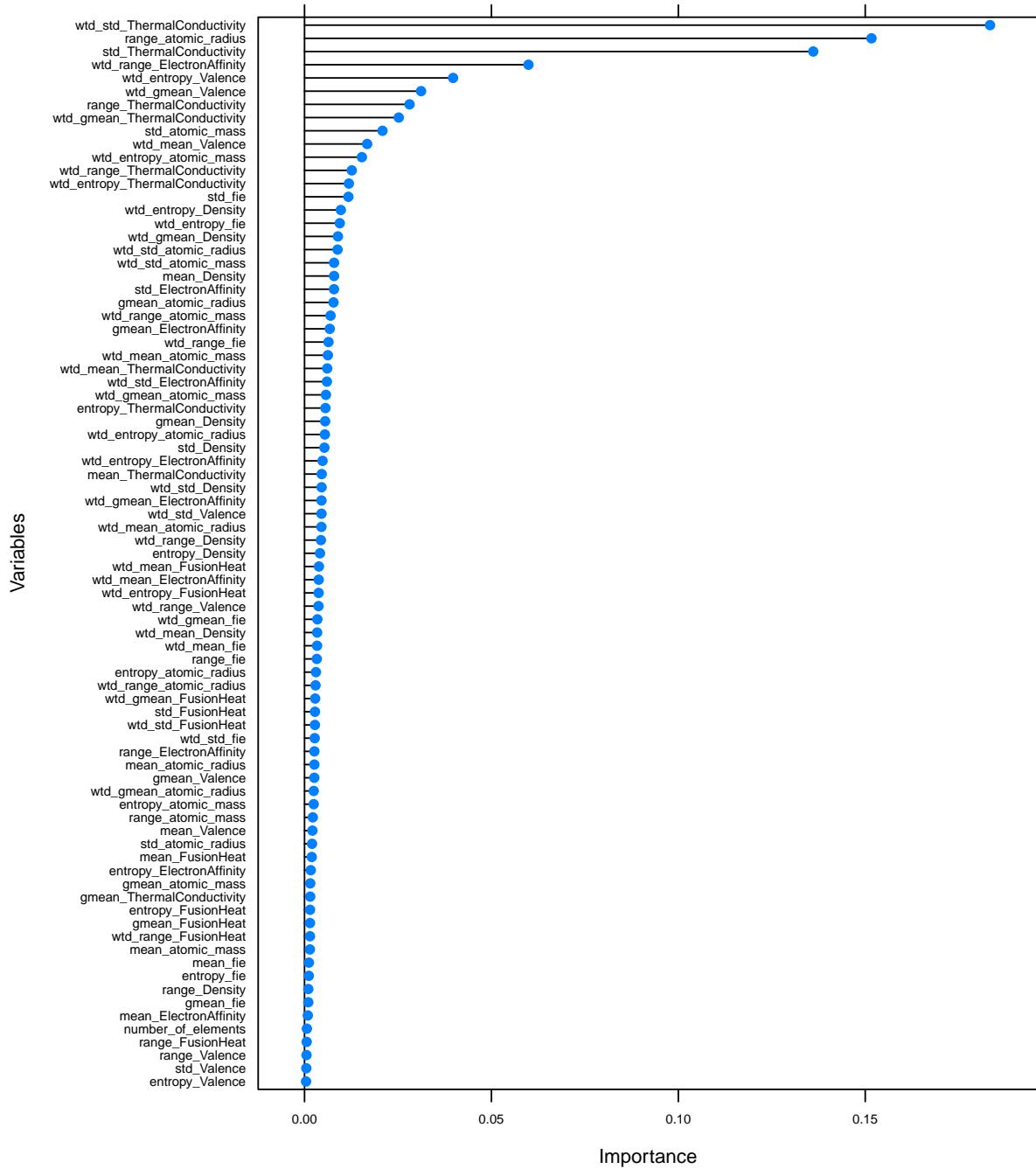


Figure 63: Variables Importance for XG-Boost

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `entropy_Valence` is the least important variable for this model.

## 3.2 Transformed Dataset

### 3.2.1 Linear Regression with All Variables (81)

Linear regression is a linear approach to model the relationship between a scalar response (or dependent variable) and one or more explanatory variables (or independent variables). First, we will create a model with all the features (81 features), later we will improve the model with the finding from the previous section and stepwise technique.

```
set.seed(seed)

# this is control for all dataset, we perform 10-folds cross validation
control <- trainControl(method = "cv", number = 10)

# Linear Model
linear_model1_trans <- train(critical_temp ~.,
                               data = train.data,
                               method = "lm",
                               preProc = c("center", "scale", "BoxCox"),
                               trControl = control
                             )

summary(linear_model1_trans)

## 
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -84.664  -9.697   0.700  11.007 182.205
##
## Coefficients:
##                               Estimate Std. Error t value Pr(>|t|)    
## (Intercept)                34.4441   0.1358 253.657 < 2e-16 ***
## number_of_elements          -2.3482   1.1827 -1.985 0.047112 *  
## mean_atomic_mass            -0.3564   1.9080 -0.187 0.851809    
## wtd_mean_atomic_mass       10.6096   2.6837  3.953 7.74e-05 ***
## gmean_atomic_mass          4.6361   2.2420  2.068 0.038668 *  
## wtd_gmean_atomic_mass     -14.4942   2.4234 -5.981 2.26e-09 ***
## entropy_atomic_mass        -6.1964   2.2648 -2.736 0.006227 ** 
## wtd_entropy_atomic_mass    5.3393   1.8800  2.840 0.004515 ** 
## range_atomic_mass          9.9552   1.0205  9.755 < 2e-16 ***
## wtd_range_atomic_mass     -0.2163   0.5588 -0.387 0.698647    
## std_atomic_mass             -2.0052   1.1918 -1.682 0.092504 .  
## wtd_std_atomic_mass        -5.0799   0.9089 -5.589 2.32e-08 ***
## mean_fie                   -14.7346   5.4980 -2.680 0.007370 ** 
## wtd_mean_fie               -0.7544   7.7518 -0.097 0.922471    
## gmean_fie                  13.8073   4.8081  2.872 0.004088 ** 
## wtd_gmean_fie              2.0544   6.0334  0.341 0.733479    
## entropy_fie                 -44.7067  12.6107 -3.545 0.000393 *** 
## wtd_entropy_fie            10.4974   1.7575  5.973 2.38e-09 *** 
## range_fie                  17.7985   2.3311  7.635 2.37e-14 *** 
## wtd_range_fie              4.6452   0.9067  5.123 3.03e-07 ***
```

## std_fie	-12.1748	2.4316	-5.007	5.58e-07	***
## wtd_std_fie	-5.5566	2.0645	-2.692	0.007120	**
## mean_atomic_radius	17.5182	2.3940	7.317	2.64e-13	***
## wtd_mean_atomic_radius	19.1194	4.3980	4.347	1.39e-05	***
## gmean_atomic_radius	-27.4699	3.0955	-8.874	< 2e-16	***
## wtd_gmean_atomic_radius	-11.4437	6.3070	-1.814	0.069627	.
## entropy_atomic_radius	12.0003	9.4181	1.274	0.202618	
## wtd_entropy_atomic_radius	9.8678	2.5123	3.928	8.61e-05	***
## range_atomic_radius	17.7829	1.6681	10.661	< 2e-16	***
## wtd_range_atomic_radius	-2.7233	0.5865	-4.643	3.46e-06	***
## std_atomic_radius	-21.8518	1.8385	-11.886	< 2e-16	***
## wtd_std_atomic_radius	6.9725	1.4811	4.708	2.53e-06	***
## mean_Density	-3.9123	1.1363	-3.443	0.000577	***
## wtd_mean_Density	0.2731	1.5809	0.173	0.862860	
## gmean_Density	0.7821	1.7457	0.448	0.654155	
## wtd_gmean_Density	13.9476	3.1797	4.387	1.16e-05	***
## entropy_Density	1.2111	1.5450	0.784	0.433096	
## wtd_entropy_Density	-10.3163	1.0617	-9.717	< 2e-16	***
## range_Density	-6.8143	0.9676	-7.043	1.96e-12	***
## wtd_range_Density	-2.4585	0.5209	-4.720	2.38e-06	***
## std_Density	10.6892	1.1937	8.955	< 2e-16	***
## wtd_std_Density	-6.2720	0.7836	-8.004	1.28e-15	***
## mean_ElectronAffinity	-1.4787	1.1974	-1.235	0.216877	
## wtd_mean_ElectronAffinity	14.9244	1.7048	8.754	< 2e-16	***
## gmean_ElectronAffinity	6.3645	1.1560	5.506	3.73e-08	***
## wtd_gmean_ElectronAffinity	-16.7773	1.3325	-12.591	< 2e-16	***
## entropy_ElectronAffinity	-3.7161	1.2892	-2.882	0.003951	**
## wtd_entropy_ElectronAffinity	-5.7820	0.6928	-8.346	< 2e-16	***
## range_ElectronAffinity	-23.0264	1.1728	-19.634	< 2e-16	***
## wtd_range_ElectronAffinity	-3.5616	0.6439	-5.531	3.22e-08	***
## std_ElectronAffinity	23.0198	1.3969	16.479	< 2e-16	***
## wtd_std_ElectronAffinity	-8.4007	0.8328	-10.087	< 2e-16	***
## mean_FusionHeat	-17.7638	1.8973	-9.362	< 2e-16	***
## wtd_mean_FusionHeat	17.5647	1.6643	10.554	< 2e-16	***
## gmean_FusionHeat	21.1243	2.5839	8.175	3.15e-16	***
## wtd_gmean_FusionHeat	-17.3743	1.7980	-9.663	< 2e-16	***
## entropy_FusionHeat	-13.7804	2.0177	-6.830	8.80e-12	***
## wtd_entropy_FusionHeat	9.8876	1.0236	9.660	< 2e-16	***
## range_FusionHeat	-14.5206	1.5552	-9.337	< 2e-16	***
## wtd_range_FusionHeat	4.4471	0.6031	7.373	1.74e-13	***
## std_FusionHeat	13.4381	1.9753	6.803	1.06e-11	***
## wtd_std_FusionHeat	-5.9674	0.7462	-7.997	1.35e-15	***
## mean_ThermalConductivity	-8.9396	0.7523	-11.883	< 2e-16	***
## wtd_mean_ThermalConductivity	21.7219	1.2474	17.413	< 2e-16	***
## gmean_ThermalConductivity	-10.4236	1.1448	-9.105	< 2e-16	***
## wtd_gmean_ThermalConductivity	-11.2019	2.3382	-4.791	1.67e-06	***
## entropy_ThermalConductivity	9.8589	0.6704	14.707	< 2e-16	***
## wtd_entropy_ThermalConductivity	4.4944	0.5563	8.079	6.98e-16	***
## range_ThermalConductivity	-14.7600	2.3451	-6.294	3.17e-10	***
## wtd_range_ThermalConductivity	-10.0916	0.5877	-17.170	< 2e-16	***
## std_ThermalConductivity	23.1094	2.3964	9.643	< 2e-16	***
## wtd_std_ThermalConductivity	6.7096	1.2620	5.317	1.07e-07	***
## mean_Valence	17.1737	4.5445	3.779	0.000158	***
## wtd_mean_Valence	-28.2091	4.4669	-6.315	2.77e-10	***

```

## gmean_Valence          -15.3852   4.2747  -3.599 0.000320 ***
## wtd_gmean_Valence      17.6536   3.8377   4.600 4.26e-06 ***
## entropy_Valence        46.7417   8.2458   5.669 1.46e-08 ***
## wtd_entropy_Valence    -16.6456   2.2121  -7.525 5.55e-14 ***
## range_Valence           5.9421   1.0299   5.769 8.10e-09 ***
## wtd_range_Valence       2.3696   0.6243   3.796 0.000148 ***
## std_Valence              -0.0332   1.1777  -0.028 0.977508
## wtd_std_Valence         -5.7400   0.7126  -8.055 8.49e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 17.71 on 16929 degrees of freedom
## Multiple R-squared:  0.7339, Adjusted R-squared:  0.7326
## F-statistic: 576.3 on 81 and 16929 DF,  p-value: < 2.2e-16

cat("MSE :",linear_model1_trans$results$RMSE^2)

```

## MSE : 326.288

From above, we can see that the R-squared for the model is 0.7339 with Adjusted R-squared is 0.7326

The summary tells us about the features which are not important such as wtd\_entropy\_atomic\_mass, wtd\_range\_atomic\_mass, wtd\_mean\_fie, wtd\_gmean\_fie, wtd\_std\_fie, wtd\_mean\_Density, wtd\_range\_Density, gmean\_ThermalConductivity, wtd\_entropy\_ThermalConductivity, wtd\_std\_ThermalConductivity, and wtd\_range\_Valence.

The Train MSE for this model is 326.288

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_model1_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

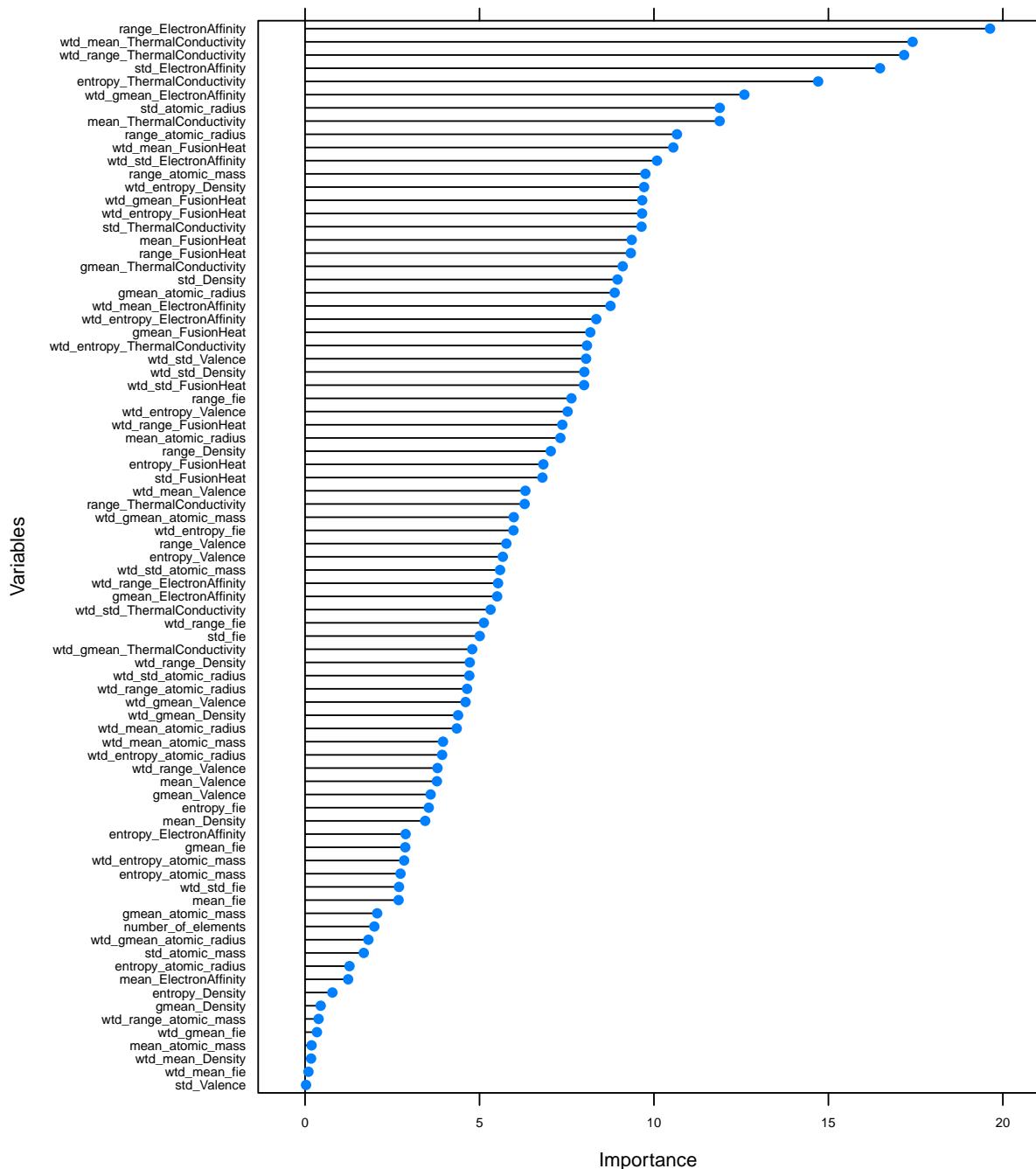


Figure 64: Variable Importance for Linear Regression Model 1 Trans

### 3.2.2 Linear Regression with Significant Variables

```
set.seed(seed)

# Store the less importance variables
```

```

less_important <- c("mean_atomic_mass", "wtd_range_atomic_mass", "wtd_mean_fie",
                  "wtd_gmean_fie", "wtd_mean_Density", "gmean_Density",
                  "entropy_Density", "mean_ElectronAffinity", "std_Valence")

# Linear Model
linear_model2_trans <- train(critical_temp ~.,
                               data = train.data[, -which(names(train.data) %in% less_important)],
                               method = "lm",
                               preProc = c("center", "scale", "BoxCox"),
                               trControl = control
)

summary(linear_model2_trans)

##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min      1Q  Median      3Q     Max 
## -84.723 -9.709   0.731  10.975 184.937 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 34.4441   0.1358 253.669 < 2e-16 ***
## number_of_elements -2.0903   1.1604 -1.801 0.071669 .
## wtd_mean_atomic_mass 10.7951   1.7461  6.183 6.45e-10 ***
## gmean_atomic_mass    3.8604   0.9662  3.996 6.48e-05 ***
## wtd_gmean_atomic_mass -14.4584  1.7337 -8.340 < 2e-16 ***
## entropy_atomic_mass   -5.1586  1.8610 -2.772 0.005578 ** 
## wtd_entropy_atomic_mass  5.8052   1.6006  3.627 0.000288 *** 
## range_atomic_mass     10.0447   1.0017 10.027 < 2e-16 ***
## std_atomic_mass       -1.8008   1.1012 -1.635 0.101983  
## wtd_std_atomic_mass   -5.4259   0.8558 -6.340 2.35e-10 ***
## mean_fie              -13.8388  4.6799 -2.957 0.003110 ** 
## gmean_fie              13.5098   4.2322  3.192 0.001415 ** 
## entropy_fie            -46.7746  11.6100 -4.029 5.63e-05 ***
## wtd_entropy_fie        10.7299   1.7070  6.286 3.34e-10 ***
## range_fie              18.7017   2.2055  8.480 < 2e-16 ***
## wtd_range_fie          4.5513   0.8632  5.273 1.36e-07 ***
## std_fie                -13.2061  2.1478 -6.149 7.99e-10 ***
## wtd_std_fie             -5.6338  1.3676 -4.119 3.82e-05 ***
## mean_atomic_radius     16.7313   2.1594  7.748 9.85e-15 *** 
## wtd_mean_atomic_radius 20.0669   3.3970  5.907 3.55e-09 *** 
## gmean_atomic_radius    -25.9188  2.8199 -9.192 < 2e-16 *** 
## wtd_gmean_atomic_radius -14.5305  4.9530 -2.934 0.003354 ** 
## entropy_atomic_radius  13.1622   8.4067  1.566 0.117440  
## wtd_entropy_atomic_radius 9.6024   2.3327  4.116 3.87e-05 *** 
## range_atomic_radius    17.7232   1.6282 10.885 < 2e-16 *** 
## wtd_range_atomic_radius -2.7670   0.5374 -5.149 2.65e-07 *** 
## std_atomic_radius      -21.4761  1.7690 -12.140 < 2e-16 *** 
## wtd_std_atomic_radius   6.8350   1.3962  4.895 9.91e-07 *** 
## mean_Density            -3.5966  0.6197 -5.803 6.62e-09 ***

```

```

## wtd_gmean_Density           15.4654   1.7337   8.920 < 2e-16 ***
## wtd_entropy_Density        -10.1807   0.7906  -12.877 < 2e-16 ***
## range_Density              -6.6899   0.9576  -6.986 2.93e-12 ***
## wtd_range_Density          -2.3630   0.3844  -6.147 8.09e-10 ***
## std_Density                 10.0528   1.1093   9.062 < 2e-16 ***
## wtd_std_Density             -5.9290   0.7229  -8.202 2.54e-16 ***
## wtd_mean_ElectronAffinity  13.4931   1.2875  10.480 < 2e-16 ***
## gmean_ElectronAffinity     5.0766   0.5785   8.776 < 2e-16 ***
## wtd_gmean_ElectronAffinity -15.8272   1.1393  -13.893 < 2e-16 ***
## entropy_ElectronAffinity   -2.7773   1.1559  -2.403 0.016287 *
## wtd_entropy_ElectronAffinity -5.9353   0.6825  -8.696 < 2e-16 ***
## range_ElectronAffinity     -23.4433   1.1149  -21.027 < 2e-16 ***
## wtd_range_ElectronAffinity -3.3526   0.6251  -5.363 8.29e-08 ***
## std_ElectronAffinity       23.0499   1.3112  17.579 < 2e-16 ***
## wtd_std_ElectronAffinity   -8.0695   0.7457  -10.822 < 2e-16 ***
## mean_FusionHeat            -18.7103   1.8076  -10.351 < 2e-16 ***
## wtd_mean_FusionHeat        18.4133   1.5260  12.066 < 2e-16 ***
## gmean_FusionHeat           21.7952   2.4073   9.054 < 2e-16 ***
## wtd_gmean_FusionHeat       -17.7193   1.7229  -10.285 < 2e-16 ***
## entropy_FusionHeat         -13.9889   2.0073  -6.969 3.31e-12 ***
## wtd_entropy_FusionHeat     10.0301   0.9742  10.296 < 2e-16 ***
## range_FusionHeat           -14.7595   1.5301  -9.646 < 2e-16 ***
## wtd_range_FusionHeat       4.4967   0.5783   7.775 7.96e-15 ***
## std_FusionHeat              13.9424   1.8963   7.353 2.03e-13 ***
## wtd_std_FusionHeat          -6.1563   0.7029  -8.758 < 2e-16 ***
## mean_ThermalConductivity  -9.4224   0.7065  -13.337 < 2e-16 ***
## wtd_mean_ThermalConductivity 22.3092   1.1900  18.747 < 2e-16 ***
## gmean_ThermalConductivity -9.7154   1.0726  -9.058 < 2e-16 ***
## wtd_gmean_ThermalConductivity -12.6222   2.1855  -5.775 7.81e-09 ***
## entropy_ThermalConductivity 9.9118   0.6573  15.079 < 2e-16 ***
## wtd_entropy_ThermalConductivity 4.4577   0.5427  8.213 2.31e-16 ***
## range_ThermalConductivity -15.3516   2.2752  -6.747 1.55e-11 ***
## wtd_range_ThermalConductivity -10.0898   0.5777  -17.466 < 2e-16 ***
## std_ThermalConductivity    24.1602   2.3213  10.408 < 2e-16 ***
## wtd_std_ThermalConductivity 5.9978   1.1967  5.012 5.44e-07 ***
## mean_Valence                16.5699   4.4357  3.736 0.000188 ***
## wtd_mean_Valence            -28.0339   4.1202  -6.804 1.05e-11 ***
## gmean_Valence               -14.4893   4.1599  -3.483 0.000497 ***
## wtd_gmean_Valence           17.3097   3.5580  4.865 1.15e-06 ***
## entropy_Valence              46.7469   7.7087  6.064 1.35e-09 ***
## wtd_entropy_Valence         -17.0720   2.0459  -8.344 < 2e-16 ***
## range_Valence                5.9296   0.6751  8.784 < 2e-16 ***
## wtd_range_Valence            2.2441   0.5951  3.771 0.000163 ***
## wtd_std_Valence              -5.7109   0.5710  -10.001 < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 17.71 on 16938 degrees of freedom
## Multiple R-squared:  0.7338, Adjusted R-squared:  0.7326
## F-statistic: 648.3 on 72 and 16938 DF,  p-value: < 2.2e-16

cat("MSE :",linear_model2_trans$results$RMSE^2)

## MSE : 315.0956

```

From above, we can see that the R-squared for the model is 0.7338 with Adjusted R-squared is 0.7326 Those 2 parameters are slightly worse than the previous model. For the R-Squared, the difference is only 0.0001, whereas the Adjusted R-squared is same. However, we decrease the number of variables from 81 variables to 72 variables, which is better in term of complexity.

The Train MSE for this model is 315.0956

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(linear_model2_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

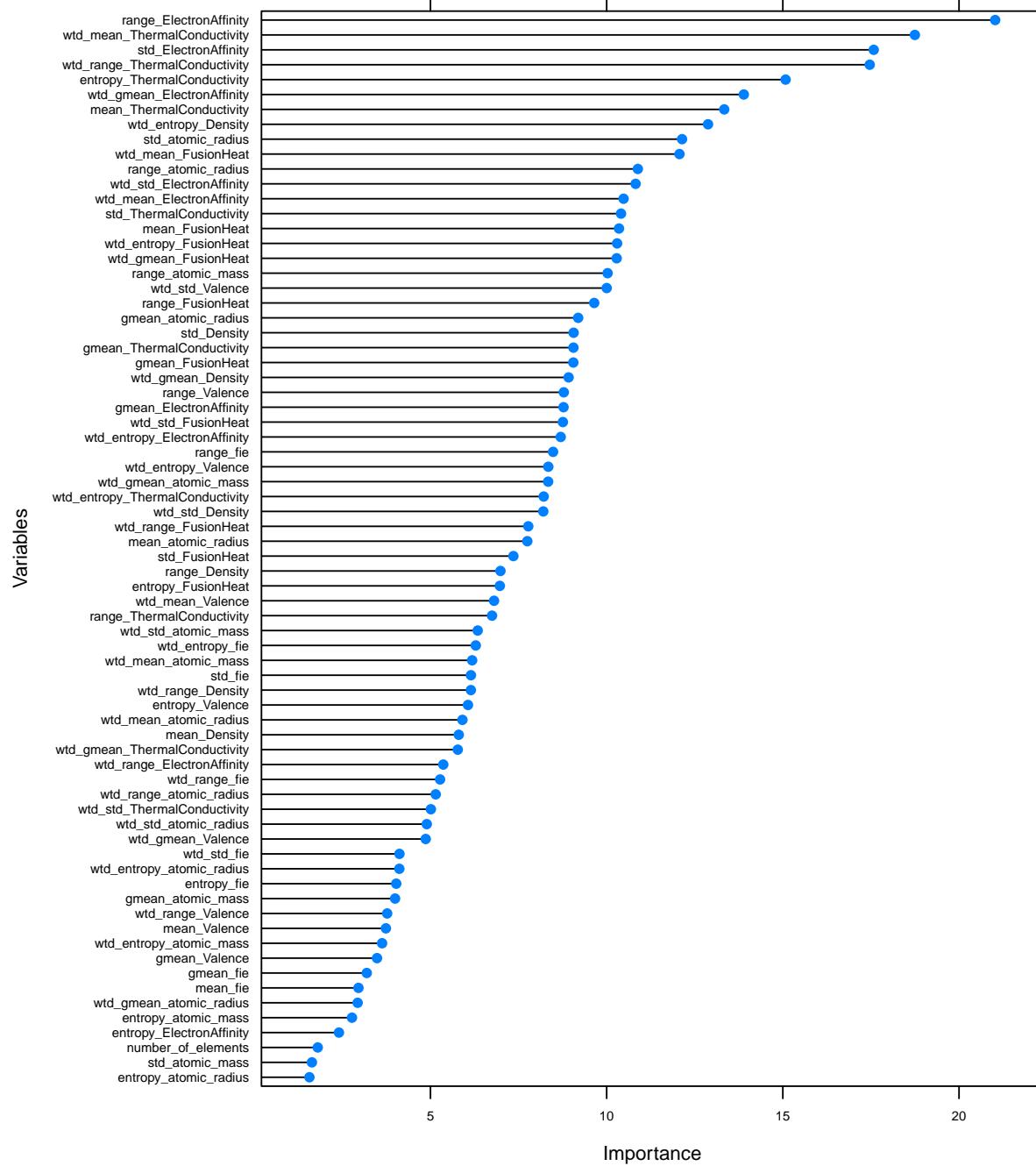


Figure 65: Variable Importance for Linear Regression Model 2 Trans

From above, it can be seen that range\_ElectronAffinity is the most important variable for this model, whereas entropy\_atomic\_radius is the least important variable for this model.

### 3.2.3 Linear Regression with Strong Correlated Variables

```

set.seed(seed)

# Linear Model
linear_model3_trans <- train(critical_temp ~.,
                               data = train.data[, -which(names(train.data) %in% less_correlated)],
                               method = "lm",
                               preProc = c("center", "scale", "BoxCox"),
                               trControl = control
                             )

summary(linear_model3_trans)

##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##    Min      1Q  Median      3Q     Max
## -82.826 -10.291   0.655  11.175 190.418
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 34.4441   0.1386 248.591 < 2e-16 ***
## number_of_elements -2.3658   1.1856 -1.995 0.046017 *
## mean_atomic_mass    4.1349   1.8789  2.201 0.027771 *
## wtd_mean_atomic_mass 12.9013   2.6559  4.858 1.20e-06 ***
## gmean_atomic_mass   -3.6349   2.2002 -1.652 0.098529 .
## wtd_gmean_atomic_mass -13.3920   2.3844 -5.616 1.98e-08 ***
## entropy_atomic_mass   1.5111   2.2782  0.663 0.507177
## wtd_entropy_atomic_mass 12.6443   1.8031  7.013 2.43e-12 ***
## range_atomic_mass    13.5979   1.0088 13.479 < 2e-16 ***
## wtd_range_atomic_mass   0.5340   0.5659  0.944 0.345422
## std_atomic_mass      -3.5244   1.1883 -2.966 0.003023 **
## wtd_std_atomic_mass   -5.3026   0.9141 -5.801 6.70e-09 ***
## mean_fie              1.0649   0.5909  1.802 0.071519 .
## wtd_mean_fie          -2.3098   6.9986 -0.330 0.741376
## wtd_gmean_fie         3.1970   5.5303  0.578 0.563207
## entropy_fie           -78.0054   9.3173 -8.372 < 2e-16 ***
## wtd_entropy_fie       15.3069   1.7134  8.933 < 2e-16 ***
## range_fie              20.7058   2.2866  9.055 < 2e-16 ***
## wtd_range_fie          5.9612   0.8862  6.727 1.79e-11 ***
## std_fie                -19.7117   2.2016 -8.953 < 2e-16 ***
## wtd_std_fie            -6.3761   2.0156 -3.163 0.001563 **
## wtd_mean_atomic_radius 15.6916   3.7492  4.185 2.86e-05 ***
## gmean_atomic_radius    -5.5334   0.7615 -7.266 3.86e-13 ***
## wtd_gmean_atomic_radius -6.1397   5.0961 -1.205 0.228301
## entropy_atomic_radius   31.2266   8.2860  3.769 0.000165 ***
## wtd_entropy_atomic_radius 7.5093   2.3365  3.214 0.001312 **
## range_atomic_radius     17.9607   1.6590 10.826 < 2e-16 ***
## wtd_range_atomic_radius  -2.1402   0.5867 -3.648 0.000265 ***
## std_atomic_radius        -17.2839   1.7339 -9.968 < 2e-16 ***

```

```

## wtd_std_atomic_radius      5.6047   1.4334   3.910 9.26e-05 ***
## mean_Density              -2.5577   1.1113  -2.301 0.021379 *
## wtd_mean_Density          -2.4799   1.5477  -1.602 0.109103
## gmean_Density             -0.8378   1.5964  -0.525 0.599715
## wtd_gmean_Density         13.5531   2.8158   4.813 1.50e-06 ***
## entropy_Density            0.7752   1.5289   0.507 0.612148
## wtd_entropy_Density       -13.7897   1.0505  -13.126 < 2e-16 ***
## range_Density              -6.2304   0.9671  -6.442 1.21e-10 ***
## wtd_range_Density          -2.9006   0.5247  -5.528 3.28e-08 ***
## std_Density                10.6150   1.2004   8.843 < 2e-16 ***
## wtd_std_Density            -8.0206   0.7857  -10.209 < 2e-16 ***
## wtd_mean_ElectronAffinity -1.8016   0.6384  -2.822 0.004777 **
## gmean_ElectronAffinity     4.2540   0.5805   7.328 2.44e-13 ***
## entropy_ElectronAffinity  -3.2633   1.1825  -2.760 0.005795 **
## wtd_entropy_ElectronAffinity -10.2912   0.6715  -15.325 < 2e-16 ***
## range_ElectronAffinity    -20.9725   1.1477  -18.273 < 2e-16 ***
## wtd_range_ElectronAffinity -4.5884   0.6389  -7.182 7.17e-13 ***
## std_ElectronAffinity       22.0341   1.3457  16.374 < 2e-16 ***
## wtd_std_ElectronAffinity  -4.0570   0.6075  -6.679 2.49e-11 ***
## mean_FusionHeat            -8.1899   1.6900  -4.846 1.27e-06 ***
## wtd_mean_FusionHeat        21.9396   1.6244  13.507 < 2e-16 ***
## gmean_FusionHeat           -0.0883   2.0834  -0.042 0.966195
## wtd_gmean_FusionHeat       -16.1460   1.7763  -9.090 < 2e-16 ***
## entropy_FusionHeat         3.2415   1.3255  2.446 0.014473 *
## wtd_entropy_FusionHeat     15.4665   0.9214  16.786 < 2e-16 ***
## wtd_range_FusionHeat       4.5131   0.4701  9.601 < 2e-16 ***
## mean_ThermalConductivity -7.8065   0.7195  -10.851 < 2e-16 ***
## wtd_mean_ThermalConductivity 22.7367   1.2336  18.432 < 2e-16 ***
## gmean_ThermalConductivity -10.2485   1.0990  -9.326 < 2e-16 ***
## wtd_gmean_ThermalConductivity -13.6272   2.3170  -5.881 4.15e-09 ***
## entropy_ThermalConductivity 11.9679   0.5867  20.399 < 2e-16 ***
## range_ThermalConductivity -11.3267   2.3114  -4.900 9.66e-07 ***
## wtd_range_ThermalConductivity -12.4780   0.5667  -22.020 < 2e-16 ***
## std_ThermalConductivity    24.2803   2.2830  10.635 < 2e-16 ***
## wtd_std_ThermalConductivity 1.7898   1.2150  1.473 0.140726
## mean_Valence               28.7752   3.8615  7.452 9.64e-14 ***
## wtd_mean_Valence           -56.4186   3.2856  -17.172 < 2e-16 ***
## gmean_Valence              -21.6018   3.5300  -6.120 9.59e-10 ***
## wtd_gmean_Valence          38.6193   2.8994  13.320 < 2e-16 ***
## entropy_Valence            28.0897   5.4546  5.150 2.64e-07 ***
## wtd_entropy_Valence        -17.0785   2.1472  -7.954 1.92e-15 ***
## wtd_range_Valence          3.4452   0.5996  5.746 9.28e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.07 on 16940 degrees of freedom
## Multiple R-squared:  0.7227, Adjusted R-squared:  0.7216
## F-statistic: 630.8 on 70 and 16940 DF,  p-value: < 2.2e-16

cat("MSE :",linear_model3_trans$results$RMSE^2)

```

```
## MSE : 334.3684
```

From above, we can see that the R-squared for the model is 0.7338 with Adjusted R-squared is 0.7216 Those

2 parameters are slightly worse than the previous model. For the R-Squared, the difference is only 0.0112, whereas for the Adjusted R-squared the different is 0.0110. However, we decrease the number of variables from 81 variables to 70 variables, which is better in term of complexity.

The Train MSE for this model is 334.3684

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance
plot(varImp(linear_model3_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

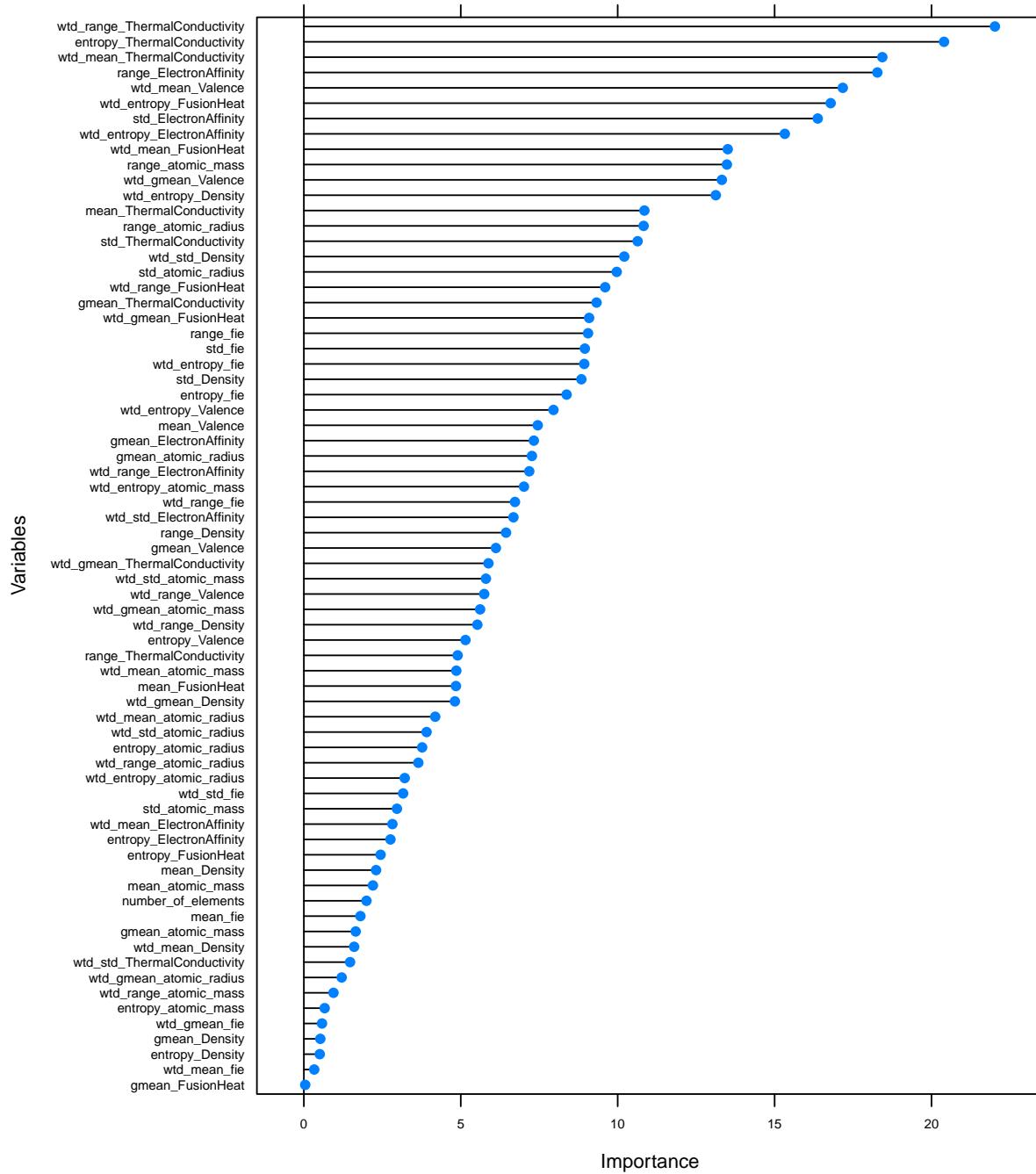


Figure 66: Variable Importance for Linear Regression Model 3 Trans

From above, it can be seen that wtd\_range\_ThermalConductivity is the most important variable for this model, whereas gmean\_FusionHeat is the least important variable for this model.

### 3.2.4 Linear Regression with Backwards Selection

The stepwise regression (or stepwise selection) consists of iteratively adding and removing predictors, in the predictive model, in order to find the subset of variables in the data set resulting in the best performing model, that is a model that lowers prediction error.

There are three strategies of stepwise regression [Bruce and Bruce, 2017]

- Backward selection (or backward elimination), which starts with all predictors in the model (full model), iteratively removes the least contributive predictors, and stops when you have a model where all predictors are statistically significant.
- Forward selection, which starts with no predictors in the model, iteratively adds the most contributive predictors, and stops when the improvement is no longer statistically significant.
- Stepwise selection (or sequential replacement), which is a combination of forward and backward selections. You start with no predictors, then sequentially add the most contributive predictors (like forward selection). After adding each new variable, remove any variables that no longer provide an improvement in the model fit (like backward selection).

In this sub section, we will perform the backward selection and in the next subsections, we will perform forward and stepwise selection.

```
# Helper Function for Plotting Metrics
plot_metrics <- function(model, x_axis, x_label) {
  par(mfrow = c(2, 2))
  plot(y = model$results$Rsquared, x = x_axis, xlab = x_label,
    ylab = "R-Squared", type = "l")
  points(x_axis[max(which(model$results$Rsquared == max(model$results$Rsquared)))],
    max(model$results$Rsquared),
    col = "red", cex = 2, pch = 20)
  plot(model$results$RMSE^2, x = x_axis, xlab = x_label, ylab = "MSE", type = "l")
  points(x_axis[max(which(model$results$RMSE == min(model$results$RMSE)))],
    min(model$results$RMSE)^2,
    col = "red", cex = 2, pch = 20)
  plot(model$results$MAE, x = x_axis, xlab = x_label, ylab = "MAE", type = "l")
  points(x_axis[max(which(model$results$MAE == min(model$results$MAE)))],
    min(model$results$MAE),
    col = "red", cex = 2, pch = 20)
}
```

```
set.seed(seed)

# Linear Regression with Backward Selection
linear_backward_trans <- train(critical_temp ~., data = train.data,
  method = "leapBackward",
  tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
  trControl = control,
  preProc = c("center", "scale", "BoxCox")
)
summary(linear_backward_trans)
```

```
## Subset selection object
## 81 Variables  (and intercept)
```

	Forced in	Forced out
##		
## number_of_elements	FALSE	FALSE
## mean_atomic_mass	FALSE	FALSE
## wtd_mean_atomic_mass	FALSE	FALSE
## gmean_atomic_mass	FALSE	FALSE
## wtd_gmean_atomic_mass	FALSE	FALSE
## entropy_atomic_mass	FALSE	FALSE
## wtd_entropy_atomic_mass	FALSE	FALSE
## range_atomic_mass	FALSE	FALSE
## wtd_range_atomic_mass	FALSE	FALSE
## std_atomic_mass	FALSE	FALSE
## wtd_std_atomic_mass	FALSE	FALSE
## mean_fie	FALSE	FALSE
## wtd_mean_fie	FALSE	FALSE
## gmean_fie	FALSE	FALSE
## wtd_gmean_fie	FALSE	FALSE
## entropy_fie	FALSE	FALSE
## wtd_entropy_fie	FALSE	FALSE
## range_fie	FALSE	FALSE
## wtd_range_fie	FALSE	FALSE
## std_fie	FALSE	FALSE
## wtd_std_fie	FALSE	FALSE
## mean_atomic_radius	FALSE	FALSE
## wtd_mean_atomic_radius	FALSE	FALSE
## gmean_atomic_radius	FALSE	FALSE
## wtd_gmean_atomic_radius	FALSE	FALSE
## entropy_atomic_radius	FALSE	FALSE
## wtd_entropy_atomic_radius	FALSE	FALSE
## range_atomic_radius	FALSE	FALSE
## wtd_range_atomic_radius	FALSE	FALSE
## std_atomic_radius	FALSE	FALSE
## wtd_std_atomic_radius	FALSE	FALSE
## mean_Density	FALSE	FALSE
## wtd_mean_Density	FALSE	FALSE
## gmean_Density	FALSE	FALSE
## wtd_gmean_Density	FALSE	FALSE
## entropy_Density	FALSE	FALSE
## wtd_entropy_Density	FALSE	FALSE
## range_Density	FALSE	FALSE
## wtd_range_Density	FALSE	FALSE
## std_Density	FALSE	FALSE
## wtd_std_Density	FALSE	FALSE
## mean_ElectronAffinity	FALSE	FALSE
## wtd_mean_ElectronAffinity	FALSE	FALSE
## gmean_ElectronAffinity	FALSE	FALSE
## wtd_gmean_ElectronAffinity	FALSE	FALSE
## entropy_ElectronAffinity	FALSE	FALSE
## wtd_entropy_ElectronAffinity	FALSE	FALSE
## range_ElectronAffinity	FALSE	FALSE
## wtd_range_ElectronAffinity	FALSE	FALSE
## std_ElectronAffinity	FALSE	FALSE
## wtd_std_ElectronAffinity	FALSE	FALSE
## mean_FusionHeat	FALSE	FALSE
## wtd_mean_FusionHeat	FALSE	FALSE

```

## gmean_FusionHeat           FALSE  FALSE
## wtd_gmean_FusionHeat      FALSE  FALSE
## entropy_FusionHeat        FALSE  FALSE
## wtd_entropy_FusionHeat    FALSE  FALSE
## range_FusionHeat          FALSE  FALSE
## wtd_range_FusionHeat      FALSE  FALSE
## std_FusionHeat            FALSE  FALSE
## wtd_std_FusionHeat        FALSE  FALSE
## mean_ThermalConductivity FALSE  FALSE
## wtd_mean_ThermalConductivity FALSE FALSE
## gmean_ThermalConductivity FALSE  FALSE
## wtd_gmean_ThermalConductivity FALSE FALSE
## entropy_ThermalConductivity FALSE FALSE
## wtd_entropy_ThermalConductivity FALSE FALSE
## range_ThermalConductivity FALSE  FALSE
## wtd_range_ThermalConductivity FALSE FALSE
## std_ThermalConductivity   FALSE  FALSE
## wtd_std_ThermalConductivity FALSE FALSE
## mean_Valence               FALSE  FALSE
## wtd_mean_Valence          FALSE  FALSE
## gmean_Valence              FALSE  FALSE
## wtd_gmean_Valence          FALSE FALSE
## entropy_Valence            FALSE FALSE
## wtd_entropy_Valence        FALSE FALSE
## range_Valence              FALSE  FALSE
## wtd_range_Valence          FALSE FALSE
## std_Valence                FALSE  FALSE
## wtd_std_Valence            FALSE FALSE

## 1 subsets of each size up to 54
## Selection Algorithm: backward
##             number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1  ( 1 )      " "           " "           " "
## 2  ( 1 )      " "           " "           " "
## 3  ( 1 )      " "           " "           " "
## 4  ( 1 )      " "           " "           " "
## 5  ( 1 )      " "           " "           " "
## 6  ( 1 )      " "           " "           " "
## 7  ( 1 )      " "           " "           " "
## 8  ( 1 )      " "           " "           " "
## 9  ( 1 )      " "           " "           " "
## 10 ( 1 )      " "           " "           " "
## 11 ( 1 )      " "           " "           " "
## 12 ( 1 )      " "           " "           " "
## 13 ( 1 )      " "           " "           " "
## 14 ( 1 )      " "           " "           " "
## 15 ( 1 )      " "           " "           " "
## 16 ( 1 )      " "           " "           " "
## 17 ( 1 )      " "           " "           " "
## 18 ( 1 )      " "           " "           " "
## 19 ( 1 )      " "           " "           " "
## 20 ( 1 )      " "           " "           " "
## 21 ( 1 )      " "           " "           " "
## 22 ( 1 )      " "           " "           " "
## 23 ( 1 )      " "           " "           " "

```

```

## 24  ( 1 ) " "      " "
## 25  ( 1 ) " "      " "
## 26  ( 1 ) " "      " "
## 27  ( 1 ) " "      " "
## 28  ( 1 ) " "      " "
## 29  ( 1 ) " "      " "
## 30  ( 1 ) " "      " "
## 31  ( 1 ) " "      " "
## 32  ( 1 ) " "      " "
## 33  ( 1 ) " "      " "
## 34  ( 1 ) " "      " "
## 35  ( 1 ) " "      " "
## 36  ( 1 ) " "      " "
## 37  ( 1 ) " "      " "
## 38  ( 1 ) " "      " "
## 39  ( 1 ) " "      " "
## 40  ( 1 ) " "      " "
## 41  ( 1 ) " "      " "
## 42  ( 1 ) " "      " "
## 43  ( 1 ) " "      " "
## 44  ( 1 ) " "      " "
## 45  ( 1 ) " "      "*"
## 46  ( 1 ) " "      "*"
## 47  ( 1 ) " "      "*"
## 48  ( 1 ) " "      "*"
## 49  ( 1 ) " "      "*"
## 50  ( 1 ) " "      "*"
## 51  ( 1 ) " "      "*"
## 52  ( 1 ) " "      "*"
## 53  ( 1 ) " "      "*"
## 54  ( 1 ) " "      "*"
##          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1  ( 1 ) " "      " "      " "
## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      " "
## 20 ( 1 ) " "      " "      " "
## 21 ( 1 ) " "      " "      " "
## 22 ( 1 ) " "      " "      " "

```

```

## 23 ( 1 ) " "      " "
## 24 ( 1 ) " "      " "
## 25 ( 1 ) " "      " "
## 26 ( 1 ) " "      " "
## 27 ( 1 ) " "      " "
## 28 ( 1 ) " "      " "
## 29 ( 1 ) " "      " "
## 30 ( 1 ) " "      " "
## 31 ( 1 ) " "      " "
## 32 ( 1 ) " "      " "
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## 40 ( 1 ) " "      " "
## 41 ( 1 ) " "      " "
## 42 ( 1 ) " "      " "
## 43 ( 1 ) " "      " "
## 44 ( 1 ) " "      " "
## 45 ( 1 ) " "      " "
## 46 ( 1 ) " "      "*" "
## 47 ( 1 ) " "      "*" "
## 48 ( 1 ) " "      "*" "
## 49 ( 1 ) " "      "*" "
## 50 ( 1 ) " "      "*" "
## 51 ( 1 ) " "      "*" "
## 52 ( 1 ) " "      "*" "
## 53 ( 1 ) " "      "*" "
## 54 ( 1 ) " "      "*" "
##          wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1 ( 1 ) " "      " "      " "
## 2 ( 1 ) " "      " "      " "
## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "
## 6 ( 1 ) " "      " "      " "
## 7 ( 1 ) " "      " "      " "
## 8 ( 1 ) " "      " "      " "
## 9 ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) "*" "
## 18 ( 1 ) "*" "
## 19 ( 1 ) "*" "
## 20 ( 1 ) "*" "
## 21 ( 1 ) "*" "

```

```

## 22  ( 1 ) "*"      "*"      " " "
## 23  ( 1 ) "*"      "*"      " " "
## 24  ( 1 ) "*"      "*"      " " "
## 25  ( 1 ) "*"      "*"      " " "
## 26  ( 1 ) "*"      "*"      " " "
## 27  ( 1 ) "*"      "*"      " " "
## 28  ( 1 ) "*"      "*"      " " "
## 29  ( 1 ) "*"      "*"      " " "
## 30  ( 1 ) "*"      "*"      " " "
## 31  ( 1 ) "*"      "*"      " " "
## 32  ( 1 ) "*"      "*"      " " "
## 33  ( 1 ) "*"      "*"      " " "
## 34  ( 1 ) "*"      "*"      " " "
## 35  ( 1 ) "*"      "*"      " " "
## 36  ( 1 ) "*"      "*"      " " "
## 37  ( 1 ) "*"      "*"      " " "
## 38  ( 1 ) "*"      "*"      " " "
## 39  ( 1 ) "*"      "*"      " " "
## 40  ( 1 ) "*"      "*"      " " "
## 41  ( 1 ) "*"      "*"      " " "
## 42  ( 1 ) "*"      "*"      " " "
## 43  ( 1 ) "*"      "*"      " " "
## 44  ( 1 ) "*"      "*"      " " "
## 45  ( 1 ) "*"      "*"      " " "
## 46  ( 1 ) "*"      "*"      " " "
## 47  ( 1 ) "*"      "*"      " " "
## 48  ( 1 ) "*"      "*"      " " "
## 49  ( 1 ) "*"      "*"      " " "
## 50  ( 1 ) "*"      "*"      " " "
## 51  ( 1 ) "*"      "*"      " " "
## 52  ( 1 ) "*"      "*"      " " "
## 53  ( 1 ) "*"      "*"      " " "
## 54  ( 1 ) "*"      "*"      " " "
##          std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie
## 1  ( 1 ) " "       " "       " " " "
## 2  ( 1 ) " "       " "       " " " "
## 3  ( 1 ) " "       " "       " " " "
## 4  ( 1 ) " "       " "       " " " "
## 5  ( 1 ) " "       " "       " " " "
## 6  ( 1 ) " "       " "       " " " "
## 7  ( 1 ) " "       " "       " " " "
## 8  ( 1 ) " "       " "       " " " "
## 9  ( 1 ) " "       " "       " " " "
## 10 ( 1 ) " "       " "       " " " "
## 11 ( 1 ) " "       " "       " " " "
## 12 ( 1 ) " "       " "       " " " "
## 13 ( 1 ) " "       " "       " " " "
## 14 ( 1 ) " "       " "       " " " "
## 15 ( 1 ) " "       " "       " " " "
## 16 ( 1 ) " "       " "       " " " "
## 17 ( 1 ) " "       " "       " " " "
## 18 ( 1 ) " "       " "       " " " "
## 19 ( 1 ) " "       " "       " " " "
## 20 ( 1 ) " "       " "       " " " "

```

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## 21  ( 1 ) " "      "*"      " "      " "
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## 51  ( 1 ) " "      "*"
## 52  ( 1 ) " "      "*"
## 53  ( 1 ) " "      "*"
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##          gmean_ElectronAffinity wtd_gmean_ElectronAffinity
## 1  ( 1 ) " "          " "
## 2  ( 1 ) " "          "*"
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## 4  ( 1 ) " "          "*"
## 5  ( 1 ) " "          "*"
## 6  ( 1 ) " "          "*"
## 7  ( 1 ) " "          "*"
## 8  ( 1 ) " "          "*"
## 9  ( 1 ) " "          "*"

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## 10  ( 1 ) " "      "*"
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## 26  ( 1 ) " "      "*"
## 27  ( 1 ) " "      "*"
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## 30  ( 1 ) " "      "*"
## 31  ( 1 ) " "      "*"
## 32  ( 1 ) " "      "*"
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## 34  ( 1 ) " "      "*"
## 35  ( 1 ) " "      "*"
## 36  ( 1 ) " "      "*"
## 37  ( 1 ) " "      "*"
## 38  ( 1 ) " "      "*"
## 39  ( 1 ) "*"      "*"
## 40  ( 1 ) "*"      "*"
## 41  ( 1 ) "*"      "*"
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## 45  ( 1 ) "*"      "*"
## 46  ( 1 ) "*"      "*"
## 47  ( 1 ) "*"      "*"
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## 49  ( 1 ) "*"      "*"
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## 51  ( 1 ) "*"      "*"
## 52  ( 1 ) "*"      "*"
## 53  ( 1 ) "*"      "*"
## 54  ( 1 ) "*"      "*"
##          entropy_ElectronAffinity wtd_entropy_ElectronAffinity
## 1  ( 1 ) " "      " "
## 2  ( 1 ) " "      " "
## 3  ( 1 ) " "      " "
## 4  ( 1 ) " "      " "
## 5  ( 1 ) " "      " "
## 6  ( 1 ) " "      " "
## 7  ( 1 ) " "      " "
## 8  ( 1 ) " "      " "

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## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
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## 40 ( 1 )   " "
## 41 ( 1 )   " "
## 42 ( 1 )   " "
## 43 ( 1 )   " "
## 44 ( 1 )   " "
## 45 ( 1 )   " "
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## 47 ( 1 )   " "
## 48 ( 1 )   " "
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## 53 ( 1 )   " "
## 54 ( 1 )   " "
##          range_ElectronAffinity wtd_range_ElectronAffinity
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## 2  ( 1 )   " "
## 3  ( 1 )   " "
## 4  ( 1 )   " "
## 5  ( 1 )   " "
## 6  ( 1 )   " "
## 7  ( 1 )   "*"

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## 32 ( 1 ) "*"          " "
## 33 ( 1 ) "*"          " "
## 34 ( 1 ) "*"          " "
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## 52 ( 1 ) "*"          "*"
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## 54 ( 1 ) "*"          "*"
##
##           std_ElectronAffinity wtd_std_ElectronAffinity mean_FusionHeat
## 1  ( 1 ) " "          " "          " "
## 2  ( 1 ) " "          " "          " "
## 3  ( 1 ) " "          " "          " "
## 4  ( 1 ) " "          " "          " "
## 5  ( 1 ) " "          " "          " "
## 6  ( 1 ) " "          " "          " "

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## 21 ( 1 )   "*" 
## 22 ( 1 )   "*" 
## 23 ( 1 )   "*" 
## 24 ( 1 )   "*" 
## 25 ( 1 )   "*" 
## 26 ( 1 )   "*" 
## 27 ( 1 )   "*" 
## 28 ( 1 )   "*" 
## 29 ( 1 )   "*" 
## 30 ( 1 )   "*" 
## 31 ( 1 )   "*" 
## 32 ( 1 )   "*" 
## 33 ( 1 )   "*" 
## 34 ( 1 )   "*" 
## 35 ( 1 )   "*" 
## 36 ( 1 )   "*" 
## 37 ( 1 )   "*" 
## 38 ( 1 )   "*" 
## 39 ( 1 )   "*" 
## 40 ( 1 )   "*" 
## 41 ( 1 )   "*" 
## 42 ( 1 )   "*" 
## 43 ( 1 )   "*" 
## 44 ( 1 )   "*" 
## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   "*" 
## 48 ( 1 )   "*" 
## 49 ( 1 )   "*" 
## 50 ( 1 )   "*" 
## 51 ( 1 )   "*" 
## 52 ( 1 )   "*" 
## 53 ( 1 )   "*" 
## 54 ( 1 )   "*"
##          wtd_mean_FusionHeat gmean_FusionHeat wtd_gmean_FusionHeat
## 1  ( 1 )   " "           " "           " "
## 2  ( 1 )   " "           " "           " "
## 3  ( 1 )   " "           " "           " "
## 4  ( 1 )   " "           " "           " "
## 5  ( 1 )   " "           " "           " "

```

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## 11 ( 1 )   " "
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## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
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## 30 ( 1 )   "*"
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## 32 ( 1 )   "*"
## 33 ( 1 )   "*"
## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
##          entropy_FusionHeat wtd_entropy_FusionHeat range_FusionHeat
## 1  ( 1 )   " "           " "           " "
## 2  ( 1 )   " "           " "           " "
## 3  ( 1 )   " "           " "           " "
## 4  ( 1 )   " "

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## 5  ( 1 )   " "
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## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   "*"
## 25 ( 1 )   "*"
## 26 ( 1 )   "*"
## 27 ( 1 )   "*"
## 28 ( 1 )   "*"
## 29 ( 1 )   "*"
## 30 ( 1 )   "*"
## 31 ( 1 )   "*"
## 32 ( 1 )   "*"
## 33 ( 1 )   "*"
## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
##          wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
## 1  ( 1 )   " "           " "           " "
## 2  ( 1 )   " "           " "           " "
## 3  ( 1 )   " "           " "           " "

```

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## 4  ( 1 )   " "
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## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   "*"
## 27 ( 1 )   "*"
## 28 ( 1 )   "*"
## 29 ( 1 )   "*"
## 30 ( 1 )   "*"
## 31 ( 1 )   "*"
## 32 ( 1 )   "*"
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## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
##               mean_ThermalConductivity wtd_mean_ThermalConductivity
## 1  ( 1 )   " "
## 2  ( 1 )   " "

```

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## 3  ( 1 )   " "
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## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
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## 13 ( 1 )   "*"
## 14 ( 1 )   "*"
## 15 ( 1 )   "*"
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## 17 ( 1 )   "*"
## 18 ( 1 )   "*"
## 19 ( 1 )   "*"
## 20 ( 1 )   "*"
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## 22 ( 1 )   "*"
## 23 ( 1 )   "*"
## 24 ( 1 )   "*"
## 25 ( 1 )   "*"
## 26 ( 1 )   "*"
## 27 ( 1 )   "*"
## 28 ( 1 )   "*"
## 29 ( 1 )   "*"
## 30 ( 1 )   "*"
## 31 ( 1 )   "*"
## 32 ( 1 )   "*"
## 33 ( 1 )   "*"
## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
##          gmean_ThermalConductivity wtd_gmean_ThermalConductivity
## 1  ( 1 )   " "

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## 2  ( 1 )   " "
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## 4  ( 1 )   " "
## 5  ( 1 )   " "
## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
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## 23 ( 1 )   "*" 
## 24 ( 1 )   "*" 
## 25 ( 1 )   "*" 
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## 27 ( 1 )   "*" 
## 28 ( 1 )   "*" 
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## 32 ( 1 )   "*" 
## 33 ( 1 )   "*" 
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## 37 ( 1 )   "*" 
## 38 ( 1 )   "*" 
## 39 ( 1 )   "*" 
## 40 ( 1 )   "*" 
## 41 ( 1 )   "*" 
## 42 ( 1 )   "*" 
## 43 ( 1 )   "*" 
## 44 ( 1 )   "*" 
## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   "*" 
## 48 ( 1 )   "*" 
## 49 ( 1 )   "*" 
## 50 ( 1 )   "*" 
## 51 ( 1 )   "*" 
## 52 ( 1 )   "*" 
## 53 ( 1 )   "*" 
## 54 ( 1 )   "*"
##          entropy_ThermalConductivity wtd_entropy_ThermalConductivity

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## 4 ( 1 ) " "
## 5 ( 1 ) " "
## 6 ( 1 ) " "
## 7 ( 1 ) " "
## 8 ( 1 ) " "
## 9 ( 1 ) " "
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## 22 ( 1 ) " "
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## 24 ( 1 ) " "
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## 44 ( 1 ) "*"
## 45 ( 1 ) "*"
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## 47 ( 1 ) "*"
## 48 ( 1 ) "*"
## 49 ( 1 ) "*"
## 50 ( 1 ) "*"
## 51 ( 1 ) "*"
## 52 ( 1 ) "*"
## 53 ( 1 ) "*"
## 54 ( 1 ) "*"

```

```

##          range_ThermalConductivity wtd_range_ThermalConductivity
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## 3      ( 1 )   " "                  " "
## 4      ( 1 )   " "                  " "
## 5      ( 1 )   " "                  " "
## 6      ( 1 )   " "                  " "
## 7      ( 1 )   " "                  " "
## 8      ( 1 )   " "                  " "
## 9      ( 1 )   " "                  " "
## 10     ( 1 )   " "                  " "
## 11     ( 1 )   " "                  " "
## 12     ( 1 )   " "                  " "
## 13     ( 1 )   " "                  " "
## 14     ( 1 )   " "                  " "
## 15     ( 1 )   " "                  " "
## 16     ( 1 )   " "                  " "
## 17     ( 1 )   " "                  " "
## 18     ( 1 )   " "                  " "
## 19     ( 1 )   " "                  " "
## 20     ( 1 )   " "                  " "
## 21     ( 1 )   " "                  " "
## 22     ( 1 )   " "                  "*" "
## 23     ( 1 )   " "                  "*" "
## 24     ( 1 )   " "                  "*" "
## 25     ( 1 )   " "                  "*" "
## 26     ( 1 )   " "                  "*" "
## 27     ( 1 )   " "                  "*" "
## 28     ( 1 )   " "                  "*" "
## 29     ( 1 )   " "                  "*" "
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## 31     ( 1 )   " "                  "*" "
## 32     ( 1 )   " "                  "*" "
## 33     ( 1 )   " "                  "*" "
## 34     ( 1 )   " "                  "*" "
## 35     ( 1 )   " "                  "*" "
## 36     ( 1 )   " "                  "*" "
## 37     ( 1 )   "*"                 "*" "
## 38     ( 1 )   "*"                 "*" "
## 39     ( 1 )   "*"                 "*" "
## 40     ( 1 )   "*"                 "*" "
## 41     ( 1 )   "*"                 "*" "
## 42     ( 1 )   "*"                 "*" "
## 43     ( 1 )   "*"                 "*" "
## 44     ( 1 )   "*"                 "*" "
## 45     ( 1 )   "*"                 "*" "
## 46     ( 1 )   "*"                 "*" "
## 47     ( 1 )   "*"                 "*" "
## 48     ( 1 )   "*"                 "*" "
## 49     ( 1 )   "*"                 "*" "
## 50     ( 1 )   "*"                 "*" "
## 51     ( 1 )   "*"                 "*" "
## 52     ( 1 )   "*"                 "*" "
## 53     ( 1 )   "*"                 "*" "

```

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## 54  ( 1 ) "*"          "*"
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## 6  ( 1 ) " "          "*"          " "
## 7  ( 1 ) " "          "*"          " "
## 8  ( 1 ) " "          "*"          " "
## 9  ( 1 ) " "          "*"          " "
## 10 ( 1 ) " "          "*"          " "
## 11 ( 1 ) " "          "*"          " "
## 12 ( 1 ) " "          "*"          " "
## 13 ( 1 ) " "          "*"          " "
## 14 ( 1 ) " "          "*"          " "
## 15 ( 1 ) " "          "*"          " "
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## 17 ( 1 ) " "          "*"          " "
## 18 ( 1 ) " "          "*"          " "
## 19 ( 1 ) " "          "*"          " "
## 20 ( 1 ) " "          "*"          " "
## 21 ( 1 ) " "          "*"          " "
## 22 ( 1 ) " "          "*"          " "
## 23 ( 1 ) " "          "*"          " "
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## 26 ( 1 ) " "          "*"          " "
## 27 ( 1 ) " "          "*"          " "
## 28 ( 1 ) " "          "*"          " "
## 29 ( 1 ) " "          "*"          " "
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## 31 ( 1 ) " "          "*"          " "
## 32 ( 1 ) " "          "*"          " "
## 33 ( 1 ) " "          "*"          " "
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## 40 ( 1 ) "*"          "*"          " "
## 41 ( 1 ) "*"          "*"          " "
## 42 ( 1 ) "*"          "*"          " "
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## 45 ( 1 ) "*"          "*"          " "
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## 48 ( 1 ) "*"          "*"          " "
## 49 ( 1 ) "*"          "*"          " "
## 50 ( 1 ) "*"          "*"          " "
## 51 ( 1 ) "*"          "*"          " "
## 52 ( 1 ) "*"          "*"          " "

```

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## 53  ( 1 ) "*"          "*"          " "
## 54  ( 1 ) "*"          "*"          " "
##           wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
## 1  ( 1 ) " "           " "           " "           " "
## 2  ( 1 ) " "           " "           " "           " "
## 3  ( 1 ) " "           " "           " "           " "
## 4  ( 1 ) " "           " "           " "           " "
## 5  ( 1 ) " "           " "           " "           " "
## 6  ( 1 ) " "           " "           " "           " "
## 7  ( 1 ) " "           " "           " "           " "
## 8  ( 1 ) " "           " "           " "           " "
## 9  ( 1 ) " "           " "           " "           " "
## 10 ( 1 ) " "           " "           " "           " "
## 11 ( 1 ) " "           " "           " "           " "
## 12 ( 1 ) " "           " "           " "           " "
## 13 ( 1 ) " "           " "           " "           " "
## 14 ( 1 ) " "           " "           " "           " "
## 15 ( 1 ) " "           " "           " "           " "
## 16 ( 1 ) " "           " "           " "           " "
## 17 ( 1 ) " "           " "           " "           " "
## 18 ( 1 ) " "           " "           " "           " "
## 19 ( 1 ) " "           " "           " "           " "
## 20 ( 1 ) " "           " "           " "           " "
## 21 ( 1 ) " "           " "           " "           " "
## 22 ( 1 ) " "           " "           " "           " "
## 23 ( 1 ) " "           " "           " "           " "
## 24 ( 1 ) " "           " "           " "           " "
## 25 ( 1 ) "*"          " "           " "           " "
## 26 ( 1 ) "*"          " "           " "           " "
## 27 ( 1 ) "*"          " "           " "           " "
## 28 ( 1 ) "*"          " "           " "           " "
## 29 ( 1 ) "*"          " "           " "           " "
## 30 ( 1 ) "*"          " "           " "           " "
## 31 ( 1 ) "*"          " "           " "           " "
## 32 ( 1 ) "*"          " "           " "           " "
## 33 ( 1 ) "*"          " "           " "           " "
## 34 ( 1 ) "*"          " "           " "           " "
## 35 ( 1 ) "*"          " "           " "           " "
## 36 ( 1 ) "*"          " "           " "           " "
## 37 ( 1 ) "*"          " "           " "           " "
## 38 ( 1 ) "*"          " "           " "           " "
## 39 ( 1 ) "*"          " "           " "           " "
## 40 ( 1 ) "*"          " "           " "           " "
## 41 ( 1 ) "*"          " "           " "           " "
## 42 ( 1 ) "*"          " "           " "           " "
## 43 ( 1 ) "*"          " "           " "           " "
## 44 ( 1 ) "*"          " "           " "           " "
## 45 ( 1 ) "*"          " "           " "           " "
## 46 ( 1 ) "*"          " "           " "           " "
## 47 ( 1 ) "*"          " "           " "           " "
## 48 ( 1 ) "*"          " "           " "           " "
## 49 ( 1 ) "*"          " "           " "           "*"
## 50 ( 1 ) "*"          " "           " "           "*"
## 51 ( 1 ) "*"          " "           " "           "*"

```

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## 52  ( 1 ) "*"          " "          " "          "*"
## 53  ( 1 ) "*"          " "          " "          "*"
## 54  ( 1 ) "*"          " "          " "          "*"
##           wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
## 1  ( 1 ) " "          " "          " "          " "
## 2  ( 1 ) " "          " "          " "          " "
## 3  ( 1 ) " "          " "          " "          " "
## 4  ( 1 ) " "          " "          " "          " "
## 5  ( 1 ) " "          " "          " "          " "
## 6  ( 1 ) " "          " "          " "          " "
## 7  ( 1 ) " "          " "          " "          " "
## 8  ( 1 ) " "          " "          " "          " "
## 9  ( 1 ) " "          " "          " "          " "
## 10 ( 1 ) " "          " "          " "          " "
## 11 ( 1 ) " "          " "          " "          " "
## 12 ( 1 ) " "          " "          " "          " "
## 13 ( 1 ) " "          " "          " "          " "
## 14 ( 1 ) " "          " "          " "          " "
## 15 ( 1 ) " "          " "          " "          " "
## 16 ( 1 ) "*"          " "          " "          " "
## 17 ( 1 ) "*"          " "          " "          " "
## 18 ( 1 ) "*"          " "          " "          " "
## 19 ( 1 ) "*"          " "          " "          " "
## 20 ( 1 ) "*"          " "          " "          " "
## 21 ( 1 ) "*"          " "          " "          " "
## 22 ( 1 ) "*"          " "          " "          " "
## 23 ( 1 ) "*"          " "          " "          " "
## 24 ( 1 ) "*"          " "          " "          " "
## 25 ( 1 ) "*"          " "          " "          " "
## 26 ( 1 ) "*"          " "          " "          " "
## 27 ( 1 ) "*"          " "          " "          " "
## 28 ( 1 ) "*"          " "          " "          " "
## 29 ( 1 ) "*"          " "          " "          " "
## 30 ( 1 ) "*"          " "          " "          " "
## 31 ( 1 ) "*"          " "          " "          " "
## 32 ( 1 ) "*"          " "          " "          " "
## 33 ( 1 ) "*"          "*"          " "          " "
## 34 ( 1 ) "*"          "*"          " "          " "
## 35 ( 1 ) "*"          "*"          " "          " "
## 36 ( 1 ) "*"          "*"          " "          " "
## 37 ( 1 ) "*"          "*"          " "          " "
## 38 ( 1 ) "*"          "*"          " "          " "
## 39 ( 1 ) "*"          "*"          " "          " "
## 40 ( 1 ) "*"          "*"          " "          " "
## 41 ( 1 ) "*"          "*"          " "          " "
## 42 ( 1 ) "*"          "*"          " "          " "
## 43 ( 1 ) "*"          "*"          " "          " "
## 44 ( 1 ) "*"          "*"          " "          " "
## 45 ( 1 ) "*"          "*"          " "          " "
## 46 ( 1 ) "*"          "*"          " "          " "
## 47 ( 1 ) "*"          "*"          " "          " "
## 48 ( 1 ) "*"          "*"          " "          " "
## 49 ( 1 ) "*"          "*"          " "          " "
## 50 ( 1 ) "*"          "*"          " "          " "

```

```

## 51  ( 1 ) "*"          "*"          " "          " "
## 52  ( 1 ) "*"          "*"          " "          " "
## 53  ( 1 ) "*"          "*"          " "          " "
## 54  ( 1 ) "*"          "*"          " "          " "
##           wtd_std_Valence
## 1  ( 1 ) " "
## 2  ( 1 ) " "
## 3  ( 1 ) " "
## 4  ( 1 ) "*"
## 5  ( 1 ) "*"
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## 46 ( 1 ) "*"
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```

```

## 50  ( 1 ) "*"
## 51  ( 1 ) "*"
## 52  ( 1 ) "*"
## 53  ( 1 ) "*"
## 54  ( 1 ) "*"

linear_backward_trans$results

##    nvmax      RMSE   Rsquared      MAE     RMSESD   RsquaredSD     MAESD
## 1      1 25.93167 0.4216497 20.26440 2.8621566 0.128255182 2.5314159
## 2      2 23.89115 0.5127856 19.00127 1.2119880 0.047127514 1.2788874
## 3      3 22.89275 0.5528923 18.16486 0.9449030 0.036151299 0.9051762
## 4      4 22.38400 0.5724783 17.68889 1.0013055 0.036760940 0.9296192
## 5      5 21.79328 0.5949606 17.18128 0.7535117 0.028085320 0.6532132
## 6      6 21.34132 0.6116654 16.76130 0.6816226 0.025303765 0.5393792
## 7      7 20.99817 0.6240711 16.48582 0.5940483 0.023527614 0.4811235
## 8      8 20.72510 0.6338308 16.26058 0.5640843 0.021510193 0.4890920
## 9      9 20.55009 0.6400560 16.07480 0.4944134 0.018117474 0.4499438
## 10    10 20.33840 0.6474575 15.86069 0.4709145 0.017873406 0.4140876
## 11    11 20.24113 0.6508179 15.76336 0.4877613 0.017800963 0.4502045
## 12    12 19.95947 0.6605102 15.51677 0.3761339 0.014221493 0.3354929
## 13    13 19.72788 0.6683591 15.30558 0.2741525 0.011263635 0.3052952
## 14    14 19.60961 0.6723260 15.21278 0.2988178 0.011550238 0.3113576
## 15    15 19.42225 0.6785477 14.98207 0.2904438 0.010817455 0.2922397
## 16    16 19.24752 0.6842853 14.80091 0.2367340 0.009819959 0.2531044
## 17    17 19.13369 0.6879815 14.67076 0.2630604 0.010885418 0.2740114
## 18    18 19.04561 0.6908622 14.58529 0.2600940 0.010707643 0.2709114
## 19    19 18.98245 0.6928947 14.51707 0.2851538 0.011428053 0.2852518
## 20    20 18.92178 0.6948447 14.46380 0.3094358 0.011900296 0.3231981
## 21    21 18.86342 0.6967252 14.40779 0.3077167 0.011792298 0.3172803
## 22    22 18.80934 0.6984603 14.36724 0.3002447 0.011459479 0.3059536
## 23    23 18.77923 0.6994270 14.34538 0.3036920 0.011414153 0.2969871
## 24    24 18.75683 0.7001369 14.32101 0.3071288 0.011574132 0.2826561
## 25    25 18.70623 0.7017535 14.26497 0.2897658 0.010892310 0.2546601
## 26    26 18.66978 0.7029266 14.23470 0.2792719 0.010428505 0.2222065
## 27    27 18.63039 0.7041621 14.21922 0.2812975 0.010475345 0.2166586
## 28    28 18.61366 0.7047013 14.20279 0.2814343 0.010776489 0.2054524
## 29    29 18.54500 0.7068687 14.15217 0.2680509 0.010192067 0.2177878
## 30    30 18.49846 0.7083324 14.11324 0.2944237 0.011101081 0.2290138
## 31    31 18.47170 0.7091882 14.08258 0.3025964 0.010982461 0.2350609
## 32    32 18.41317 0.7110169 14.04578 0.3018380 0.010651660 0.2414300
## 33    33 18.37703 0.7121614 14.00938 0.3062766 0.010515696 0.2518999
## 34    34 18.33858 0.7133556 13.98462 0.3028108 0.010783612 0.2265766
## 35    35 18.28383 0.7150380 13.94379 0.3224155 0.011244108 0.2335227
## 36    36 18.25946 0.7157991 13.93614 0.3225595 0.011039020 0.2470838
## 37    37 18.23396 0.7165971 13.90612 0.3274141 0.010895561 0.2386135
## 38    38 18.21061 0.7173206 13.86959 0.3286426 0.011088908 0.2204510
## 39    39 18.19327 0.7178667 13.85096 0.3352543 0.011237901 0.2239688
## 40    40 18.17415 0.7184623 13.83430 0.3426592 0.011350225 0.2287565
## 41    41 18.14159 0.7194801 13.81037 0.3493897 0.011251742 0.2332754
## 42    42 18.11590 0.7202753 13.79603 0.3492848 0.011156076 0.2238414
## 43    43 18.07977 0.7213807 13.76813 0.3385752 0.010932280 0.2255438
## 44    44 18.06154 0.7219491 13.73699 0.3374202 0.010851458 0.2196077
## 45    45 18.04649 0.7224167 13.72061 0.3274280 0.010687990 0.2135746

```

```

## 46 46 18.03294 0.7228395 13.71307 0.3342054 0.010780768 0.2208750
## 47 47 18.01975 0.7232512 13.68969 0.3389380 0.010962015 0.2231504
## 48 48 17.99780 0.7239226 13.67213 0.3372902 0.010861069 0.2232909
## 49 49 17.96699 0.7248676 13.64376 0.3408686 0.010890739 0.2303357
## 50 50 17.94723 0.7254734 13.63032 0.3422120 0.010745070 0.2382962
## 51 51 17.94353 0.7255852 13.64028 0.3376645 0.010793743 0.2396358
## 52 52 17.91425 0.7264752 13.61955 0.3409623 0.010816609 0.2425700
## 53 53 17.90469 0.7267698 13.60985 0.3480189 0.010894774 0.2384678
## 54 54 17.88182 0.7274711 13.60426 0.3415999 0.010731082 0.2291324
## 55 55 17.93503 0.7259626 13.59165 0.4351080 0.014420056 0.2393383
## 56 56 18.22593 0.7181701 13.58733 1.2932809 0.037639732 0.2640444
## 57 57 18.37664 0.7145287 13.57611 1.7859261 0.049667193 0.2722000
## 58 58 18.33760 0.7155038 13.57015 1.6934525 0.047518953 0.2753117
## 59 59 18.38138 0.7145149 13.55747 1.8510725 0.051217909 0.2670961
## 60 60 18.39897 0.7141065 13.55060 1.9122507 0.052663572 0.2656385
## 61 61 18.41660 0.7137462 13.53777 1.9846906 0.054290080 0.2698884
## 62 62 18.37846 0.7147315 13.52132 1.9008250 0.052309342 0.2765713
## 63 63 18.24610 0.7179513 13.51777 1.5122438 0.043037230 0.2688104
## 64 64 18.27049 0.7173835 13.51409 1.6056005 0.045318603 0.2767186
## 65 65 18.26119 0.7176874 13.50461 1.6168971 0.045587636 0.2761052
## 66 66 18.27874 0.7172995 13.49656 1.6930704 0.047450624 0.2748862
## 67 67 18.14775 0.7205230 13.49408 1.2771886 0.037200659 0.2606376
## 68 68 18.07834 0.7223309 13.48666 1.0743944 0.031952720 0.2591624
## 69 69 18.08631 0.7221159 13.48678 1.0998103 0.032637758 0.2586231
## 70 70 18.09918 0.7217898 13.48146 1.1465937 0.033853671 0.2568815
## 71 71 18.10489 0.7216486 13.47993 1.1687574 0.034432656 0.2565617
## 72 72 18.14546 0.7206285 13.47603 1.2993972 0.037739500 0.2576732
## 73 73 18.11405 0.7214425 13.47188 1.2130019 0.035540957 0.2600231
## 74 74 18.09353 0.7219649 13.47135 1.1465273 0.033832983 0.2599225
## 75 75 18.06745 0.7226503 13.47075 1.0699564 0.031837248 0.2593106
## 76 76 18.07354 0.7224963 13.47077 1.0878654 0.032288960 0.2588139
## 77 77 18.06497 0.7227212 13.47071 1.0644665 0.031681667 0.2589973
## 78 78 18.05469 0.7229865 13.47060 1.0301944 0.030790304 0.2582255
## 79 79 18.05892 0.7228750 13.47098 1.0417478 0.031088229 0.2582815
## 80 80 18.06192 0.7227953 13.47116 1.0495913 0.031290460 0.2589526
## 81 81 18.06344 0.7227549 13.47126 1.0536750 0.031395839 0.2587849

```

From the above results, we can see how backward selection works and the corresponding errors to the number of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_backward_trans, linear_backward_trans$results$nvmax, "Number of Variables")
```

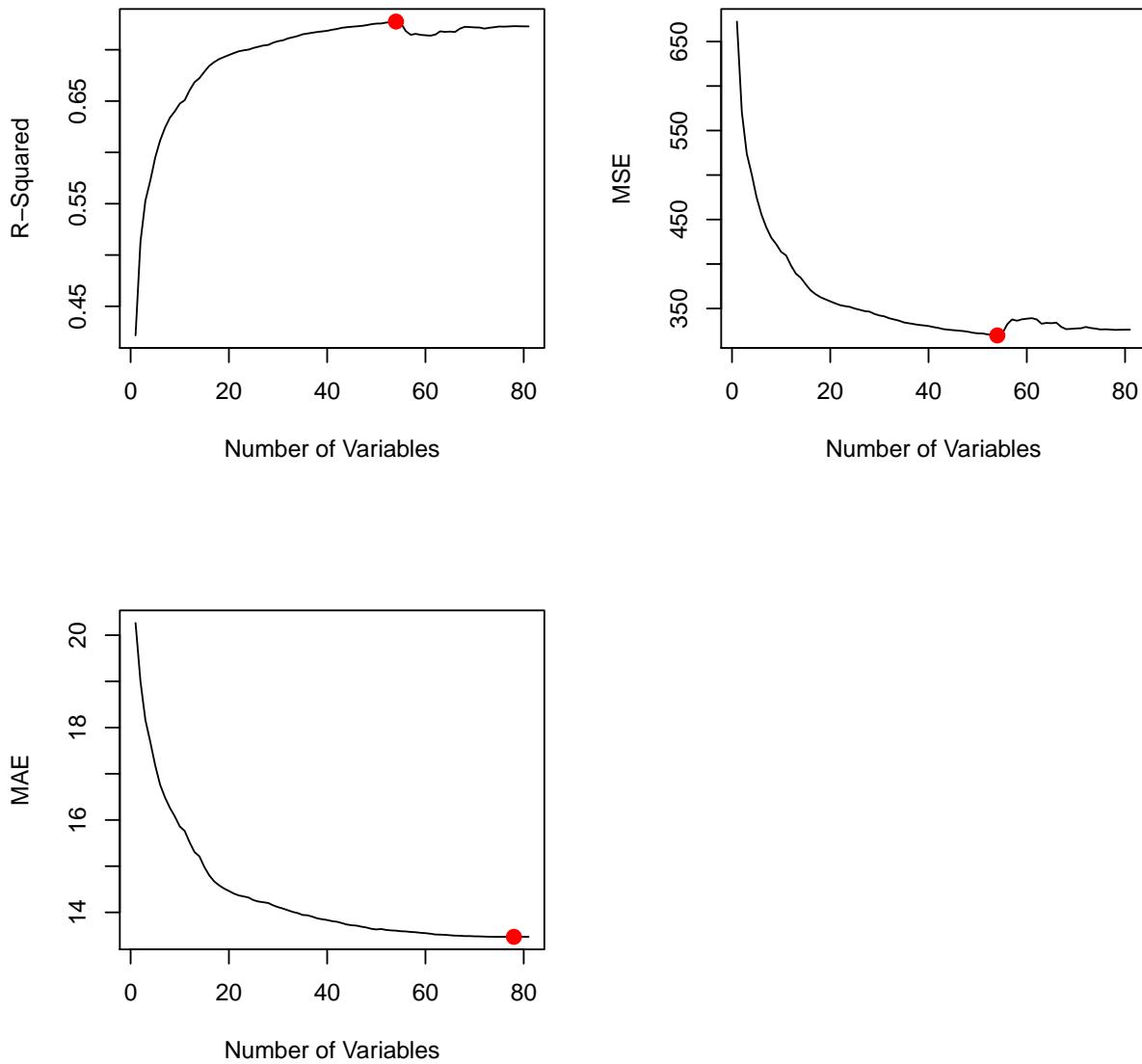


Figure 67: R-Squared, MSE, and MAE for Backward Selection Trans

```
linear_backward_trans$bestTune
```

```
##      nvmax
## 54      54
```

```
coef(linear_backward_trans$finalModel, linear_backward_trans$bestTune$nvmax)
```

```
##                               (Intercept)          wtd_mean_atomic_mass
##                               34.444109                      9.365299
## wtd_gmean_atomic_mass          wtd_entropy_atomic_mass
```

```

##          -11.752310         9.386529
## range_atomic_mass      8.946642      wtd_std_atomic_mass      -5.058029
##          entropy_fie      -30.711517     wtd_entropy_fie      13.340745
##          range_fie       19.803934      wtd_range_fie       6.903149
##          std_fie        -20.290814     mean_atomic_radius    15.600660
##          wtd_mean_atomic_radius 10.449693   gmean_atomic_radius  -24.187840
##          range_atomic_radius 18.158619   wtd_range_atomic_radius -4.492265
##          std_atomic_radius -16.220715   wtd_gmean_Density     9.377910
##          wtd_entropy_Density -8.536552   range_Density      -5.872693
##          std_Density       7.596935      wtd_std_Density      -5.112605
##          wtd_mean_ElectronAffinity 15.470910   gmean_ElectronAffinity 4.555943
##          wtd_gmean_ElectronAffinity -16.678416   wtd_entropy_ElectronAffinity -7.758636
##          range_ElectronAffinity -26.339064   wtd_range_ElectronAffinity -4.770660
##          std_ElectronAffinity  27.631871   wtd_std_ElectronAffinity -9.338356
##          mean_FusionHeat     -18.444724   wtd_mean_FusionHeat    17.304183
##          gmean_FusionHeat    20.598024   wtd_gmean_FusionHeat   -15.120797
##          entropy_FusionHeat -15.406352   wtd_entropy_FusionHeat 11.857945
##          range_FusionHeat    -15.601722   wtd_range_FusionHeat   5.256458
##          std_FusionHeat      12.759175   wtd_std_FusionHeat    -3.684415
##          mean_ThermalConductivity -9.022749   wtd_mean_ThermalConductivity 20.458649
##          gmean_ThermalConductivity -8.504769   wtd_gmean_ThermalConductivity -13.949509
##          entropy_ThermalConductivity 9.365643   wtd_entropy_ThermalConductivity 4.755024
##          range_ThermalConductivity -19.212678   wtd_range_ThermalConductivity -9.689626
##          std_ThermalConductivity 24.684274   wtd_std_ThermalConductivity 9.670127
##          wtd_mean_Valence    -7.275137   entropy_Valence      37.845794
##          wtd_entropy_Valence -17.905937   range_Valence       7.735316
##          wtd_std_Valence     -7.762618

```

```

getTrainPerf(linear_backward_trans)

##   TrainRMSE TrainRsquared TrainMAE      method
## 1  17.88182     0.7274711 13.60426  leapBackward

```

From the above metrics, it can be seen that based on R-Squared and MSE, the best model is the model with 54 variables, however, MAE choose a model with more variables. By using the feature from caret package, we can decide that the best model is the model with 54 variables. The list of 54 variables is provided above. The R-Squared for this model is 0.7274711 with Train MSE is 319.69. Those metrics are slightly lower than the original linear regression, however, this model decrease the number of variables from 81 to only 54, which is good in term of model complexity.

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_backward_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

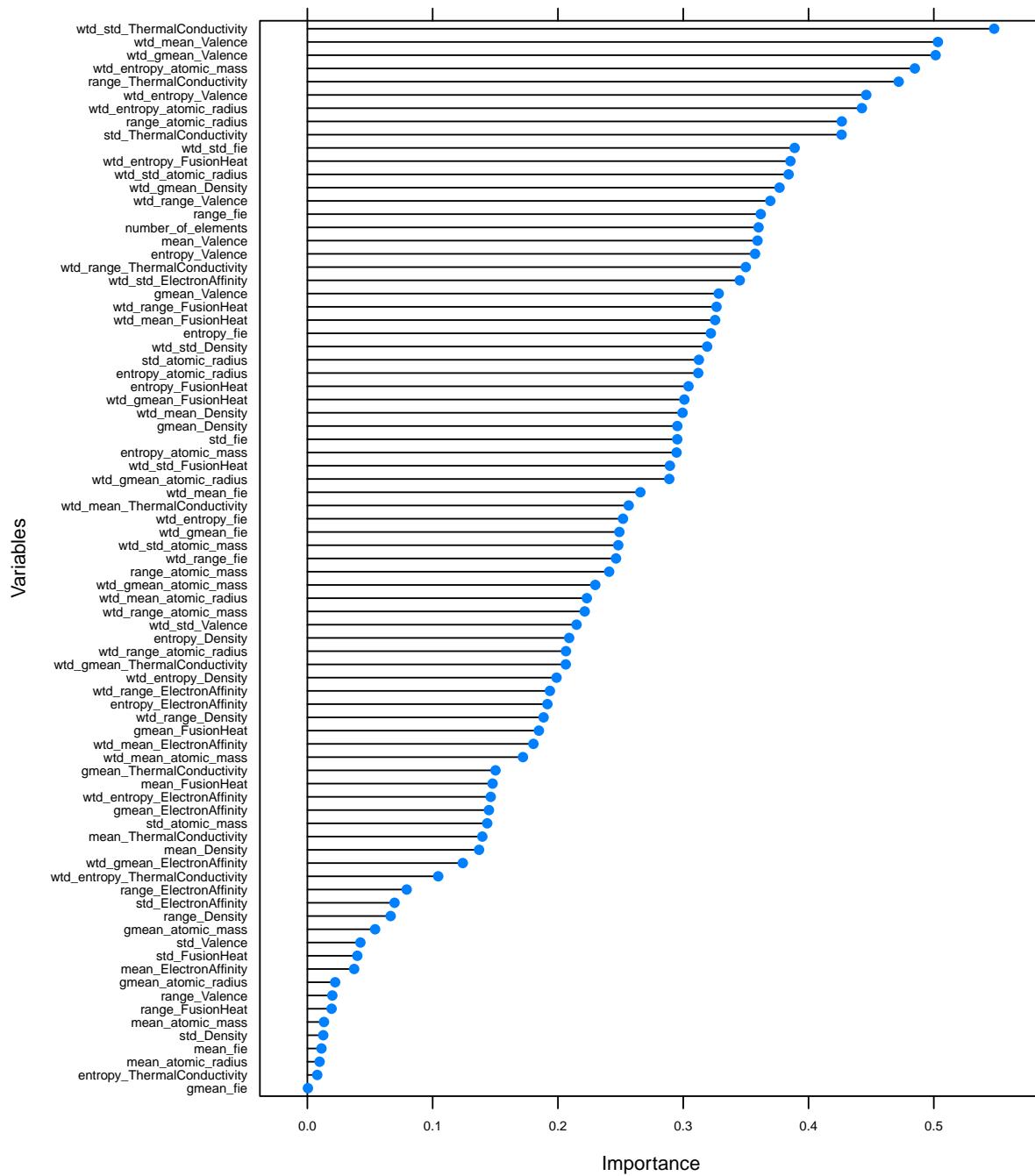


Figure 68: Variable Importance for Backward Selection Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.5 Linear Regression with Forward Selection

In this sub section, we will perform the forward selection and in the next subsection, we will perform stepwise selection.

```
set.seed(seed)

# Linear Regression with Forward Selection
linear_forward_trans <- train(critical_temp ~., data = train.data,
                               method = "leapForward",
                               tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
                               trControl = control,
                               preProc = c("center", "scale", "BoxCox")
)
summary(linear_forward_trans)

## Subset selection object
## 81 Variables  (and intercept)
##                                     Forced in    Forced out
## number_of_elements                 FALSE       FALSE
## mean_atomic_mass                  FALSE       FALSE
## wtd_mean_atomic_mass              FALSE       FALSE
## gmean_atomic_mass                 FALSE       FALSE
## wtd_gmean_atomic_mass             FALSE       FALSE
## entropy_atomic_mass               FALSE       FALSE
## wtd_entropy_atomic_mass           FALSE       FALSE
## range_atomic_mass                 FALSE       FALSE
## wtd_range_atomic_mass              FALSE       FALSE
## std_atomic_mass                  FALSE       FALSE
## wtd_std_atomic_mass               FALSE       FALSE
## mean_fie                         FALSE       FALSE
## wtd_mean_fie                     FALSE       FALSE
## gmean_fie                        FALSE       FALSE
## wtd_gmean_fie                    FALSE       FALSE
## entropy_fie                      FALSE       FALSE
## wtd_entropy_fie                  FALSE       FALSE
## range_fie                        FALSE       FALSE
## wtd_range_fie                    FALSE       FALSE
## std_fie                          FALSE       FALSE
## wtd_std_fie                      FALSE       FALSE
## mean_atomic_radius                FALSE       FALSE
## wtd_mean_atomic_radius            FALSE       FALSE
## gmean_atomic_radius               FALSE       FALSE
## wtd_gmean_atomic_radius           FALSE       FALSE
## entropy_atomic_radius             FALSE       FALSE
## wtd_entropy_atomic_radius         FALSE       FALSE
## range_atomic_radius               FALSE       FALSE
## wtd_range_atomic_radius           FALSE       FALSE
## std_atomic_radius                 FALSE       FALSE
## wtd_std_atomic_radius             FALSE       FALSE
## mean_Density                      FALSE       FALSE
## wtd_mean_Density                  FALSE       FALSE
## gmean_Density                     FALSE       FALSE
## wtd_gmean_Density                 FALSE       FALSE
```

```

## entropy_Density FALSE FALSE
## wtd_entropy_Density FALSE FALSE
## range_Density FALSE FALSE
## wtd_range_Density FALSE FALSE
## std_Density FALSE FALSE
## wtd_std_Density FALSE FALSE
## mean_ElectronAffinity FALSE FALSE
## wtd_mean_ElectronAffinity FALSE FALSE
## gmean_ElectronAffinity FALSE FALSE
## wtd_gmean_ElectronAffinity FALSE FALSE
## entropy_ElectronAffinity FALSE FALSE
## wtd_entropy_ElectronAffinity FALSE FALSE
## range_ElectronAffinity FALSE FALSE
## wtd_range_ElectronAffinity FALSE FALSE
## std_ElectronAffinity FALSE FALSE
## wtd_std_ElectronAffinity FALSE FALSE
## mean_FusionHeat FALSE FALSE
## wtd_mean_FusionHeat FALSE FALSE
## gmean_FusionHeat FALSE FALSE
## wtd_gmean_FusionHeat FALSE FALSE
## entropy_FusionHeat FALSE FALSE
## wtd_entropy_FusionHeat FALSE FALSE
## range_FusionHeat FALSE FALSE
## wtd_range_FusionHeat FALSE FALSE
## std_FusionHeat FALSE FALSE
## wtd_std_FusionHeat FALSE FALSE
## mean_ThermalConductivity FALSE FALSE
## wtd_mean_ThermalConductivity FALSE FALSE
## gmean_ThermalConductivity FALSE FALSE
## wtd_gmean_ThermalConductivity FALSE FALSE
## entropy_ThermalConductivity FALSE FALSE
## wtd_entropy_ThermalConductivity FALSE FALSE
## range_ThermalConductivity FALSE FALSE
## wtd_range_ThermalConductivity FALSE FALSE
## std_ThermalConductivity FALSE FALSE
## wtd_std_ThermalConductivity FALSE FALSE
## mean_Valence FALSE FALSE
## wtd_mean_Valence FALSE FALSE
## gmean_Valence FALSE FALSE
## wtd_gmean_Valence FALSE FALSE
## entropy_Valence FALSE FALSE
## wtd_entropy_Valence FALSE FALSE
## range_Valence FALSE FALSE
## wtd_range_Valence FALSE FALSE
## std_Valence FALSE FALSE
## wtd_std_Valence FALSE FALSE

## 1 subsets of each size up to 80
## Selection Algorithm: forward
##      number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1  ( 1 )   "   "           "   "           "   "
## 2  ( 1 )   "   "           "   "           "   "
## 3  ( 1 )   "   "           "   "           "   "
## 4  ( 1 )   "   "           "   "           "   "
## 5  ( 1 )   "   "           "   "           "   "

```

```

## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   " "
## 32 ( 1 )   " "
## 33 ( 1 )   " "
## 34 ( 1 )   " "
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 60  ( 1 ) "*"      "*"      " "
## 61  ( 1 ) "*"      "*"      " "
## 62  ( 1 ) "*"      "*"      " "
## 63  ( 1 ) "*"      "*"      "*"
## 64  ( 1 ) "*"      "*"      "*"
## 65  ( 1 ) "*"      "*"      "*"
## 66  ( 1 ) "*"      "*"      "*"
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## 69  ( 1 ) "*"      "*"      "*"
## 70  ( 1 ) "*"      "*"      "*"
## 71  ( 1 ) "*"      "*"      "*"
## 72  ( 1 ) "*"      "*"      "*"
## 73  ( 1 ) "*"      "*"      "*"
## 74  ( 1 ) "*"      "*"      "*"
## 75  ( 1 ) "*"      "*"      "*"
## 76  ( 1 ) "*"      "*"      "*"
## 77  ( 1 ) "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"
## 79  ( 1 ) "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"
##          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1  ( 1 ) " "      " "      " "
## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      "*"
## 20 ( 1 ) " "      " "      "*"
## 21 ( 1 ) " "      " "      "*"
## 22 ( 1 ) " "      " "      "*"
## 23 ( 1 ) " "      " "      "*"
## 24 ( 1 ) " "      " "      "*"
## 25 ( 1 ) " "      " "      "*"
## 26 ( 1 ) " "      " "      "*"
## 27 ( 1 ) " "      " "      "*"
## 28 ( 1 ) " "      " "      "*"
## 29 ( 1 ) " "      " "      "*"
## 30 ( 1 ) " "      " "      "*"
## 31 ( 1 ) " "      " "      "*"
## 32 ( 1 ) " "      " "      "*"

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## 33 ( 1 ) " "      " "      "*"
## 34 ( 1 ) " "      " "      "*"
## 35 ( 1 ) " "      " "      "*"
## 36 ( 1 ) " "      " "      "*"
## 37 ( 1 ) " "      " "      "*"
## 38 ( 1 ) " "      " "      "*"
## 39 ( 1 ) " "      " "      "*"
## 40 ( 1 ) " "      " "      "*"
## 41 ( 1 ) " "      " "      "*"
## 42 ( 1 ) " "      " "      "*"
## 43 ( 1 ) " "      " "      "*"
## 44 ( 1 ) " "      " "      "*"
## 45 ( 1 ) " "      " "      "*"
## 46 ( 1 ) " "      " "      "*"
## 47 ( 1 ) " "      " "      "*"
## 48 ( 1 ) " "      " "      "*"
## 49 ( 1 ) " "      " "      "*"
## 50 ( 1 ) " "      " "      "*"
## 51 ( 1 ) " "      " "      "*"
## 52 ( 1 ) " "      " "      "*"
## 53 ( 1 ) " "      " "      "*"
## 54 ( 1 ) " "      "*"     "*"
## 55 ( 1 ) " "      "*"     "*"
## 56 ( 1 ) " "      "*"     "*"
## 57 ( 1 ) " "      "*"     "*"
## 58 ( 1 ) " "      "*"     "*"
## 59 ( 1 ) " "      "*"     "*"
## 60 ( 1 ) " "      "*"     "*"
## 61 ( 1 ) " "      "*"     "*"
## 62 ( 1 ) " "      "*"     "*"
## 63 ( 1 ) " "      "*"     "*"
## 64 ( 1 ) " "      "*"     "*"
## 65 ( 1 ) " "      "*"     "*"
## 66 ( 1 ) " "      "*"     "*"
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## 69 ( 1 ) " "      "*"     "*"
## 70 ( 1 ) " "      "*"     "*"
## 71 ( 1 ) " "      "*"     "*"
## 72 ( 1 ) " "      "*"     "*"
## 73 ( 1 ) " "      "*"     "*"
## 74 ( 1 ) "*"     "*"     "*"
## 75 ( 1 ) "*"     "*"     "*"
## 76 ( 1 ) "*"     "*"     "*"
## 77 ( 1 ) "*"     "*"     "*"
## 78 ( 1 ) "*"     "*"     "*"
## 79 ( 1 ) "*"     "*"     "*"
## 80 ( 1 ) "*"     "*"     "*"
##
##          wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1 ( 1 ) " "      " "      " "
## 2 ( 1 ) " "      " "      " "
## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "

```

```

## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   " "
## 32 ( 1 )   " "
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## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 60  ( 1 ) "*"      "*"      " "
## 61  ( 1 ) "*"      "*"      " "
## 62  ( 1 ) "*"      "*"      " "
## 63  ( 1 ) "*"      "*"      " "
## 64  ( 1 ) "*"      "*"      " "
## 65  ( 1 ) "*"      "*"      " "
## 66  ( 1 ) "*"      "*"      " "
## 67  ( 1 ) "*"      "*"      " "
## 68  ( 1 ) "*"      "*"      " "
## 69  ( 1 ) "*"      "*"      " "
## 70  ( 1 ) "*"      "*"      " "
## 71  ( 1 ) "*"      "*"      " "
## 72  ( 1 ) "*"      "*"      " "
## 73  ( 1 ) "*"      "*"      " "
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## 75  ( 1 ) "*"      "*"      " "
## 76  ( 1 ) "*"      "*"      " "
## 77  ( 1 ) "*"      "*"      " "
## 78  ( 1 ) "*"      "*"      " "
## 79  ( 1 ) "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"

##          std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie
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## 2  ( 1 ) " "      " "      " "      " "
## 3  ( 1 ) " "      " "      " "      " "
## 4  ( 1 ) " "      " "      " "      " "
## 5  ( 1 ) " "      " "      " "      " "
## 6  ( 1 ) " "      " "      " "      " "
## 7  ( 1 ) " "      " "      " "      " "
## 8  ( 1 ) " "      " "      " "      " "
## 9  ( 1 ) " "      " "      " "      " "
## 10 ( 1 ) " "      " "      " "      " "
## 11 ( 1 ) " "      " "      " "      " "
## 12 ( 1 ) " "      " "      " "      " "
## 13 ( 1 ) " "      " "      " "      " "
## 14 ( 1 ) " "      " "      " "      " "
## 15 ( 1 ) " "      "*"      " "      " "
## 16 ( 1 ) " "      "*"      " "      " "
## 17 ( 1 ) " "      "*"      " "      " "
## 18 ( 1 ) " "      "*"      " "      " "
## 19 ( 1 ) " "      "*"      " "      " "
## 20 ( 1 ) " "      "*"      "*"      " "
## 21 ( 1 ) " "      "*"      "*"      " "
## 22 ( 1 ) " "      "*"      "*"      " "
## 23 ( 1 ) " "      "*"      "*"      " "
## 24 ( 1 ) " "      "*"      "*"      " "
## 25 ( 1 ) " "      "*"      "*"      " "
## 26 ( 1 ) " "      "*"      "*"      " "
## 27 ( 1 ) " "      "*"      "*"      " "
## 28 ( 1 ) " "      "*"      "*"      " "
## 29 ( 1 ) " "      "*"      "*"      " "
## 30 ( 1 ) " "      "*"      "*"      " "
## 31 ( 1 ) " "      "*"      "*"      " "
## 32 ( 1 ) " "      "*"      "*"      " "

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## 33 ( 1 ) " "      "*"      "*"      " "
## 34 ( 1 ) " "      "*"      "*"      " "
## 35 ( 1 ) " "      "*"      "*"      " "
## 36 ( 1 ) " "      "*"      "*"      " "
## 37 ( 1 ) " "      "*"      "*"      " "
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## 39 ( 1 ) " "      "*"      "*"      " "
## 40 ( 1 ) " "      "*"      "*"      " "
## 41 ( 1 ) " "      "*"      "*"      " "
## 42 ( 1 ) " "      "*"      "*"      " "
## 43 ( 1 ) " "      "*"      "*"      " "
## 44 ( 1 ) " "      "*"      "*"      " "
## 45 ( 1 ) " "      "*"      "*"      " "
## 46 ( 1 ) " "      "*"      "*"      " "
## 47 ( 1 ) " "      "*"      "*"      " "
## 48 ( 1 ) " "      "*"      "*"      " "
## 49 ( 1 ) " "      "*"      "*"      " "
## 50 ( 1 ) " "      "*"      "*"      " "
## 51 ( 1 ) " "      "*"      "*"      " "
## 52 ( 1 ) " "      "*"      "*"      " "
## 53 ( 1 ) " "      "*"      "*"      " "
## 54 ( 1 ) " "      "*"      "*"      " "
## 55 ( 1 ) " "      "*"      "*"      " "
## 56 ( 1 ) " "      "*"      "*"      " "
## 57 ( 1 ) " "      "*"      "*"      " "
## 58 ( 1 ) " "      "*"      "*"      " "
## 59 ( 1 ) " "      "*"      "*"      " "
## 60 ( 1 ) " "      "*"      "*"      " "
## 61 ( 1 ) " "      "*"      "*"      " "
## 62 ( 1 ) " "      "*"      "*"      " "
## 63 ( 1 ) " "      "*"      "*"      " "
## 64 ( 1 ) " "      "*"      "*"      " "
## 65 ( 1 ) " "      "*"      "*"      " "
## 66 ( 1 ) " "      "*"      "*"      " "
## 67 ( 1 ) " "      "*"      "*"      " "
## 68 ( 1 ) " "      "*"      "*"      " "
## 69 ( 1 ) " "      "*"      "*"      " "
## 70 ( 1 ) "*"      "*"      "*"      " "
## 71 ( 1 ) "*"      "*"      "*"      " "
## 72 ( 1 ) "*"      "*"      "*"      " "
## 73 ( 1 ) "*"      "*"      "*"      " "
## 74 ( 1 ) "*"      "*"      "*"      " "
## 75 ( 1 ) "*"      "*"      "*"      " "
## 76 ( 1 ) "*"      "*"      "*"      " "
## 77 ( 1 ) "*"      "*"      "*"      " "
## 78 ( 1 ) "*"      "*"      "*"      " "
## 79 ( 1 ) "*"      "*"      "*"      " "
## 80 ( 1 ) "*"      "*"      "*"      " *"
##          gmean_fie wtd_gmean_fie entropy_fie wtd_entropy_fie range_fie
## 1 ( 1 ) " "      " "      " "      " "      " "
## 2 ( 1 ) " "      " "      " "      " "      " "
## 3 ( 1 ) " "      " "      " "      " "      " "
## 4 ( 1 ) " "      " "      " "      " "      " "
## 5 ( 1 ) " "      " "      " "      " "      " "

```

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## 6  ( 1 )   " "   " "   " "   " "   " "
## 7  ( 1 )   " "   " "   " "   " "   " "
## 8  ( 1 )   " "   " "   " "   " "   " "
## 9  ( 1 )   " "   " "   " "   " "   " "
## 10 ( 1 )   " "   " "   " "   " "   " "
## 11 ( 1 )   " "   " "   " "   " "   " "
## 12 ( 1 )   " "   " "   " "   " "   " "
## 13 ( 1 )   " "   " "   " "   " "   " "
## 14 ( 1 )   " "   " "   " "   " "   " "
## 15 ( 1 )   " "   " "   " "   " "   " "
## 16 ( 1 )   " "   " "   " "   " "   " "
## 17 ( 1 )   " "   " "   " "   " "   " "
## 18 ( 1 )   " "   " "   " "   " "   " "
## 19 ( 1 )   " "   " "   " "   " "   " "
## 20 ( 1 )   " "   " "   " "   " "   " "
## 21 ( 1 )   " "   " "   " "   " "   " "
## 22 ( 1 )   " "   " "   " "   " "   " "
## 23 ( 1 )   " "   " "   " "   " "   " "
## 24 ( 1 )   " "   " "   " "   " "   " "
## 25 ( 1 )   " "   " "   " "   " "   " "
## 26 ( 1 )   " "   " "   " "   " "   " "
## 27 ( 1 )   " "   " "   " "   " "   " "
## 28 ( 1 )   " "   " "   " "   " "   " "
## 29 ( 1 )   " "   " "   " "   " "   " "
## 30 ( 1 )   " "   " "   " "   " "   " "
## 31 ( 1 )   " "   " "   " "   " "   " "
## 32 ( 1 )   " "   " "   " "   " "   " "
## 33 ( 1 )   " "   " "   " "   " "   " "
## 34 ( 1 )   " "   " "   "*"  " "   " "
## 35 ( 1 )   " "   " "   "*"  " "   " "
## 36 ( 1 )   " "   " "   "*"  " "   " "
## 37 ( 1 )   " "   " "   "*"  " "   " "
## 38 ( 1 )   " "   " "   "*"  " "   " "
## 39 ( 1 )   " "   " "   "*"  " "   " "
## 40 ( 1 )   " "   " "   "*"  " "   " "
## 41 ( 1 )   " "   " "   "*"  " "   " "
## 42 ( 1 )   " "   " "   "*"  " "   " "
## 43 ( 1 )   " "   " "   "*"  " "   " "
## 44 ( 1 )   " "   " "   "*"  " "   " "
## 45 ( 1 )   " "   " "   "*"  " "   " "
## 46 ( 1 )   " "   " "   "*"  " "   " "
## 47 ( 1 )   " "   " "   "*"  " "   " "
## 48 ( 1 )   " "   " "   "*"  " "   " "
## 49 ( 1 )   " "   " "   "*"  " "   " "
## 50 ( 1 )   " "   " "   "*"  " "   " "
## 51 ( 1 )   " "   " "   "*"  " "   " "
## 52 ( 1 )   " "   " "   "*"  " "   " "
## 53 ( 1 )   " "   " "   "*"  " "   " "
## 54 ( 1 )   " "   " "   "*"  " "   " "
## 55 ( 1 )   " "   " "   "*"  " "   " "
## 56 ( 1 )   " "   " "   "*"  " "   " "
## 57 ( 1 )   " "   " "   "*"  " "   " "
## 58 ( 1 )   " "   " "   "*"  " "   "*"
## 59 ( 1 )   " "   " "   "*"  " "   "*"

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## 60  ( 1 ) " "      " "      "*"      " "      "*"
## 61  ( 1 ) " "      " "      "*"      " "      "*"
## 62  ( 1 ) " "      " "      "*"      " "      "*"
## 63  ( 1 ) " "      " "      "*"      " "      "*"
## 64  ( 1 ) " "      " "      "*"      " "      "*"
## 65  ( 1 ) " "      " "      "*"      " "      "*"
## 66  ( 1 ) " "      " "      "*"      " "      "*"
## 67  ( 1 ) " "      " "      "*"      " "      "*"
## 68  ( 1 ) " "      " "      "*"      " "      "*"
## 69  ( 1 ) " "      " "      "*"      " "      "*"
## 70  ( 1 ) " "      " "      "*"      " "      "*"
## 71  ( 1 ) " "      " "      "*"      " "      "*"
## 72  ( 1 ) " "      " "      "*"      " "      "*"
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## 75  ( 1 ) "*"      " "      "*"      " "      "*"
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## 77  ( 1 ) "*"      " "      "*"      " "      "*"
## 78  ( 1 ) "*"      " "      "*"      " "      "*"
## 79  ( 1 ) "*"      " "      "*"      " "      "*"
## 80  ( 1 ) "*"      " "      "*"      " "      "*"

##          wtd_range_fie std_fie wtd_std_fie mean_atomic_radius
## 1  ( 1 ) " "      " "      " "      " "
## 2  ( 1 ) " "      " "      " "      " "
## 3  ( 1 ) " "      " "      " "      " "
## 4  ( 1 ) " "      " "      " "      " "
## 5  ( 1 ) " "      " "      " "      " "
## 6  ( 1 ) " "      " "      " "      " "
## 7  ( 1 ) " "      " "      " "      " "
## 8  ( 1 ) " "      " "      " "      " "
## 9  ( 1 ) " "      " "      " "      " "
## 10 ( 1 ) " "      " "      " "      " "
## 11 ( 1 ) " "      " "      " "      " "
## 12 ( 1 ) " "      " "      " "      " "
## 13 ( 1 ) " "      " "      " "      " "
## 14 ( 1 ) " "      " "      " "      " "
## 15 ( 1 ) " "      " "      " "      " "
## 16 ( 1 ) " "      " "      " "      " "
## 17 ( 1 ) " "      " "      " "      " "
## 18 ( 1 ) " "      " "      " "      " "
## 19 ( 1 ) " "      " "      " "      " "
## 20 ( 1 ) " "      " "      " "      " "
## 21 ( 1 ) " "      " "      " "      " "
## 22 ( 1 ) " "      " "      " "      " "
## 23 ( 1 ) " "      " "      " "      " "
## 24 ( 1 ) " "      " "      " "      " "
## 25 ( 1 ) " "      " "      " "      " "
## 26 ( 1 ) " "      " "      " "      " "
## 27 ( 1 ) " "      " "      " "      " "
## 28 ( 1 ) " "      " "      " "      " "
## 29 ( 1 ) " "      " "      " "      " "
## 30 ( 1 ) " "      " "      " "      " "
## 31 ( 1 ) " "      " "      " "      " "
## 32 ( 1 ) " "      " "      " "      " "

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## 33 ( 1 ) " "      " "      " "
## 34 ( 1 ) " "      " "      " "
## 35 ( 1 ) " "      " "      " "
## 36 ( 1 ) " "      " "      " "
## 37 ( 1 ) " "      " "      " "
## 38 ( 1 ) " "      " "      " "
## 39 ( 1 ) " "      " "      " "
## 40 ( 1 ) " "      " "      " "
## 41 ( 1 ) " "      " "      " "
## 42 ( 1 ) " "      " "      " "
## 43 ( 1 ) " "      " "      " "
## 44 ( 1 ) " "      " "      " "
## 45 ( 1 ) " "      " "      " "
## 46 ( 1 ) " "      " "      "*"
## 47 ( 1 ) " "      " "      "*"
## 48 ( 1 ) " "      " "      "*"
## 49 ( 1 ) " "      " "      "*"
## 50 ( 1 ) " "      " "      "*"
## 51 ( 1 ) " "      " "      "*"
## 52 ( 1 ) " "      " "      "*"
## 53 ( 1 ) " "      " "      "*"
## 54 ( 1 ) " "      " "      "*"
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## 56 ( 1 ) " "      " "      "*"
## 57 ( 1 ) " "      " "      "*"
## 58 ( 1 ) " "      " "      "*"
## 59 ( 1 ) " "      "*"      "*"
## 60 ( 1 ) " "      "*"      "*"
## 61 ( 1 ) " "      "*"      "*"
## 62 ( 1 ) " "      "*"      "*"
## 63 ( 1 ) " "      "*"      "*"
## 64 ( 1 ) " "      "*"      "*"
## 65 ( 1 ) " "      "*"      "*"
## 66 ( 1 ) " "      "*"      "*"
## 67 ( 1 ) " "      "*"      "*"
## 68 ( 1 ) " "      "*"      "*"
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## 70 ( 1 ) "*"      "*"      "*"
## 71 ( 1 ) "*"      "*"      "*"
## 72 ( 1 ) "*"      "*"      "*"
## 73 ( 1 ) "*"      "*"      "*"
## 74 ( 1 ) "*"      "*"      "*"
## 75 ( 1 ) "*"      "*"      "*"
## 76 ( 1 ) "*"      "*"      "*"
## 77 ( 1 ) "*"      "*"      "*"
## 78 ( 1 ) "*"      "*"      "*"
## 79 ( 1 ) "*"      "*"      "*"
## 80 ( 1 ) "*"      "*"      "*"
##
##          wtd_mean_atomic_radius gmean_atomic_radius
## 1 ( 1 ) " "                  " "
## 2 ( 1 ) " "                  " "
## 3 ( 1 ) " "                  " "
## 4 ( 1 ) " "                  " "
## 5 ( 1 ) " "                  " "

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## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
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##           wtd_gmean_atomic_radius entropy_atomic_radius
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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
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## 5 ( 1 ) " "           "*"

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##           wtd_range_atomic_radius std_atomic_radius wtd_std_atomic_radius
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## 11 ( 1 ) " "          "*"         " "
## 12 ( 1 ) " "          "*"         " "
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## 15 ( 1 ) " "          "*"         " "
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## 17 ( 1 ) " "          "*"         " "
## 18 ( 1 ) " "          "*"         " "
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## 23 ( 1 ) " "          "*"         " "
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## 26 ( 1 ) " "          "*"         " "
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## 32 ( 1 ) "*"          "*"         " "

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## 4 ( 1 ) " "        " "        " "        " "
## 5 ( 1 ) " "        " "        " "        " "

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## 14 ( 1 )   " "
## 15 ( 1 )   " "
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## 17 ( 1 )   "*" "
## 18 ( 1 )   "*" "
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## 21 ( 1 )   "*" "
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## 25 ( 1 )   "*" "
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## 37 ( 1 )   "*" "
## 38 ( 1 )   "*" "
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## 51 ( 1 )   "*" "
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## 65  ( 1 ) "*"      " *"     "*"      "*" 
## 66  ( 1 ) "*"      " *"     "*"      "*" 
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## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
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## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      " "
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## 23 ( 1 ) " "      " *"     "*" 
## 24 ( 1 ) " "      " *"     "*" 
## 25 ( 1 ) " "      " *"     "*" 
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## 28 ( 1 ) " "      " *"     "*" 
## 29 ( 1 ) " "      " *"     "*" 
## 30 ( 1 ) " "      " *"     "*" 
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## 80 ( 1 ) "*"      "*"      "*"
##          wtd_range_Density std_Density wtd_std_Density
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## 2 ( 1 ) " "      " "      " "
## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "

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## 80 ( 1 ) "*"
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## 4 ( 1 ) "*"                 " "
## 5 ( 1 ) "*"                 " "

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## 42 ( 1 ) "*"      "*"
## 43 ( 1 ) "*"      "*"
## 44 ( 1 ) "*"      "*"
## 45 ( 1 ) "*"      "*"
## 46 ( 1 ) "*"      "*"
## 47 ( 1 ) "*"      "*"
## 48 ( 1 ) "*"      "*"
## 49 ( 1 ) "*"      "*"
## 50 ( 1 ) "*"      "*"
## 51 ( 1 ) "*"      "*"
## 52 ( 1 ) "*"      "*"
## 53 ( 1 ) "*"      "*"
## 54 ( 1 ) "*"      "*"
## 55 ( 1 ) "*"      "*"
## 56 ( 1 ) "*"      "*"
## 57 ( 1 ) "*"      "*"
## 58 ( 1 ) "*"      "*"
## 59 ( 1 ) "*"      "*"

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## 60  ( 1 ) "*"          "*"
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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
## 66  ( 1 ) "*"          "*"
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## 68  ( 1 ) "*"          "*"
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## 70  ( 1 ) "*"          "*"
## 71  ( 1 ) "*"          "*"
## 72  ( 1 ) "*"          "*"
## 73  ( 1 ) "*"          "*"
## 74  ( 1 ) "*"          "*"
## 75  ( 1 ) "*"          "*"
## 76  ( 1 ) "*"          "*"
## 77  ( 1 ) "*"          "*"
## 78  ( 1 ) "*"          "*"
## 79  ( 1 ) "*"          "*"
## 80  ( 1 ) "*"          "*"
##           entropy_ElectronAffinity wtd_entropy_ElectronAffinity
## 1  ( 1 ) " "          " "
## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) "*"          " "
## 6  ( 1 ) "*"          " "
## 7  ( 1 ) "*"          " "
## 8  ( 1 ) "*"          " "
## 9  ( 1 ) "*"          " "
## 10 ( 1 ) "*"          " "
## 11 ( 1 ) "*"          " "
## 12 ( 1 ) "*"          " "
## 13 ( 1 ) "*"          " "
## 14 ( 1 ) "*"          " "
## 15 ( 1 ) "*"          " "
## 16 ( 1 ) "*"          " "
## 17 ( 1 ) "*"          " "
## 18 ( 1 ) "*"          " "
## 19 ( 1 ) "*"          " "
## 20 ( 1 ) "*"          " "
## 21 ( 1 ) "*"          " "
## 22 ( 1 ) "*"          " "
## 23 ( 1 ) "*"          " "
## 24 ( 1 ) "*"          " "
## 25 ( 1 ) "*"          " "
## 26 ( 1 ) "*"          " "
## 27 ( 1 ) "*"          " "
## 28 ( 1 ) "*"          " "
## 29 ( 1 ) "*"          "*"
## 30 ( 1 ) "*"          "*"
## 31 ( 1 ) "*"          "*"
## 32 ( 1 ) "*"          "*"

```

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## 33 ( 1 ) "*"      "*"
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## 35 ( 1 ) "*"      "*"
## 36 ( 1 ) "*"      "*"
## 37 ( 1 ) "*"      "*"
## 38 ( 1 ) "*"      "*"
## 39 ( 1 ) "*"      "*"
## 40 ( 1 ) "*"      "*"
## 41 ( 1 ) "*"      "*"
## 42 ( 1 ) "*"      "*"
## 43 ( 1 ) "*"      "*"
## 44 ( 1 ) "*"      "*"
## 45 ( 1 ) "*"      "*"
## 46 ( 1 ) "*"      "*"
## 47 ( 1 ) "*"      "*"
## 48 ( 1 ) "*"      "*"
## 49 ( 1 ) "*"      "*"
## 50 ( 1 ) "*"      "*"
## 51 ( 1 ) "*"      "*"
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## 53 ( 1 ) "*"      "*"
## 54 ( 1 ) "*"      "*"
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## 56 ( 1 ) "*"      "*"
## 57 ( 1 ) "*"      "*"
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## 59 ( 1 ) "*"      "*"
## 60 ( 1 ) "*"      "*"
## 61 ( 1 ) "*"      "*"
## 62 ( 1 ) "*"      "*"
## 63 ( 1 ) "*"      "*"
## 64 ( 1 ) "*"      "*"
## 65 ( 1 ) "*"      "*"
## 66 ( 1 ) "*"      "*"
## 67 ( 1 ) "*"      "*"
## 68 ( 1 ) "*"      "*"
## 69 ( 1 ) "*"      "*"
## 70 ( 1 ) "*"      "*"
## 71 ( 1 ) "*"      "*"
## 72 ( 1 ) "*"      "*"
## 73 ( 1 ) "*"      "*"
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## 75 ( 1 ) "*"      "*"
## 76 ( 1 ) "*"      "*"
## 77 ( 1 ) "*"      "*"
## 78 ( 1 ) "*"      "*"
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## 80 ( 1 ) "*"      "*"
##          range_ElectronAffinity wtd_range_ElectronAffinity
## 1 ( 1 ) " "           " "
## 2 ( 1 ) " "           " "
## 3 ( 1 ) " "           " "
## 4 ( 1 ) " "           " "
## 5 ( 1 ) " "           " "

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## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   "*"
## 31 ( 1 )   "*"
## 32 ( 1 )   "*"
## 33 ( 1 )   "*"
## 34 ( 1 )   "*"
## 35 ( 1 )   "*"
## 36 ( 1 )   "*"
## 37 ( 1 )   "*"
## 38 ( 1 )   "*"
## 39 ( 1 )   "*"
## 40 ( 1 )   "*"
## 41 ( 1 )   "*"
## 42 ( 1 )   "*"
## 43 ( 1 )   "*"
## 44 ( 1 )   "*"
## 45 ( 1 )   "*"
## 46 ( 1 )   "*"
## 47 ( 1 )   "*"
## 48 ( 1 )   "*"
## 49 ( 1 )   "*"
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 62  ( 1 ) "*"      "*"
## 63  ( 1 ) "*"      "*"
## 64  ( 1 ) "*"      "*"
## 65  ( 1 ) "*"      "*"
## 66  ( 1 ) "*"      "*"
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## 70  ( 1 ) "*"      "*"
## 71  ( 1 ) "*"      "*"
## 72  ( 1 ) "*"      "*"
## 73  ( 1 ) "*"      "*"
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## 75  ( 1 ) "*"      "*"
## 76  ( 1 ) "*"      "*"
## 77  ( 1 ) "*"      "*"
## 78  ( 1 ) "*"      "*"
## 79  ( 1 ) "*"      "*"
## 80  ( 1 ) "*"      "*"
##          std_ElectronAffinity wtd_std_ElectronAffinity mean_FusionHeat
## 1  ( 1 ) " "      " "      " "
## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      "*"      " "
## 10 ( 1 ) " "      "*"      " "
## 11 ( 1 ) " "      "*"      " "
## 12 ( 1 ) " "      "*"      " "
## 13 ( 1 ) " "      "*"      " "
## 14 ( 1 ) " "      "*"      " "
## 15 ( 1 ) " "      "*"      " "
## 16 ( 1 ) " "      "*"      " "
## 17 ( 1 ) " "      "*"      " "
## 18 ( 1 ) " "      "*"      " "
## 19 ( 1 ) " "      "*"      " "
## 20 ( 1 ) " "      "*"      " "
## 21 ( 1 ) " "      "*"      " "
## 22 ( 1 ) " "      "*"      " "
## 23 ( 1 ) " "      "*"      " "
## 24 ( 1 ) " "      "*"      " "
## 25 ( 1 ) " "      "*"      " "
## 26 ( 1 ) " "      "*"      " "
## 27 ( 1 ) " "      "*"      " "
## 28 ( 1 ) " "      "*"      " "
## 29 ( 1 ) " "      "*"      " "
## 30 ( 1 ) " "      "*"      " "
## 31 ( 1 ) " "      "*"      " "
## 32 ( 1 ) " "      "*"      " "

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## 33 ( 1 ) " "
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## 37 ( 1 ) " "
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## 39 ( 1 ) " "
## 40 ( 1 ) " "
## 41 ( 1 ) " "
## 42 ( 1 ) " "
## 43 ( 1 ) " "
## 44 ( 1 ) " "
## 45 ( 1 ) "*"
## 46 ( 1 ) "*"
## 47 ( 1 ) "*"
## 48 ( 1 ) "*"
## 49 ( 1 ) "*"
## 50 ( 1 ) "*"
## 51 ( 1 ) "*"
## 52 ( 1 ) "*"
## 53 ( 1 ) "*"
## 54 ( 1 ) "*"
## 55 ( 1 ) "*"
## 56 ( 1 ) "*"
## 57 ( 1 ) "*"
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## 59 ( 1 ) "*"
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## 62 ( 1 ) "*"
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## 64 ( 1 ) "*"
## 65 ( 1 ) "*"
## 66 ( 1 ) "*"
## 67 ( 1 ) "*"
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## 73 ( 1 ) "*"
## 74 ( 1 ) "*"
## 75 ( 1 ) "*"
## 76 ( 1 ) "*"
## 77 ( 1 ) "*"
## 78 ( 1 ) "*"
## 79 ( 1 ) "*"
## 80 ( 1 ) "*"
##          wtd_mean_FusionHeat gmean_FusionHeat wtd_gmean_FusionHeat
## 1 ( 1 ) " "           " "           " "
## 2 ( 1 ) " "           " "           " "
## 3 ( 1 ) " "           " "           " "
## 4 ( 1 ) " "           " "           " "
## 5 ( 1 ) " "           " "           " "

```

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## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   " "
## 32 ( 1 )   " "
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## 34 ( 1 )   " "
## 35 ( 1 )   " "
## 36 ( 1 )   " "
## 37 ( 1 )   " "
## 38 ( 1 )   " "
## 39 ( 1 )   " "
## 40 ( 1 )   " "
## 41 ( 1 )   " "
## 42 ( 1 )   " "
## 43 ( 1 )   " "
## 44 ( 1 )   " "
## 45 ( 1 )   " "
## 46 ( 1 )   " "
## 47 ( 1 )   " "
## 48 ( 1 )   " "
## 49 ( 1 )   " "
## 50 ( 1 )   "*"
## 51 ( 1 )   "*"
## 52 ( 1 )   "*"
## 53 ( 1 )   "*"
## 54 ( 1 )   "*"
## 55 ( 1 )   "*"
## 56 ( 1 )   "*"
## 57 ( 1 )   "*"
## 58 ( 1 )   "*"
## 59 ( 1 )   "*"

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## 60  ( 1 ) "*"      " "      "*"
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## 62  ( 1 ) "*"      " "      "*"
## 63  ( 1 ) "*"      " "      "*"
## 64  ( 1 ) "*"      " "      "*"
## 65  ( 1 ) "*"      " "      "*"
## 66  ( 1 ) "*"      "*"     "*"
## 67  ( 1 ) "*"      "*"     "*"
## 68  ( 1 ) "*"      "*"     "*"
## 69  ( 1 ) "*"      "*"     "*"
## 70  ( 1 ) "*"      "*"     "*"
## 71  ( 1 ) "*"      "*"     "*"
## 72  ( 1 ) "*"      "*"     "*"
## 73  ( 1 ) "*"      "*"     "*"
## 74  ( 1 ) "*"      "*"     "*"
## 75  ( 1 ) "*"      "*"     "*"
## 76  ( 1 ) "*"      "*"     "*"
## 77  ( 1 ) "*"      "*"     "*"
## 78  ( 1 ) "*"      "*"     "*"
## 79  ( 1 ) "*"      "*"     "*"
## 80  ( 1 ) "*"      "*"     "*"

##          entropy_FusionHeat wtd_entropy_FusionHeat range_FusionHeat
## 1  ( 1 ) " "      " "      " "
## 2  ( 1 ) " "      " "      " "
## 3  ( 1 ) " "      " "      " "
## 4  ( 1 ) " "      " "      " "
## 5  ( 1 ) " "      " "      " "
## 6  ( 1 ) " "      " "      " "
## 7  ( 1 ) " "      " "      " "
## 8  ( 1 ) " "      " "      " "
## 9  ( 1 ) " "      " "      " "
## 10 ( 1 ) " "      " "      " "
## 11 ( 1 ) " "      " "      " "
## 12 ( 1 ) " "      " "      " "
## 13 ( 1 ) " "      " "      " "
## 14 ( 1 ) " "      " "      " "
## 15 ( 1 ) " "      " "      " "
## 16 ( 1 ) " "      " "      " "
## 17 ( 1 ) " "      " "      " "
## 18 ( 1 ) " "      " "      " "
## 19 ( 1 ) " "      " "      " "
## 20 ( 1 ) " "      " "      " "
## 21 ( 1 ) " "      " "      " "
## 22 ( 1 ) " "      " "      " "
## 23 ( 1 ) " "      " "      " "
## 24 ( 1 ) " "      " "      " "
## 25 ( 1 ) " "      " "      " "
## 26 ( 1 ) " "      " "      " "
## 27 ( 1 ) " "      " "      " "
## 28 ( 1 ) " "      " "      " "
## 29 ( 1 ) " "      " "      " "
## 30 ( 1 ) " "      " "      " "
## 31 ( 1 ) " "      " "      " "
## 32 ( 1 ) " "      "*"     " "

```

```

## 33 ( 1 ) " "      "*"      " "
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## 35 ( 1 ) " "      "*"      " "
## 36 ( 1 ) " "      "*"      " "
## 37 ( 1 ) " "      "*"      " "
## 38 ( 1 ) " "      "*"      " "
## 39 ( 1 ) " "      "*"      " "
## 40 ( 1 ) " "      "*"      " "
## 41 ( 1 ) " "      "*"      " "
## 42 ( 1 ) " "      "*"      " "
## 43 ( 1 ) " "      "*"      " "
## 44 ( 1 ) " "      "*"      " "
## 45 ( 1 ) " "      "*"      " "
## 46 ( 1 ) " "      "*"      " "
## 47 ( 1 ) " "      "*"      "*"
## 48 ( 1 ) " "      "*"      "*"
## 49 ( 1 ) " "      "*"      "*"
## 50 ( 1 ) " "      "*"      "*"
## 51 ( 1 ) " "      "*"      "*"
## 52 ( 1 ) " "      "*"      "*"
## 53 ( 1 ) " "      "*"      "*"
## 54 ( 1 ) " "      "*"      "*"
## 55 ( 1 ) " "      "*"      "*"
## 56 ( 1 ) " "      "*"      "*"
## 57 ( 1 ) " "      "*"      "*"
## 58 ( 1 ) " "      "*"      "*"
## 59 ( 1 ) " "      "*"      "*"
## 60 ( 1 ) " "      "*"      "*"
## 61 ( 1 ) " "      "*"      "*"
## 62 ( 1 ) " "      "*"      "*"
## 63 ( 1 ) " "      "*"      "*"
## 64 ( 1 ) " "      "*"      "*"
## 65 ( 1 ) " "      "*"      "*"
## 66 ( 1 ) " "      "*"      "*"
## 67 ( 1 ) "*"      "*"      "*"
## 68 ( 1 ) "*"      "*"      "*"
## 69 ( 1 ) "*"      "*"      "*"
## 70 ( 1 ) "*"      "*"      "*"
## 71 ( 1 ) "*"      "*"      "*"
## 72 ( 1 ) "*"      "*"      "*"
## 73 ( 1 ) "*"      "*"      "*"
## 74 ( 1 ) "*"      "*"      "*"
## 75 ( 1 ) "*"      "*"      "*"
## 76 ( 1 ) "*"      "*"      "*"
## 77 ( 1 ) "*"      "*"      "*"
## 78 ( 1 ) "*"      "*"      "*"
## 79 ( 1 ) "*"      "*"      "*"
## 80 ( 1 ) "*"      "*"      "*"

##          wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
## 1 ( 1 ) " "      " "      " "
## 2 ( 1 ) " "      " "      " "
## 3 ( 1 ) " "      " "      " "
## 4 ( 1 ) " "      " "      " "
## 5 ( 1 ) " "      " "      " "

```

```

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## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 ) "*" 
## 27 ( 1 ) "*" 
## 28 ( 1 ) "*" 
## 29 ( 1 ) "*" 
## 30 ( 1 ) "*" 
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## 32 ( 1 ) "*" 
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## 41 ( 1 ) "*" 
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## 43 ( 1 ) "*" 
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## 54 ( 1 ) "*" 
## 55 ( 1 ) "*" 
## 56 ( 1 ) "*" 
## 57 ( 1 ) "*" 
## 58 ( 1 ) "*" 
## 59 ( 1 ) "*"

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## 62  ( 1 ) "*"      "*"      "*"
## 63  ( 1 ) "*"      "*"      "*"
## 64  ( 1 ) "*"      "*"      "*"
## 65  ( 1 ) "*"      "*"      "*"
## 66  ( 1 ) "*"      "*"      "*"
## 67  ( 1 ) "*"      "*"      "*"
## 68  ( 1 ) "*"      "*"      "*"
## 69  ( 1 ) "*"      "*"      "*"
## 70  ( 1 ) "*"      "*"      "*"
## 71  ( 1 ) "*"      "*"      "*"
## 72  ( 1 ) "*"      "*"      "*"
## 73  ( 1 ) "*"      "*"      "*"
## 74  ( 1 ) "*"      "*"      "*"
## 75  ( 1 ) "*"      "*"      "*"
## 76  ( 1 ) "*"      "*"      "*"
## 77  ( 1 ) "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"
## 79  ( 1 ) "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"

##          mean_ThermalConductivity wtd_mean_ThermalConductivity
## 1  ( 1 ) " "      " "
## 2  ( 1 ) " "      " "
## 3  ( 1 ) " "      " "
## 4  ( 1 ) " "      " "
## 5  ( 1 ) " "      " "
## 6  ( 1 ) " "      " "
## 7  ( 1 ) " "      " "
## 8  ( 1 ) " "      " "
## 9  ( 1 ) " "      " "
## 10 ( 1 ) " "      " "
## 11 ( 1 ) " "      " "
## 12 ( 1 ) " "      " "
## 13 ( 1 ) " "      " "
## 14 ( 1 ) " "      " "
## 15 ( 1 ) " "      " "
## 16 ( 1 ) " "      " "
## 17 ( 1 ) " "      " "
## 18 ( 1 ) " "      " "
## 19 ( 1 ) " "      " "
## 20 ( 1 ) " "      " "
## 21 ( 1 ) " "      " "
## 22 ( 1 ) " "      " "
## 23 ( 1 ) " "      " "
## 24 ( 1 ) " "      " "
## 25 ( 1 ) " "      " "
## 26 ( 1 ) " "      " "
## 27 ( 1 ) " "      " "
## 28 ( 1 ) " "      " "
## 29 ( 1 ) " "      " "
## 30 ( 1 ) " "      " "
## 31 ( 1 ) " "      " "
## 32 ( 1 ) " "      " "

```

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## 35 ( 1 ) " "
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## 42 ( 1 ) "*"
## 43 ( 1 ) "*"
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## 52 ( 1 ) "*"
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## 55 ( 1 ) "*"
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## 57 ( 1 ) "*"
## 58 ( 1 ) "*"
## 59 ( 1 ) "*"
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## 74 ( 1 ) "*"
## 75 ( 1 ) "*"
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## 77 ( 1 ) "*"
## 78 ( 1 ) "*"
## 79 ( 1 ) "*"
## 80 ( 1 ) "*"
##          gmean_ThermalConductivity wtd_gmean_ThermalConductivity
## 1 ( 1 ) " "
## 2 ( 1 ) " "
## 3 ( 1 ) " "
## 4 ( 1 ) " "
## 5 ( 1 ) " "

```

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## 6  ( 1 )   " "
## 7  ( 1 )   " "
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## 9  ( 1 )   " "
## 10 ( 1 )   " "
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## 13 ( 1 )   " "
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## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
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## 32 ( 1 )   "*" 
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## 34 ( 1 )   "*" 
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## 40 ( 1 )   "*" 
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## 42 ( 1 )   "*" 
## 43 ( 1 )   "*" 
## 44 ( 1 )   "*" 
## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   "*" 
## 48 ( 1 )   "*" 
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## 50 ( 1 )   "*" 
## 51 ( 1 )   "*" 
## 52 ( 1 )   "*" 
## 53 ( 1 )   "*" 
## 54 ( 1 )   "*" 
## 55 ( 1 )   "*" 
## 56 ( 1 )   "*" 
## 57 ( 1 )   "*" 
## 58 ( 1 )   "*" 
## 59 ( 1 )   "*"

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## 62  ( 1 ) "*"          "*"
## 63  ( 1 ) "*"          "*"
## 64  ( 1 ) "*"          "*"
## 65  ( 1 ) "*"          "*"
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##           entropy_ThermalConductivity wtd_entropy_ThermalConductivity
## 1  ( 1 ) " "          " "
## 2  ( 1 ) " "          " "
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##          range_ThermalConductivity wtd_range_ThermalConductivity
## 1 ( 1 ) " "                      " "
## 2 ( 1 ) " "                      " "
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## 80  ( 1 ) "*"          "*"

##           std_ThermalConductivity wtd_std_ThermalConductivity mean_Valence
## 1  ( 1 ) " "          "*"          " "
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## 3  ( 1 ) " "          "*"          " "
## 4  ( 1 ) " "          "*"          " "
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## 80 ( 1 ) "*"
##          wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
## 1 ( 1 ) " "           " "           " "           " "
## 2 ( 1 ) " "           " "           " "           " "
## 3 ( 1 ) " "           " "           " "           " "
## 4 ( 1 ) " "           " "           " "           " "
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## 60  ( 1 ) "*"      " "      "*"      "*"
## 61  ( 1 ) "*"      " "      "*"      "*"
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## 67  ( 1 ) "*"      " "      "*"      "*"
## 68  ( 1 ) "*"      " "      "*"      "*"
## 69  ( 1 ) "*"      " "      "*"      "*"
## 70  ( 1 ) "*"      " "      "*"      "*"
## 71  ( 1 ) "*"      " "      "*"      "*"
## 72  ( 1 ) "*"      "*"      "*"      "*"
## 73  ( 1 ) "*"      "*"      "*"      "*"
## 74  ( 1 ) "*"      "*"      "*"      "*"
## 75  ( 1 ) "*"      "*"      "*"      "*"
## 76  ( 1 ) "*"      "*"      "*"      "*"
## 77  ( 1 ) "*"      "*"      "*"      "*"
## 78  ( 1 ) "*"      "*"      "*"      "*"
## 79  ( 1 ) "*"      "*"      "*"      "*"
## 80  ( 1 ) "*"      "*"      "*"      "*"

##          wtd_entropy_Valence range_Valence wtd_range_Valence std_Valence
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## 2  ( 1 ) " "           " "           " "           " "
## 3  ( 1 ) " "           " "           " "           " "
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## 23 ( 1 ) " "           "*"          "*"          " "
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## 25 ( 1 ) " "           "*"          "*"          " "
## 26 ( 1 ) " "           "*"          "*"          " "
## 27 ( 1 ) " "           "*"          "*"          " "
## 28 ( 1 ) " "           "*"          "*"          " "
## 29 ( 1 ) " "           "*"          "*"          " "
## 30 ( 1 ) " "           "*"          "*"          " "
## 31 ( 1 ) " "           "*"          "*"          " "
## 32 ( 1 ) " "           "*"          "*"          " "

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##          wtd_std_Valence
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```
linear_forward_trans$results
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	nvmax	RMSE	Rsquared	MAE	RMSESD	RsquaredSD	MAESD
## 1	1	23.73833	0.5198107	18.24597	0.2467303	0.008466076	0.2298375
## 2	2	22.77972	0.5577446	17.59998	0.2190986	0.009593824	0.2049417
## 3	3	22.01319	0.5870264	17.23048	0.2361849	0.009907962	0.2699336
## 4	4	21.73861	0.5972449	16.88196	0.2273257	0.010163606	0.2294816
## 5	5	21.39575	0.6098494	16.58364	0.2681439	0.011668609	0.2613956
## 6	6	21.04490	0.6225622	16.44033	0.2952996	0.012676057	0.3247834
## 7	7	20.81886	0.6306289	16.15551	0.2805978	0.011958508	0.3273314
## 8	8	20.57609	0.6392197	16.04812	0.2393283	0.010941893	0.3393630
## 9	9	20.30645	0.6486416	15.79772	0.1994125	0.009735672	0.2493824
## 10	10	20.07535	0.6565385	15.50183	0.2066536	0.009283046	0.1605920
## 11	11	19.93184	0.6614510	15.42278	0.2385750	0.010372171	0.2090526
## 12	12	19.77182	0.6668821	15.26017	0.2747978	0.011090266	0.2231507
## 13	13	19.68432	0.6698091	15.21525	0.3206886	0.012248773	0.2781926
## 14	14	19.46664	0.6770047	15.07365	0.3745011	0.013791474	0.3184126
## 15	15	19.27853	0.6832451	14.86116	0.2962089	0.011822644	0.2297602
## 16	16	19.20351	0.6857282	14.79685	0.2790403	0.011001313	0.2281997
## 17	17	19.14855	0.6875292	14.75662	0.3034635	0.011285268	0.2236084
## 18	18	19.10176	0.6890595	14.70142	0.2909735	0.010892776	0.2519570
## 19	19	19.05308	0.6906330	14.70246	0.3077775	0.011343942	0.2638267
## 20	20	19.19876	0.6864091	14.65461	0.7252819	0.024346481	0.2913257
## 21	21	19.32346	0.6832203	14.63325	1.1923352	0.036843124	0.2833353
## 22	22	19.24604	0.6855229	14.59416	1.1202275	0.035069646	0.3187539
## 23	23	19.26525	0.6852330	14.55644	1.2800528	0.039153706	0.3212744
## 24	24	19.25422	0.6858331	14.52387	1.3997115	0.042156201	0.3127539
## 25	25	19.23656	0.6865332	14.48814	1.4373794	0.043018531	0.3105368
## 26	26	19.18209	0.6882002	14.45970	1.3820180	0.041417609	0.3085727
## 27	27	19.15211	0.6891498	14.44362	1.3812285	0.041330722	0.2933049
## 28	28	19.07336	0.6916481	14.35412	1.3077718	0.039049390	0.2710434
## 29	29	18.77329	0.6999072	14.31659	0.4844461	0.016765936	0.2661330

```

## 30 30 18.69493 0.7023023 14.28927 0.4199555 0.014728281 0.2746684
## 31 31 18.83569 0.6984434 14.27836 0.8670728 0.027402952 0.2651204
## 32 32 18.75371 0.7008892 14.24465 0.7972794 0.025618587 0.2794460
## 33 33 18.73651 0.7015500 14.19914 0.8527474 0.027072397 0.2405193
## 34 34 18.71651 0.7022442 14.17310 0.8973683 0.028302002 0.2383385
## 35 35 18.61063 0.7053194 14.14494 0.6731538 0.022031661 0.2239013
## 36 36 18.65575 0.7042342 14.11759 0.9299754 0.028903708 0.2248136
## 37 37 18.64960 0.7044928 14.11493 0.9891651 0.030592265 0.2245867
## 38 38 18.58857 0.7063328 14.06714 0.9682395 0.030165806 0.2170313
## 39 39 18.49561 0.7089844 14.02939 0.7831178 0.025120128 0.2300129
## 40 40 18.44948 0.7103529 14.01621 0.7029098 0.022787254 0.2307366
## 41 41 18.39613 0.7119386 13.97959 0.6358111 0.020977142 0.2215511
## 42 42 18.33779 0.7136473 13.95494 0.5192623 0.017710554 0.2277488
## 43 43 18.40745 0.7117436 13.95007 0.7724002 0.024684408 0.2456737
## 44 44 18.35566 0.7133216 13.91090 0.7636617 0.024522866 0.2388690
## 45 45 18.17215 0.7186163 13.88083 0.3792329 0.013663199 0.2396020
## 46 46 18.37832 0.7128766 13.87535 0.9803927 0.030324542 0.2373041
## 47 47 18.39347 0.7125877 13.86155 1.0880973 0.033071876 0.2462799
## 48 48 18.39468 0.7126264 13.84673 1.1435237 0.034516599 0.2454852
## 49 49 18.41340 0.7122142 13.83581 1.2412489 0.036943298 0.2551442
## 50 50 18.41562 0.7122951 13.80626 1.3032269 0.038378689 0.2528737
## 51 51 18.18214 0.7185942 13.77523 0.6709044 0.021730979 0.2429212
## 52 52 18.34247 0.7143544 13.76717 1.1970440 0.035585118 0.2649469
## 53 53 18.39788 0.7130726 13.75256 1.4296555 0.041358947 0.2806139
## 54 54 18.48278 0.7110775 13.75685 1.7223374 0.048398271 0.2831715
## 55 55 18.48489 0.7111175 13.74116 1.7704064 0.049541236 0.2934953
## 56 56 18.44921 0.7120470 13.72820 1.6940494 0.047693461 0.2779263
## 57 57 18.47111 0.7116596 13.71223 1.8153570 0.050514528 0.2826241
## 58 58 18.50459 0.7109880 13.69992 1.9622137 0.053906323 0.2826685
## 59 59 18.42340 0.7129757 13.67811 1.7418726 0.048760698 0.2722019
## 60 60 18.43489 0.7127264 13.67157 1.7808628 0.049648068 0.2754469
## 61 61 18.41450 0.7133667 13.64599 1.7806598 0.049610640 0.2598923
## 62 62 18.54140 0.7105817 13.63297 2.2364188 0.060018307 0.2706660
## 63 63 18.55666 0.7103250 13.61383 2.3136759 0.061724779 0.2687453
## 64 64 18.44234 0.7129724 13.60738 1.9819126 0.054242459 0.2708415
## 65 65 18.27110 0.7171676 13.57390 1.4985067 0.042773868 0.2450521
## 66 66 18.18865 0.7192974 13.55772 1.2856368 0.037464027 0.2449238
## 67 67 18.16794 0.7198980 13.54243 1.2716587 0.037093857 0.2548742
## 68 68 18.19325 0.7193026 13.52624 1.3742622 0.039661181 0.2478534
## 69 69 18.20232 0.7190929 13.51914 1.4135133 0.040642430 0.2489291
## 70 70 18.23675 0.7182516 13.51865 1.5266670 0.043417604 0.2494714
## 71 71 18.18389 0.7195785 13.51066 1.3698787 0.039514112 0.2528976
## 72 72 18.10757 0.7215277 13.50050 1.1412878 0.033718813 0.2565873
## 73 73 18.06264 0.7227128 13.49100 1.0101205 0.030293146 0.2531586
## 74 74 18.07059 0.7225166 13.48971 1.0388901 0.031021978 0.2585994
## 75 75 18.09065 0.7220056 13.49101 1.1030883 0.032657932 0.2593553
## 76 76 18.10988 0.7215186 13.48364 1.1714629 0.034432834 0.2540787
## 77 77 18.07890 0.7223411 13.47401 1.0924888 0.032412091 0.2591445
## 78 78 18.08052 0.7223123 13.47073 1.1062257 0.032759177 0.2588667
## 79 79 18.07121 0.7225548 13.47029 1.0786395 0.032044703 0.2580894
## 80 80 18.06173 0.7228009 13.47109 1.0496071 0.031290171 0.2582926
## 81 81 18.06344 0.7227549 13.47126 1.0536750 0.031395839 0.2587849

```

From the above results, we can see how forward selection works and the corresponding errors to the number

of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_forward_trans, linear_forward_trans$results$nvmax, "Number of Variables")
```

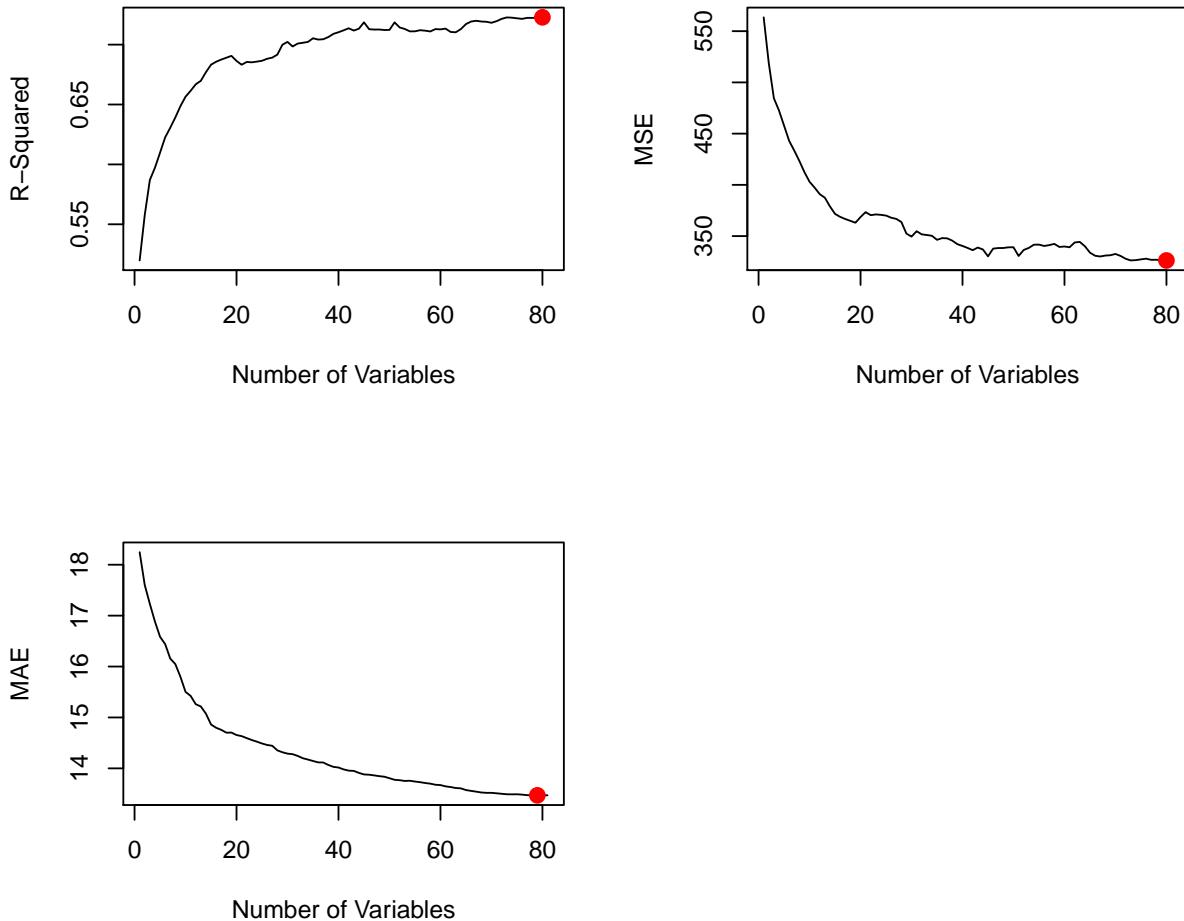


Figure 69: R-Squared, MSE, and MAE for Forward Selection Trans

```
linear_forward_trans$bestTune
```

```
##      nvmax
## 80      80
```

```
coef(linear_forward_trans$finalModel, linear_forward_trans$bestTune$nvmax)
```

```
##                               (Intercept)          number_of_elements
##                               34.4441094                  -2.3462576
## mean_atomic_mass           -0.3493471                   wtd_mean_atomic_mass
##                                         10.6010932
```

```

##          gmean_atomic_mass           wtd_gmean_atomic_mass
##                      4.6283093                  -14.4840844
##          entropy_atomic_mass         wtd_entropy_atomic_mass
##                      -6.1942826                   5.3355092
##          range_atomic_mass          wtd_range_atomic_mass
##                      9.9581982                  -0.2168921
##          std_atomic_mass           wtd_std_atomic_mass
##                      -2.0094355                  -5.0772790
##          mean_fie                  wtd_mean_fie
##                      -14.7226971                 -0.7646974
##          gmean_fie                  wtd_gmean_fie
##                      13.7968410                  2.0623784
##          entropy_fie                wtd_entropy_fie
##                      -44.7283289                 10.5034920
##          range_fie                  wtd_range_fie
##                      17.8087938                  4.6478424
##          std_fie                    wtd_std_fie
##                      -12.1855018                 -5.5551711
##          mean_atomic_radius        wtd_mean_atomic_radius
##                      17.5177860                  19.1082509
##          gmean_atomic_radius        wtd_gmean_atomic_radius
##                      -27.4677529                 -11.4295997
##          entropy_atomic_radius      wtd_entropy_atomic_radius
##                      11.9596226                  9.8744536
##          range_atomic_radius        wtd_range_atomic_radius
##                      17.7756756                 -2.7227117
##          std_atomic_radius         wtd_std_atomic_radius
##                      -21.8518636                  6.9767026
##          mean_Density               wtd_mean_Density
##                      -3.9151265                  0.2768287
##          gmean_Density               wtd_gmean_Density
##                      0.7883830                  13.9337704
##          entropy_Density             wtd_entropy_Density
##                      1.2075288                 -10.3136994
##          range_Density               wtd_range_Density
##                      -6.8141044                 -2.4578380
##          std_Density                 wtd_std_Density
##                      10.6899956                 -6.2741996
##          mean_ElectronAffinity       wtd_mean_ElectronAffinity
##                      -1.4756475                  14.9212649
##          gmean_ElectronAffinity       wtd_gmean_ElectronAffinity
##                      6.3625161                 -16.7757532
##          entropy_ElectronAffinity    wtd_entropy_ElectronAffinity
##                      -3.7137282                 -5.7827485
##          range_ElectronAffinity       wtd_range_ElectronAffinity
##                      -23.0234216                 -3.5613322
##          std_ElectronAffinity         wtd_std_ElectronAffinity
##                      23.0152108                 -8.3984750
##          mean_FusionHeat              wtd_mean_FusionHeat
##                      -17.7663529                  17.5669027
##          gmean_FusionHeat              wtd_gmean_FusionHeat
##                      21.1263950                 -17.3762940
##          entropy_FusionHeat            wtd_entropy_FusionHeat
##                      -13.7800045                  9.8885896

```

```

##          range_FusionHeat      wtd_range_FusionHeat
##                  -14.5156730        4.4466319
##          std_FusionHeat       wtd_std_FusionHeat
##                  13.4325037        -5.9664992
##          mean_ThermalConductivity  wtd_mean_ThermalConductivity
##                  -8.9395266        21.7210488
##          gmean_ThermalConductivity  wtd_gmean_ThermalConductivity
##                  -10.4250911       -11.1961674
##          entropy_ThermalConductivity  wtd_entropy_ThermalConductivity
##                  9.8595419         4.4944976
##          range_ThermalConductivity  wtd_range_ThermalConductivity
##                  -14.7660820       -10.0922047
##          std_ThermalConductivity   wtd_std_ThermalConductivity
##                  23.1133167        6.7111089
##          mean_Valence           wtd_mean_Valence
##                  17.1663329        -28.1639820
##          gmean_Valence          wtd_gmean_Valence
##                  -15.3827859        17.6163793
##          entropy_Valence        wtd_entropy_Valence
##                  46.8051805        -16.6576560
##          range_Valence          wtd_range_Valence
##                  5.9205966         2.3658486
##          wtd_std_Valence
##                  -5.7515839

```

```
getTrainPerf(linear_forward_trans)
```

```

##    TrainRMSE TrainRsquared TrainMAE      method
## 1  18.06173     0.7228009 13.47109  leapForward

```

From the above metrics, the best model is model with 80 variables, this is more than the one from backward selection. This is because the algorithm find the best model randomly. The R-Squared for this model is 0.7228009 with Train MSE is 326.1636

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_forward_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

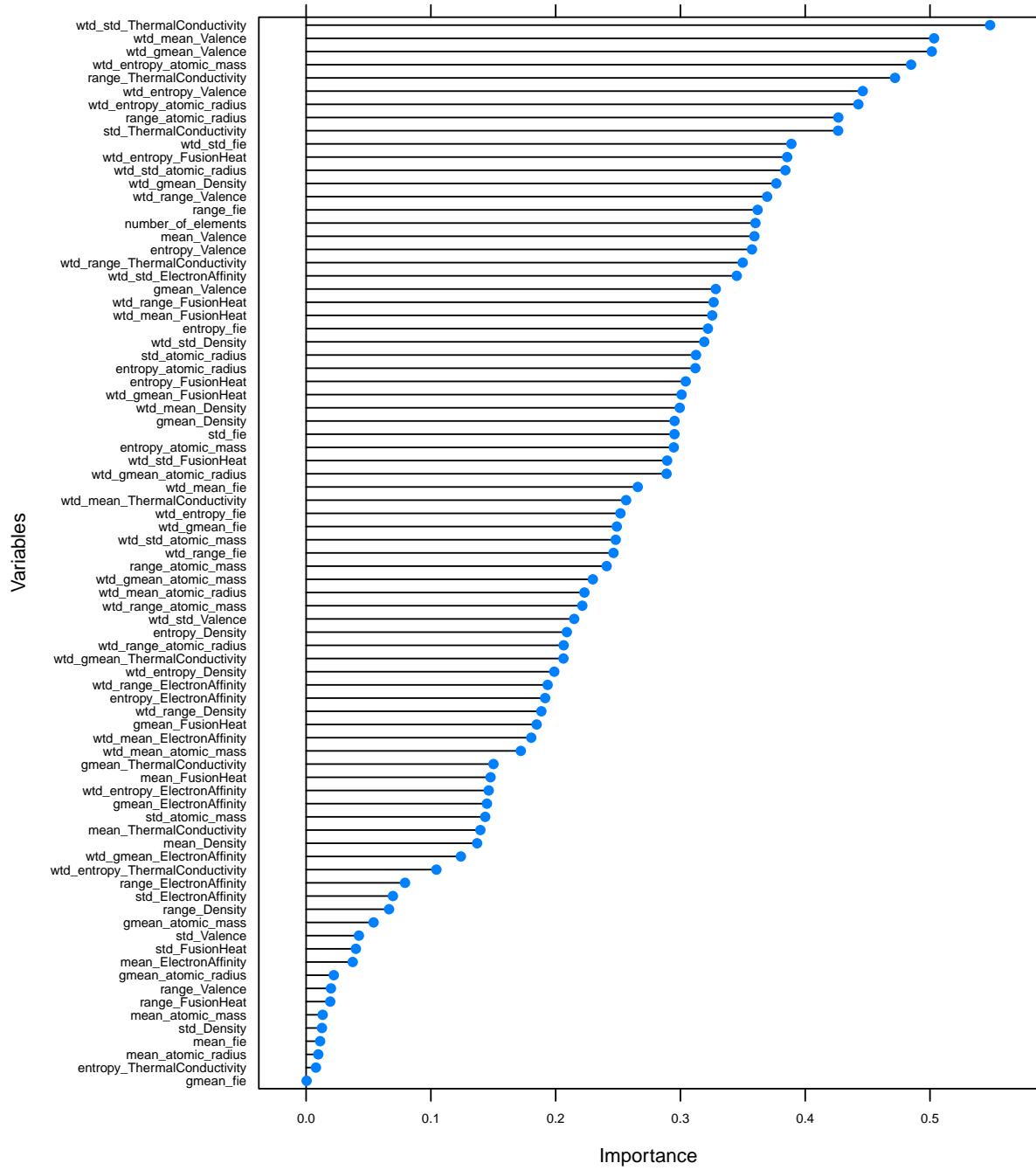


Figure 70: Variables Importance for Forward Selection Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.6 Linear Regression with Stepwise Selection

In this sub section, we will perform the stepwise selection which is the combination of forward and backward selections.

```
set.seed(seed)

# Linear Regression with Stepwise Selection
linear_stepwise_trans <- train(critical_temp ~., data = train.data,
                                method = "leapSeq",
                                tuneGrid = data.frame(nvmax = 1:(ncol(train.data)-1)),
                                trControl = control,
                                preProc = c("center", "scale", "BoxCox")
                                )

summary(linear_stepwise_trans)

## Subset selection object
## 81 Variables  (and intercept)
##                                     Forced in    Forced out
## number_of_elements             FALSE      FALSE
## mean_atomic_mass              FALSE      FALSE
## wtd_mean_atomic_mass          FALSE      FALSE
## gmean_atomic_mass             FALSE      FALSE
## wtd_gmean_atomic_mass         FALSE      FALSE
## entropy_atomic_mass           FALSE      FALSE
## wtd_entropy_atomic_mass       FALSE      FALSE
## range_atomic_mass             FALSE      FALSE
## wtd_range_atomic_mass         FALSE      FALSE
## std_atomic_mass               FALSE      FALSE
## wtd_std_atomic_mass           FALSE      FALSE
## mean_fie                      FALSE      FALSE
## wtd_mean_fie                 FALSE      FALSE
## gmean_fie                     FALSE      FALSE
## wtd_gmean_fie                FALSE      FALSE
## entropy_fie                   FALSE      FALSE
## wtd_entropy_fie               FALSE      FALSE
## range_fie                     FALSE      FALSE
## wtd_range_fie                FALSE      FALSE
## std_fie                       FALSE      FALSE
## wtd_std_fie                  FALSE      FALSE
## mean_atomic_radius            FALSE      FALSE
## wtd_mean_atomic_radius        FALSE      FALSE
## gmean_atomic_radius           FALSE      FALSE
## wtd_gmean_atomic_radius       FALSE      FALSE
## entropy_atomic_radius         FALSE      FALSE
## wtd_entropy_atomic_radius     FALSE      FALSE
## range_atomic_radius           FALSE      FALSE
## wtd_range_atomic_radius       FALSE      FALSE
## std_atomic_radius             FALSE      FALSE
## wtd_std_atomic_radius         FALSE      FALSE
## mean_Density                  FALSE      FALSE
## wtd_mean_Density              FALSE      FALSE
## gmean_Density                 FALSE      FALSE
```

```

## wtd_gmean_Density           FALSE  FALSE
## entropy_Density             FALSE  FALSE
## wtd_entropy_Density         FALSE  FALSE
## range_Density               FALSE  FALSE
## wtd_range_Density           FALSE  FALSE
## std_Density                 FALSE  FALSE
## wtd_std_Density              FALSE  FALSE
## mean_ElectronAffinity       FALSE  FALSE
## wtd_mean_ElectronAffinity   FALSE  FALSE
## gmean_ElectronAffinity      FALSE  FALSE
## wtd_gmean_ElectronAffinity  FALSE  FALSE
## entropy_ElectronAffinity    FALSE  FALSE
## wtd_entropy_ElectronAffinity FALSE  FALSE
## range_ElectronAffinity      FALSE  FALSE
## wtd_range_ElectronAffinity  FALSE  FALSE
## std_ElectronAffinity        FALSE  FALSE
## wtd_std_ElectronAffinity    FALSE  FALSE
## mean_FusionHeat              FALSE  FALSE
## wtd_mean_FusionHeat          FALSE  FALSE
## gmean_FusionHeat             FALSE  FALSE
## wtd_gmean_FusionHeat         FALSE  FALSE
## entropy_FusionHeat           FALSE  FALSE
## wtd_entropy_FusionHeat        FALSE  FALSE
## range_FusionHeat              FALSE  FALSE
## wtd_range_FusionHeat          FALSE  FALSE
## std_FusionHeat                FALSE  FALSE
## wtd_std_FusionHeat            FALSE  FALSE
## mean_ThermalConductivity    FALSE  FALSE
## wtd_mean_ThermalConductivity FALSE  FALSE
## gmean_ThermalConductivity   FALSE  FALSE
## wtd_gmean_ThermalConductivity FALSE  FALSE
## entropy_ThermalConductivity FALSE  FALSE
## wtd_entropy_ThermalConductivity FALSE  FALSE
## range_ThermalConductivity   FALSE  FALSE
## wtd_range_ThermalConductivity FALSE  FALSE
## std_ThermalConductivity     FALSE  FALSE
## wtd_std_ThermalConductivity  FALSE  FALSE
## mean_Valence                 FALSE  FALSE
## wtd_mean_Valence             FALSE  FALSE
## gmean_Valence                FALSE  FALSE
## wtd_gmean_Valence            FALSE  FALSE
## entropy_Valence              FALSE  FALSE
## wtd_entropy_Valence          FALSE  FALSE
## range_Valence                FALSE  FALSE
## wtd_range_Valence            FALSE  FALSE
## std_Valence                  FALSE  FALSE
## wtd_std_Valence              FALSE  FALSE
## 1 subsets of each size up to 58
## Selection Algorithm: 'sequential replacement'
##          number_of_elements mean_atomic_mass wtd_mean_atomic_mass
## 1  ( 1 )    " "           " "           " "
## 2  ( 1 )    " "           " "           " "
## 3  ( 1 )    " "           " "           " "
## 4  ( 1 )    " "           " "           " "

```

```

## 5  ( 1 )   " "
## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 ) "*" "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 ) "*" "
## 17 ( 1 )   " "
## 18 ( 1 )   " "
## 19 ( 1 )   " "
## 20 ( 1 )   " "
## 21 ( 1 )   " "
## 22 ( 1 )   " "
## 23 ( 1 )   " "
## 24 ( 1 )   " "
## 25 ( 1 )   " "
## 26 ( 1 )   " "
## 27 ( 1 )   " "
## 28 ( 1 )   " "
## 29 ( 1 )   " "
## 30 ( 1 )   " "
## 31 ( 1 )   " "
## 32 ( 1 )   " "
## 33 ( 1 ) "*" "
## 34 ( 1 )   " "
## 35 ( 1 )   " "
## 36 ( 1 )   " "
## 37 ( 1 )   " "
## 38 ( 1 ) "*" "
## 39 ( 1 )   " "
## 40 ( 1 ) "*" "
## 41 ( 1 )   " "
## 42 ( 1 )   " "
## 43 ( 1 )   " "
## 44 ( 1 ) "*" "
## 45 ( 1 )   " "
## 46 ( 1 )   " "
## 47 ( 1 ) "*" "
## 48 ( 1 )   " "
## 49 ( 1 )   " "
## 50 ( 1 )   " "
## 51 ( 1 )   " "
## 52 ( 1 ) "*" "
## 53 ( 1 )   " "
## 54 ( 1 )   " "
## 55 ( 1 )   " "
## 56 ( 1 ) "*" "
## 57 ( 1 ) "*" "
## 58 ( 1 ) "*" "

```

```

##          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
## 1      " "                 " "                  " "
## 2      ( 1 )               " "                  " "
## 3      ( 1 )               " "                  " "
## 4      ( 1 )               " "                  " "
## 5      ( 1 )               " "                  " "
## 6      ( 1 )               " "                  " "
## 7      ( 1 )               " "                  " "
## 8      ( 1 )               " "                  " "
## 9      ( 1 )               " "                  " "
## 10     ( 1 )              " "                  " "
## 11     ( 1 )              " "                  " "
## 12     ( 1 )              " "                  "*" 
## 13     ( 1 )              "*"                "*" 
## 14     ( 1 )              " "                  "*" 
## 15     ( 1 )              " "                  "*" 
## 16     ( 1 )              "*"                "*" 
## 17     ( 1 )              " "                  "*" 
## 18     ( 1 )              " "                  "*" 
## 19     ( 1 )              " "                  "*" 
## 20     ( 1 )              " "                  "*" 
## 21     ( 1 )              " "                  "*" 
## 22     ( 1 )              " "                  "*" 
## 23     ( 1 )              " "                  "*" 
## 24     ( 1 )              " "                  " " 
## 25     ( 1 )              " "                  " " 
## 26     ( 1 )              " "                  " " 
## 27     ( 1 )              " "                  " " 
## 28     ( 1 )              " "                  " " 
## 29     ( 1 )              " "                  " " 
## 30     ( 1 )              " "                  " " 
## 31     ( 1 )              " "                  " " 
## 32     ( 1 )              " "                  " " 
## 33     ( 1 )              "*"                "*" 
## 34     ( 1 )              " "                  "*" 
## 35     ( 1 )              " "                  "*" 
## 36     ( 1 )              " "                  "*" 
## 37     ( 1 )              " "                  "*" 
## 38     ( 1 )              "*"                "*" 
## 39     ( 1 )              " "                  "*" 
## 40     ( 1 )              "*"                "*" 
## 41     ( 1 )              " "                  "*" 
## 42     ( 1 )              " "                  "*" 
## 43     ( 1 )              " "                  "*" 
## 44     ( 1 )              "*"                "*" 
## 45     ( 1 )              " "                  "*" 
## 46     ( 1 )              " "                  "*" 
## 47     ( 1 )              "*"                "*" 
## 48     ( 1 )              " "                  "*" 
## 49     ( 1 )              " "                  "*" 
## 50     ( 1 )              " "                  "*" 
## 51     ( 1 )              " "                  "*" 
## 52     ( 1 )              "*"                "*" 
## 53     ( 1 )              " "                  "*"

```

```

## 54  ( 1 ) " "          " "          "*"
## 55  ( 1 ) " "          " "          "*"
## 56  ( 1 ) " "          "*"         " "
## 57  ( 1 ) "*"         "*"         "*"
## 58  ( 1 ) " "          "*"         " "
##           wtd_entropy_atomic_mass range_atomic_mass wtd_range_atomic_mass
## 1  ( 1 ) " "          " "          " "
## 2  ( 1 ) " "          " "          " "
## 3  ( 1 ) " "          " "          " "
## 4  ( 1 ) " "          " "          " "
## 5  ( 1 ) " "          " "          " "
## 6  ( 1 ) " "          " "          " "
## 7  ( 1 ) " "          " "          " "
## 8  ( 1 ) " "          " "          " "
## 9  ( 1 ) " "          " "          " "
## 10 ( 1 ) " "          " "          " "
## 11 ( 1 ) " "          " "          " "
## 12 ( 1 ) " "          " "          " "
## 13 ( 1 ) "*"         "*"         "*"
## 14 ( 1 ) " "          " "          " "
## 15 ( 1 ) " "          " "          " "
## 16 ( 1 ) "*"         "*"         "*"
## 17 ( 1 ) " "          " "          " "
## 18 ( 1 ) " "          " "          " "
## 19 ( 1 ) " "          " "          " "
## 20 ( 1 ) "*"         " "          " "
## 21 ( 1 ) "*"         " "          " "
## 22 ( 1 ) "*"         " "          " "
## 23 ( 1 ) "*"         "*"         " "
## 24 ( 1 ) " "          "*"         " "
## 25 ( 1 ) " "          "*"         " "
## 26 ( 1 ) " "          "*"         " "
## 27 ( 1 ) " "          "*"         " "
## 28 ( 1 ) " "          "*"         " "
## 29 ( 1 ) " "          "*"         " "
## 30 ( 1 ) " "          "*"         " "
## 31 ( 1 ) " "          "*"         " "
## 32 ( 1 ) " "          "*"         " "
## 33 ( 1 ) "*"         "*"         "*"
## 34 ( 1 ) "*"         "*"         " "
## 35 ( 1 ) "*"         "*"         " "
## 36 ( 1 ) "*"         "*"         " "
## 37 ( 1 ) "*"         "*"         " "
## 38 ( 1 ) "*"         "*"         "*"
## 39 ( 1 ) "*"         "*"         " "
## 40 ( 1 ) "*"         "*"         "*"
## 41 ( 1 ) "*"         "*"         " "
## 42 ( 1 ) "*"         "*"         " "
## 43 ( 1 ) "*"         "*"         " "
## 44 ( 1 ) "*"         "*"         "*"
## 45 ( 1 ) "*"         "*"         " "
## 46 ( 1 ) "*"         "*"         " "
## 47 ( 1 ) "*"         "*"         "*"
## 48 ( 1 ) "*"         "*"         " "

```

```

## 49  ( 1 ) "*"      "*"      " "
## 50  ( 1 ) "*"      "*"      " "
## 51  ( 1 ) "*"      "*"      " "
## 52  ( 1 ) "*"      "*"      "*"
## 53  ( 1 ) "*"      "*"      " "
## 54  ( 1 ) "*"      "*"      " "
## 55  ( 1 ) " "      "*"      " "
## 56  ( 1 ) " "      "*"      " "
## 57  ( 1 ) "*"      "*"      "*"
## 58  ( 1 ) " "      "*"      " "

##          std_atomic_mass wtd_std_atomic_mass mean_fie wtd_mean_fie
## 1  ( 1 ) " "        " "        " "        " "
## 2  ( 1 ) " "        " "        " "        " "
## 3  ( 1 ) " "        " "        " "        " "
## 4  ( 1 ) " "        " "        " "        " "
## 5  ( 1 ) " "        " "        " "        " "
## 6  ( 1 ) " "        " "        " "        " "
## 7  ( 1 ) " "        " "        " "        " "
## 8  ( 1 ) " "        " "        " "        " "
## 9  ( 1 ) " "        " "        " "        " "
## 10 ( 1 ) " "        " "        " "        " "
## 11 ( 1 ) " "        " "        " "        " "
## 12 ( 1 ) " "        " "        " "        " "
## 13 ( 1 ) "*"      "*"      "*"
## 14 ( 1 ) " "        " "        " "        " "
## 15 ( 1 ) " "        " "        " "        " "
## 16 ( 1 ) "*"      "*"      "*"
## 17 ( 1 ) " "        " "        " "        " "
## 18 ( 1 ) " "        " "        " "        " "
## 19 ( 1 ) " "        " "        " "        " "
## 20 ( 1 ) " "        " "        " "        " "
## 21 ( 1 ) " "        " "        " "        " "
## 22 ( 1 ) " "        " "        " "        " "
## 23 ( 1 ) " "        " "        " "        " "
## 24 ( 1 ) " "        " "        " "        " "
## 25 ( 1 ) " "        " "        " "        " "
## 26 ( 1 ) " "        "*"      " "
## 27 ( 1 ) " "        "*"      " "
## 28 ( 1 ) " "        "*"      " "
## 29 ( 1 ) " "        "*"      " "
## 30 ( 1 ) " "        "*"      " "
## 31 ( 1 ) " "        "*"      " "
## 32 ( 1 ) " "        "*"      " "
## 33 ( 1 ) "*"      "*"      "*"
## 34 ( 1 ) " "        " "        " "
## 35 ( 1 ) " "        "*"      " "
## 36 ( 1 ) " "        "*"      " "
## 37 ( 1 ) " "        " "        " "
## 38 ( 1 ) "*"      "*"      "*"
## 39 ( 1 ) " "        "*"      " "
## 40 ( 1 ) "*"      "*"      "*"
## 41 ( 1 ) " "        "*"      " "
## 42 ( 1 ) " "        "*"      " "
## 43 ( 1 ) " "        "*"      " "

```

```

## 44  ( 1 ) "*"      "*"      "*"      "*"      "*"
## 45  ( 1 ) " "     "*"      " "      " "      " "
## 46  ( 1 ) " "     "*"      " "      " "      " "
## 47  ( 1 ) "*"      "*"      "*"      "*"      "*"
## 48  ( 1 ) " "     "*"      " "      " "      " "
## 49  ( 1 ) " "     "*"      " "      " "      " "
## 50  ( 1 ) " "     "*"      " "      " "      " "
## 51  ( 1 ) " "     "*"      " "      " "      " "
## 52  ( 1 ) "*"      "*"      "*"      "*"      "*"
## 53  ( 1 ) " "     "*"      " "      " "      " "
## 54  ( 1 ) " "     "*"      " "      " "      " "
## 55  ( 1 ) " "     "*"      " "      " "      " "
## 56  ( 1 ) " "     "*"      " "      " "      " "
## 57  ( 1 ) "*"      "*"      "*"      "*"      "*"
## 58  ( 1 ) " "     "*"      " "      " "      " "
##          gmean_fie wtd_gmean_fie entropy_fie wtd_entropy_fie range_fie
## 1  ( 1 ) " "     " "      " "      " "      " "
## 2  ( 1 ) " "     " "      " "      " "      " "
## 3  ( 1 ) " "     " "      " "      " "      " "
## 4  ( 1 ) " "     " "      " "      " "      " "
## 5  ( 1 ) " "     " "      " "      " "      " "
## 6  ( 1 ) " "     " "      " "      " "      " "
## 7  ( 1 ) " "     " "      " "      " "      " "
## 8  ( 1 ) " "     " "      " "      " "      " "
## 9  ( 1 ) " "     " "      " "      " "      " "
## 10 ( 1 ) " "     " "      " "      " "      " "
## 11 ( 1 ) " "     " "      " "      " "      " "
## 12 ( 1 ) " "     " "      " "      " "      " "
## 13 ( 1 ) " "     " "      " "      " "      " "
## 14 ( 1 ) " "     " "      " "      " "      " "
## 15 ( 1 ) " "     " "      " "      " "      " "
## 16 ( 1 ) "*"      "*"      "*"      " "      " "
## 17 ( 1 ) " "     " "      " "      " "      " "
## 18 ( 1 ) " "     " "      " "      " "      " "
## 19 ( 1 ) " "     " "      " "      " "      " "
## 20 ( 1 ) " "     " "      " "      " "      " "
## 21 ( 1 ) " "     " "      " "      " "      " "
## 22 ( 1 ) " "     " "      " "      " "      " "
## 23 ( 1 ) " "     " "      " "      " "      " "
## 24 ( 1 ) " "     " "      " "      " "      " "
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## 37 ( 1 ) " "     " "      " "      " "      " "
## 38 ( 1 ) "*"      "*"      "*"      "*"      "*"

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##          wtd_range_fie std_fie wtd_std_fie mean_atomic_radius
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## 16 ( 1 ) " "      " "      " "      " "
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## 27 ( 1 ) " "      " "      " "      " "
## 28 ( 1 ) " "      " "      " "      " "
## 29 ( 1 ) " "      " "      " "      " "
## 30 ( 1 ) " "      " "      " "      " "
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## 16 ( 1 ) " "      " "
## 17 ( 1 ) " "      " "
## 18 ( 1 ) " "      " "
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## 21 ( 1 ) " "      " "
## 22 ( 1 ) " "      " "
## 23 ( 1 ) " "      " "
## 24 ( 1 ) " "      " "
## 25 ( 1 ) " "      " "
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## 27 ( 1 ) " "      " "
## 28 ( 1 ) " "      " "

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## 6  ( 1 ) " "
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## 8  ( 1 ) " "
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## 21 ( 1 ) " "
## 22 ( 1 ) " "
## 23 ( 1 ) " "

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## 9  ( 1 ) " "          "*"         " "
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## 11 ( 1 ) " "          " "          " "
## 12 ( 1 ) " "          "*"         " "
## 13 ( 1 ) " "          " "          " "

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## 3  ( 1 ) " "      " "      " "      " "
## 4  ( 1 ) " "      " "      " "      " "
## 5  ( 1 ) " "      " "      " "      " "
## 6  ( 1 ) " "      " "      " "      " "
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## 8  ( 1 ) " "      " "      " "      " "

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## 14 ( 1 )   " "      " "      " "
## 15 ( 1 )   " "      " "      " "
## 16 ( 1 )   " "      " "      " "
## 17 ( 1 )   " "      " "      " "
## 18 ( 1 )   " "      " "      " "
## 19 ( 1 )   " "      " "      " "
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## 42 ( 1 )   " "      " "      "*"
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## 49 ( 1 )   " "      " "      "*"
## 50 ( 1 )   " "      " "      "*"
## 51 ( 1 )   " "      " "      "*"
## 52 ( 1 )   "*"     "*"     "*"     "*"
## 53 ( 1 )   " "      " "      "*"
## 54 ( 1 )   " "      " "      "*"
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## 57 ( 1 )   "*"     "*"     "*"     "*"
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## 3  ( 1 )   " "      " "      " "

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## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   " "
## 16 ( 1 )   " "
## 17 ( 1 )   " "
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## 19 ( 1 )   " "
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## 43 ( 1 )   "*"
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## 46 ( 1 )   "*"
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## 51 ( 1 )   "*"
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## 56 ( 1 )   "*"
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## 6  ( 1 ) " "          " "          " "
## 7  ( 1 ) " "          " "          " "
## 8  ( 1 ) " "          " "          " "
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## 10 ( 1 ) " "          " "          " "
## 11 ( 1 ) " "          " "          " "
## 12 ( 1 ) " "          " "          " "
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## 15 ( 1 ) " "          " "          " "
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## 51 ( 1 ) " "          " "          "*"
## 52 ( 1 ) "*"          "*"          "*"

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## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          "*"          "
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## 7  ( 1 ) " "          "*"          "
## 8  ( 1 ) " "          "*"          "
## 9  ( 1 ) " "          "*"          "
## 10 ( 1 ) " "          "*"          "
## 11 ( 1 ) " "          "*"          "
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## 15 ( 1 ) " "          "*"          "
## 16 ( 1 ) " "          " "
## 17 ( 1 ) " "          "*"          "
## 18 ( 1 ) " "          "*"          "
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## 21 ( 1 ) " "          "*"          "
## 22 ( 1 ) " "          "*"          "
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## 42 ( 1 ) " "          "*"          "
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## 45 ( 1 ) " "          "*"          "
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## 47 ( 1 ) "*"          "*"          "

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## 57  ( 1 ) "*"          "*"
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## 2  ( 1 ) "*"          " "
## 3  ( 1 ) "*"          " "
## 4  ( 1 ) " "          "*"
## 5  ( 1 ) " "          "*"
## 6  ( 1 ) " "          "*"
## 7  ( 1 ) " "          "*"
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## 9  ( 1 ) " "          "*"
## 10 ( 1 ) " "          "*"
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## 33 ( 1 ) " "          " "
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## 35 ( 1 ) "*"          "*"
## 36 ( 1 ) "*"          "*"
## 37 ( 1 ) "*"          "*"
## 38 ( 1 ) " "          " "
## 39 ( 1 ) "*"          "*"
## 40 ( 1 ) " "          " "
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## 42 ( 1 ) "*"          "*"

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## 55  ( 1 ) "*"          "*"
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## 57  ( 1 ) "*"          "*"
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## 1  ( 1 ) " "          " "
## 2  ( 1 ) " "          " "
## 3  ( 1 ) " "          " "
## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "
## 11 ( 1 ) " "          " "
## 12 ( 1 ) " "          " "
## 13 ( 1 ) " "          " "
## 14 ( 1 ) " "          " "
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## 16 ( 1 ) " "          " "
## 17 ( 1 ) " "          " "
## 18 ( 1 ) " "          " "
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## 20 ( 1 ) " "          " "
## 21 ( 1 ) " "          " "
## 22 ( 1 ) " "          " "
## 23 ( 1 ) " "          " "
## 24 ( 1 ) " "          " "
## 25 ( 1 ) " "          " "
## 26 ( 1 ) " "          " "
## 27 ( 1 ) " "          " "
## 28 ( 1 ) " "          "*"
## 29 ( 1 ) " "          " "
## 30 ( 1 ) " "          " "
## 31 ( 1 ) "*"          " "
## 32 ( 1 ) " "          "*"
## 33 ( 1 ) " "          " "
## 34 ( 1 ) " "          "*"
## 35 ( 1 ) " "          "*"
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## 37 ( 1 ) " "          "*"

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## 32 ( 1 ) "*"

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##           std_ElectronAffinity wtd_std_ElectronAffinity mean_FusionHeat
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## 4 ( 1 ) " "          " "          " "
## 5 ( 1 ) " "          " "          " "
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## 7 ( 1 ) " "          "*" "
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## 22 ( 1 ) "*" "
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## 24 ( 1 ) "*" "
## 25 ( 1 ) "*" "
## 26 ( 1 ) "*" "
## 27 ( 1 ) "*" "

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## 34  ( 1 ) "*"          "*"
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## 37  ( 1 ) "*"          "*"
## 38  ( 1 ) " "          " "
## 39  ( 1 ) "*"          "*"
## 40  ( 1 ) " "          " "
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## 42  ( 1 ) "*"          "*"
## 43  ( 1 ) "*"          "*"
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## 45  ( 1 ) "*"          "*"
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## 49  ( 1 ) "*"          "*"
## 50  ( 1 ) "*"          "*"
## 51  ( 1 ) "*"          "*"
## 52  ( 1 ) "*"          "*"
## 53  ( 1 ) "*"          "*"
## 54  ( 1 ) "*"          "*"
## 55  ( 1 ) "*"          "*"
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##           wtd_mean_FusionHeat gmean_FusionHeat wtd_gmean_FusionHeat
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## 4  ( 1 ) " "          " "          " "
## 5  ( 1 ) " "          " "          " "
## 6  ( 1 ) " "          " "          " "
## 7  ( 1 ) " "          " "          " "
## 8  ( 1 ) " "          " "          " "
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## 11 ( 1 ) " "          " "          " "
## 12 ( 1 ) " "          " "          " "
## 13 ( 1 ) " "          " "          " "
## 14 ( 1 ) " "          " "          " "
## 15 ( 1 ) " "          " "          " "
## 16 ( 1 ) " "          " "          " "
## 17 ( 1 ) " "          " "          " "
## 18 ( 1 ) " "          " "          " "
## 19 ( 1 ) " "          " "          " "
## 20 ( 1 ) " "          " "          " "
## 21 ( 1 ) " "          " "          " "
## 22 ( 1 ) " "          " "          " "

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## 36 ( 1 ) "*"
## 37 ( 1 ) "*"
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## 49 ( 1 ) "*"
## 50 ( 1 ) "*"
## 51 ( 1 ) "*"
## 52 ( 1 ) " "
## 53 ( 1 ) "*"
## 54 ( 1 ) "*"
## 55 ( 1 ) "*"
## 56 ( 1 ) "*"
## 57 ( 1 ) "*"
## 58 ( 1 ) "*"
##          entropy_FusionHeat wtd_entropy_FusionHeat range_FusionHeat
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## 2 ( 1 ) " "
## 3 ( 1 ) " "
## 4 ( 1 ) " "
## 5 ( 1 ) " "
## 6 ( 1 ) " "
## 7 ( 1 ) " "
## 8 ( 1 ) " "
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## 10 ( 1 ) " "
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## 13 ( 1 ) " "
## 14 ( 1 ) " "
## 15 ( 1 ) " "
## 16 ( 1 ) " "
## 17 ( 1 ) " "

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## 22 ( 1 ) " "      " "      "*"
## 23 ( 1 ) " "      " "      "*"
## 24 ( 1 ) " "      " "      "*"
## 25 ( 1 ) " "      " "      "*"
## 26 ( 1 ) " "      " "      "*"
## 27 ( 1 ) " "      " "      "*"
## 28 ( 1 ) " "      "*"     "*"
## 29 ( 1 ) " "      "*"     "*"
## 30 ( 1 ) " "      "*"     "*"
## 31 ( 1 ) " "      "*"     "*"
## 32 ( 1 ) " "      "*"     "*"
## 33 ( 1 ) " "      " "      "
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## 36 ( 1 ) " "      "*"     "*"
## 37 ( 1 ) " "      "*"     "*"
## 38 ( 1 ) " "      " "      "
## 39 ( 1 ) " "      "*"     "*"
## 40 ( 1 ) " "      " "      "
## 41 ( 1 ) " "      "*"     "*"
## 42 ( 1 ) " "      "*"     "*"
## 43 ( 1 ) " "      "*"     "*"
## 44 ( 1 ) " "      " "      "
## 45 ( 1 ) " "      "*"     "*"
## 46 ( 1 ) " "      "*"     "*"
## 47 ( 1 ) " "      " "      "
## 48 ( 1 ) " "      "*"     "*"
## 49 ( 1 ) " "      "*"     "*"
## 50 ( 1 ) " "      "*"     "*"
## 51 ( 1 ) "*"     "*"     "*"
## 52 ( 1 ) " "      " "      "
## 53 ( 1 ) "*"     "*"     "*"
## 54 ( 1 ) "*"     "*"     "*"
## 55 ( 1 ) "*"     "*"     "*"
## 56 ( 1 ) "*"     "*"     "*"
## 57 ( 1 ) "*"     "*"     "
## 58 ( 1 ) "*"     "*"     "*"
##          wtd_range_FusionHeat std_FusionHeat wtd_std_FusionHeat
## 1 ( 1 ) " "      " "      "
## 2 ( 1 ) " "      " "      "
## 3 ( 1 ) " "      " "      "
## 4 ( 1 ) " "      " "      "
## 5 ( 1 ) " "      " "      "
## 6 ( 1 ) " "      " "      "
## 7 ( 1 ) " "      " "      "
## 8 ( 1 ) " "      " "      "
## 9 ( 1 ) " "      " "      "
## 10 ( 1 ) " "     " "      "
## 11 ( 1 ) " "     " "      "*"
## 12 ( 1 ) " "     " "      "*"

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## 15 ( 1 ) " "      " "
## 16 ( 1 ) " "      " "
## 17 ( 1 ) " "      " "
## 18 ( 1 ) " "      " "
## 19 ( 1 ) " "      " "
## 20 ( 1 ) " "      " "
## 21 ( 1 ) " "      " "
## 22 ( 1 ) " "      " "
## 23 ( 1 ) " "      " "
## 24 ( 1 ) " "      " "
## 25 ( 1 ) " "      " "
## 26 ( 1 ) " "      " "
## 27 ( 1 ) " "      " "
## 28 ( 1 ) " "      " "
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## 30 ( 1 ) " "      "*"
## 31 ( 1 ) " "      "*"
## 32 ( 1 ) " "      "*"
## 33 ( 1 ) " "      " "
## 34 ( 1 ) "*"      " "
## 35 ( 1 ) "*"      " "
## 36 ( 1 ) " "      "*"
## 37 ( 1 ) " "      "*"
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## 40 ( 1 ) " "      " "
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## 44 ( 1 ) " "      " "
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## 46 ( 1 ) "*"      "*"
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## 49 ( 1 ) "*"      "*"
## 50 ( 1 ) "*"      "*"
## 51 ( 1 ) "*"      "*"
## 52 ( 1 ) " "      " "
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## 54 ( 1 ) "*"      "*"
## 55 ( 1 ) "*"      "*"
## 56 ( 1 ) "*"      "*"
## 57 ( 1 ) " "      " "
## 58 ( 1 ) "*"      "*"
##               mean_ThermalConductivity wtd_mean_ThermalConductivity
## 1 ( 1 ) " "      " "
## 2 ( 1 ) " "      " "
## 3 ( 1 ) " "      " "
## 4 ( 1 ) " "      " "
## 5 ( 1 ) " "      " "
## 6 ( 1 ) " "      " "
## 7 ( 1 ) " "      " "

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## 12 ( 1 )   " "
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## 17 ( 1 )   "*" 
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## 21 ( 1 )   "*" 
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## 33 ( 1 )   " "
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## 36 ( 1 )   "*" 
## 37 ( 1 )   "*" 
## 38 ( 1 )   " "
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## 40 ( 1 )   " "
## 41 ( 1 )   "*" 
## 42 ( 1 )   "*" 
## 43 ( 1 )   "*" 
## 44 ( 1 )   " "
## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   " "
## 48 ( 1 )   "*" 
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## 50 ( 1 )   "*" 
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## 54 ( 1 )   "*" 
## 55 ( 1 )   "*" 
## 56 ( 1 )   "*" 
## 57 ( 1 )   " "
## 58 ( 1 )   "*" 
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## 1  ( 1 )   " "
## 2  ( 1 )   " "

```

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## 3  ( 1 )   " "
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## 5  ( 1 )   " "
## 6  ( 1 )   " "
## 7  ( 1 )   " "
## 8  ( 1 )   " "
## 9  ( 1 )   " "
## 10 ( 1 )   " "
## 11 ( 1 )   " "
## 12 ( 1 )   " "
## 13 ( 1 )   " "
## 14 ( 1 )   " "
## 15 ( 1 )   "*" 
## 16 ( 1 )   " "
## 17 ( 1 )   "*" 
## 18 ( 1 )   "*" 
## 19 ( 1 )   "*" 
## 20 ( 1 )   "*" 
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## 22 ( 1 )   "*" 
## 23 ( 1 )   "*" 
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## 27 ( 1 )   "*" 
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## 29 ( 1 )   "*" 
## 30 ( 1 )   "*" 
## 31 ( 1 )   "*" 
## 32 ( 1 )   "*" 
## 33 ( 1 )   " "
## 34 ( 1 )   "*" 
## 35 ( 1 )   "*" 
## 36 ( 1 )   "*" 
## 37 ( 1 )   "*" 
## 38 ( 1 )   " "
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## 44 ( 1 )   " "
## 45 ( 1 )   "*" 
## 46 ( 1 )   "*" 
## 47 ( 1 )   " "
## 48 ( 1 )   "*" 
## 49 ( 1 )   "*" 
## 50 ( 1 )   "*" 
## 51 ( 1 )   "*" 
## 52 ( 1 )   " "
## 53 ( 1 )   "*" 
## 54 ( 1 )   "*" 
## 55 ( 1 )   "*" 
## 56 ( 1 )   "*"

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## 4  ( 1 ) " "          " "
## 5  ( 1 ) " "          " "
## 6  ( 1 ) " "          " "
## 7  ( 1 ) " "          " "
## 8  ( 1 ) " "          " "
## 9  ( 1 ) " "          " "
## 10 ( 1 ) " "          " "
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## 12 ( 1 ) " "          "*"
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## 21 ( 1 ) "*"          "*"
## 22 ( 1 ) "*"          "*"
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## 34 ( 1 ) "*"          "*"
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## 38 ( 1 ) " "          " "
## 39 ( 1 ) "*"          "*"
## 40 ( 1 ) " "          " "
## 41 ( 1 ) "*"          "*"
## 42 ( 1 ) "*"          "*"
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## 44 ( 1 ) " "          " "
## 45 ( 1 ) "*"          "*"
## 46 ( 1 ) "*"          "*"
## 47 ( 1 ) " "          " "
## 48 ( 1 ) "*"          "*"
## 49 ( 1 ) "*"          "*"
## 50 ( 1 ) "*"          "*"
## 51 ( 1 ) "*"          "*"

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## 56  ( 1 ) "*"
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## 58  ( 1 ) "*"
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## 2  ( 1 ) " "
## 3  ( 1 ) " "
## 4  ( 1 ) " "
## 5  ( 1 ) " "
## 6  ( 1 ) " "
## 7  ( 1 ) " "
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## 11 ( 1 ) "*"
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## 27 ( 1 ) " "
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## 45 ( 1 ) "*"
## 46 ( 1 ) "*"

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## 8  ( 1 ) " "           "*" "
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## 14 ( 1 ) " "           "*" "
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## 16 ( 1 ) " "           " "
## 17 ( 1 ) " "           "*" "
## 18 ( 1 ) " "           "*" "
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## 20 ( 1 ) " "           "*" "
## 21 ( 1 ) " "           "*" "
## 22 ( 1 ) " "           "*" "
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## 34 ( 1 ) " "           "*" "
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## 39 ( 1 ) "*" "
## 40 ( 1 ) " "           " "
## 41 ( 1 ) "*" "

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## 42 ( 1 ) "*"      "*"      " "
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## 51 ( 1 ) "*"      "*"      " "
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##          wtd_mean_Valence gmean_Valence wtd_gmean_Valence entropy_Valence
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linear_stepwise_trans$results

##      nvmax      RMSE   Rsquared      MAE     RMSESD   RsquaredSD     MAESD
## 1       1 23.73833 0.5198107 18.24597 0.2467303 0.008466076 0.2298375
## 2       2 22.77972 0.5577446 17.59998 0.2190986 0.009593824 0.2049417
## 3       3 22.01319 0.5870264 17.23048 0.2361849 0.009907962 0.2699336
## 4       4 21.44967 0.6079547 16.80859 0.1902049 0.009495616 0.1626152
## 5       5 20.94882 0.6260647 16.48752 0.1811812 0.009939315 0.1866227
## 6       6 20.65791 0.6363753 16.15813 0.1497790 0.008627713 0.1621507
## 7       7 20.42467 0.6444857 15.77413 0.1506396 0.007452758 0.1722256
## 8       8 20.19085 0.6525663 15.53950 0.1727360 0.008070484 0.2021921
## 9       9 20.08628 0.6561573 15.37467 0.1733370 0.008073159 0.2081623
## 10    10 19.95712 0.6605658 15.27684 0.2204478 0.009785714 0.2431182
## 11    11 19.83290 0.6648455 15.28049 0.2120748 0.009505936 0.2221913
## 12    12 20.21563 0.6491633 15.65851 1.7238990 0.068864303 1.3462794
## 13    13 21.69837 0.5926830 16.84487 2.9508396 0.109367158 2.4028491
## 14    14 19.87655 0.6609574 15.35584 1.6518801 0.064461055 1.3971909
## 15    15 19.32663 0.6816361 14.92684 0.3262955 0.012939107 0.3074274
## 16    16 20.52003 0.6367927 15.92885 2.2191309 0.084775318 1.8136520
## 17    17 19.10012 0.6890674 14.74872 0.2880812 0.011321498 0.2645709
## 18    18 18.97166 0.6932544 14.60046 0.2631660 0.011148373 0.2001065

```

```

## 19 19 20.84686 0.6248986 16.19422 2.6826603 0.094013489 2.2232729
## 20 20 18.82767 0.6978462 14.50014 0.2793265 0.011091446 0.2260402
## 21 21 18.78733 0.6991347 14.51079 0.2784994 0.010581343 0.2156906
## 22 22 18.75357 0.7002605 14.43084 0.2823154 0.010412037 0.2051394
## 23 23 20.42073 0.6410731 15.84276 2.2064910 0.076933533 1.9319837
## 24 24 18.63908 0.7038804 14.35473 0.2683192 0.010278532 0.2099186
## 25 25 18.55793 0.7064509 14.27405 0.2843836 0.010296714 0.2085286
## 26 26 18.51445 0.7078523 14.23606 0.2952845 0.010425173 0.2371643
## 27 27 18.85725 0.6959709 14.50935 1.4110177 0.044501681 1.0847976
## 28 28 18.44616 0.7099900 14.15611 0.2873639 0.010486341 0.2453747
## 29 29 18.40001 0.7114465 14.12219 0.2976418 0.010466511 0.2441590
## 30 30 18.62735 0.7038306 14.29813 0.8027488 0.027252447 0.6472537
## 31 31 18.34456 0.7131748 14.05357 0.3144470 0.011120294 0.2447821
## 32 32 18.58979 0.7046742 14.27322 0.9180330 0.034190392 0.8314472
## 33 33 18.79788 0.6980128 14.42021 1.2178320 0.038677474 0.9177170
## 34 34 18.48748 0.7082586 14.16353 0.7431865 0.026640616 0.5738093
## 35 35 18.21546 0.7172295 13.92322 0.3219818 0.011123526 0.2440779
## 36 36 18.19198 0.7179483 13.89863 0.3201801 0.011475644 0.2633434
## 37 37 18.61087 0.7043065 14.24735 0.9303195 0.030213219 0.7484784
## 38 38 18.58787 0.7045503 14.21410 1.0257954 0.036614177 0.7262742
## 39 39 18.98218 0.6931352 14.21453 2.0943813 0.067288504 0.7136752
## 40 40 18.54266 0.7060880 14.13325 1.0686064 0.035808361 0.7900066
## 41 41 19.51827 0.6761921 14.57854 2.3250574 0.073503833 0.9591431
## 42 42 18.67549 0.7030449 13.96372 2.0125200 0.064028922 0.6158027
## 43 43 18.27867 0.7147599 13.99094 0.7504749 0.026641543 0.5143094
## 44 44 18.43888 0.7093131 14.12363 1.0208529 0.035744884 0.8592826
## 45 45 18.24085 0.7163586 13.95169 0.5495711 0.014933011 0.5474653
## 46 46 18.20627 0.7170078 13.90231 0.7646978 0.026695429 0.5581931
## 47 47 18.20625 0.7171199 13.91931 0.6457801 0.022810652 0.4556426
## 48 48 18.18847 0.7177542 13.88909 0.7105439 0.022332131 0.5758834
## 49 49 18.15976 0.7187623 13.86351 0.6364853 0.019593209 0.5325272
## 50 50 18.09445 0.7207112 13.80639 0.5239422 0.018523224 0.3592336
## 51 51 18.11366 0.7202075 13.79702 0.7208480 0.020115765 0.5247142
## 52 52 18.08337 0.7213506 13.76968 0.3656274 0.008594298 0.3910421
## 53 53 17.90727 0.7266692 13.63562 0.3195754 0.010973428 0.1924238
## 54 54 18.89743 0.6967568 14.06302 1.8271308 0.055845912 0.6019598
## 55 55 18.77616 0.7009741 13.94801 1.9580621 0.058606773 0.5766184
## 56 56 17.84143 0.7286841 13.57587 0.3348299 0.011014459 0.2235424
## 57 57 18.38732 0.7118725 13.80003 1.4063800 0.045202078 0.5412456
## 58 58 17.80655 0.7297433 13.54902 0.3349053 0.010804777 0.2538353
## 59 59 18.79092 0.7010698 13.90156 2.2515068 0.065926231 0.6655683
## 60 60 17.90769 0.7265616 13.62736 0.4479740 0.015306774 0.2834832
## 61 61 17.93239 0.7258420 13.62709 0.5469123 0.016374756 0.4469859
## 62 62 18.41064 0.7128432 13.62070 2.0089033 0.058361718 0.4212771
## 63 63 18.11586 0.7208265 13.62510 0.7902345 0.024562420 0.2821729
## 64 64 18.11138 0.7209960 13.59631 0.9289858 0.027420044 0.4036824
## 65 65 18.08228 0.7221415 13.52586 1.0351277 0.030999676 0.2477799
## 66 66 18.09222 0.7218917 13.52026 1.0757438 0.032061782 0.2482453
## 67 67 18.20101 0.7183752 13.65306 0.9844554 0.028815106 0.4514264
## 68 68 18.21396 0.7184610 13.56093 1.2854928 0.037009868 0.3609844
## 69 69 18.17496 0.7194148 13.58772 1.0942742 0.032313125 0.3736568
## 70 70 17.88078 0.7273924 13.57359 0.4198472 0.014985192 0.3247162
## 71 71 18.15466 0.7199596 13.56549 1.0911161 0.032179153 0.3822446
## 72 72 18.15249 0.7204152 13.48578 1.2986493 0.037723712 0.2662976

```

```

## 73 73 18.06549 0.7225661 13.49457 0.9672402 0.029382016 0.2621734
## 74 74 18.11004 0.7214744 13.48808 1.1497655 0.033793124 0.2845690
## 75 75 17.82593 0.7291726 13.49680 0.3749279 0.012594848 0.2471028
## 76 76 18.10071 0.7216580 13.49721 1.0807438 0.032105298 0.2614887
## 77 77 18.09191 0.7219553 13.48161 1.0983212 0.032554076 0.2620113
## 78 78 18.08517 0.7220692 13.48386 1.0189629 0.030470944 0.2621218
## 79 79 18.02872 0.7236107 13.47565 0.9321811 0.028328354 0.2524276
## 80 80 17.98800 0.7247080 13.47118 0.8005527 0.024768474 0.2571303
## 81 81 18.06344 0.7227549 13.47126 1.0536750 0.031395839 0.2587849

```

From the above results, we can see how stepwise selection works and the corresponding errors to the number of variables. Here, we will plot and see the optimal number of variables.

```
plot_metrics(linear_stepwise_trans, linear_stepwise_trans$results$nvmax, "Number of Variables")
```

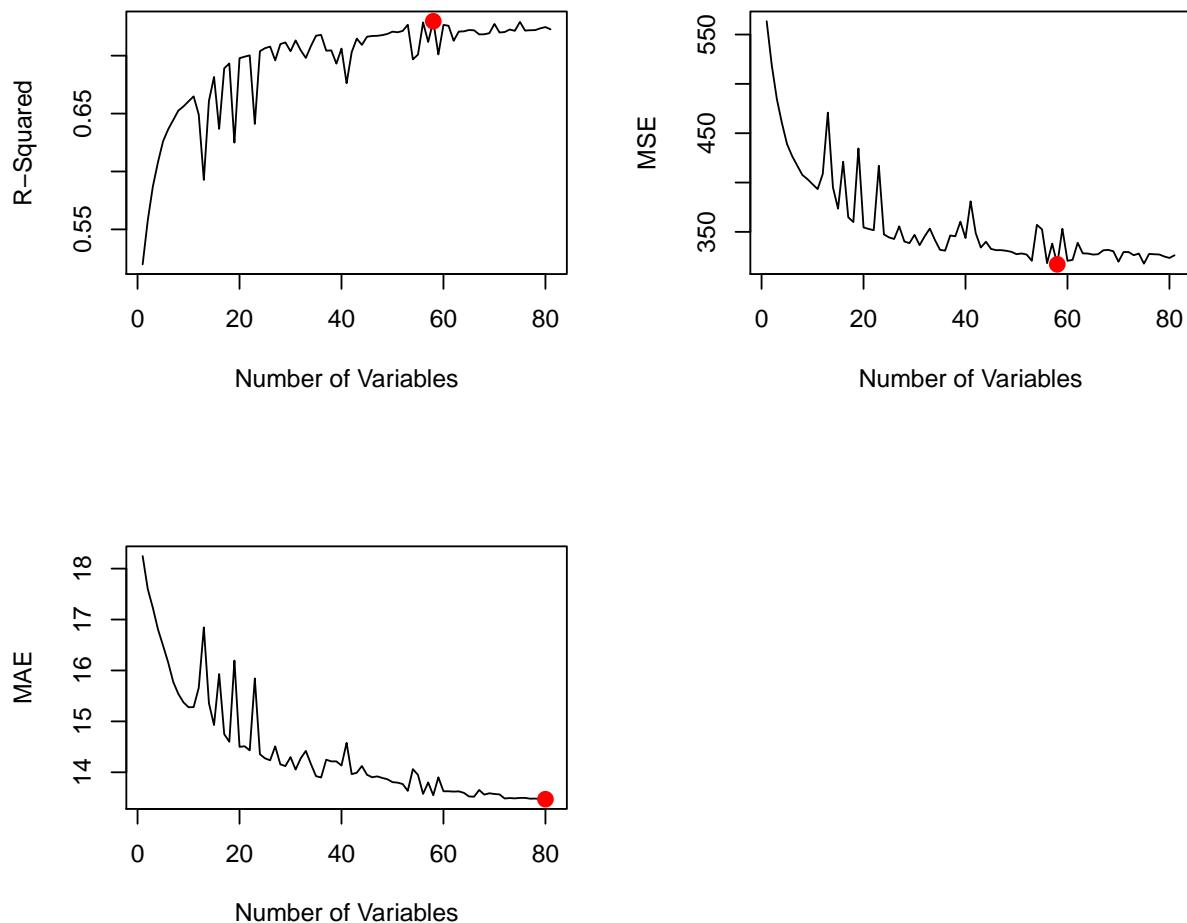


Figure 71: R-Squared, MSE, and MAE for Stepwise Selection Trans

```

linear_stepwise_trans$bestTune

##      nvmax
## 58      58

coef(linear_stepwise_trans$finalModel, linear_stepwise_trans$bestTune$nvmax)

##              (Intercept)          mean_atomic_mass
##                  34.444109           3.989050
##      wtd_gmean_atomic_mass range_atomic_mass
##                  -4.806391           9.194657
##      wtd_std_atomic_mass  entropy_fie
##                  -5.642161          -31.117085
##      wtd_entropy_fie     range_fie
##                  9.067704           19.678035
##      wtd_range_fie       std_fie
##                  5.437904          -15.697471
##      wtd_std_fie         mean_atomic_radius
##                  -6.909015           18.365051
##      wtd_mean_atomic_radius gmean_atomic_radius
##                  11.344534          -28.834430
##      wtd_entropy_atomic_radius range_atomic_radius
##                  15.565216           17.493569
##      wtd_range_atomic_radius std_atomic_radius
##                  -2.846926          -23.765248
##      wtd_std_atomic_radius wtd_gmean_Density
##                  10.172287           9.527348
##      wtd_entropy_Density   range_Density
##                  -9.742499          -6.709820
##      wtd_range_Density    std_Density
##                  -1.888567           8.622692
##      wtd_std_Density      wtd_mean_ElectronAffinity
##                  -5.050572           14.471037
##      gmean_ElectronAffinity wtd_gmean_ElectronAffinity
##                  3.685746          -15.262041
##      wtd_entropy_ElectronAffinity range_ElectronAffinity
##                  -6.362706          -26.209650
##      wtd_range_ElectronAffinity std_ElectronAffinity
##                  -4.769657           26.505366
##      wtd_std_ElectronAffinity mean_FusionHeat
##                  -7.715554          -17.599811
##      wtd_mean_FusionHeat   gmean_FusionHeat
##                  16.658681           20.708055
##      wtd_gmean_FusionHeat  entropy_FusionHeat
##                  -15.853736          -14.280561
##      wtd_entropy_FusionHeat range_FusionHeat
##                  10.637585          -15.639459
##      wtd_range_FusionHeat  std_FusionHeat
##                  5.263980           14.544540
##      wtd_std_FusionHeat   mean_ThermalConductivity
##                  -5.665764          -8.935898
##      wtd_mean_ThermalConductivity gmean_ThermalConductivity

```

```

##          20.445634          -9.702490
##   wtd_gmean_ThermalConductivity      10.059669
##          -11.278138          range_ThermalConductivity
##          3.972564          -16.869594
##   wtd_range_ThermalConductivity      std_ThermalConductivity
##          -9.378631          24.564701
##   wtd_std_ThermalConductivity      wtd_mean_Valence
##          6.975725          -7.802747
##   entropy_Valence      wtd_entropy_Valence
##          34.571499          -15.153236
##   range_Valence      wtd_range_Valence
##          6.986828          1.866188
##   wtd_std_Valence
##          -7.523263

getTrainPerf(linear_stepwise_trans)

##   TrainRMSE TrainRsquared TrainMAE   method
## 1  17.80655     0.7297433 13.54902  leapSeq

```

From the above metrics, it can be seen that based on R-Squared and MSE, the best model is the model with 58 variables, however, MAE choose a model with more variables. By using the feature from caret package, we can decide that the best model is the model with 54 variables. The list of 54 variables is provided above. The R-Squared for this model is 0.7297433 with Train MSE is 316.84. Those metrics are slightly lower than the original linear regression, however, this model decrease the number of variables from 81 to only 58, which is good in term of model complexity. In addition, this model is relatively better compared to the other stepwise models.

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(linear_stepwise_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

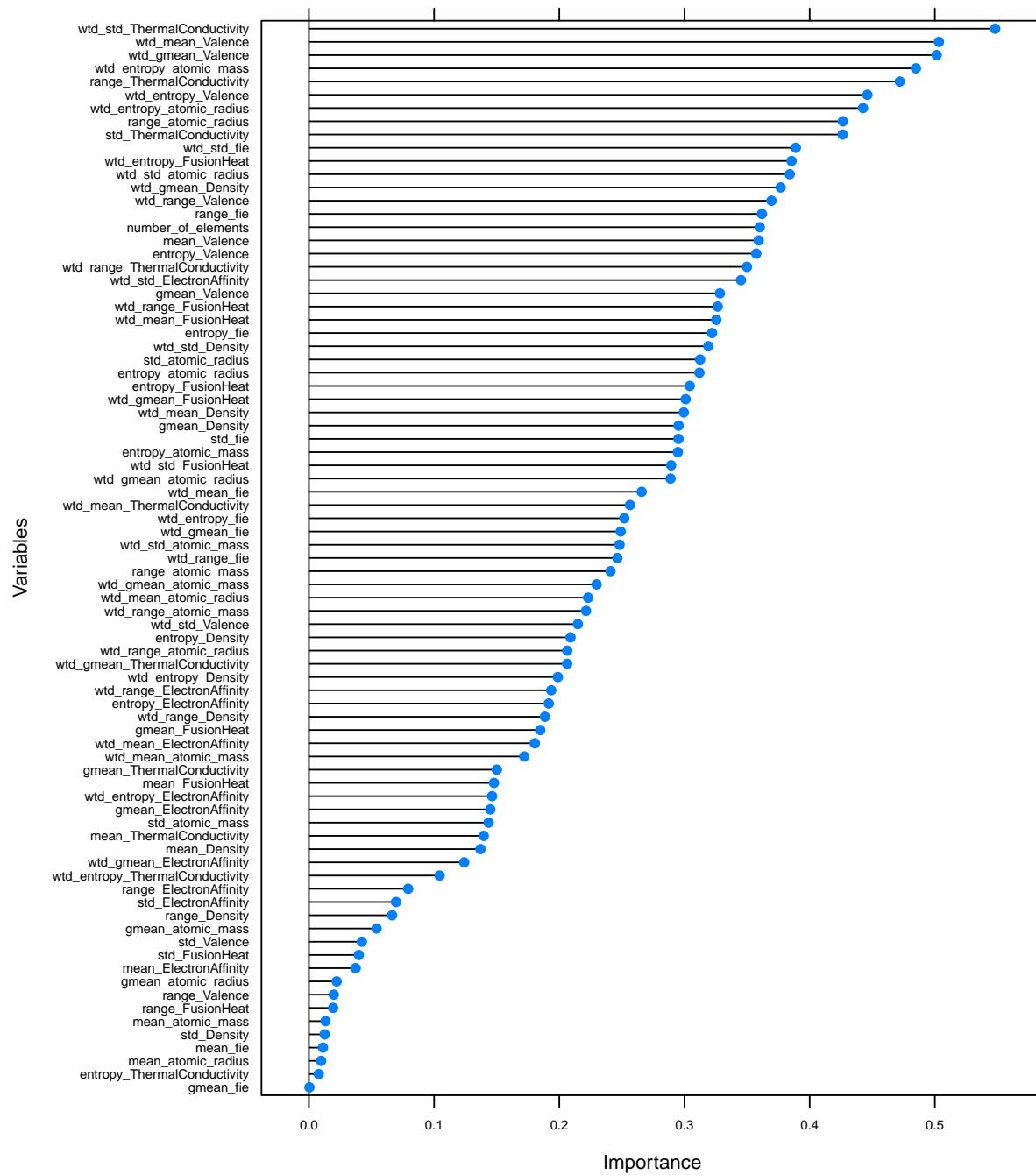


Figure 72: Variables Importance for Stepwise Selection Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.7 Ridge Regression

The standard linear model performs poorly in a situation, where you have a large multivariate data set containing a number of variables superior to the number of samples.

A better alternative is the penalized regression allowing to create a linear regression model that is penalized, for having too many variables in the model, by adding a constraint in the equation [Bruce and Bruce, 2017]. This is also known as shrinkage or regularization methods.

The consequence of imposing this penalty, is to reduce the coefficient values towards zero. This allows the less contributive variables to have a coefficient close to zero or equal zero.

Note that, the shrinkage requires the selection of a tuning parameter (lambda) that determines the amount of shrinkage.

In this sub section, we will perform Ridge regression. Ridge regression shrinks the regression coefficients, so that variables, with minor contribution to the outcome, have their coefficients close to zero.

The shrinkage of the coefficients is achieved by penalizing the regression model with a penalty term called L2-norm, which is the sum of the squared coefficients.

The amount of the penalty can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

lambda_seq <- seq(0.01, 1, length = 15)

# Ridge Regression
ridge_model_trans <- train(
  critical_temp ~.,
  data = train.data,
  method = "ridge",
  trControl = control,
  tuneGrid = expand.grid(lambda = lambda_seq),
  preProc = c("center", "scale", "BoxCox")
)

ridge_model_trans$results

##          lambda      RMSE   Rsquared       MAE     RMSESD   RsquaredSD     MAESD
## 1  0.01000000 18.43636  0.7108181 13.92396  0.8153076  0.026567892 0.2165090
## 2  0.08071429 19.20489  0.6866190 14.91797  0.2049529  0.009600148 0.1574312
## 3  0.15142857 19.78270  0.6726782 15.55765  0.1994404  0.009213196 0.1638558
## 4  0.22214286 20.37342  0.6627789 16.17002  0.2151865  0.009204032 0.1784139
## 5  0.29285714 21.02048  0.6552387 16.80031  0.2367739  0.009206516 0.1926451
## 6  0.36357143 21.73708  0.6492246 17.46130  0.2604786  0.009194458 0.2131727
## 7  0.43428571 22.52488  0.6442642 18.16121  0.2846503  0.009169931 0.2353071
## 8  0.50500000 23.38052  0.6400665 18.90126  0.3084491  0.009137224 0.2583965
## 9  0.57571429 24.29845  0.6364408 19.67914  0.3314419  0.009099695 0.2828544
## 10 0.64642857 25.27229  0.6332568 20.49734  0.3534250  0.009059668 0.3063202
## 11 0.71714286 26.29558  0.6304219 21.35559  0.3743297  0.009018706 0.3253212
## 12 0.78785714 27.36216  0.6278684 22.25044  0.3941663  0.008977849 0.3422981
## 13 0.85857143 28.46635  0.6255455 23.17467  0.4129897  0.008937791 0.3614098
## 14 0.92928571 29.60303  0.6234144 24.12814  0.4308780  0.008898985 0.3821459
## 15 1.00000000 30.76763  0.6214450 25.10896  0.4479184  0.008861726 0.4006238
```

From the above results, we can see the corresponding errors to the lambda values. Here, we will plot and see the optimal lambda.

```
plot_metrics(ridge_model_trans, ridge_model_trans$results$lambda, "Lambda")
```

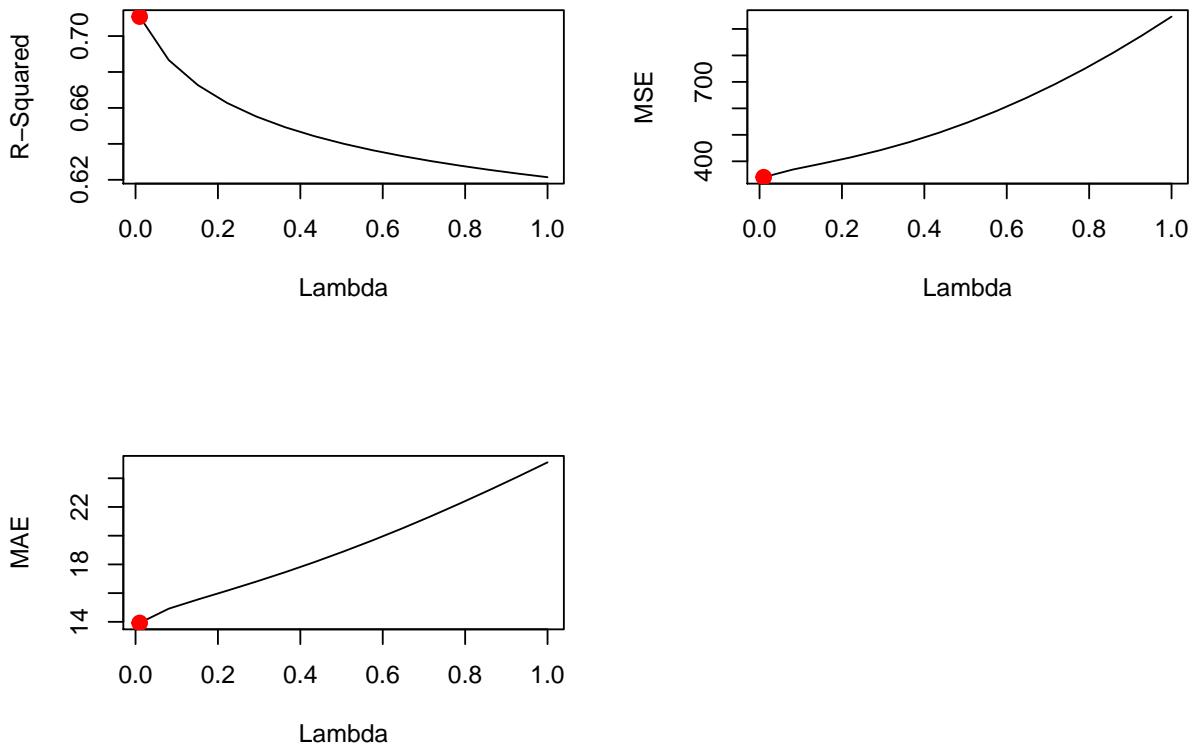


Figure 73: R-Squared, MSE, and MAE for Ridge Regression Trans

```
ridge_model_trans$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next we will show the coefficient after regularization.

```
varImp(ridge_model_trans)$importance
```

```
##                                     Overall
## number_of_elements                 65.666830
## mean_atomic_mass                  2.340670
## wtd_mean_atomic_mass              31.332214
## gmean_atomic_mass                9.789289
## wtd_gmean_atomic_mass             41.873592
## entropy_atomic_mass               53.717397
## wtd_entropy_atomic_mass           88.439537
## range_atomic_mass                 43.896261
## wtd_range_atomic_mass              40.332190
```

```

## std_atomic_mass           26.126408
## wtd_std_atomic_mass      45.220901
## mean_fie                  1.969445
## wtd_mean_fie              48.444039
## gmean_fie                 0.000000
## wtd_gmean_fie             45.381919
## entropy_fie                58.711572
## wtd_entropy_fie            45.914068
## range_fie                  65.983263
## wtd_range_fie              44.894401
## std_fie                     53.815465
## wtd_std_fie                 70.925237
## mean_atomic_radius          1.702301
## wtd_mean_atomic_radius     40.639964
## gmean_atomic_radius          3.970195
## wtd_gmean_atomic_radius     52.658746
## entropy_atomic_radius        56.874572
## wtd_entropy_atomic_radius   80.723038
## range_atomic_radius          77.791891
## wtd_range_atomic_radius     37.603038
## std_atomic_radius            56.967153
## wtd_std_atomic_radius       70.044923
## mean_Density                 24.938698
## wtd_mean_Density             54.589447
## gmean_Density                 53.827694
## wtd_gmean_Density             68.720521
## entropy_Density               38.066656
## wtd_entropy_Density            36.228805
## range_Density                  12.054532
## wtd_range_Density              34.339177
## std_Density                   2.232043
## wtd_std_Density                 58.173311
## mean_ElectronAffinity         6.736804
## wtd_mean_ElectronAffinity     32.860649
## gmean_ElectronAffinity         26.375327
## wtd_gmean_ElectronAffinity     22.565659
## entropy_ElectronAffinity       34.896012
## wtd_entropy_ElectronAffinity    26.634459
## range_ElectronAffinity          14.392845
## wtd_range_ElectronAffinity     35.260218
## std_ElectronAffinity            12.620594
## wtd_std_ElectronAffinity       62.926880
## mean_FusionHeat                  26.907726
## wtd_mean_FusionHeat              59.338381
## gmean_FusionHeat                  33.655417
## wtd_gmean_FusionHeat              54.858189
## entropy_FusionHeat                 55.457733
## wtd_entropy_FusionHeat            70.307323
## range_FusionHeat                  3.449967
## wtd_range_FusionHeat              59.540820
## std_FusionHeat                      7.198470
## wtd_std_FusionHeat                 52.743087
## mean_ThermalConductivity        25.413098
## wtd_mean_ThermalConductivity     46.740051

```

```

## gmean_ThermalConductivity      27.335587
## wtd_gmean_ThermalConductivity 37.572795
## entropy_ThermalConductivity   1.354467
## wtd_entropy_ThermalConductivity 18.985751
## range_ThermalConductivity     86.084589
## wtd_range_ThermalConductivity 63.805474
## std_ThermalConductivity       77.761604
## wtd_std_ThermalConductivity   100.000000
## mean_Valence                  65.510304
## wtd_mean_Valence              91.800565
## gmean_Valence                 59.856849
## wtd_gmean_Valence             91.469039
## entropy_Valence               65.156151
## wtd_entropy_Valence           81.364893
## range_Valence                 3.552174
## wtd_range_Valence             67.378506
## std_Valence                   7.647729
## wtd_std_Valence               39.144031

```

```
getTrainPerf(ridge_model_trans)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 18.43636    0.7108181 13.92396 ridge

```

From the above metrics, the R-Squared for this model is 0.7108181 with Train MSE is 339.66

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(ridge_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

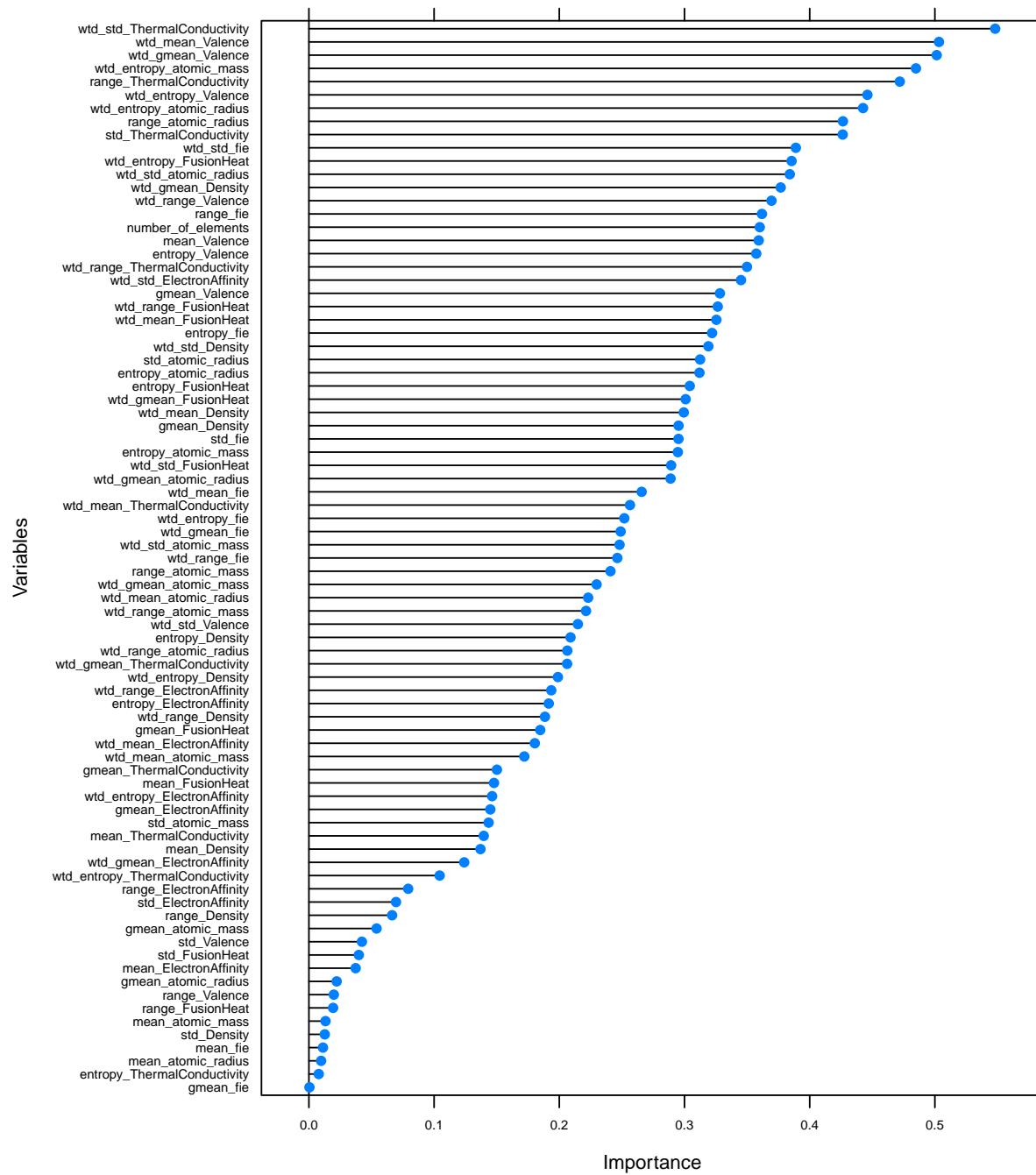


Figure 74: Variables Importance for Ridge Regression Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.8 Lasso Regression

Lasso shrinks the regression coefficients toward zero by penalizing the regression model with a penalty term called L1-norm, which is the sum of the absolute coefficients.

In the case of lasso regression, the penalty has the effect of forcing some of the coefficient estimates, with a minor contribution to the model, to be exactly equal to zero. This means that, lasso can be also seen as an alternative to the subset selection methods for performing variable selection in order to reduce the complexity of the model.

The amount of the penalty for Lasso also can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

# Lasso Regression
lasso_model_trans <- train(
  critical_temp ~., data = train.data, method = "glmnet",
  trControl = control,
  tuneGrid = expand.grid(alpha = 1, lambda = lambda_seq),
  preProc = c("center", "scale", "BoxCox")
)

lasso_model_trans$results

##     alpha    lambda      RMSE   Rsquared      MAE     RMSESD  RsquaredSD
## 1  0.01000000 18.28933 0.7164220 13.59093 1.4981499 0.043468600
## 2  0.08071429 18.43008 0.7107697 14.05731 0.2887385 0.011900916
## 3  0.15142857 18.84976 0.6976178 14.47612 0.2094707 0.009788531
## 4  0.22214286 19.14368 0.6882935 14.76952 0.1808481 0.009042110
## 5  0.29285714 19.37106 0.6810140 15.00250 0.1707993 0.009091814
## 6  0.36357143 19.59893 0.6735719 15.23470 0.1676915 0.009370997
## 7  0.43428571 19.82433 0.6660706 15.45581 0.1636822 0.009368206
## 8  0.50500000 19.96541 0.6614310 15.57062 0.1644913 0.009384342
## 9  0.57571429 20.09488 0.6571620 15.67094 0.1636040 0.009322640
## 10 0.64642857 20.19913 0.6537596 15.75263 0.1628233 0.009291537
## 11 0.71714286 20.30199 0.6503754 15.83693 0.1636132 0.009273845
## 12 0.78785714 20.40738 0.6468769 15.92638 0.1631790 0.009186215
## 13 0.85857143 20.48963 0.6441863 16.00015 0.1629335 0.009060677
## 14 0.92928571 20.54673 0.6424416 16.04647 0.1640705 0.009011886
## 15 1.00000000 20.60371 0.6406956 16.09099 0.1669912 0.009037111
##     MAESD
## 1  0.2602107
## 2  0.1932017
## 3  0.1450347
## 4  0.1270633
## 5  0.1203201
## 6  0.1212970
## 7  0.1320259
## 8  0.1372033
## 9  0.1392758
## 10 0.1412385
## 11 0.1440127
## 12 0.1447196
## 13 0.1434385
```

```

## 14 0.1439201
## 15 0.1442124

plot_metrics(lasso_model_trans, lasso_model_trans$results$lambda, "Lambda")

```

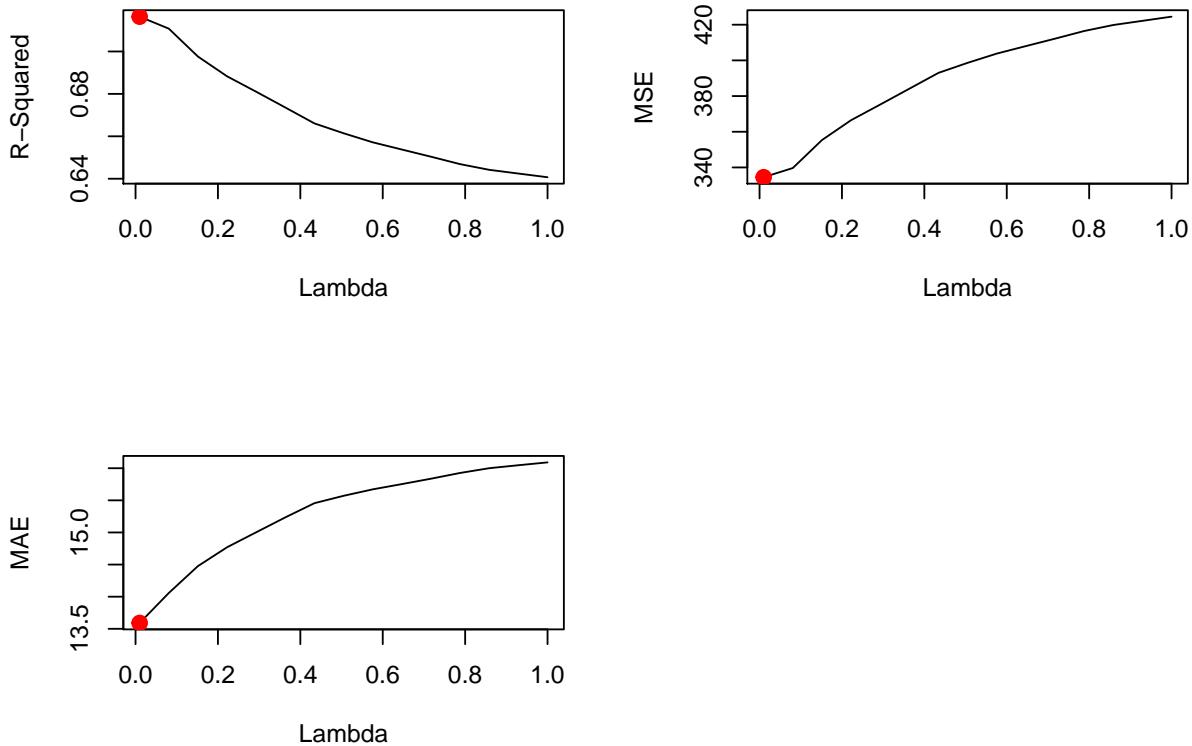


Figure 75: R-Squared, MSE, and MAE for Lasso Regression Trans

```
lasso_model_trans$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next, we will plot the list of coefficients for this model.

```
coef(lasso_model_trans$finalModel, lasso_model_trans$bestTune$lambda)
```

```

## 82 x 1 sparse Matrix of class "dgCMatrix"
##                                         1
## (Intercept)          34.4441094
## number_of_elements -4.0235029
## mean_atomic_mass   4.8013658
## wtd_mean_atomic_mass 2.6193714
## gmean_atomic_mass  -0.9912732

```

```

## wtd_gmean_atomic_mass           -5.7096652
## entropy_atomic_mass            -5.7882715
## wtd_entropy_atomic_mass        4.8891079
## range_atomic_mass              9.2202235
## wtd_range_atomic_mass          -0.1007548
## std_atomic_mass                -1.4469505
## wtd_std_atomic_mass            -4.8166733
## mean_fie                       .
## wtd_mean_fie                  .
## gmean_fie                      0.2556477
## wtd_gmean_fie                 1.5479407
## entropy_fie                   .
## wtd_entropy_fie               5.4397069
## range_fie                      17.0447134
## wtd_range_fie                 3.2920165
## std_fie                        -10.8147914
## wtd_std_fie                   -6.7351527
## mean_atomic_radius             10.9055452
## wtd_mean_atomic_radius         10.4360899
## gmean_atomic_radius            -18.6287862
## wtd_gmean_atomic_radius        .
## entropy_atomic_radius          .
## wtd_entropy_atomic_radius      6.7911695
## range_atomic_radius            16.2321865
## wtd_range_atomic_radius        -3.4729787
## std_atomic_radius              -19.8225051
## wtd_std_atomic_radius          7.9506014
## mean_Density                   -5.0714202
## wtd_mean_Density               2.3476287
## gmean_Density                  5.3817234
## wtd_gmean_Density              3.5431534
## entropy_Density                1.0102991
## wtd_entropy_Density            -8.9305111
## range_Density                  -5.4235354
## wtd_range_Density              -1.9401561
## std_Density                     8.1029031
## wtd_std_Density                -5.2954796
## mean_ElectronAffinity          -0.9151014
## wtd_mean_ElectronAffinity      13.4688579
## gmean_ElectronAffinity         5.0785121
## wtd_gmean_ElectronAffinity     -14.6639905
## entropy_ElectronAffinity       -2.9703896
## wtd_entropy_ElectronAffinity   -5.6794276
## range_ElectronAffinity         -22.6218051
## wtd_range_ElectronAffinity     -4.0209049
## std_ElectronAffinity           22.3420612
## wtd_std_ElectronAffinity       -6.6017761
## mean_FusionHeat                -6.0235761
## wtd_mean_FusionHeat             11.0713964
## gmean_FusionHeat                7.7322993
## wtd_gmean_FusionHeat            -13.0431526
## entropy_FusionHeat              -3.6067616
## wtd_entropy_FusionHeat          8.0987667
## range_FusionHeat                -9.3762832

```

```

## wtd_range_FusionHeat           4.5206284
## std_FusionHeat                7.5727547
## wtd_std_FusionHeat            -3.7134373
## mean_ThermalConductivity     -6.7503408
## wtd_mean_ThermalConductivity 17.1273646
## gmean_ThermalConductivity    -11.4297612
## wtd_gmean_ThermalConductivity -5.1946830
## entropy_ThermalConductivity  7.7088017
## wtd_entropy_ThermalConductivity 5.2281646
## range_ThermalConductivity   -4.9466387
## wtd_range_ThermalConductivity -8.2708358
## std_ThermalConductivity      10.1076895
## wtd_std_ThermalConductivity   10.8112451
## mean_Valence                  -4.3884707
## wtd_mean_Valence              -11.1135987
## gmean_Valence                 3.4419288
## wtd_gmean_Valence             4.4714735
## entropy_Valence               4.7584171
## wtd_entropy_Valence           -8.9714961
## range_Valence                 4.7407264
## wtd_range_Valence             3.7254815
## std_Valence                   .
## wtd_std_Valence               -7.1446992

```

```
getTrainPerf(lasso_model_trans)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 18.28933      0.716422 13.59093 glmnet

```

From the above metrics, the R-Squared for this model is 0.716422 with Train MSE is 334.48

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(lasso_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables", cex=0.75))

```

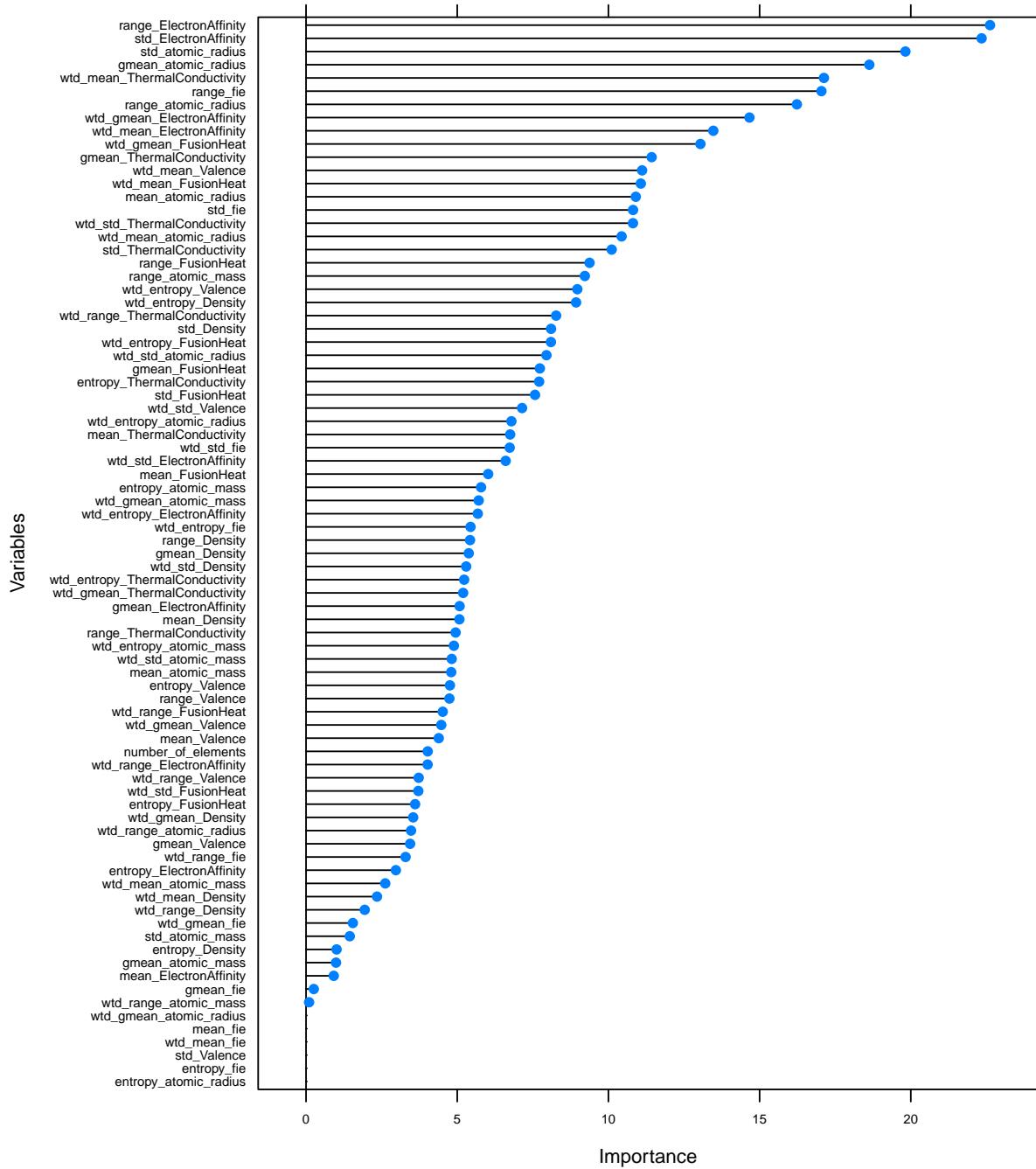


Figure 76: Variables Importance for Lasso Regression Trans

From the plot, we can see that some variables have zero importance, this is because lasso some of the variables' coefficient to zero, which is different compared to ridge regression. In addition, the most important variable is range\_ElectronAffinity.

### 3.2.9 Elastic Net

Elastic Net produces a regression model that is penalized with both the L1 and L2 regularizations. The consequence of this is to effectively shrink coefficients and to set some coefficients to zero.

The amount of the penalty for Elastic Net also can be fine-tuned using a constant called lambda. Here we provide a sequence of lambda values, later we will find which value gives the best result.

```
set.seed(seed)

# Elastic Net Regression
elastic_net_model_trans <- train(
  critical_temp ~., data = train.data, method = "glmnet",
  trControl = control,
  tuneGrid = expand.grid(alpha = 0.5, lambda = lambda_seq),
  preProc = c("center", "scale", "BoxCox")
)

elastic_net_model_trans$results

##   alpha     lambda      RMSE    Rsquared      MAE      RMSESD  RsquaredSD
## 1  0.5 0.01000000 18.22402  0.7182826 13.56322 1.3987900 0.040772602
## 2  0.5 0.08071429 18.27206  0.7156505 13.87353 0.4357409 0.016038019
## 3  0.5 0.15142857 18.48465  0.7090958 14.10413 0.2943325 0.012237913
## 4  0.5 0.22214286 18.70372  0.7022666 14.33094 0.2323351 0.010439978
## 5  0.5 0.29285714 18.90529  0.6959128 14.52835 0.2070124 0.009791507
## 6  0.5 0.36357143 19.06531  0.6908579 14.69259 0.1885486 0.009223855
## 7  0.5 0.43428571 19.20468  0.6864195 14.83266 0.1786797 0.009082853
## 8  0.5 0.50500000 19.33104  0.6823739 14.96302 0.1734545 0.009096381
## 9  0.5 0.57571429 19.44042  0.6788643 15.07919 0.1705800 0.009197978
## 10 0.5 0.64642857 19.55399  0.6751719 15.19539 0.1683583 0.009307409
## 11 0.5 0.71714286 19.67607  0.6711469 15.31663 0.1673754 0.009428616
## 12 0.5 0.78785714 19.79731  0.6671108 15.43041 0.1642518 0.009424222
## 13 0.5 0.85857143 19.89357  0.6639157 15.51500 0.1610808 0.009345763
## 14 0.5 0.92928571 19.96499  0.6615819 15.57356 0.1612296 0.009323110
## 15 0.5 1.00000000 20.03122  0.6594227 15.62494 0.1621493 0.009349012
##           MAESD
## 1  0.2585685
## 2  0.2122923
## 3  0.1882493
## 4  0.1633473
## 5  0.1445750
## 6  0.1346372
## 7  0.1265970
## 8  0.1236948
## 9  0.1238354
## 10 0.1250466
## 11 0.1287192
## 12 0.1321630
## 13 0.1338647
## 14 0.1354916
## 15 0.1360695
```

From the above results, we can see the corresponding errors to the lambda values. Here, we will plot and see the optimal lambda.

```
plot_metrics(elastic_net_model_trans, elastic_net_model_trans$results$lambda, "Lambda")
```

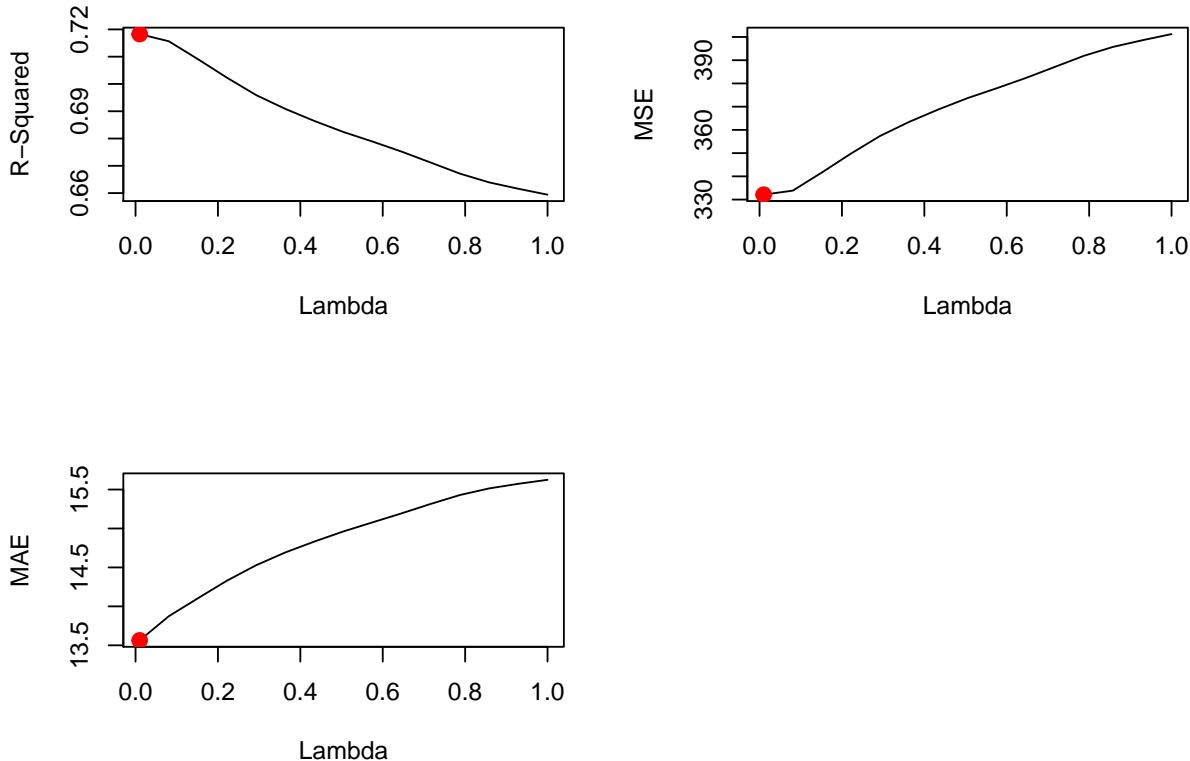


Figure 77: R-Squared, MSE, and MAE for Elastic Net Regression Trans

```
elastic_net_model_trans$bestTune$lambda
```

```
## [1] 0.01
```

From above, we know that the best lambda is 0.01. Next, we will plot the list of coefficients for this model.

```
coef(elastic_net_model_trans$finalModel, elastic_net_model_trans$bestTune$lambda)
```

```
## 82 x 1 sparse Matrix of class "dgCMatrix"
##                                     1
## (Intercept)           34.4441094
## number_of_elements   -3.6146083
## mean_atomic_mass     5.0513589
## wtd_mean_atomic_mass 4.2954978
## gmean_atomic_mass   -1.5673406
## wtd_gmean_atomic_mass -7.2714433
## entropy_atomic_mass -5.2726571
## wtd_entropy_atomic_mass 5.3676349
```

```

## range_atomic_mass           9.6966888
## wtd_range_atomic_mass      -0.1530216
## std_atomic_mass            -2.0234866
## wtd_std_atomic_mass        -4.7563457
## mean_fie                   .
## wtd_mean_fie               .
## gmean_fie                  0.2825284
## wtd_gmean_fie              1.6189289
## entropy_fie                .
## wtd_entropy_fie             5.9992267
## range_fie                  16.3314571
## wtd_range_fie              3.6731220
## std_fie                    -10.2651188
## wtd_std_fie                -6.6291912
## mean_atomic_radius          11.2564992
## wtd_mean_atomic_radius     10.5399495
## gmean_atomic_radius         -18.9689425
## wtd_gmean_atomic_radius    .
## entropy_atomic_radius       .
## wtd_entropy_atomic_radius   7.3339349
## range_atomic_radius          16.8116095
## wtd_range_atomic_radius     -3.3052468
## std_atomic_radius            -20.9380448
## wtd_std_atomic_radius       8.4753872
## mean_Density                -5.1436781
## wtd_mean_Density             2.0851698
## gmean_Density                5.4197798
## wtd_gmean_Density            5.0841829
## entropy_Density              1.6393438
## wtd_entropy_Density          -9.8812215
## range_Density                -6.0608431
## wtd_range_Density             -2.1958108
## std_Density                  9.3080115
## wtd_std_Density              -5.8687396
## mean_ElectronAffinity        -1.2595956
## wtd_mean_ElectronAffinity    13.7097788
## gmean_ElectronAffinity        5.7542109
## wtd_gmean_ElectronAffinity   -15.0144023
## entropy_ElectronAffinity     -3.4823866
## wtd_entropy_ElectronAffinity -5.7541723
## range_ElectronAffinity        -22.3593681
## wtd_range_ElectronAffinity   -3.9982774
## std_ElectronAffinity          22.2239348
## wtd_std_ElectronAffinity     -6.8874602
## mean_FusionHeat               -6.8149682
## wtd_mean_FusionHeat            11.9503493
## gmean_FusionHeat               8.3074950
## wtd_gmean_FusionHeat           -13.4764259
## entropy_FusionHeat              -4.6546825
## wtd_entropy_FusionHeat          8.5384897
## range_FusionHeat                 -10.1667474
## wtd_range_FusionHeat              4.5791784
## std_FusionHeat                  8.5269854
## wtd_std_FusionHeat              -4.1359910

```

```

## mean_ThermalConductivity      -7.1997937
## wtd_mean_ThermalConductivity 18.1507294
## gmean_ThermalConductivity    -11.3833289
## wtd_gmean_ThermalConductivity -6.4727639
## entropy_ThermalConductivity  8.1109289
## wtd_entropy_ThermalConductivity 5.2174463
## range_ThermalConductivity   -7.0831525
## wtd_range_ThermalConductivity -8.6864045
## std_ThermalConductivity     12.6429166
## wtd_std_ThermalConductivity  10.3574738
## mean_Valence                 -6.0195332
## wtd_mean_Valence             -11.4743284
## gmean_Valence                5.2031078
## wtd_gmean_Valence            4.6266923
## entropy_Valence              4.4460538
## wtd_entropy_Valence          -9.6081148
## range_Valence                4.9143021
## wtd_range_Valence            3.5320218
## std_Valence                  .
## wtd_std_Valence              -7.1381806

```

```
getTrainPerf(elastic_net_model_trans)
```

```

## TrainRMSE TrainRsquared TrainMAE method
## 1 18.22402 0.7182826 13.56322 glmnet

```

From the above metrics, the R-Squared for this model is 0.7182826 with Train MSE is 331.96

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(elastic_net_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

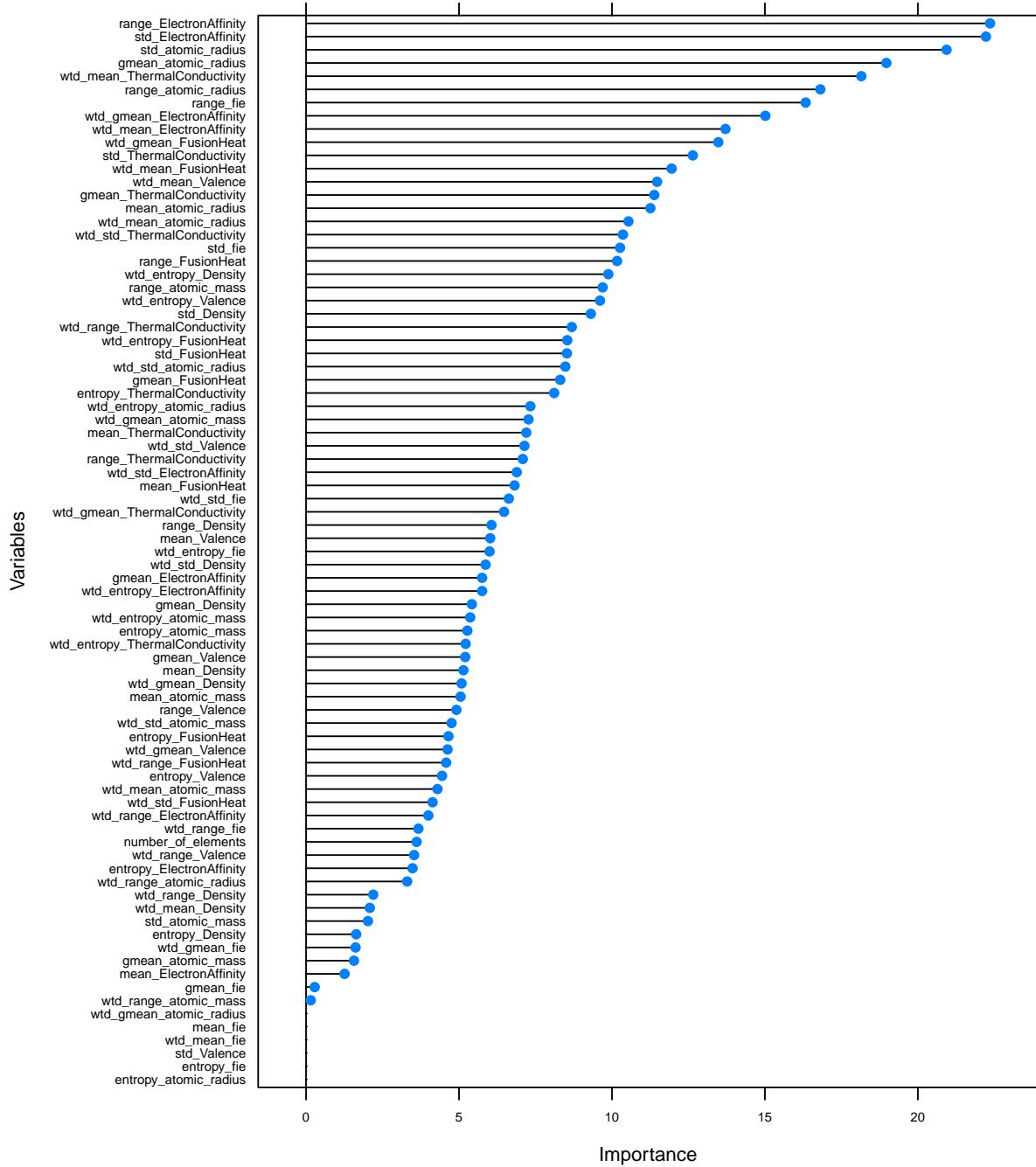


Figure 78: Variables Importance for Elastic Net Regression Trans

From the plot, we can see that some variables have zero importance, however, compared to lasso regression, the number of zero importance is less. This is because elastic net is the combination between ridge and lasso regressions. In addition, the most important variable for this model is range\_ElectronAffinity.

### 3.2.10 Principal Component Regression

The principal component regression (PCR) first applies Principal Component Analysis on the data set to summarize the original predictor variables into few new variables also known as principal components (PCs), which are a linear combination of the original data.

These PCs are then used to build the linear regression model. The number of principal components, to incorporate in the model, is chosen by cross-validation (cv).

```
set.seed(seed)

# Principal Component Regression
pcr_model_trans <- train(critical_temp ~ .,
  data      = train.data,
  method    = "pcr",
  tuneGrid  = expand.grid(ncomp = seq(2,40,2)),
  trControl = control,
  preProc  = c("center", "scale", "BoxCox"))
summary(pcr_model_trans)

## Data: X dimension: 17011 81
## Y dimension: 17011 1
## Fit method: svdpc
## Number of components considered: 38
## TRAINING: % variance explained
##          1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X        39.14    50.51    60.28    68.16    73.66    77.63    81.28
## .outcome 43.22    43.34    50.09    52.60    53.63    58.00    58.05
##          8 comps  9 comps 10 comps 11 comps 12 comps 13 comps
## X        84.26    86.48    88.46    90.27    91.52    92.60
## .outcome 58.09    58.10    58.10    59.32    59.40    59.49
##          14 comps 15 comps 16 comps 17 comps 18 comps 19 comps
## X       93.58    94.41    95.08    95.71    96.21    96.59
## .outcome 59.72    60.26    60.40    60.90    60.98    61.61
##          20 comps 21 comps 22 comps 23 comps 24 comps 25 comps
## X       96.94    97.25    97.54    97.76    97.97    98.16
## .outcome 61.62    61.78    62.91    63.65    64.06    64.82
##          26 comps 27 comps 28 comps 29 comps 30 comps 31 comps
## X       98.34    98.48    98.62    98.74    98.84    98.95
## .outcome 66.61    66.63    66.64    66.71    67.70    67.75
##          32 comps 33 comps 34 comps 35 comps 36 comps 37 comps
## X       99.04    99.13    99.22    99.29    99.36    99.43
## .outcome 68.12    68.12    68.17    68.21    68.21    68.34
##          38 comps
## X       99.48
## .outcome 69.46

pcr_model_trans$results

##   ncomp    RMSE  Rsquared      MAE    RMSESD  RsquaredSD     MAESD
## 1     2 25.78395 0.4333389 20.99659 0.3865687 0.012818176 0.2767409
## 2     4 23.59660 0.5254559 18.74677 0.2627282 0.008167231 0.2295490
## 3     6 22.20221 0.5799332 17.65958 0.1901349 0.008814111 0.1664551
```

```

## 4     8 22.18025 0.5807716 17.52641 0.1861584 0.008772845 0.1550329
## 5    10 22.17855 0.5808330 17.51611 0.1904561 0.008847307 0.1539704
## 6    12 21.83674 0.5936690 17.17750 0.2118288 0.010755545 0.2296573
## 7    14 21.75285 0.5967572 17.10077 0.2115913 0.010917738 0.2121527
## 8    16 21.56877 0.6035331 16.99367 0.1966415 0.010500570 0.2015958
## 9    18 21.41788 0.6090851 16.84166 0.2296112 0.011372079 0.2025066
## 10   20 21.24356 0.6153745 16.75516 0.2291370 0.012116389 0.1849129
## 11   22 20.93324 0.6266041 16.67015 0.2457245 0.012787902 0.1820839
## 12   24 20.56423 0.6396888 16.25868 0.3131246 0.014639363 0.1892303
## 13   26 19.87862 0.6632743 15.61734 0.2924232 0.013907699 0.2003327
## 14   28 19.86409 0.6637658 15.60758 0.2759575 0.013412127 0.2035207
## 15   30 19.60593 0.6725073 15.20644 0.3923380 0.016203928 0.2155193
## 16   32 19.48605 0.6765255 15.09381 0.4424449 0.017462927 0.2119547
## 17   34 19.47820 0.6767916 15.09615 0.4571033 0.017834900 0.2158762
## 18   36 19.40758 0.6790767 15.04642 0.3086941 0.013213554 0.2023607
## 19   38 19.17264 0.6872938 14.57579 0.7100325 0.023990004 0.1869270
## 20   40 19.21838 0.6860360 14.58317 0.8603940 0.028112845 0.1903371

```

```
plot_metrics(pcr_model_trans, pcr_model_trans$results$ncomp, "Number of Component")
```

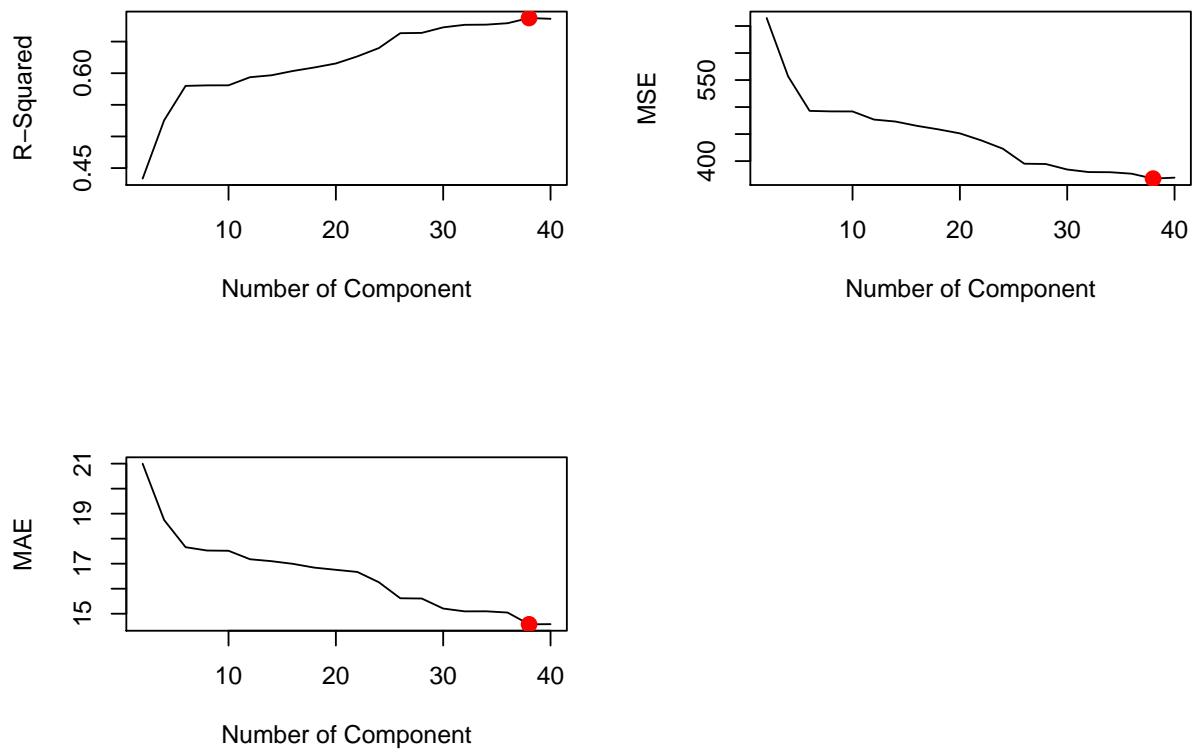


Figure 79: R-Squared, MSE, and MAE for Principal Component Regression Trans

```
pcr_model_trans$bestTune
```

```
##      ncomp  
## 19     38
```

From the above results, we can see the corresponding errors to the number of principal components. Here, we will plot and see the optimal number of principal components.

```
getTrainPerf(pcr_model_trans)
```

```
##   TrainRMSE TrainRsquared TrainMAE method  
## 1 19.17264    0.6872938 14.57579   pcr
```

```
varImp(pcr_model_trans)$importance
```

	Overall
## number_of_elements	65.666830
## mean_atomic_mass	2.340670
## wtd_mean_atomic_mass	31.332214
## gmean_atomic_mass	9.789289
## wtd_gmean_atomic_mass	41.873592
## entropy_atomic_mass	53.717397
## wtd_entropy_atomic_mass	88.439537
## range_atomic_mass	43.896261
## wtd_range_atomic_mass	40.332190
## std_atomic_mass	26.126408
## wtd_std_atomic_mass	45.220901
## mean_fie	1.969445
## wtd_mean_fie	48.444039
## gmean_fie	0.000000
## wtd_gmean_fie	45.381919
## entropy_fie	58.711572
## wtd_entropy_fie	45.914068
## range_fie	65.983263
## wtd_range_fie	44.894401
## std_fie	53.815465
## wtd_std_fie	70.925237
## mean_atomic_radius	1.702301
## wtd_mean_atomic_radius	40.639964
## gmean_atomic_radius	3.970195
## wtd_gmean_atomic_radius	52.658746
## entropy_atomic_radius	56.874572
## wtd_entropy_atomic_radius	80.723038
## range_atomic_radius	77.791891
## wtd_range_atomic_radius	37.603038
## std_atomic_radius	56.967153
## wtd_std_atomic_radius	70.044923
## mean_Density	24.938698
## wtd_mean_Density	54.589447
## gmean_Density	53.827694
## wtd_gmean_Density	68.720521

```

## entropy_Density           38.066656
## wtd_entropy_Density       36.228805
## range_Density             12.054532
## wtd_range_Density          34.339177
## std_Density                2.232043
## wtd_std_Density            58.173311
## mean_ElectronAffinity      6.736804
## wtd_mean_ElectronAffinity   32.860649
## gmean_ElectronAffinity     26.375327
## wtd_gmean_ElectronAffinity  22.565659
## entropy_ElectronAffinity    34.896012
## wtd_entropy_ElectronAffinity 26.634459
## range_ElectronAffinity      14.392845
## wtd_range_ElectronAffinity   35.260218
## std_ElectronAffinity         12.620594
## wtd_std_ElectronAffinity     62.926880
## mean_FusionHeat              26.907726
## wtd_mean_FusionHeat          59.338381
## gmean_FusionHeat              33.655417
## wtd_gmean_FusionHeat          54.858189
## entropy_FusionHeat            55.457733
## wtd_entropy_FusionHeat         70.307323
## range_FusionHeat               3.449967
## wtd_range_FusionHeat          59.540820
## std_FusionHeat                 7.198470
## wtd_std_FusionHeat             52.743087
## mean_ThermalConductivity      25.413098
## wtd_mean_ThermalConductivity   46.740051
## gmean_ThermalConductivity      27.335587
## wtd_gmean_ThermalConductivity  37.572795
## entropy_ThermalConductivity    1.354467
## wtd_entropy_ThermalConductivity 18.985751
## range_ThermalConductivity      86.084589
## wtd_range_ThermalConductivity   63.805474
## std_ThermalConductivity        77.761604
## wtd_std_ThermalConductivity     100.000000
## mean_Valence                  65.510304
## wtd_mean_Valence                91.800565
## gmean_Valence                  59.856849
## wtd_gmean_Valence                91.469039
## entropy_Valence                  65.156151
## wtd_entropy_Valence                81.364893
## range_Valence                   3.552174
## wtd_range_Valence                  67.378506
## std_Valence                      7.647729
## wtd_std_Valence                  39.144031

```

From the above metrics, the R-Squared for this model is 0.6872938 with Train MSE is 367.4889 However, now the model only has 40 variables as the predictors which is far from the original model.

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(pcr_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

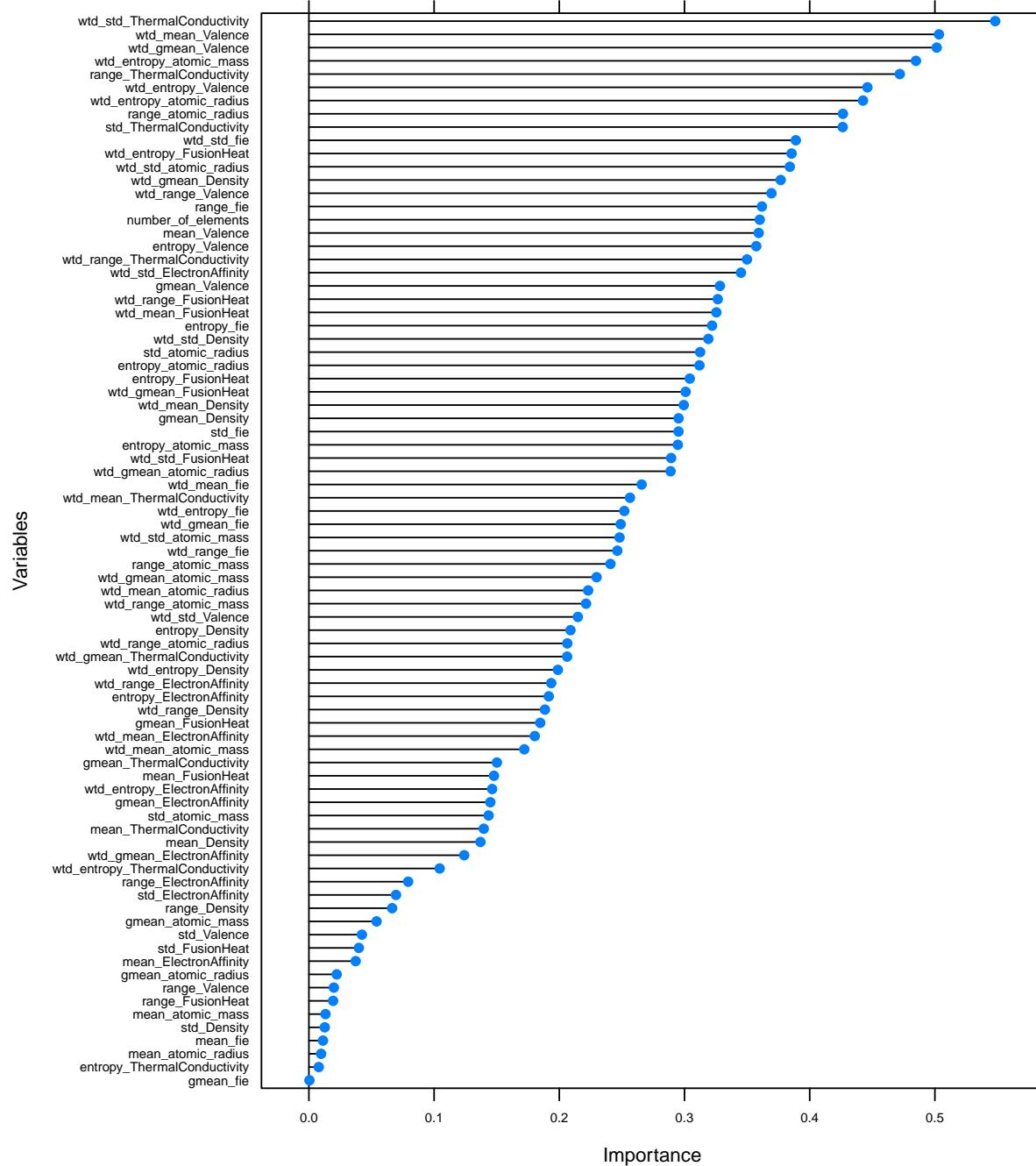


Figure 80: Variables Importance for Principal Component Regression Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.11 K-Nearest Neighbor Regression

K-Nearest Neighbor is a non-parametric method used for classification and regression. In both cases, the input consists of the k closest training examples in the feature space. For regression, the prediction is the average of the response variable of the closest neighbors.

```
set.seed(seed)

# K-Nearest Neighbor Regression
knn_model_trans <- train(critical_temp ~ .,
  method      = "knn",
  tuneGrid    = expand.grid(k = c(1:5)),
  trControl   = control,
  data        = train.data,
  preProc    = c("center", "scale", "BoxCox"))

knn_model_trans$results

##   k     RMSE  Rsquared      MAE     RMSESD  RsquaredSD      MAESD
## 1 1 10.88461 0.9010050 5.638316 0.4351285 0.007601759 0.1744774
## 2 2 10.59921 0.9052090 5.551922 0.3678790 0.006416985 0.1739438
## 3 3 10.64152 0.9040196 5.756087 0.3668278 0.006264945 0.2050375
## 4 4 10.84530 0.9001417 5.979875 0.3502730 0.006312116 0.2125334
## 5 5 11.04566 0.8962893 6.173404 0.3478482 0.006388241 0.2080974
```

From the above results, we can see the corresponding errors to the number of k. Here, we will plot and see the optimal number of k.

```
plot_metrics(knn_model_trans, knn_model_trans$results$k, "k")
```

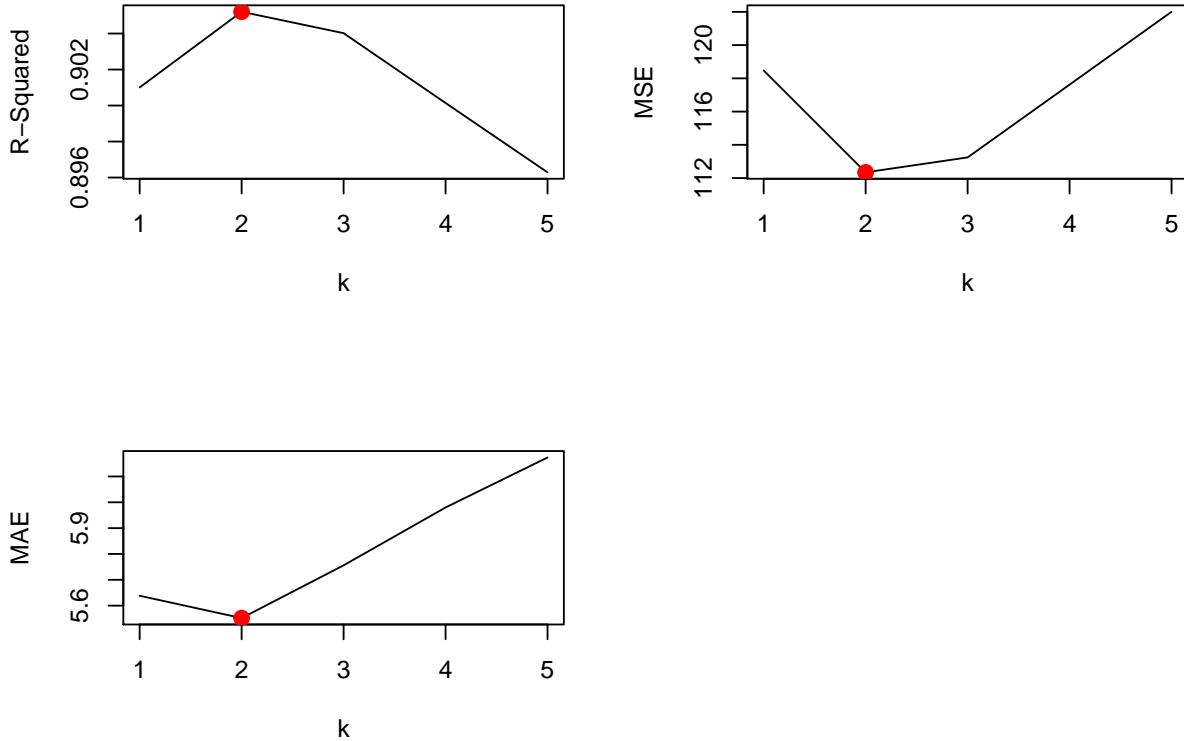


Figure 81: R-Squared, MSE, and MAE for KNN Regression Trans

```
# Best tuning parameter k that minimize the RMSE
knn_model_trans$bestTune
```

```
##      k
## 2 2
```

```
getTrainPerf(knn_model_trans)
```

```
##      TrainRMSE TrainRsquared TrainMAE method
## 1 10.59921     0.905209 5.551922    knn
```

From the result, we know that the best  $k$  is 2 with R-Squared 0.905209 and MSE 112.36 So far, this is the best model we have.

Here, we show the variable importance for this model.

```
varImp(knn_model_trans, scale = FALSE)$importance
```

```
##                                              Overall
## number_of_elements                      0.3601224431
## mean_atomic_mass                       0.0132644523
```

```

## wtd_mean_atomic_mass          0.1720605759
## gmean_atomic_mass            0.0540629652
## wtd_gmean_atomic_mass        0.2297991342
## entropy_atomic_mass          0.2946715118
## wtd_entropy_atomic_mass      0.4848559723
## range_atomic_mass            0.2408779512
## wtd_range_atomic_mass        0.2213563770
## std_atomic_mass              0.1435466804
## wtd_std_atomic_mass          0.2481334360
## mean_fie                      0.0112311343
## wtd_mean_fie                 0.2657876103
## gmean_fie                     0.0004438412
## wtd_gmean_fie                0.2490153844
## entropy_fie                  0.3220262349
## wtd_entropy_fie              0.2519301375
## range_fie                     0.3618556522
## wtd_range_fie                0.2463450900
## std_fie                       0.2952086611
## wtd_std_fie                  0.3889244539
## mean_atomic_radius            0.0097678961
## wtd_mean_atomic_radius        0.2230421516
## gmean_atomic_radius           0.0221898933
## wtd_gmean_atomic_radius       0.2888729368
## entropy_atomic_radius         0.3119643880
## wtd_entropy_atomic_radius     0.4425901964
## range_atomic_radius           0.4265353533
## wtd_range_atomic_radius       0.2064079194
## std_atomic_radius             0.3124714830
## wtd_std_atomic_radius         0.3841026869
## mean_Density                  0.1370412057
## wtd_mean_Density              0.2994480102
## gmean_Density                 0.2952756440
## wtd_gmean_Density             0.3768485038
## entropy_Density               0.2089473062
## wtd_entropy_Density           0.1988808014
## range_Density                 0.0664704367
## wtd_range_Density             0.1885306934
## std_Density                   0.0126694694
## wtd_std_Density               0.3190780045
## mean_ElectronAffinity         0.0373435119
## wtd_mean_ElectronAffinity     0.1804323136
## gmean_ElectronAffinity        0.1449100944
## wtd_gmean_ElectronAffinity    0.1240433001
## entropy_ElectronAffinity      0.1915806587
## wtd_entropy_ElectronAffinity   0.1463294443
## range_ElectronAffinity        0.0792781409
## wtd_range_ElectronAffinity    0.1935755341
## std_ElectronAffinity          0.0695709452
## wtd_std_ElectronAffinity      0.3451148458
## mean_FusionHeat               0.1478262170
## wtd_mean_FusionHeat            0.3254594685
## gmean_FusionHeat               0.1847855168
## wtd_gmean_FusionHeat           0.3009200017
## entropy_FusionHeat             0.3042038971

```

```

## wtd_entropy_FusionHeat          0.3855399384
## range_FusionHeat               0.0193404344
## wtd_range_FusionHeat           0.3265682914
## std_FusionHeat                 0.0398722031
## wtd_std_FusionHeat              0.2893349003
## mean_ThermalConductivity      0.1396396530
## wtd_mean_ThermalConductivity   0.2564543149
## gmean_ThermalConductivity     0.1501697502
## wtd_gmean_ThermalConductivity  0.2062422695
## entropy_ThermalConductivity   0.0078626971
## wtd_entropy_ThermalConductivity 0.1044349818
## range_ThermalConductivity     0.4719571565
## wtd_range_ThermalConductivity  0.3499271935
## std_ThermalConductivity       0.4263694613
## wtd_std_ThermalConductivity    0.5481763933
## mean_Valence                  0.3592651026
## wtd_mean_Valence              0.5032654171
## gmean_Valence                 0.3282992890
## wtd_gmean_Valence             0.5014495452
## entropy_Valence               0.3573252876
## wtd_entropy_Valence            0.4461058445
## range_Valence                 0.0199002543
## wtd_range_Valence              0.3694978531
## std_Valence                   0.0423329431
## wtd_std_Valence                0.2148484399

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(knn_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

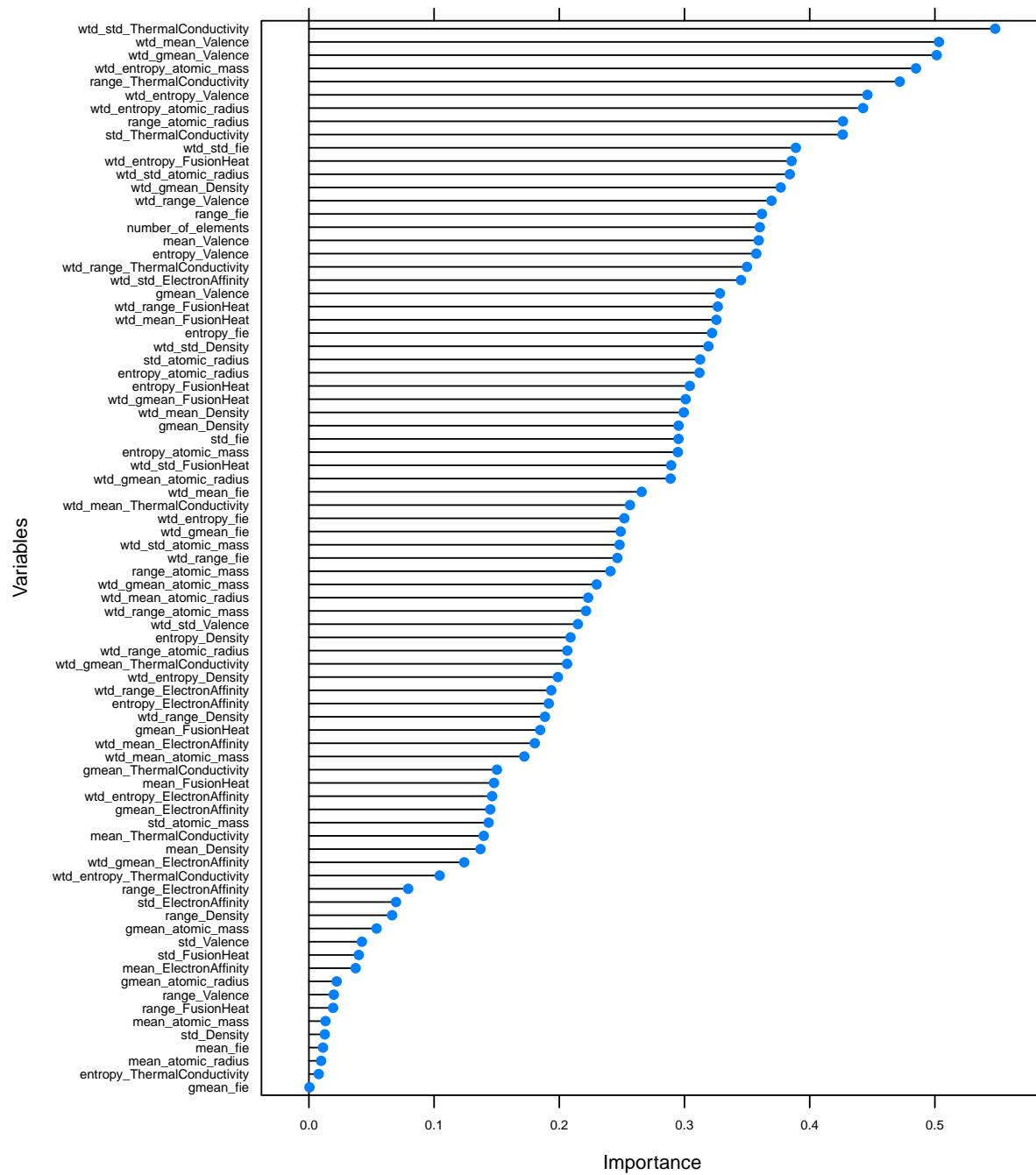


Figure 82: Variables Importance for KNN Regression Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `gmean_fie` is the least important variable for this model.

### 3.2.12 Random Forest

Random forest provides a strong improvement, which consists of applying bagging to the data and bootstrap sampling to the predictor variables at each split [Bruce and Bruce, 2017]. This means that at each splitting step of the tree algorithm, a random sample of n predictors is chosen as split candidates from the full set of the predictors.

Here, we will perform a random forest algorithm by using ranger library, there are three main parameter to be tuned which are mtry, splrule and min.node.size. mtry is number of variables to possibly split at in each node. Default is the (rounded down) square root of the number variables.

```
set.seed(seed)

# Random Forest
random_forest_model_trans <- train(
  critical_temp ~.,
  data = train.data,
  trControl = trainControl( method = "cv", number = 10, search = "random"),
  tuneLength = 5,
  method = "ranger",
  importance = 'impurity',
  preProc = c("center", "scale", "BoxCox")
)

## Growing trees.. Progress: 88%. Estimated remaining time: 4 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 85%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 5 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 89%. Estimated remaining time: 3 seconds.
## Growing trees.. Progress: 84%. Estimated remaining time: 6 seconds.

random_forest_model_trans$results

##   min.node.size mtry    splrule      RMSE  Rsquared       MAE     RMSESD
## 1             13     1  extratrees 12.075879 0.8797300 7.798733 0.2450494
## 2             13    19  variance   9.543068 0.9226579 5.445209 0.2624370
## 5             18    42  variance   9.597666 0.9217708 5.492564 0.2453484
## 3             13    54  maxstat  9.999160 0.9154141 5.780316 0.3131273
## 4             13    57  maxstat 10.009396 0.9152444 5.792905 0.3090393
##   RsquaredSD     MAESD
```

```

## 1 0.005350989 0.1874913
## 2 0.005064541 0.1288124
## 5 0.004812328 0.1331354
## 3 0.005655636 0.1374879
## 4 0.005533801 0.1380031

```

From the above results, we can see the corresponding errors to the number of mtry, splitrule, and minimum node size. Here, we will plot and see the optimal number of those three parameters.

```

random_forest_model_trans$bestTune

##   mtry splitrule min.node.size
## 2    19      variance         13

getTrainPerf(random_forest_model_trans)

##   TrainRMSE TrainRsquared TrainMAE method
## 1  9.543068     0.9226579  5.445209 ranger

```

From above, we can see that the optimal model is the model with mtry = 19, splitrule = variance and min.node.size = 13 with R-Squared = 0.9226579 and MSE = 91.01

Here, we show the variable importance for this model.

```

varImp(random_forest_model_trans, scale = FALSE)$importance

##                                     Overall
## number_of_elements            3370.912
## mean_atomic_mass              49252.025
## wtd_mean_atomic_mass          112798.578
## gmean_atomic_mass             40825.979
## wtd_gmean_atomic_mass          80466.449
## entropy_atomic_mass           51235.752
## wtd_entropy_atomic_mass        600720.554
## range_atomic_mass              69787.020
## wtd_range_atomic_mass          92415.769
## std_atomic_mass                311201.101
## wtd_std_atomic_mass            126772.867
## mean_fie                       35351.225
## wtd_mean_fie                  67228.426
## gmean_fie                      33698.918
## wtd_gmean_fie                 57744.653
## entropy_fie                   49340.391
## wtd_entropy_fie                189371.651
## range_fie                      296136.947
## wtd_range_fie                  149702.848
## std_fie                        112353.017
## wtd_std_fie                    79802.962
## mean_atomic_radius              39862.538
## wtd_mean_atomic_radius          75523.993
## gmean_atomic_radius             34555.079
## wtd_gmean_atomic_radius         80236.282

```

```

## entropy_atomic_radius           43087.270
## wtd_entropy_atomic_radius      169081.441
## range_atomic_radius            1569768.692
## wtd_range_atomic_radius        69257.159
## std_atomic_radius              68295.800
## wtd_std_atomic_radius          88890.202
## mean_Density                   72116.022
## wtd_mean_Density               70587.401
## gmean_Density                  281841.601
## wtd_gmean_Density              155560.560
## entropy_Density                76121.071
## wtd_entropy_Density             114341.200
## range_Density                  27588.321
## wtd_range_Density              64895.691
## std_Density                     118851.733
## wtd_std_Density                80458.053
## mean_ElectronAffinity          39800.487
## wtd_mean_ElectronAffinity       91623.719
## gmean_ElectronAffinity          133933.456
## wtd_gmean_ElectronAffinity      365207.856
## entropy_ElectronAffinity        35890.793
## wtd_entropy_ElectronAffinity    73185.264
## range_ElectronAffinity          60244.870
## wtd_range_ElectronAffinity      284180.427
## std_ElectronAffinity            137247.349
## wtd_std_ElectronAffinity         457015.218
## mean_FusionHeat                 33550.602
## wtd_mean_FusionHeat              60658.364
## gmean_FusionHeat                26059.260
## wtd_gmean_FusionHeat             118263.376
## entropy_FusionHeat              47790.220
## wtd_entropy_FusionHeat            135578.988
## range_FusionHeat                 14799.419
## wtd_range_FusionHeat              71945.970
## std_FusionHeat                  35628.268
## wtd_std_FusionHeat                77878.787
## mean_ThermalConductivity        112410.094
## wtd_mean_ThermalConductivity     427809.651
## gmean_ThermalConductivity        45882.033
## wtd_gmean_ThermalConductivity    483466.242
## entropy_ThermalConductivity      64610.578
## wtd_entropy_ThermalConductivity   208998.858
## range_ThermalConductivity        2604644.221
## wtd_range_ThermalConductivity     228001.726
## std_ThermalConductivity          1017119.457
## wtd_std_ThermalConductivity       2399536.041
## mean_Valence                     131505.487
## wtd_mean_Valence                 823342.098
## gmean_Valence                    166134.035
## wtd_gmean_Valence                 688857.015
## entropy_Valence                  294596.298
## wtd_entropy_Valence                1130612.252
## range_Valence                      10038.878
## wtd_range_Valence                  123637.932

```

```
## std_Valence          36987.362  
## wtd_std_Valence    200239.724
```

Next, we will plot the variable importance for this model.

```
# Plot the Variable Importance  
plot(varImp(random_forest_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),  
     xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))
```

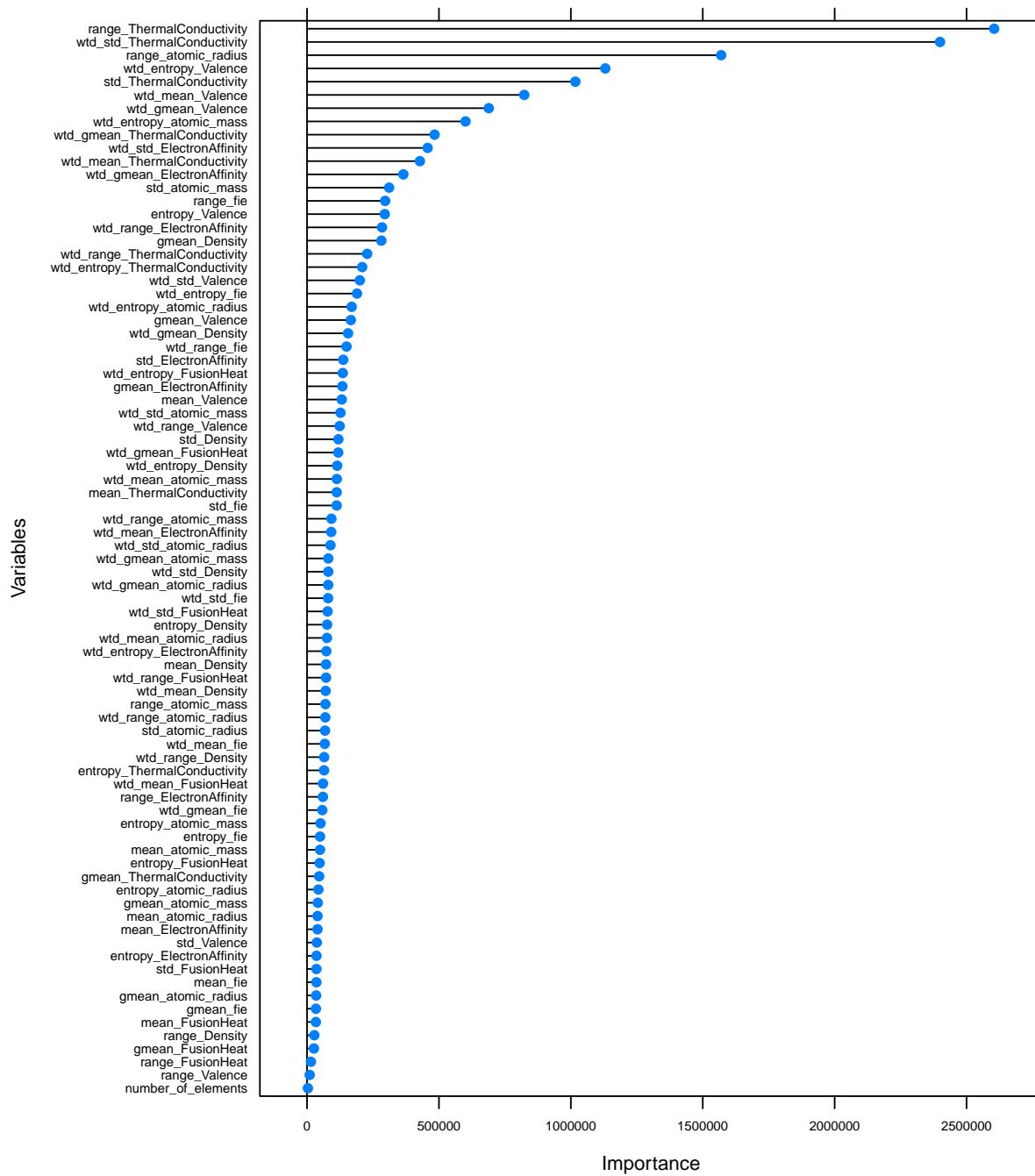


Figure 83: Variables Importance for Random Forest Trans

From above, it can be seen that range\_ThermalConductivity is the most important variable for this model, whereas number\_of\_elements is the least important variable for this model.

### 3.2.13 Gradient Boosting Machine

Compared to random forests which build an ensemble of deep independent trees, GBMs build an ensemble of shallow and weak successive trees with each tree learning and improving on the previous. When combined, these many weak successive trees produce a powerful combination that are often hard to beat with other algorithms.

For a gradient boosting machine (GBM) model, there are four main tuning parameters, n.trees (number of iterations), interaction.depth (complexity of the tree), shrinkage (learning rate), and m.minobsinnode (the minimum number of training set samples in a node to commence splitting).

For the parameters tuning process, we can use apply manual grid search, random grid search or random search tuning. Grid search technique for some cases are more effective, however, it is very time consuming and need much computational cost. Therefore, for this assignment purpose, we will only apply random search tuning with tune length = 2.

```
set.seed(seed)

# Gradient Boosting Machine
gbm_model_trans <- train(critical_temp ~ .,
                         data = train.data,
                         method = "gbm",
                         tuneLength = 4,
                         preProc = c("center", "scale", "BoxCox"),
                         trControl = trainControl( method = "cv", number = 10, search = "random"),
                         verbose = FALSE
                       )

gbm_model_trans$results

##   shrinkage interaction.depth n.minobsinnode n.trees      RMSE    Rsquared
## 4 0.4164612                 1             11     3046 12.17813 0.8736013
## 2 0.3090364                 7             24     3111 10.45755 0.9072912
## 3 0.3274399                 3             22     3117 10.45700 0.9070904
## 1 0.1703574                 7             11     4304 10.00986 0.9147804
##           MAE      RMSESD  RsquaredSD       MAESD
## 4 8.177155 0.2497581 0.005741453 0.21176984
## 2 6.244750 0.2884086 0.005717800 0.14338786
## 3 6.441774 0.3250856 0.006553769 0.16934170
## 1 5.896819 0.3336993 0.006162329 0.09614653

gbm_model_trans$finalModel

## A gradient boosted model with gaussian loss function.
## 4304 iterations were performed.
## There were 81 predictors of which 80 had non-zero influence.

gbm_model_trans$bestTune

##   n.trees interaction.depth shrinkage n.minobsinnode
## 1     4304                  7 0.1703574            11
```

```
getTrainPerf(gbm_model_trans)
```

```
##   TrainRMSE TrainRsquared TrainMAE method
## 1 10.00986    0.9147804 5.896819    gbm
```

From above, we can see that the optimal model is the model with shrinkage = 0.1703574, n.trees = 4304, interaction.depth = 7, and m.minobsinnode = 11. The R-Squared and MSE are 0.9147804 and 100 consecutively.

Here, we show the variable importance for this model.

```
varImp(gbm_model_trans, scale = FALSE)$importance
```

	Overall
## number_of_elements	0.000
## mean_atomic_mass	108700.127
## wtd_mean_atomic_mass	370233.350
## gmean_atomic_mass	203818.924
## wtd_gmean_atomic_mass	395550.690
## entropy_atomic_mass	111653.525
## wtd_entropy_atomic_mass	1070500.658
## range_atomic_mass	99505.143
## wtd_range_atomic_mass	287924.028
## std_atomic_mass	846691.930
## wtd_std_atomic_mass	387564.396
## mean_fie	133799.360
## wtd_mean_fie	232071.918
## gmean_fie	80538.237
## wtd_gmean_fie	267752.781
## entropy_fie	161057.906
## wtd_entropy_fie	274010.385
## range_fie	262487.057
## wtd_range_fie	299259.723
## std_fie	182966.190
## wtd_std_fie	660242.043
## mean_atomic_radius	384108.631
## wtd_mean_atomic_radius	652449.298
## gmean_atomic_radius	117031.396
## wtd_gmean_atomic_radius	190858.091
## entropy_atomic_radius	179576.843
## wtd_entropy_atomic_radius	307006.887
## range_atomic_radius	2541667.378
## wtd_range_atomic_radius	263566.250
## std_atomic_radius	217291.922
## wtd_std_atomic_radius	784638.227
## mean_Density	329333.418
## wtd_mean_Density	454090.477
## gmean_Density	357671.007
## wtd_gmean_Density	205615.921
## entropy_Density	164355.155
## wtd_entropy_Density	597368.997
## range_Density	7510.862
## wtd_range_Density	135635.730

```

## std_Density           80376.804
## wtd_std_Density      343895.300
## mean_ElectronAffinity 77253.099
## wtd_mean_ElectronAffinity 238963.093
## gmean_ElectronAffinity 756485.875
## wtd_gmean_ElectronAffinity 326649.943
## entropy_ElectronAffinity 98903.446
## wtd_entropy_ElectronAffinity 273120.011
## range_ElectronAffinity 99801.653
## wtd_range_ElectronAffinity 164201.595
## std_ElectronAffinity 117097.365
## wtd_std_ElectronAffinity 445127.169
## mean_FusionHeat       169751.159
## wtd_mean_FusionHeat   419015.028
## gmean_FusionHeat      213840.811
## wtd_gmean_FusionHeat  298165.358
## entropy_FusionHeat    103526.396
## wtd_entropy_FusionHeat 267895.277
## range_FusionHeat      44811.632
## wtd_range_FusionHeat  303170.198
## std_FusionHeat         107598.380
## wtd_std_FusionHeat    178809.521
## mean_ThermalConductivity 241406.474
## wtd_mean_ThermalConductivity 609965.765
## gmean_ThermalConductivity 89970.612
## wtd_gmean_ThermalConductivity 3522323.458
## entropy_ThermalConductivity 129539.341
## wtd_entropy_ThermalConductivity 676601.488
## range_ThermalConductivity 11525867.279
## wtd_range_ThermalConductivity 376441.863
## std_ThermalConductivity 227192.008
## wtd_std_ThermalConductivity 1882088.282
## mean_Valence          67137.065
## wtd_mean_Valence      664830.665
## gmean_Valence          208707.518
## wtd_gmean_Valence     950449.517
## entropy_Valence        43903.446
## wtd_entropy_Valence   2008614.630
## range_Valence          16108.304
## wtd_range_Valence     480762.847
## std_Valence            98345.551
## wtd_std_Valence        398108.534

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(gbm_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

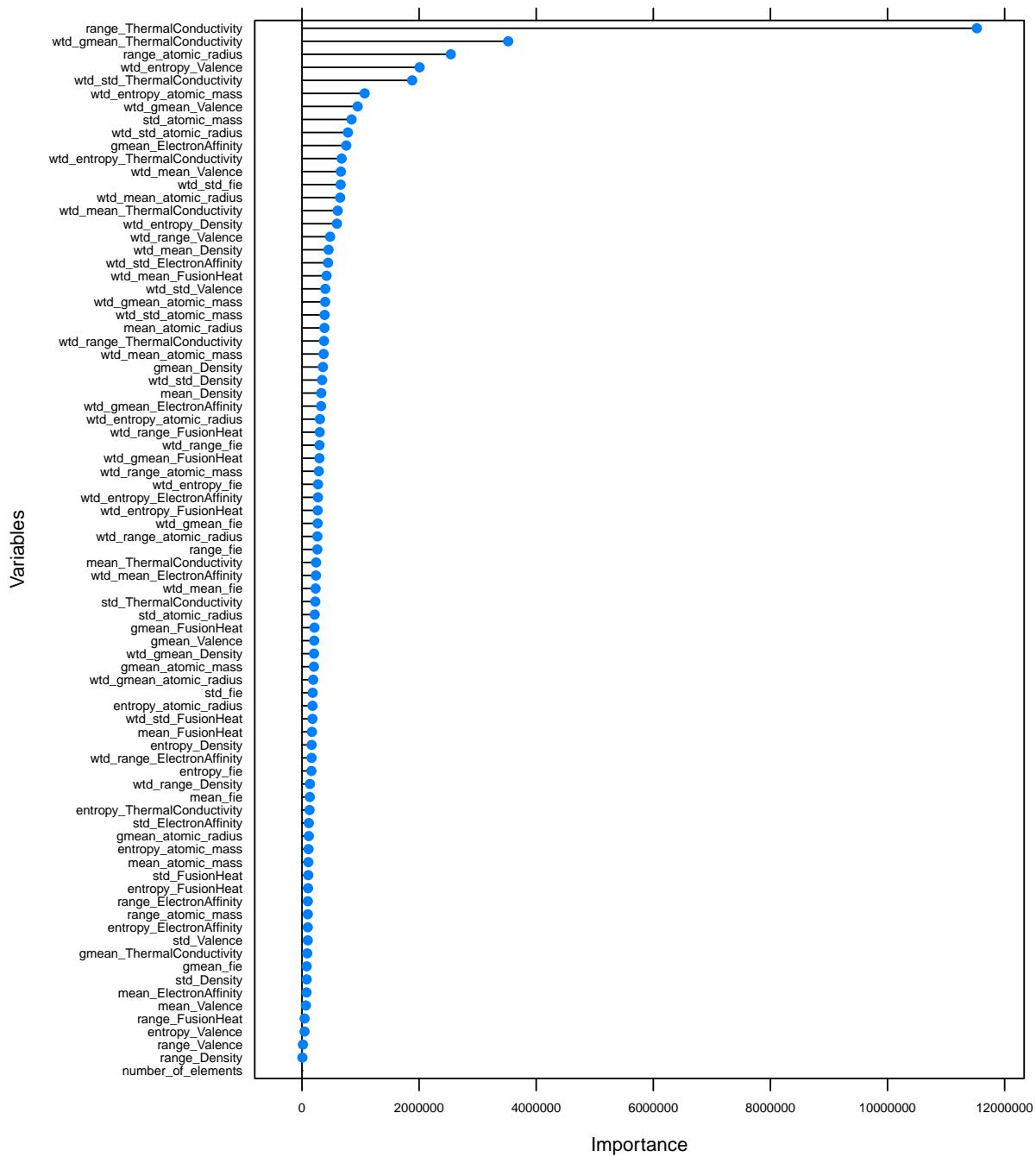


Figure 84: Variables Importance for Gradient Boosting Machine Trans

From above, it can be seen that range\_ThermalConductivity is the most important variable for this model, whereas number\_of\_elements is the least important variable for this model which is same to random forest model.

### 3.2.14 XG-Boost Regression

XG-Boost is an optimized distributed gradient boosting library designed to be highly efficient, flexible and portable. It implements machine learning algorithms under the Gradient Boosting framework. However, xgboost used a more regularized model formalization to control over-fitting, which gives it better performance.

For this algorithm, the main parameters for tuning are nrounds, max\_depth, eta, gamma, colsample\_bytree, min\_child\_weight, and subsample. eta is the learning rate, gamma specifies the minimum loss reduction required to make a split, colsample\_bytree denotes the fraction of columns to be randomly samples for each tree, min\_child\_weight defines the minimum sum of weights of all observations required in a child and subsample denotes the fraction of observations to be randomly samples for each tree.

For the parameters tuning process, we can use apply manual grid search, random grid search or random search tuning. Grid search technique for some cases are more effective, however, it is very time consuming and need much computational cost. Therefore, for this assignment purpose, we will only apply random search tuning with tune length = 2

```
set.seed(seed)

# XG-Boost Regression
xgb_model_trans <- train(
  critical_temp ~., data = train.data,
  trControl = trainControl( method = "cv", number = 10, search = "random"),
  tuneLength = 4,
  method = "xgbTree",
  verbose = FALSE,
  preProc = c("center", "scale", "BoxCox"),
  nthread = 1
)

xgb_model_trans$results

##          eta max_depth     gamma colsample_bytree min_child_weight subsample
## 4 0.4164612          1 2.923158      0.3746891            3 0.6442732
## 2 0.3090364          7 9.234335      0.4067283            6 0.8579489
## 3 0.3274399          3 8.372956      0.3928904            0 0.9359936
## 1 0.1703574          7 2.862233      0.4266450            4 0.8735088
##   nrounds      RMSE    Rsquared      MAE      RMSESD    RsquaredSD      MAESD
## 4      610 13.373199 0.8476288 9.283276 0.3434025 0.007928769 0.2633059
## 2      623 10.169931 0.9120638 5.734965 0.3041558 0.005608927 0.1073369
## 3      624 10.417263 0.9075371 6.407527 0.2614438 0.005009245 0.1466841
## 1      861  9.782014 0.9184236 5.476982 0.3857261 0.007258856 0.1321094

xgb_model_trans$finalModel

## ##### xgb.Booster
## raw: 3.1 Mb
## call:
##   xgboost::xgb.train(params = list(eta = param$eta, max_depth = param$max_depth,
##     gamma = param$gamma, colsample_bytree = param$colsample_bytree,
##     min_child_weight = param$min_child_weight, subsample = param$subsample),
##     data = x, nrounds = param$nrounds, verbose = FALSE, objective = "reg:linear",
##     nthread = 1)
## params (as set within xgb.train):
```

```

##   eta = "0.170357416570419", max_depth = "7", gamma = "2.86223284667358", colsample_bytree = "0.426645"
## xgb.attributes:
##   niter
## # of features: 81
## niter: 861
## nfeatures : 81
## xNames : number_of_elements mean_atomic_mass wtd_mean_atomic_mass gmean_atomic_mass wtd_gmean_atomic_
## problemType : Regression
## tuneValue :
##   nrounds max_depth      eta      gamma colsample_bytree min_child_weight
## 1     861          7 0.1703574 2.862233      0.426645          4
##   subsample
## 1 0.8735088
## obsLevels : NA
## param :
##   $verbose
## [1] FALSE
##
## $nthread
## [1] 1

```

```
xgb_model_trans$bestTune
```

```

##   nrounds max_depth      eta      gamma colsample_bytree min_child_weight
## 1     861          7 0.1703574 2.862233      0.426645          4
##   subsample
## 1 0.8735088

```

```
getTrainPerf(xgb_model_trans)
```

```

##   TrainRMSE TrainRsquared TrainMAE   method
## 1  9.782014      0.9184236 5.476982 xgbTree

```

From above, we can see that the optimal model is the model with nrounds = 861, max\_depth = 7, eta = 0.1703574, gamma = 2.862233, colsample\_bytree = 0.426645, min\_child\_weight = 4, and subsample = 0.8735088. The R-Squared and MSE are 0.9184236 and 95.64 consecutively.

Here, we show the variable importance for this model.

```
varImp(xgb_model_trans, scale = FALSE)$importance
```

	Overall
##	Overall
## wtd_std_ThermalConductivity	0.1830910211
## range_atomic_radius	0.1517557132
## std_ThermalConductivity	0.1360641888
## wtd_range_ElectronAffinity	0.0602163848
## wtd_entropy_Valence	0.0396806683
## wtd_gmean_Valence	0.0313701731
## range_ThermalConductivity	0.0281202940
## wtd_gmean_ThermalConductivity	0.0254845500
## std_atomic_mass	0.0209211612
## wtd_mean_Valence	0.0164776174

```

## wtd_entropy_atomic_mass      0.0156061305
## wtd_range_ThermalConductivity 0.0125970150
## wtd_entropy_ThermalConductivity 0.0117636234
## std_fie                      0.0116862464
## wtd_entropy_Density           0.0096396987
## wtd_std_atomic_radius         0.0091815488
## wtd_gmean_Density             0.0091298887
## wtd_entropy_fie               0.0090565862
## std_ElectronAffinity          0.0079672088
## mean_Density                  0.0077788174
## wtd_std_atomic_mass           0.0077751597
## gmean_atomic_radius           0.0076516357
## wtd_range_atomic_mass          0.0072413924
## gmean_ElectronAffinity        0.0064836719
## wtd_std_ElectronAffinity      0.0061411010
## wtd_mean_ThermalConductivity 0.0060895913
## wtd_range_fie                 0.0060506597
## wtd_mean_atomic_mass          0.0058928941
## gmean_Density                 0.0057007578
## entropy_ThermalConductivity 0.0056563727
## wtd_gmean_atomic_mass          0.0056114984
## wtd_entropy_atomic_radius      0.0055914692
## std_Density                   0.0053729569
## wtd_entropy_ElectronAffinity   0.0047607255
## wtd_mean_atomic_radius         0.0047043328
## mean_ThermalConductivity     0.0045731331
## wtd_std_Density               0.0045574484
## wtd_gmean_ElectronAffinity    0.0045298810
## wtd_range_Density              0.0043478293
## wtd_std_Valence               0.0043344389
## wtd_mean_FusionHeat            0.0042260447
## entropy_Density                0.0040446755
## wtd_range_Valence              0.0037660307
## wtd_entropy_FusionHeat          0.0037182088
## wtd_mean_ElectronAffinity      0.0035842123
## wtd_mean_fie                   0.0034767891
## wtd_mean_Density               0.0033201888
## range_fie                      0.0032664049
## entropy_atomic_radius           0.0032550020
## wtd_gmean_fie                  0.0032216343
## wtd_std_fie                     0.0029347667
## wtd_range_atomic_radius          0.0029041501
## wtd_std_FusionHeat              0.0027984601
## std_FusionHeat                  0.0027386654
## mean_atomic_radius               0.0026911923
## gmean_Valence                  0.0025664430
## range_ElectronAffinity          0.0025310819
## wtd_gmean_atomic_radius          0.0025079600
## wtd_gmean_FusionHeat             0.0024862617
## mean_Valence                    0.0021799362
## range_atomic_mass                0.0021312340
## entropy_atomic_mass              0.0021293077
## std_atomic_radius                0.0020941405
## mean_FusionHeat                  0.0020781658

```

```

## entropy_ElectronAffinity          0.0015989748
## mean_atomic_mass                 0.0015784136
## entropy_FusionHeat              0.0015664411
## gmean_FusionHeat                0.0014912156
## mean_fie                         0.0014803783
## gmean_ThermalConductivity       0.0014763310
## gmean_atomic_mass               0.0014325015
## wtd_range_FusionHeat            0.0014287167
## entropy_fie                      0.0013321488
## range_Density                    0.0009949747
## gmean_fie                        0.0009534808
## mean_ElectronAffinity           0.0008279311
## number_of_elements               0.0006238812
## range_FusionHeat                0.0005164010
## range_Valence                   0.0005141476
## entropy_Valence                 0.0004699976
## std_Valence                      0.0004076218

```

Next, we will plot the variable importance for this model.

```

# Plot the Variable Importance
plot(varImp(xgb_model_trans, scale = FALSE), scales=list(x=list(cex=0.5), y=list(cex=0.5)),
      xlab=list(cex=0.75), ylab=list(label = "Variables",cex=0.75))

```

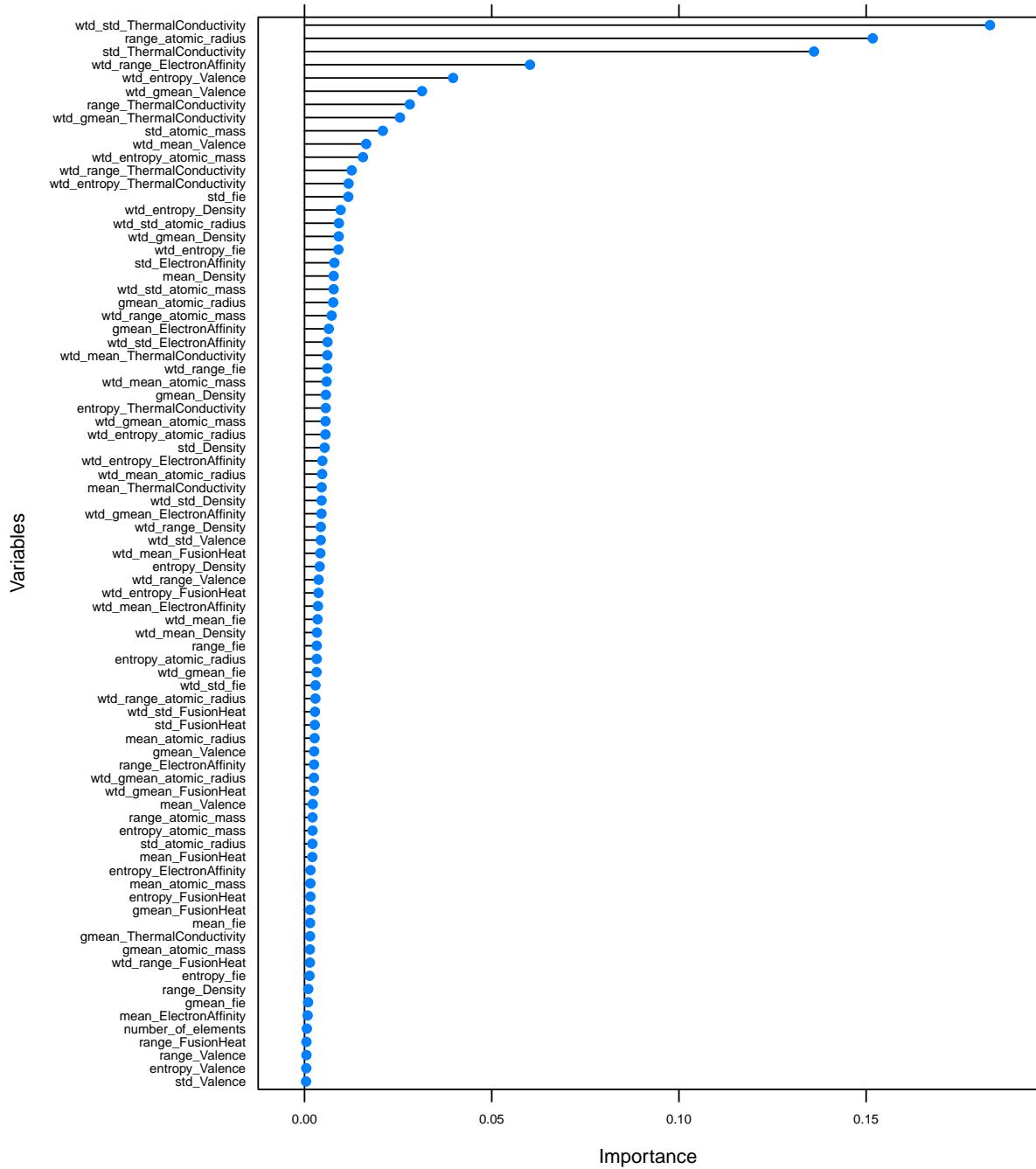


Figure 85: Variables Importance for XG-Boost Trans

From above, it can be seen that `wtd_std_ThermalConductivity` is the most important variable for this model, whereas `std_Valence` is the least important variable for this model.

From this section, we have developed in total 28 models. In the next section, we will focus on model comparison and evaluation.

## 4 Model Comparison

### 4.1 Model Explanation

In the previous section, we have performed multiple algorithms to the original dataset and transformed dataset. Based on the similarity, we can categorize those algorithms into regression algorithm, regularization algorithm, dimensionality reduction algorithm, instance-based algorithm and ensemble tree-based algorithm. Before we go into the model comparison, first we will explain about the idea behind them and their strengths and weaknesses.

#### Regression Algorithm

Regression is focus with modeling the linear relationship between variables that is iteratively refined using a loss function by the model. For this category, we performed linear regression and stepwise regression. For the linear regression, we performed three different models for each dataset which are with all variables, exclude the non-significant variables, and exclude the non-correlated variables. Meanwhile, for the stepwise, we performed forward, backward, and hybrid approach. In general, the main strength of this approach is simple, fast and easy to understand and interpret. However, this type of algorithm will perform poorly when the relationship between the predictors and response variable is non-linear. In addition, linear regression is very sensitive to outliers.

#### Regularization Algorithm

In general, a standard linear regression will fail in the case there is high collinearity among the feature variables. Collinearity is the existence of near-linear relationships among the independent variables. This condition will lead the model to have a huge variance which tends to overfit. Regularization technique discourages learning a more complex or flexible model in order to avoid the risk of overfitting by introducing some bias. For this category, we performed ridge, lasso and elastic net regression. Ridge regression shrinks the regression coefficients, so that variables, with minor contribution to the outcome, have their coefficients close to zero. The shrinkage of the coefficients is achieved by penalizing the regression model with a penalty term called L2-norm, which is the sum of the squared coefficients. Lasso shrinks the regression coefficients toward zero by penalizing the regression model with a penalty term called L1-norm, which is the sum of the absolute coefficients. In the case of lasso regression, the penalty has the effect of forcing some of the coefficient estimates, with a minor contribution to the model, to be exactly equal to zero. This means that, lasso can be also seen as an alternative to the subset selection methods for performing variable selection in order to reduce the complexity of the model. Elastic Net produces a regression model that is penalized with both the L1 and L2 regularizations. The consequence of this is to effectively shrink coefficients and to set some coefficients to zero.

#### Dimensionality Reduction Algorithm

Dimensionality reduction is a process of reducing the dimension of the features set. For this category, we performed Principal Component Regression (PCR) which popularly used for dimensionality reduction in continuous data. One of the strengths is it can reduce the number of needed features for a model, however, it only works well when the dataset contains highly correlated predictors.

#### Instance-based Algorithm

Instance-based algorithm is a decision problem with instances of training data that are deemed important and required to the model. For this category, we performed K-Nearest Neighbor Regression. In general, some of the strengths of this algorithm is pretty intuitive, simple, no assumptions, and only has 1 parameter which is the number of neighbors. However, one of the key challenges for this model is to determine the optimal number of neighbors.

#### Ensemble Tree-based Algorithm

Tree-based algorithm empower predictive models with high accuracy, stability and ease of interpretation. Unlike linear models, this type of algorithms performs well in non-linear relationships cases. There are

some ensemble methods in tree-based algorithm, namely bagging, boosting and stacking. Ensemble methods combine a of predictive models to achieve a better accuracy and model stability.

Bagging is a technique used to reduce the variance of our predictions by combining the result of multiple classifiers modelled on different sub-samples of the same dataset. One of the implementations of bagging models is random forest. This algorithm grows multiple trees in order to predict a new object. The final result is the average of outputs by different trees. One of the benefits from this algorithm is the power of handle large dataset with higher dimensionality. However, it might be over-fit for noisy dataset.

Boosting is a technique to convert weak learners to strong learners. Gradient Boosting Machine (GBM) and Extreme Gradient Boosting (XG-Boost) are two of the boosting implementations. The advantages of using GBM is often produce accuracy that cannot be beat and no data pre-processing required (often works well with categorical and numerical value). However, this algorithm is very computationally expensive and less interpretable. On the other hand, XGBoost is a specific implementation of the Gradient Boosting method which delivers more accurate approximations by using the strengths of second order derivative of the loss function, L1 and L2 regularization and parallel computing which makes it faster compared to GBM.

## 4.2 Model Evaluation

In this subsection, we will do model evaluation and comparison

```
# List of Models
models <- list(linear_model1, linear_model2, linear_model3, linear_backward,
               linear_forward, linear_stepwise, ridge_model, lasso_model,
               elastic_net_model, pcr_model, knn_model, random_forest_model,
               gbm_model, xgb_model, linear_model1_trans, linear_model2_trans,
               linear_model3_trans, linear_backward_trans, linear_forward_trans,
               linear_stepwise_trans, ridge_model_trans, lasso_model_trans,
               elastic_net_model_trans, pcr_model_trans, knn_model_trans,
               random_forest_model_trans, gbm_model_trans, xgb_model_trans)

# List of Models' Label
models.label <- c("Linear Regression Model 1", "Linear Regression Model 2",
                  "Linear regression Model 3", "Linear Regression Backward Selection",
                  "Linear Regression Forward Selection", "Linear Regression Stepwise Selection",
                  "Ridge Regression", "Lasso Regression", "Elastic Net",
                  "Principal Component Regression", "K-Nearest Neighbor Regression",
                  "Random Forest", "Gradient Boosting Machine",
                  "XG-Boost Regression", "Linear Regression Model 1 Trans",
                  "Linear Regression Model 2 Trans", "Linear regression Model 3 Trans",
                  "Linear Regression Backward Selection Trans",
                  "Linear Regression Forward Selection Trans",
                  "Linear Regression Stepwise Selection Trans",
                  "Ridge Regression Trans", "Lasso Regression Trans", "Elastic Net Trans",
                  "Principal Component Regression Trans", "K-Nearest Neighbor Regression Trans",
                  "Random Forest Trans", "Gradient Boosting Machine Trans", "XG-Boost Regression Trans")

# List of Linear Models' Label
linear.models <- c("Linear Regression Model 1", "Linear Regression Model 2",
                  "Linear regression Model 3", "Linear Regression Backward Selection",
                  "Linear Regression Forward Selection", "Linear Regression Stepwise Selection",
                  "Ridge Regression", "Lasso Regression", "Elastic Net",
                  "Principal Component Regression", "Linear Regression Model 1 Trans",
                  "Linear Regression Model 2 Trans", "Linear regression Model 3 Trans",
```

```

    "Linear Regression Backward Selection Trans",
    "Linear Regression Forward Selection Trans",
    "Linear Regression Stepwise Selection Trans",
    "Ridge Regression Trans", "Lasso Regression Trans", "Elastic Net Trans",
    "Principal Component Regression Trans")

# List of Instance-Based Models' Label
instance.models <- c("K-Nearest Neighbor Regression",
                    "K-Nearest Neighbor Regression Trans")

# List of Ensemble Tree-Based Models' Label
treebased.models <- c("Random Forest", "Gradient Boosting Machine",
                      "XG-Boost Regression", "Random Forest Trans",
                      "Gradient Boosting Machine Trans", "XG-Boost Regression Trans")

# Store the Metrics
R_Square <- c()
MSE <- c()
MAE <- c()
for (model in models){
  R_Square <- append(R_Square, round(getTrainPerf(model)$TrainRsquared,3))
  MSE <- append(MSE, round((getTrainPerf(model)$TrainRMSE)^2,3))
  MAE <- append(MAE, round(getTrainPerf(model)$TrainMAE,3))
}

```

Table 1 shows the summary of all models which contains R-Squared, MSE, and MAE. From the table, it can be seen that Random Forest on original data or transformed data outperform other models with Train R-Squared 0.923, whereas the worst model is the model with Principal Component Regression on the tranformed data with Train R-Squared 0.687. We will elaborate more about it at the end of this section.

Now, in order to visualise the matrix in the boxplots, we will resample the cross validation using resamples features from caret. The resamples function can be used to collect, summarize and contrast the resampling results [The].

```

set.seed(seed)

# Resample the Cross Validation
results <- resamples(
  list(
    "Linear Regression Model 1" = linear_model1,
    "Linear Regression Model 2" = linear_model2,
    "Linear regression Model 3" = linear_model3,
    "Linear Regression Backward Selection" = linear_backward,
    "Linear Regression Forward Selection" = linear_forward,
    "Linear Regression Stepwise Selection" = linear_stepwise,
    "Ridge Regression" = ridge_model,
    "Lasso Regression" = lasso_model,
    "Elastic Net" = elastic_net_model,
    "Princial Component Regression" = pcr_model,
    "K-Nearest Neighbor Regression" = knn_model,
    "Random Forest" = random_forest_model,
    "Gradient Boosting Machine" = gbm_model,
    "XG-Boost Regression" = xgb_model,
    "Linear Regression Model 1 Trans" = linear_model1_trans,

```

Table 1: Train Metrics Summary for All Models

models.label	R_Square	MSE	MAE
Linear Regression Model 1	0.733	313.673	13.403
Linear Regression Model 2	0.732	314.375	13.419
Linear regression Model 3	0.725	323.072	13.654
Linear Regression Backward Selection	0.733	313.661	13.405
Linear Regression Forward Selection	0.733	313.651	13.398
Linear Regression Stepwise Selection	0.733	313.673	13.403
Ridge Regression	0.715	333.869	13.927
Lasso Regression	0.729	318.452	13.510
Elastic Net	0.730	317.289	13.478
Principal Component Regression	0.692	360.840	14.550
K-Nearest Neighbor Regression	0.906	111.674	5.578
Random Forest	0.923	91.080	5.445
Gradient Boosting Machine	0.914	101.252	5.901
XG-Boost Regression	0.918	96.145	5.479
Linear Regression Model 1 Trans	0.723	326.288	13.471
Linear Regression Model 2 Trans	0.731	315.096	13.444
Linear regression Model 3 Trans	0.715	334.368	13.820
Linear Regression Backward Selection Trans	0.727	319.760	13.604
Linear Regression Forward Selection Trans	0.723	326.226	13.471
Linear Regression Stepwise Selection Trans	0.730	317.073	13.549
Ridge Regression Trans	0.711	339.899	13.924
Lasso Regression Trans	0.716	334.500	13.591
Elastic Net Trans	0.718	332.115	13.563
Principal Component Regression Trans	0.687	367.590	14.576
K-Nearest Neighbor Regression Trans	0.905	112.343	5.552
Random Forest Trans	0.923	91.070	5.445
Gradient Boosting Machine Trans	0.915	100.197	5.897
XG-Boost Regression Trans	0.918	95.688	5.477

```

"Linear Regression Model 2 Trans" = linear_model2_trans,
"Linear regression Model 3 Trans" = linear_model3_trans,
"Linear Regression Backward Selection Trans" = linear_backward_trans,
"Linear Regression Forward Selection Trans" = linear_forward_trans,
"Linear Regression Stepwise Selection Trans" = linear_stepwise_trans,
"Ridge Regression Trans" = ridge_model_trans,
"Lasso Regression Trans" = lasso_model_trans,
"Elastic Net Trans" = elastic_net_model_trans,
"Principal Component Regression Trans" = pcr_model_trans,
"K-Nearest Neighbor Regression Trans" = knn_model_trans,
"Random Forest Trans" = random_forest_model_trans,
"Gradient Boosting Machine Trans" = gbm_model_trans,
"XG-Boost Regression Trans" = xgb_model_trans)

# summarize the distributions
results$values

##      Resample Linear Regression Model 1~MAE Linear Regression Model 1~RMSE
## 1      Fold01                13.25891                17.70088

```

```

## 2 Fold02 13.29565 17.62663
## 3 Fold03 13.23059 17.14295
## 4 Fold04 13.47349 17.65272
## 5 Fold05 13.64726 18.12081
## 6 Fold06 13.25330 17.50229
## 7 Fold07 13.53133 17.86527
## 8 Fold08 13.01947 17.43296
## 9 Fold09 13.67079 18.14428
## 10 Fold10 13.64800 17.91943
## Linear Regression Model 1~Rsquared Linear Regression Model 2~MAE
## 1 0.7276638 13.30040
## 2 0.7277978 13.33926
## 3 0.7557495 13.22337
## 4 0.7370980 13.49252
## 5 0.7206884 13.67251
## 6 0.7382326 13.25697
## 7 0.7241983 13.56595
## 8 0.7367862 13.04323
## 9 0.7296482 13.64308
## 10 0.7286353 13.65738
## Linear Regression Model 2~RMSE Linear Regression Model 2~Rsquared
## 1 17.74690 0.7262372
## 2 17.65303 0.7269939
## 3 17.15273 0.7554948
## 4 17.67598 0.7364132
## 5 18.14552 0.7199165
## 6 17.52764 0.7374518
## 7 17.89206 0.7233506
## 8 17.46760 0.7357266
## 9 18.11304 0.7306134
## 10 17.93166 0.7282750
## Linear regression Model 3~MAE Linear regression Model 3~RMSE
## 1 13.38377 17.88961
## 2 13.61534 18.05109
## 3 13.59964 17.49058
## 4 13.83816 18.01002
## 5 13.91825 18.39287
## 6 13.47085 17.71522
## 7 13.66265 18.06154
## 8 13.31563 17.68705
## 9 13.91135 18.39253
## 10 13.82506 18.05151
## Linear regression Model 3~Rsquared
## 1 0.7216450
## 2 0.7145878
## 3 0.7456185
## 4 0.7263777
## 5 0.7121857
## 6 0.7318272
## 7 0.7180756
## 8 0.7290206
## 9 0.7222410
## 10 0.7246688
## Linear Regression Backward Selection~MAE

```

```

## 1          13.26018
## 2          13.29568
## 3          13.23036
## 4          13.47498
## 5          13.64507
## 6          13.25597
## 7          13.53233
## 8          13.02355
## 9          13.67762
## 10         13.65090
## Linear Regression Backward Selection~RMSE
## 1          17.70468
## 2          17.62471
## 3          17.14180
## 4          17.65129
## 5          18.11656
## 6          17.50354
## 7          17.86592
## 8          17.43629
## 9          18.14047
## 10         17.91944
## Linear Regression Backward Selection~Rsquared
## 1          0.7275506
## 2          0.7278547
## 3          0.7557824
## 4          0.7371403
## 5          0.7208145
## 6          0.7381954
## 7          0.7241765
## 8          0.7366862
## 9          0.7297624
## 10         0.7286344
## Linear Regression Forward Selection~MAE
## 1          13.25824
## 2          13.27357
## 3          13.21910
## 4          13.47997
## 5          13.64456
## 6          13.24354
## 7          13.52247
## 8          13.02035
## 9          13.67563
## 10         13.64409
## Linear Regression Forward Selection~RMSE
## 1          17.71175
## 2          17.61522
## 3          17.13753
## 4          17.66282
## 5          18.12605
## 6          17.49919
## 7          17.86206
## 8          17.42483
## 9          18.14315
## 10         17.91923

```

```

##      Linear Regression Forward Selection~Rsquared
## 1          0.7273358
## 2          0.7281540
## 3          0.7559196
## 4          0.7367964
## 5          0.7205204
## 6          0.7383236
## 7          0.7242904
## 8          0.7370270
## 9          0.7296859
## 10         0.7286400
##      Linear Regression Stepwise Selection~MAE
## 1          13.25891
## 2          13.29565
## 3          13.23059
## 4          13.47349
## 5          13.64726
## 6          13.25330
## 7          13.53133
## 8          13.01947
## 9          13.67079
## 10         13.64800
##      Linear Regression Stepwise Selection~RMSE
## 1          17.70088
## 2          17.62663
## 3          17.14295
## 4          17.65272
## 5          18.12081
## 6          17.50229
## 7          17.86527
## 8          17.43296
## 9          18.14428
## 10         17.91943
##      Linear Regression Stepwise Selection~Rsquared Ridge Regression~MAE
## 1          0.7276638          13.81863
## 2          0.7277978          13.93558
## 3          0.7557495          13.90288
## 4          0.7370980          13.85555
## 5          0.7206884          14.10568
## 6          0.7382326          13.70787
## 7          0.7241983          14.07167
## 8          0.7367862          13.58893
## 9          0.7296482          14.16283
## 10         0.7286353          14.11859
##      Ridge Regression~RMSE Ridge Regression~Rsquared Lasso Regression~MAE
## 1          18.24295          0.7104397          13.37137
## 2          18.26529          0.7077500          13.47776
## 3          17.92535          0.7330527          13.39169
## 4          18.01920          0.7263568          13.55522
## 5          18.58786          0.7057830          13.78192
## 6          18.04457          0.7220021          13.36370
## 7          18.51875          0.7033514          13.62671
## 8          18.05825          0.7175896          13.09539
## 9          18.64405          0.7147889          13.72931

```

```

## 10          18.41456          0.7136254          13.71090
## Lasso Regression~RMSE Lasso Regression~Rsquared Elastic Net~MAE
## 1           17.83460          0.7233062          13.33772
## 2           17.82009          0.7218323          13.42814
## 3           17.35311          0.7499590          13.34101
## 4           17.73799          0.7346482          13.52237
## 5           18.24843          0.7165120          13.75779
## 6           17.65159          0.7338754          13.32892
## 7           18.05482          0.7180643          13.62423
## 8           17.53861          0.7336164          13.05458
## 9           18.23011          0.7272380          13.70551
## 10          17.98293          0.7268176          13.68279
## Elastic Net~RMSE Elastic Net~Rsquared Princial Component Regression~MAE
## 1           17.80692          0.7242089          14.49177
## 2           17.77954          0.7230865          14.68089
## 3           17.29704          0.7515482          14.58995
## 4           17.71105          0.7354119          14.40131
## 5           18.22526          0.7172708          14.69409
## 6           17.61047          0.7350744          14.28358
## 7           18.04627          0.7183242          14.66100
## 8           17.50106          0.7347292          14.21322
## 9           18.18913          0.7284316          14.76461
## 10          17.95944          0.7274911          14.72071
## Princial Component Regression~RMSE
## 1           18.96102
## 2           19.06768
## 3           18.74505
## 4           18.69661
## 5           19.24868
## 6           18.66091
## 7           19.24104
## 8           18.83364
## 9           19.32361
## 10          19.17966
## Princial Component Regression~Rsquared
## 1           0.6873808
## 2           0.6815899
## 3           0.7077584
## 4           0.7053500
## 5           0.6846424
## 6           0.7025335
## 7           0.6799834
## 8           0.6927310
## 9           0.6934673
## 10          0.6891877
## K-Nearest Neighbor Regression~MAE K-Nearest Neighbor Regression~RMSE
## 1           5.519993          10.485246
## 2           5.498055          10.272284
## 3           5.279794          9.930064
## 4           5.607509          10.232325
## 5           6.000632          11.268734
## 6           5.511357          10.666385
## 7           5.608949          10.491905
## 8           5.473120          10.686955

```

```

## 9          5.734065          11.100893
## 10         5.550344          10.540989
## K-Nearest Neighbor Regression~Rsquared Random Forest~MAE
## 1          0.9053780        5.313385
## 2          0.9098300        5.426169
## 3          0.9189304        5.290154
## 4          0.9123403        5.407212
## 5          0.8927269        5.606425
## 6          0.9045103        5.446963
## 7          0.9058743        5.660868
## 8          0.9019202        5.293195
## 9          0.8991429        5.535084
## 10         0.9068798        5.472745
## Random Forest~RMSE Random Forest~Rsquared Gradient Boosting Machine~MAE
## 1          9.382288         0.9236583        5.882465
## 2          9.607786         0.9193841        5.952600
## 3          9.182999         0.9301996        5.659071
## 4          9.148167         0.9297563        5.809131
## 5          9.627553         0.9215915        6.129791
## 6          9.925006         0.9159090        6.055896
## 7          9.910527         0.9151135        5.984628
## 8          9.472286         0.9225602        5.819534
## 9          9.611148         0.9251831        5.912933
## 10         9.568057         0.9231394        5.801724
## Gradient Boosting Machine~RMSE Gradient Boosting Machine~Rsquared
## 1          10.254887        0.9089901
## 2          10.268231        0.9089349
## 3          9.550411         0.9240928
## 4          9.486169         0.9243438
## 5          10.288416        0.9099524
## 6          10.513565        0.9058233
## 7          10.224100        0.9098474
## 8          10.048445        0.9127974
## 9          10.219385        0.9143812
## 10         9.770355         0.9193639
## XG-Boost Regression~MAE XG-Boost Regression~RMSE
## 1          5.339522         10.023799
## 2          5.562819         10.030538
## 3          5.363252         9.418773
## 4          5.295091         9.057921
## 5          5.613160         9.873478
## 6          5.624130         10.356763
## 7          5.585176         10.005305
## 8          5.386574         9.746768
## 9          5.612616         9.919597
## 10         5.407134         9.620459
## XG-Boost Regression~Rsquared Linear Regression Model 1 Trans~MAE
## 1          0.9128807        13.64420
## 2          0.9126200        13.37014
## 3          0.9260859        13.28869
## 4          0.9307937        13.55345
## 5          0.9170130        13.76288
## 6          0.9084222        13.12930
## 7          0.9137248        13.49415

```

```

## 8          0.9178059      13.03329
## 9          0.9193360      13.77381
## 10         0.9218091      13.66270
##   Linear Regression Model 1 Trans~RMSE
## 1          20.89847
## 2          17.67556
## 3          17.11537
## 4          17.78550
## 5          18.20402
## 6          17.34976
## 7          17.77678
## 8          17.65561
## 9          18.24395
## 10         17.92943
##   Linear Regression Model 1 Trans~Rsquared
## 1          0.6387659
## 2          0.7262899
## 3          0.7568032
## 4          0.7331424
## 5          0.7180825
## 6          0.7427988
## 7          0.7267124
## 8          0.7299526
## 9          0.7266817
## 10         0.7283198
##   Linear Regression Model 2 Trans~MAE
## 1          13.40986
## 2          13.37233
## 3          13.27551
## 4          13.56358
## 5          13.74284
## 6          13.12360
## 7          13.50552
## 8          13.02671
## 9          13.76501
## 10         13.65656
##   Linear Regression Model 2 Trans~RMSE
## 1          17.84597
## 2          17.67476
## 3          17.10689
## 4          17.77932
## 5          18.16247
## 6          17.35333
## 7          17.78256
## 8          17.63736
## 9          18.24433
## 10         17.92233
##   Linear Regression Model 2 Trans~Rsquared
## 1          0.7232781
## 2          0.7263147
## 3          0.7570769
## 4          0.7333338
## 5          0.7193109
## 6          0.7426876

```

```

## 7          0.7265413
## 8          0.7305084
## 9          0.7266694
## 10         0.7285363
##   Linear regression Model 3 Trans~MAE
## 1          14.03602
## 2          13.74741
## 3          13.54342
## 4          13.99353
## 5          14.09325
## 6          13.41322
## 7          13.83482
## 8          13.39595
## 9          14.18938
## 10         13.95174
##   Linear regression Model 3 Trans~RMSE
## 1          20.06323
## 2          18.10375
## 3          17.41928
## 4          18.26415
## 5          18.41880
## 6          17.61064
## 7          18.15523
## 8          18.09977
## 9          18.62340
## 10         18.09919
##   Linear regression Model 3 Trans~Rsquared
## 1          0.6582403
## 2          0.7129246
## 3          0.7479731
## 4          0.7186504
## 5          0.7112060
## 6          0.7350004
## 7          0.7148884
## 8          0.7161921
## 9          0.7152204
## 10         0.7231769
##   Linear Regression Backward Selection Trans~MAE
## 1          13.51705
## 2          13.47660
## 3          13.48672
## 4          13.77515
## 5          13.89325
## 6          13.25199
## 7          13.62087
## 8          13.33163
## 9          13.90708
## 10         13.78226
##   Linear Regression Backward Selection Trans~RMSE
## 1          17.86219
## 2          17.79710
## 3          17.28304
## 4          17.94325
## 5          18.31171

```

```

## 6 17.43974
## 7 17.87318
## 8 17.86244
## 9 18.40600
## 10 18.03959
## Linear Regression Backward Selection Trans~Rsquared
## 1 0.7226445
## 2 0.7225707
## 3 0.7519915
## 4 0.7283813
## 5 0.7148494
## 6 0.7401419
## 7 0.7237426
## 8 0.7236289
## 9 0.7217954
## 10 0.7249651
## Linear Regression Forward Selection Trans~MAE
## 1 13.64371
## 2 13.36952
## 3 13.28977
## 4 13.55355
## 5 13.75984
## 6 13.12976
## 7 13.49434
## 8 13.03327
## 9 13.77361
## 10 13.66349
## Linear Regression Forward Selection Trans~RMSE
## 1 20.88459
## 2 17.67543
## 3 17.11554
## 4 17.78555
## 5 18.20242
## 6 17.34820
## 7 17.77671
## 8 17.65551
## 9 18.24374
## 10 17.92959
## Linear Regression Forward Selection Trans~Rsquared
## 1 0.6391284
## 2 0.7262938
## 3 0.7567992
## 4 0.7331409
## 5 0.7181293
## 6 0.7428443
## 7 0.7267143
## 8 0.7299555
## 9 0.7266881
## 10 0.7283149
## Linear Regression Stepwise Selection Trans~MAE
## 1 13.51717
## 2 13.50045
## 3 13.41736
## 4 13.66961

```

```

## 5 13.84205
## 6 13.17572
## 7 13.60952
## 8 13.13714
## 9 13.87876
## 10 13.74240
## Linear Regression Stepwise Selection Trans~RMSE
## 1 17.88492
## 2 17.76922
## 3 17.21586
## 4 17.82228
## 5 18.24465
## 6 17.38877
## 7 17.84836
## 8 17.64885
## 9 18.29670
## 10 17.94587
## Linear Regression Stepwise Selection Trans~Rsquared
## 1 0.7220574
## 2 0.7234305
## 3 0.7538932
## 4 0.7320360
## 5 0.7167398
## 6 0.7416455
## 7 0.7245392
## 8 0.7301646
## 9 0.7250925
## 10 0.7278338
## Ridge Regression Trans~MAE Ridge Regression Trans~RMSE
## 1 14.14707 20.64489
## 2 13.87535 18.19776
## 3 13.83447 17.76513
## 4 13.89821 18.08747
## 5 14.10682 18.46523
## 6 13.56834 17.84158
## 7 14.03300 18.32281
## 8 13.57022 18.14471
## 9 14.10211 18.55418
## 10 14.10398 18.33989
## Ridge Regression Trans~Rsquared Lasso Regression Trans~MAE
## 1 0.6399302 13.89471
## 2 0.7098804 13.51247
## 3 0.7381232 13.42804
## 4 0.7242294 13.62855
## 5 0.7096343 13.84969
## 6 0.7283815 13.23768
## 7 0.7095064 13.64026
## 8 0.7148661 13.13598
## 9 0.7176396 13.82099
## 10 0.7159903 13.76097
## Lasso Regression Trans~RMSE Lasso Regression Trans~Rsquared
## 1 22.45857 0.5962075
## 2 17.80443 0.7223079
## 3 17.26345 0.7527208

```

```

## 4          17.79399      0.7329247
## 5          18.22804      0.7171355
## 6          17.46180      0.7396155
## 7          17.95430      0.7211378
## 8          17.67582      0.7293725
## 9          18.29124      0.7253780
## 10         17.96167      0.7274195
##   Elastic Net Trans~MAE Elastic Net Trans~RMSE Elastic Net Trans~Rsquared
## 1          13.83817      22.09942      0.6060407
## 2          13.47639      17.75680      0.7237825
## 3          13.39042      17.21987      0.7539226
## 4          13.59504      17.75514      0.7340708
## 5          13.83263      18.21519      0.7175745
## 6          13.20778      17.42286      0.7407439
## 7          13.60616      17.90164      0.7227900
## 8          13.12625      17.65775      0.7299095
## 9          13.81353      18.26374      0.7261809
## 10         13.74580      17.94784      0.7278105
##   Principal Component Regression Trans~MAE
## 1          14.71631
## 2          14.65243
## 3          14.56090
## 4          14.50421
## 5          14.68592
## 6          14.22727
## 7          14.59396
## 8          14.29395
## 9          14.78585
## 10         14.73711
##   Principal Component Regression Trans~RMSE
## 1          21.09093
## 2          19.00654
## 3          18.63814
## 4          18.79531
## 5          19.12656
## 6          18.59290
## 7          19.07293
## 8          18.99094
## 9          19.30201
## 10         19.11017
##   Principal Component Regression Trans~Rsquared
## 1          0.6240535
## 2          0.6835704
## 3          0.7112804
## 4          0.7021439
## 5          0.6886266
## 6          0.7046600
## 7          0.6854646
## 8          0.6875664
## 9          0.6941065
## 10         0.6914658
##   K-Nearest Neighbor Regression Trans~MAE
## 1          5.411281
## 2          5.494471

```

```

## 3          5.388101
## 4          5.631288
## 5          5.932339
## 6          5.377543
## 7          5.543259
## 8          5.501435
## 9          5.740458
## 10         5.499044
## K-Nearest Neighbor Regression Trans~RMSE
## 1          10.26538
## 2          10.33516
## 3          10.30903
## 4          10.34560
## 5          11.26319
## 6          10.46825
## 7          10.50137
## 8          10.87978
## 9          11.16665
## 10         10.45768
## K-Nearest Neighbor Regression Trans~Rsquared Random Forest Trans~MAE
## 1          0.9089279   5.312593
## 2          0.9086628   5.426169
## 3          0.9124154   5.287369
## 4          0.9106057   5.408466
## 5          0.8930785   5.606920
## 6          0.9078416   5.447746
## 7          0.9058456   5.661633
## 8          0.8984195   5.293079
## 9          0.8979172   5.536108
## 10         0.9083760   5.472004
## Random Forest Trans~RMSE Random Forest Trans~Rsquared
## 1          9.381974    0.9236633
## 2          9.606523    0.9194046
## 3          9.178113    0.9302797
## 4          9.148425    0.9297512
## 5          9.627697    0.9215892
## 6          9.925264    0.9159046
## 7          9.913208    0.9150669
## 8          9.470723    0.9225857
## 9          9.613701    0.9251446
## 10         9.565050    0.9231898
## Gradient Boosting Machine Trans~MAE
## 1          5.822525
## 2          5.916651
## 3          5.816165
## 4          5.780141
## 5          5.988511
## 6          6.071791
## 7          5.973457
## 8          5.834098
## 9          5.945356
## 10         5.819491
## Gradient Boosting Machine Trans~RMSE
## 1          10.284100

```

```

## 2          10.103758
## 3          9.754359
## 4          9.424242
## 5          9.992584
## 6          10.474677
## 7          10.138429
## 8          10.044399
## 9          10.305994
## 10         9.576072
##   Gradient Boosting Machine Trans~Rsquared XG-Boost Regression Trans~MAE
## 1          0.9086440      5.397595
## 2          0.9120015      5.497334
## 3          0.9208849      5.327164
## 4          0.9252283      5.288206
## 5          0.9150595      5.639201
## 6          0.9063464      5.639570
## 7          0.9113558      5.648312
## 8          0.9129418      5.416894
## 9          0.9128264      5.511741
## 10         0.9225154      5.403803
##   XG-Boost Regression Trans~RMSE XG-Boost Regression Trans~Rsquared
## 1          10.082469      0.9120134
## 2          9.977100      0.9135602
## 3          9.414233      0.9261574
## 4          9.040906      0.9310877
## 5          9.767263      0.9187842
## 6          10.367552      0.9082399
## 7          10.099379      0.9120057
## 8          9.816249      0.9166534
## 9          9.756936      0.9219624
## 10         9.498055      0.9237715

```

From the above result, we can see the information about the R-Squared, MSE and MAE for each fold. Next, we will visualise them using boxplot in order to ease the interpretation.

```

# Transpose the Table
train.result <- melt(results$values, id = c("Resample"))[2:3]

train.result <- as.data.frame(
  cbind(do.call('rbind', strsplit(as.character(train.result$variable), '~', fixed=TRUE)),
    round(train.result$value,3)))

train.result$V4<- ifelse(grepl("Trans", train.result$V1), "Transformed", "Original")
colnames(train.result) <- c("Model","Metrics","Value","Type")

# Boxplot for R-Squared Metric
ggplot(train.result[train.result$Metrics == "Rsquared",], aes(x=Model,
                                                               y=as.numeric(as.character(Value)),
                                                               fill = Type)) +
  geom_boxplot() + ylab("Rsquared") + theme_bw() + scale_fill_brewer(palette = "Accent") +
  theme(legend.position = "bottom",axis.text.x = element_text(angle = 90, hjust = 1))

```

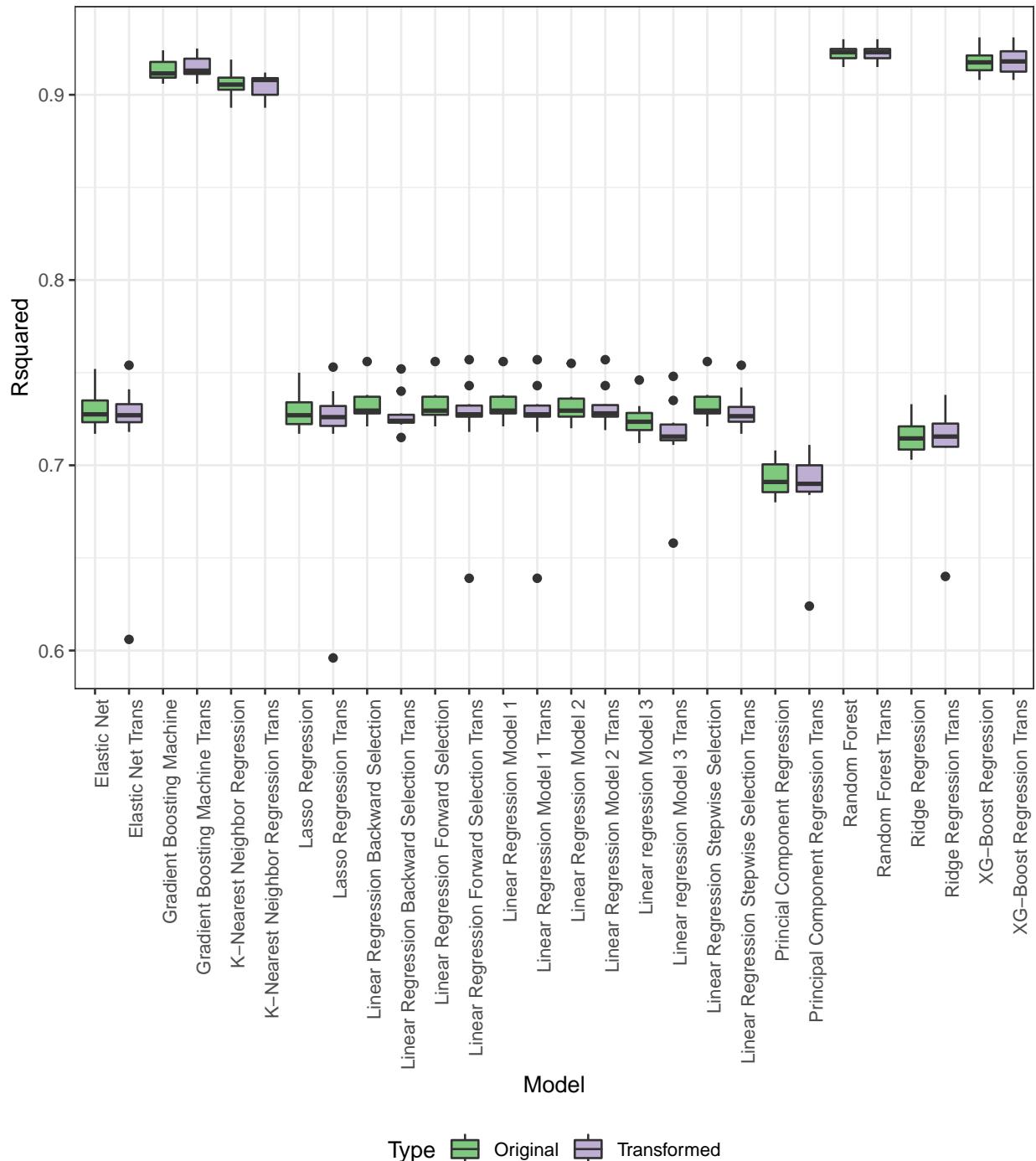


Figure 86: R-Squared Model Comparison

```
# Boxplot for MSE Metric
ggplot(train.result[train.result$Metrics == "RMSE",], aes(x=Model,
y=as.numeric(as.character(Value))^2,
fill = Type)) +
geom_boxplot() + ylab("MSE") + theme_bw() + scale_fill_brewer(palette = "Accent") +
theme(legend.position = "bottom",axis.text.x = element_text(angle = 90, hjust = 1))
```

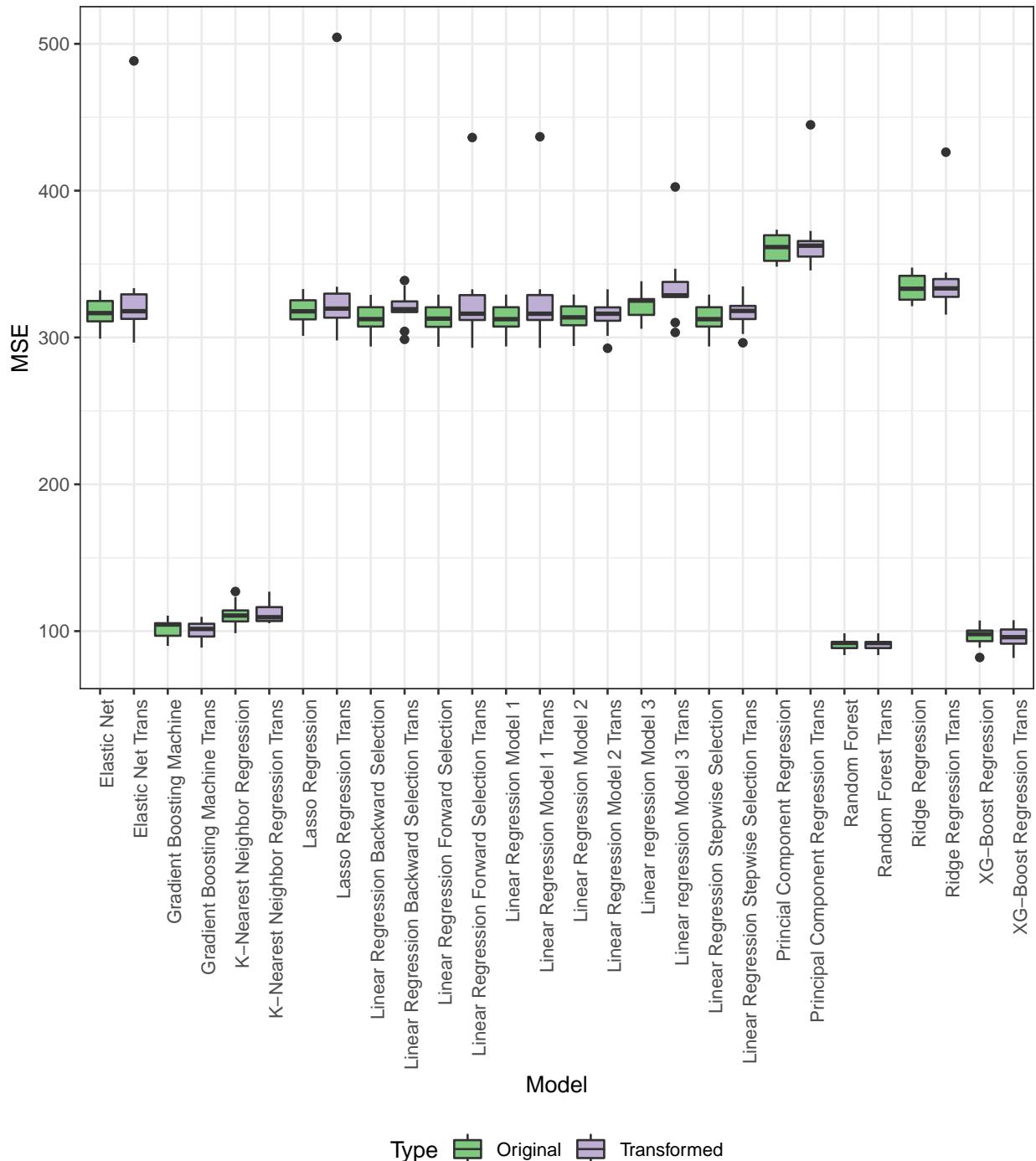


Figure 87: MSE Model Comparison

```
# Boxplot for MAE Metric
ggplot(train.result[train.result$Metrics == "MAE",], aes(x=Model,
                                                       y=as.numeric(as.character(Value)),
                                                       fill = Type)) +
  geom_boxplot() + ylab("MAE") + theme_bw() + scale_fill_brewer(palette = "Accent") +
  theme(legend.position = "bottom", axis.text.x = element_text(angle = 90, hjust = 1))
```

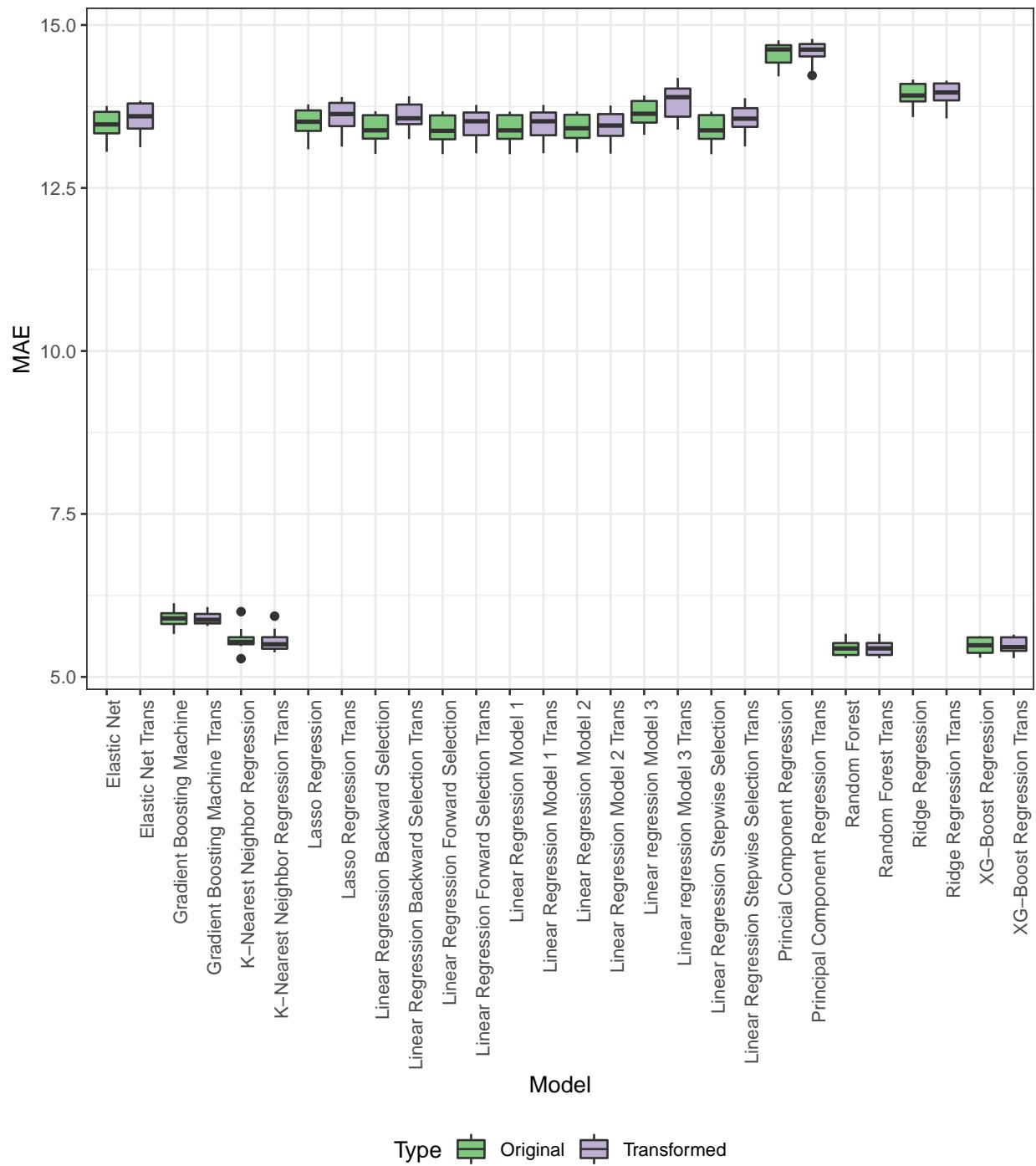


Figure 88: MAE Model Comparison

From the above visualisation, we can easily see and interpret the performance of all models. Here is the results of the model comparison.

- Principal Component Regression is the worst model. This is because PCR will perform well if the dataset contains highly correlated predictors, whereas, in our dataset the majority of the predictors has no correlation to others.

- Ridge, Lasso and Elastic Net Regression perform worse compared to the original linear regression. The is no collinearity among the feature variables in our dataset. As we know that, regularisation will help in the case there is high collinearity among the feature variables, so in this case it does not help to improve the model quality.
- In general, backward, forward, and stepwise selection regression models perform nearly similar with the original linear regression model. This is because all the variables are contributed to the model, therefore, even though we perform the selection, it will not significantly reduce the number of predictors.
- All linear regression related models have almost similar results. In term of R-Squared, all of them have around 0.73. This is because linear regression will perform well only if the solution is linear, whereas, in our dataset, most of the features has no linear relationship to the response variable. This leads us to try non-linear models.
- KNN Regression is one of the top four models. KNN Regression outperforms other linear related models. KNN regression is a nonparametric regression technique that fits regression locally based on the k nearest points to a point under consideration. Therefore, it is suitable for the problem that cannot meet all the assumption in linear regression, because of its flexibility.
- Ensemble tree-based algorithm (GBM, XGBoost and Random Forest) outperform all other models. There are many reason why they perform better among other models. First, our dataset has high dimension. As we know that ensemble tree-based algorithms perform well in handling large dataset with higher dimensionality. Second, most of the variables in our dataset have non linear relationship with the response variable. However, the weakness of these models is having more parameter to be tuned which leads to time complexity.
- In general, data transformation does not increase the performance of the model. For non-linear models, data transformation basically is not needed, because those models do not need the linear assumption, whereas for linear related models, the models with transformed data are worse, this might because some information are loss during the transformation process.

### 4.3 Prediction

In this subsection, we will predict the test data and calculate the MSE for each model.

```
pred.data <- as.data.frame(test.data$critical_temp)

mse.data <- data.frame(Model = character(),
                        MSE = numeric(),
                        stringsAsFactors=FALSE)

# Store the Prediction and Test MSE
for(i in seq(1, length(models))){
  prediction <- predict(models[i],
                        newdata = test.data[,-82])
  pred.data[,models.label[i]] <- prediction
  mse.data[nrow(mse.data) + 1,] = c(models.label[i], round(mse(as.vector(prediction[[1]])),
                                                test.data$critical_temp), 3))
}
```

Table 2 shows Test Mean Square Error (MSE). It can be seen that the test error follows the pattern of the train metrics. Random Forest has the lowest MSE 81.317, whereas PCA has the largest test MSE. For details can be seen in the table.

Next, we will visualise the test MSE for better representation.

```
mse.data$MSE <- as.numeric(as.character(mse.data$MSE))
```

Table 2: Test Metrics Summary for All Models

Model	MSE
Linear Regression Model 1	298.989
Linear Regression Model 2	299.606
Linear regression Model 3	308.133
Linear Regression Backward Selection	298.992
Linear Regression Forward Selection	299.16
Linear Regression Stepwise Selection	298.989
Ridge Regression	316.002
Lasso Regression	301.886
Elastic Net	300.826
Principal Component Regression	340.481
K-Nearest Neighbor Regression	103.392
Random Forest	81.317
Gradient Boosting Machine	93.066
XG-Boost Regression	87.77
Linear Regression Model 1 Trans	295.924
Linear Regression Model 2 Trans	296.045
Linear regression Model 3 Trans	309.612
Linear Regression Backward Selection Trans	299.708
Linear Regression Forward Selection Trans	295.927
Linear Regression Stepwise Selection Trans	298.053
Ridge Regression Trans	312.287
Lasso Regression Trans	299.064
Elastic Net Trans	298.255
Principal Component Regression Trans	338.724
K-Nearest Neighbor Regression Trans	102.917
Random Forest Trans	81.31
Gradient Boosting Machine Trans	91.446
XG-Boost Regression Trans	88.446

```
# Horizontal Barplot for MSE
ggplot(mse.data) +
  geom_bar(aes(y=MSE, x=reorder(Model, -MSE), fill = -MSE),
           stat="identity", position="dodge") + xlab("Model") +
  coord_flip() + theme_bw() + labs(fill = "MSE")
```

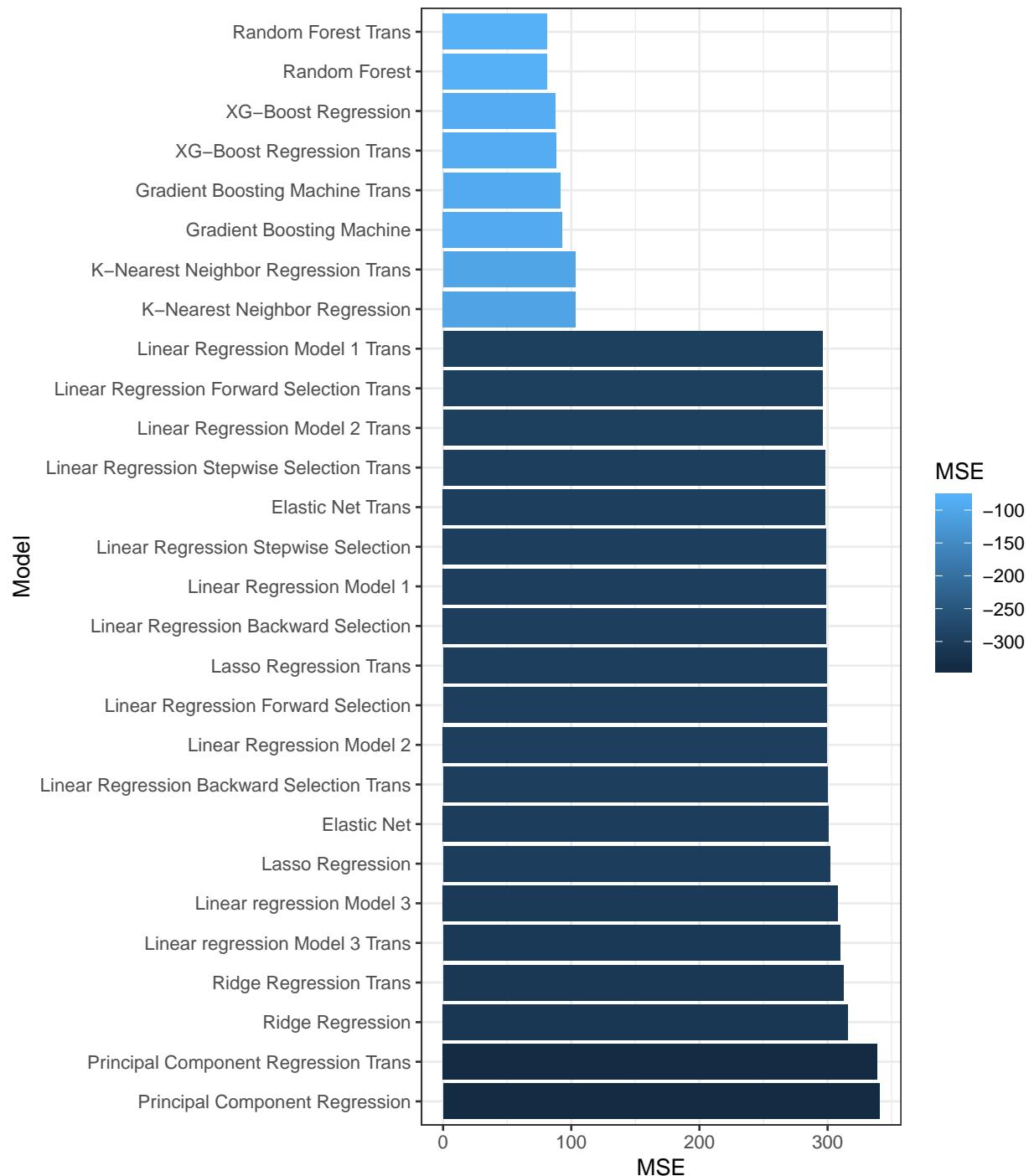


Figure 89: Model with MSE Test Data

Next we will visualise the sequence of real critical temperature compared to predicted critical temperature from each model. As shown below, for the better model, the blue line covers almost all the red lines.

```
# Visualise the Sequence of Prediction and Real Values
for(label in models.label){
  sequence_data = seq(1:length(test.data$critical_temp))
```

```

plot(sequence_data, test.data$critical_temp, type="l", col="red",
      ylab = "Critical Temperature", xlab = "Sequence of Test Data")
lines(sequence_data, pred.data[,label], col="blue", xlab="", ylab="")
legend("topleft", legend=c("critical_temp_original", "critical_temp_predicted"),
       col=c("red", "blue"), lty=1,cex=0.8)
cat('\n\n')
}

```

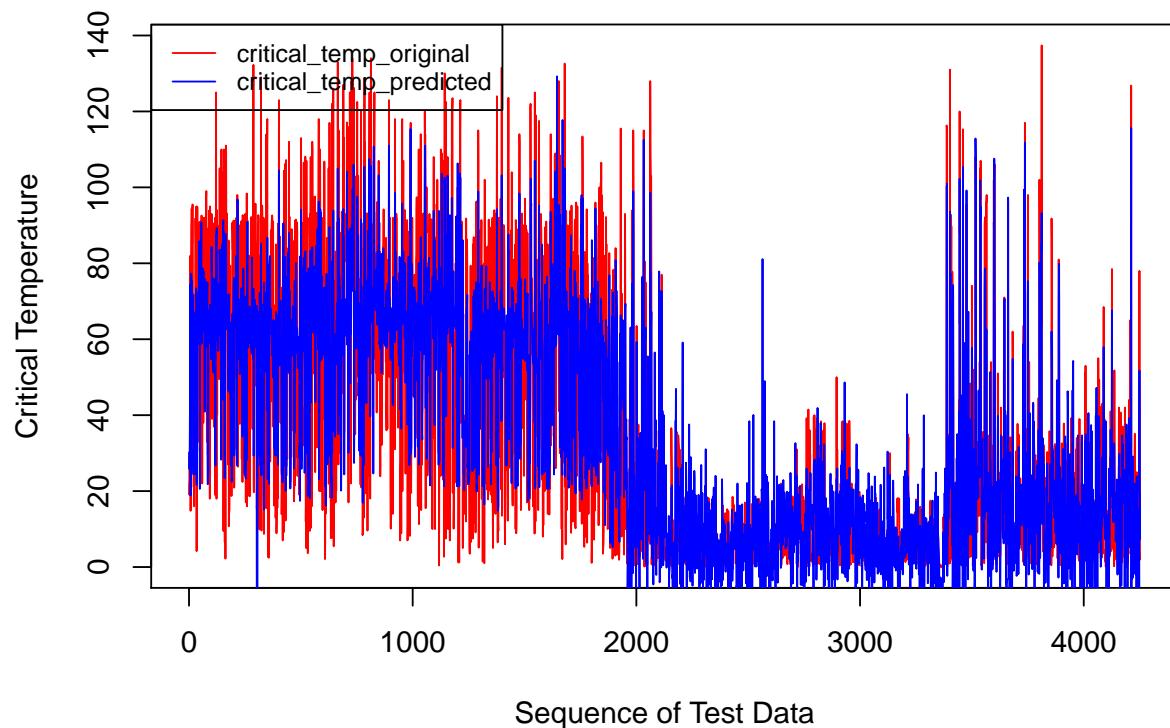


Figure 90: Sequence of Prediction vs Real Values with Linear Regression Model 1

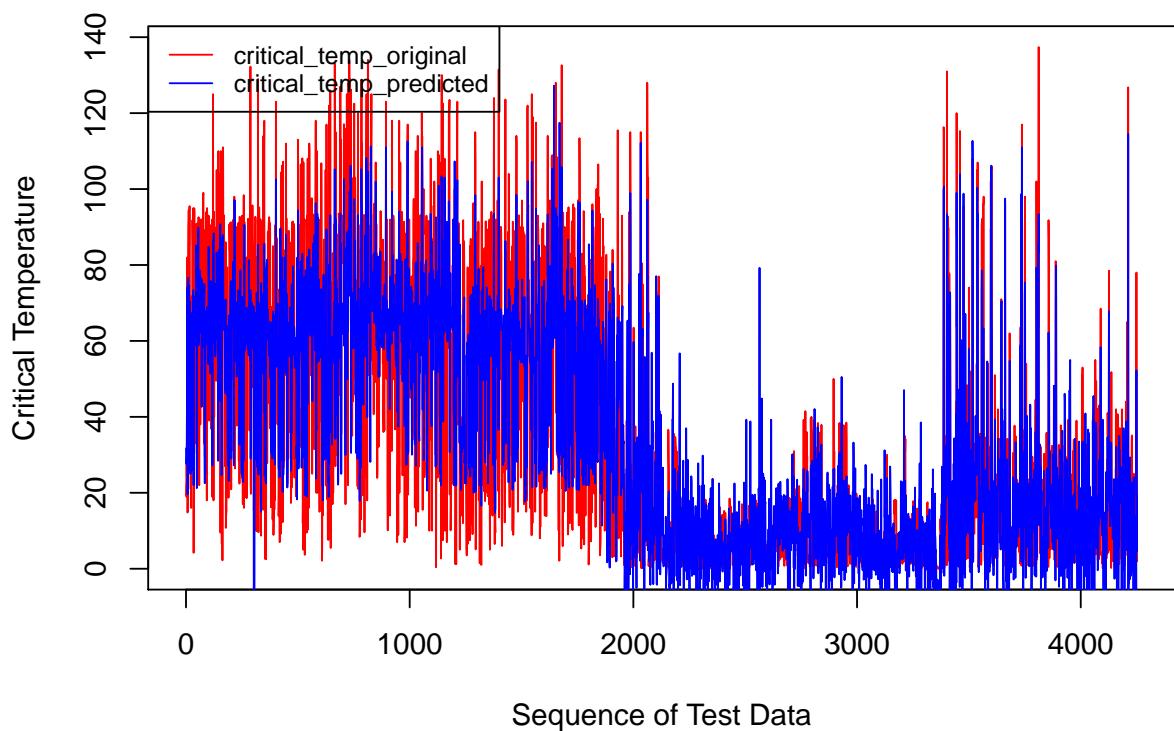


Figure 91: Sequence of Prediction vs Real Values with Linear Regression Model 2

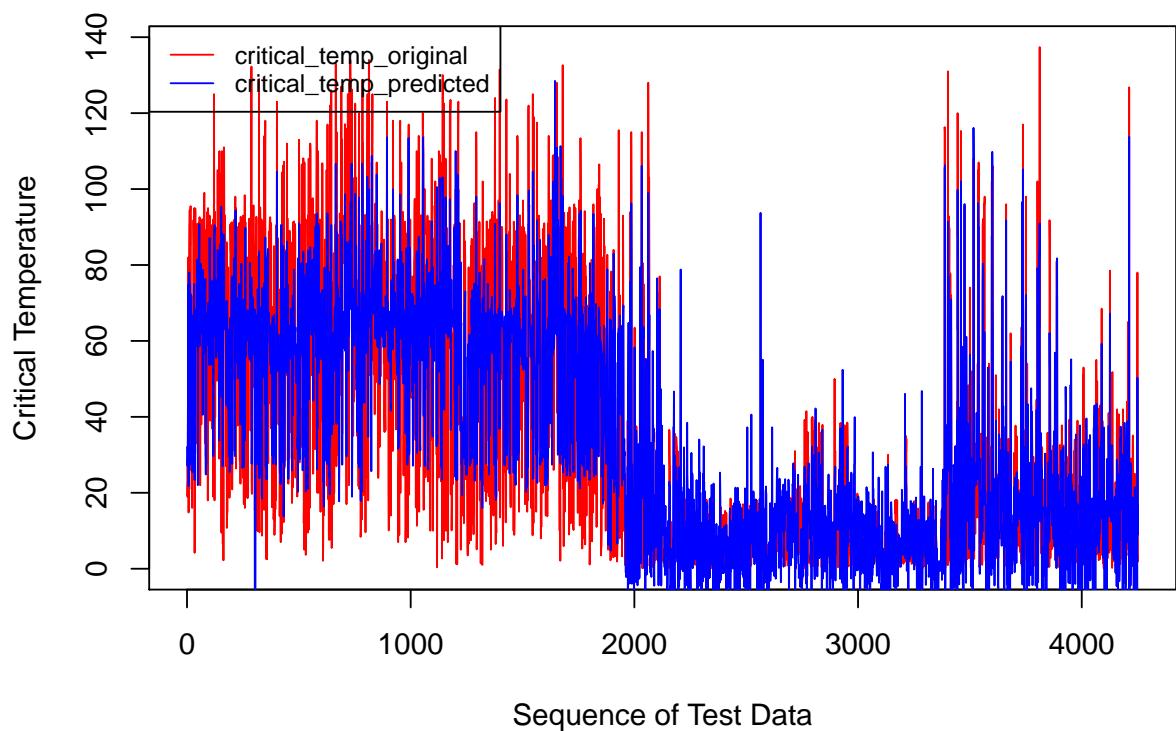


Figure 92: Sequence of Prediction vs Real Values with Linear regression Model 3

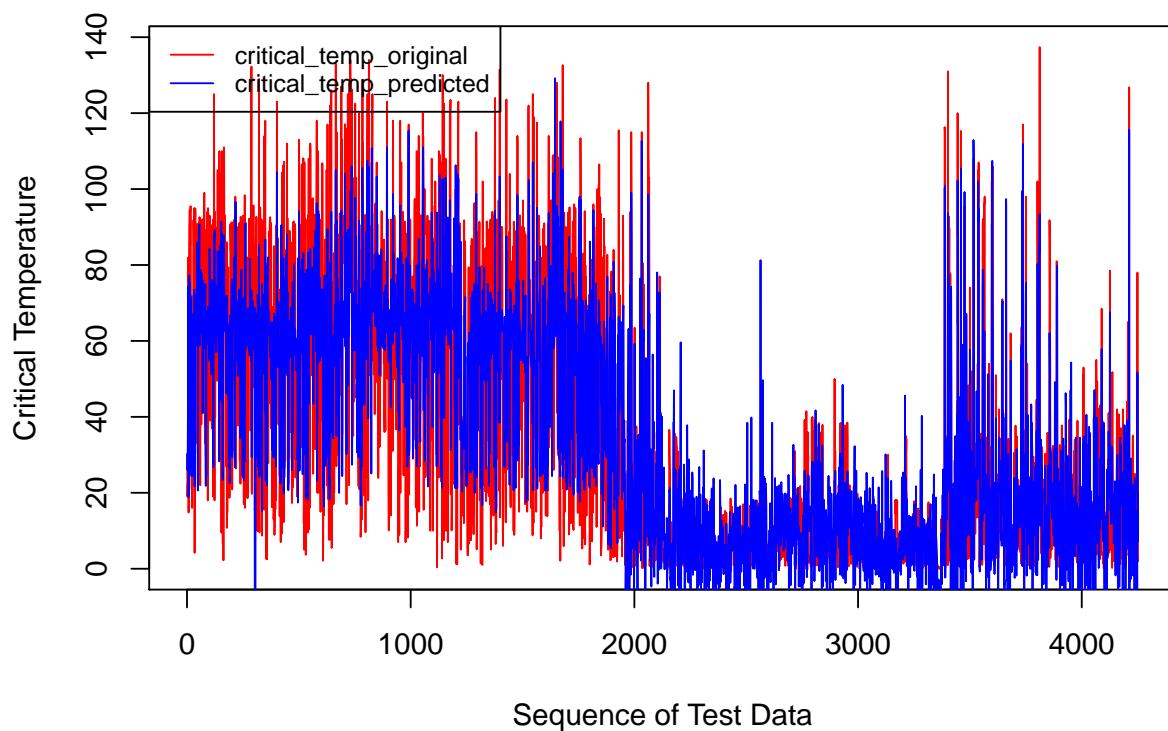


Figure 93: Sequence of Prediction vs Real Values with Linear Regression Backward Selection

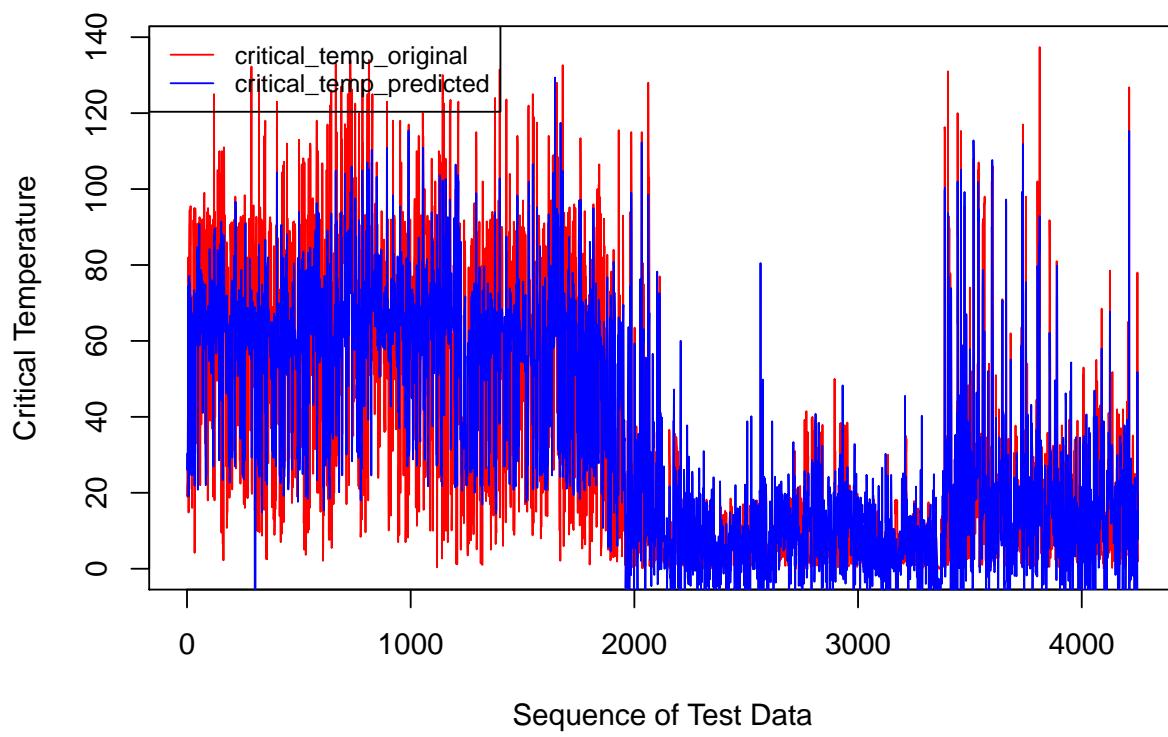


Figure 94: Sequence of Prediction vs Real Values with Linear Regression Forward Selection

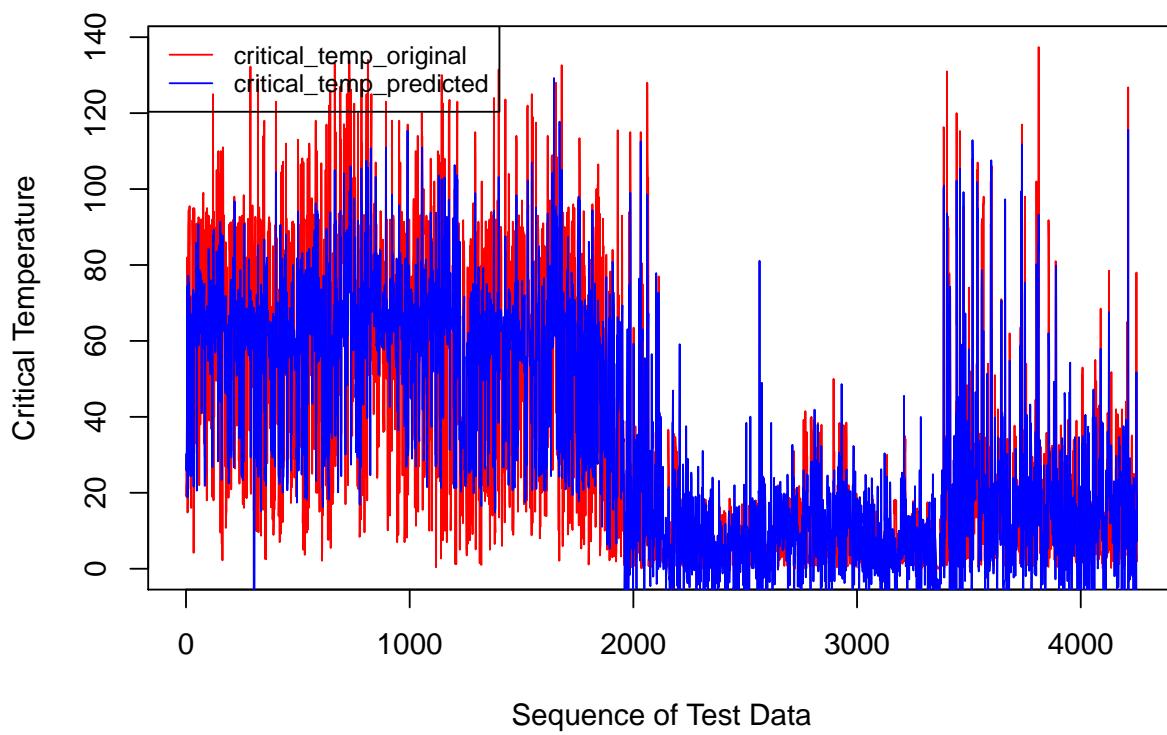


Figure 95: Sequence of Prediction vs Real Values with Linear Regression Stepwise Selection

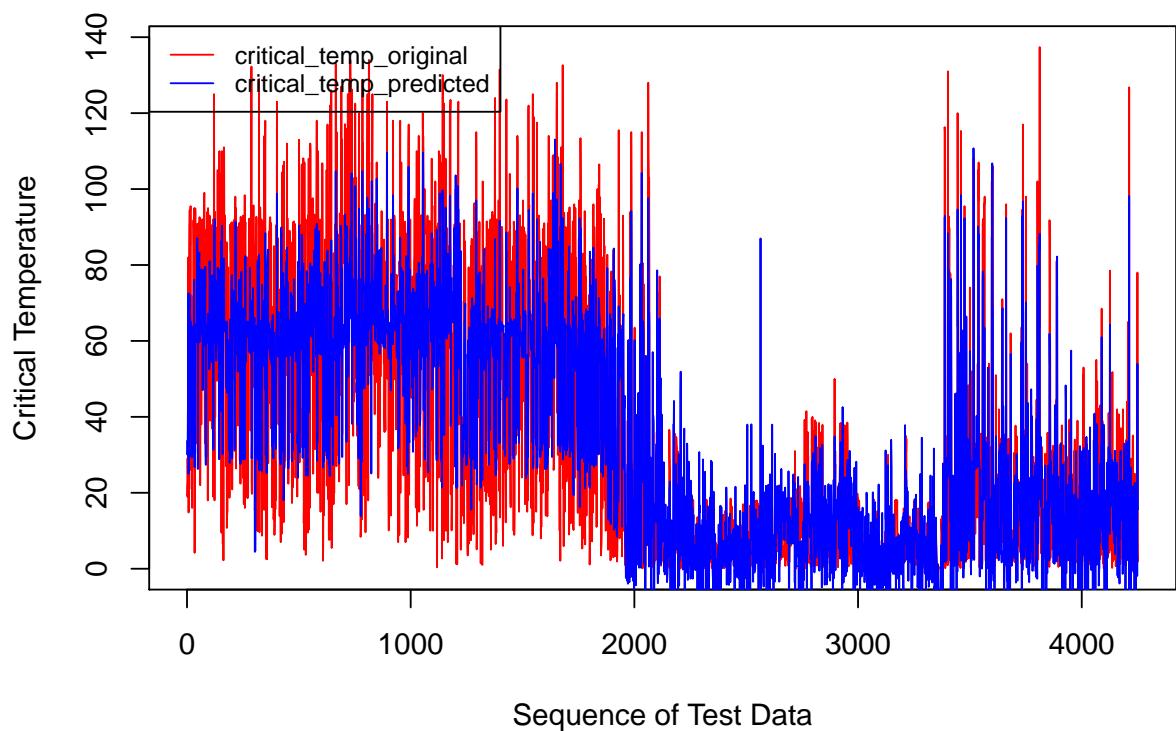


Figure 96: Sequence of Prediction vs Real Values with Ridge Regression

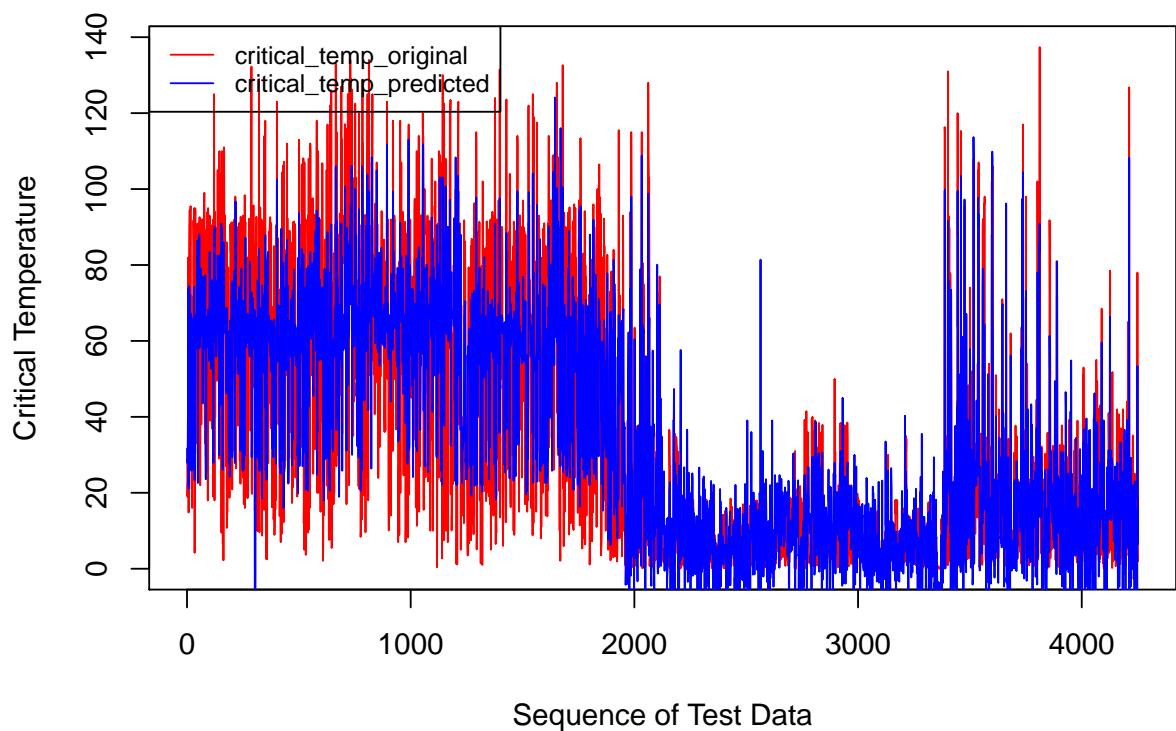


Figure 97: Sequence of Prediction vs Real Values with Lasso Regression

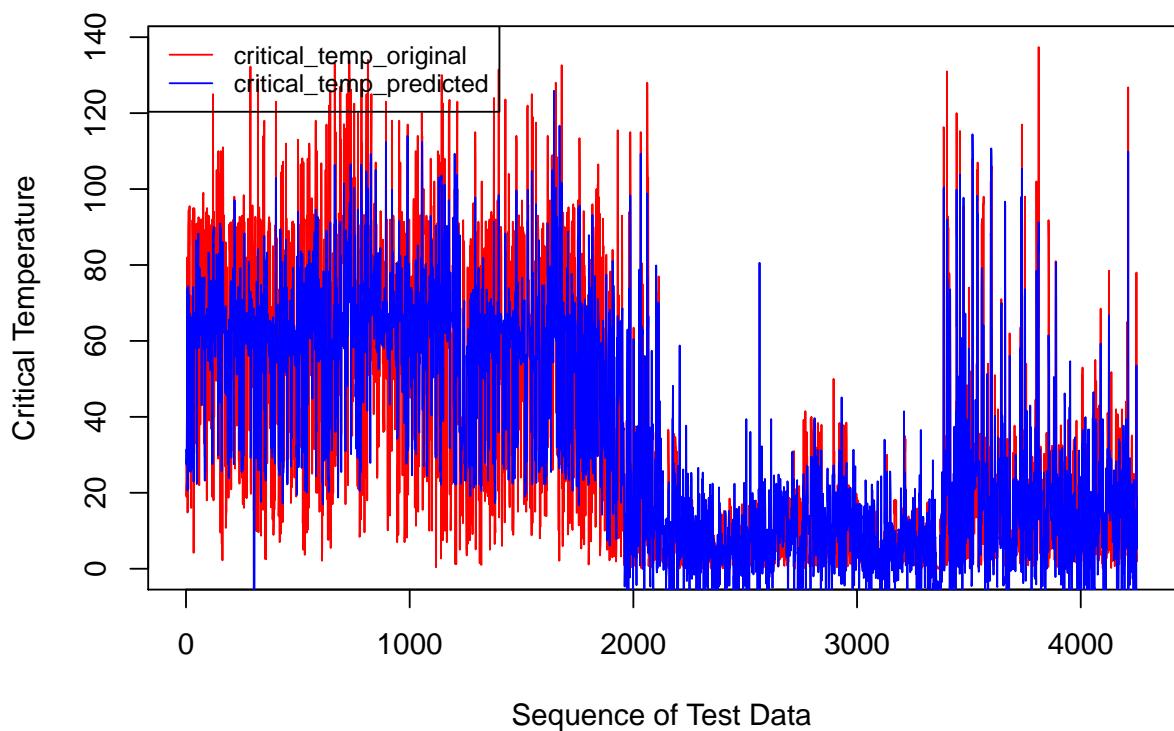


Figure 98: Sequence of Prediction vs Real Values with Elastic Net

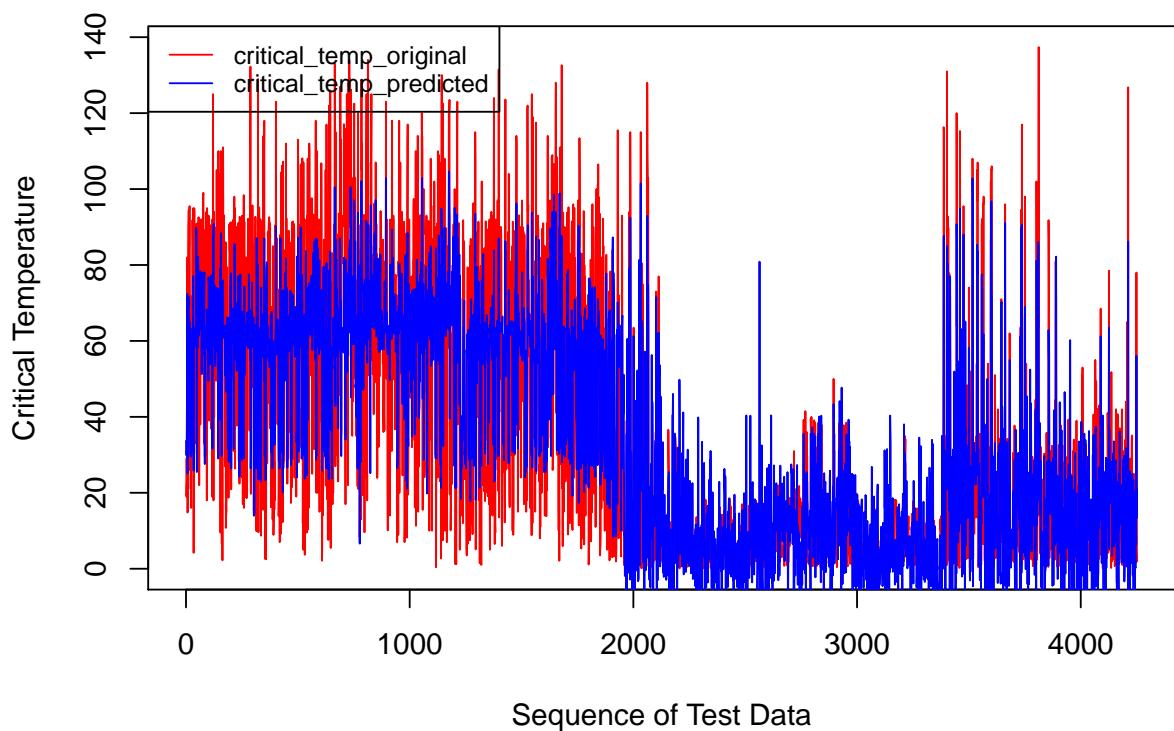


Figure 99: Sequence of Prediction vs Real Values with Principal Component Regression

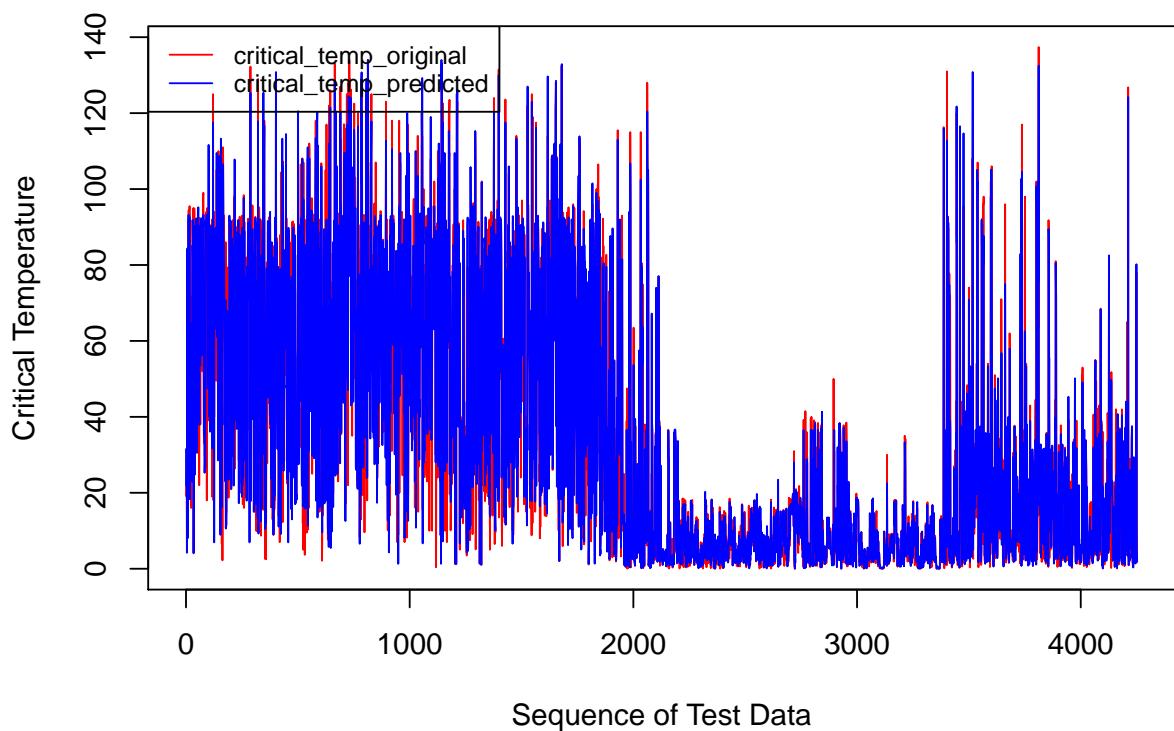


Figure 100: Sequence of Prediction vs Real Values with K-Nearest Neighbor Regression

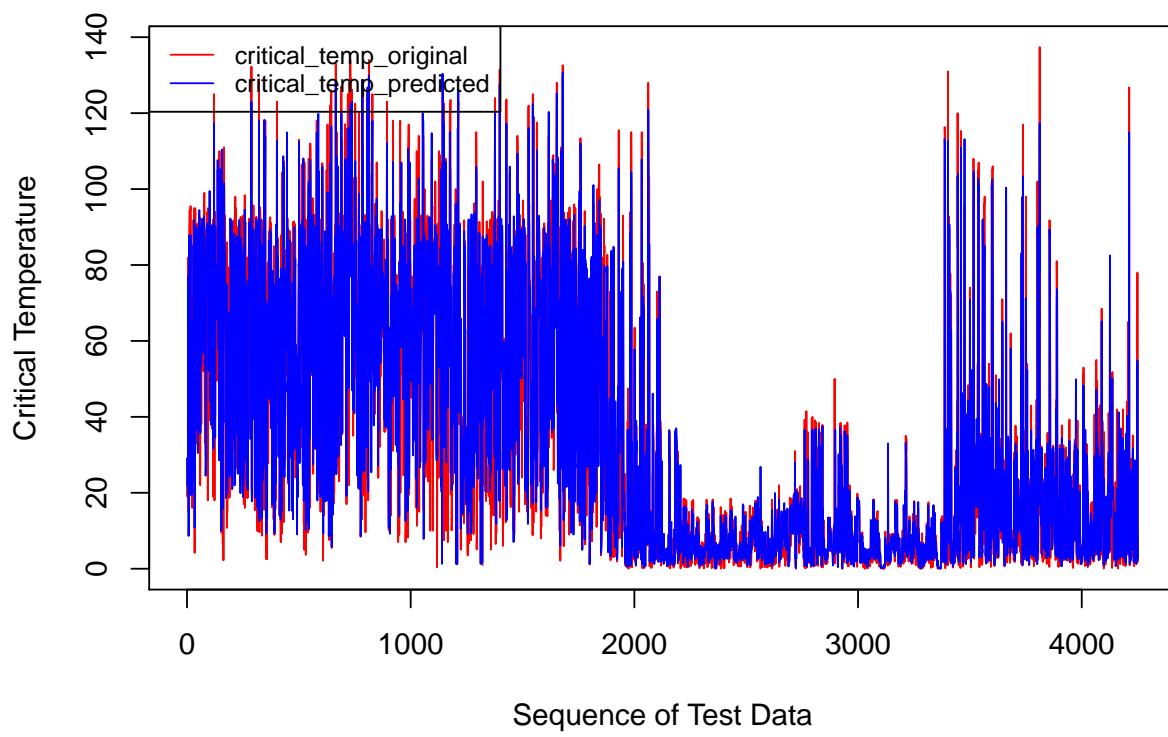


Figure 101: Sequence of Prediction vs Real Values with Random Forest

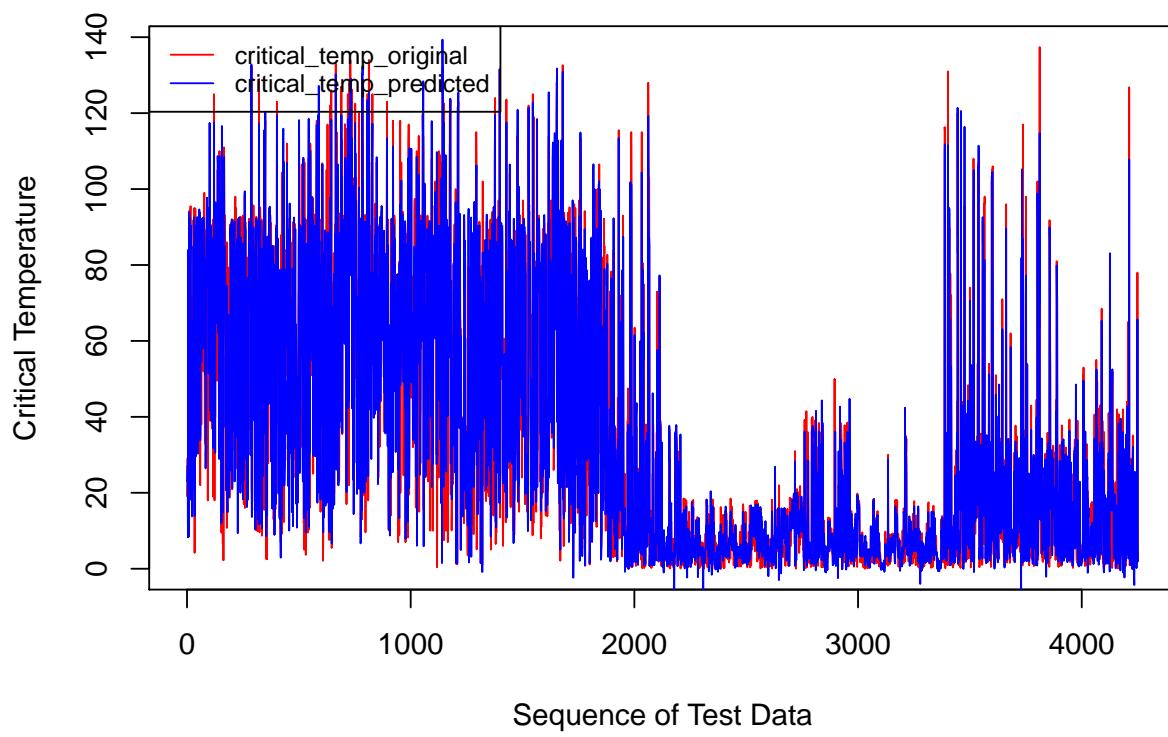


Figure 102: Sequence of Prediction vs Real Values with Gradient Boosting Machine

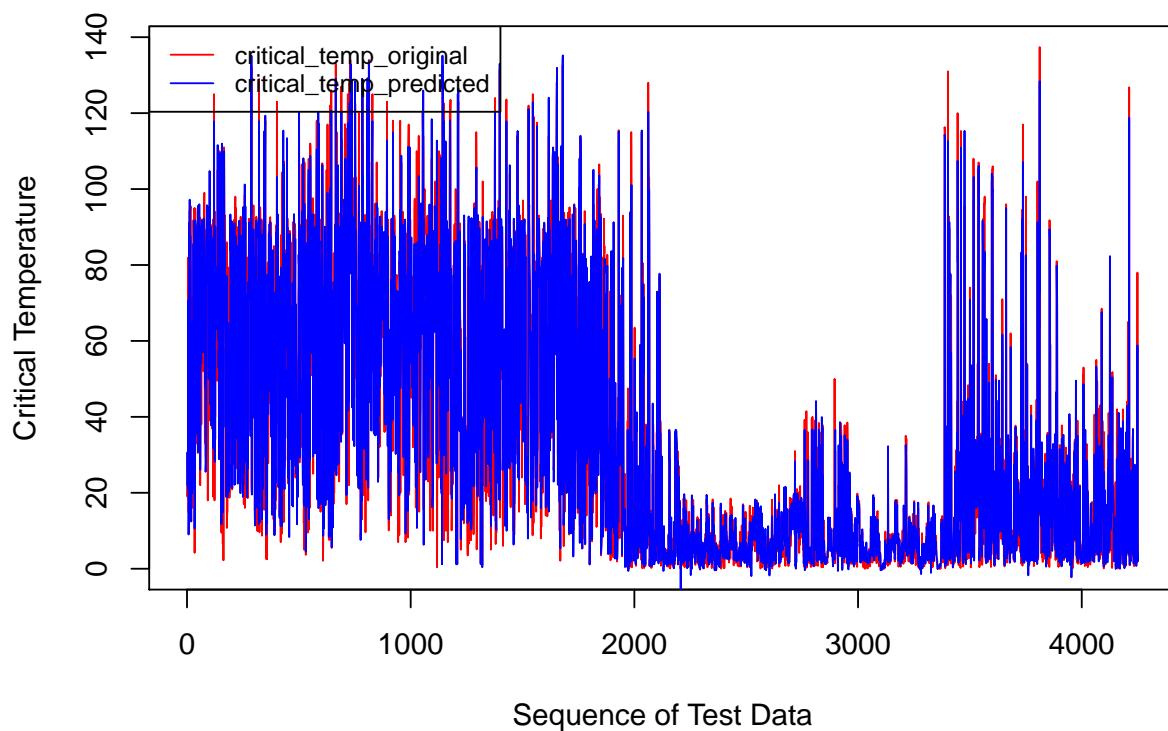


Figure 103: Sequence of Prediction vs Real Values with XG-Boost Regression

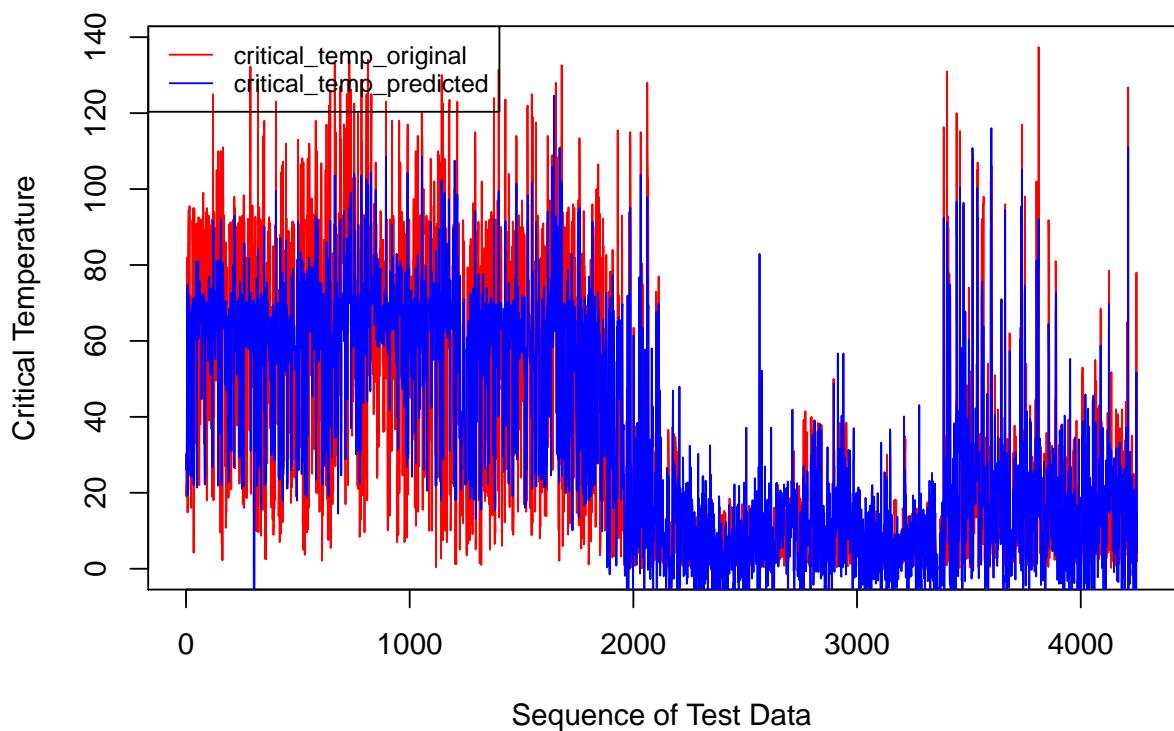


Figure 104: Sequence of Prediction vs Real Values with Linear Regression Model 1 Trans

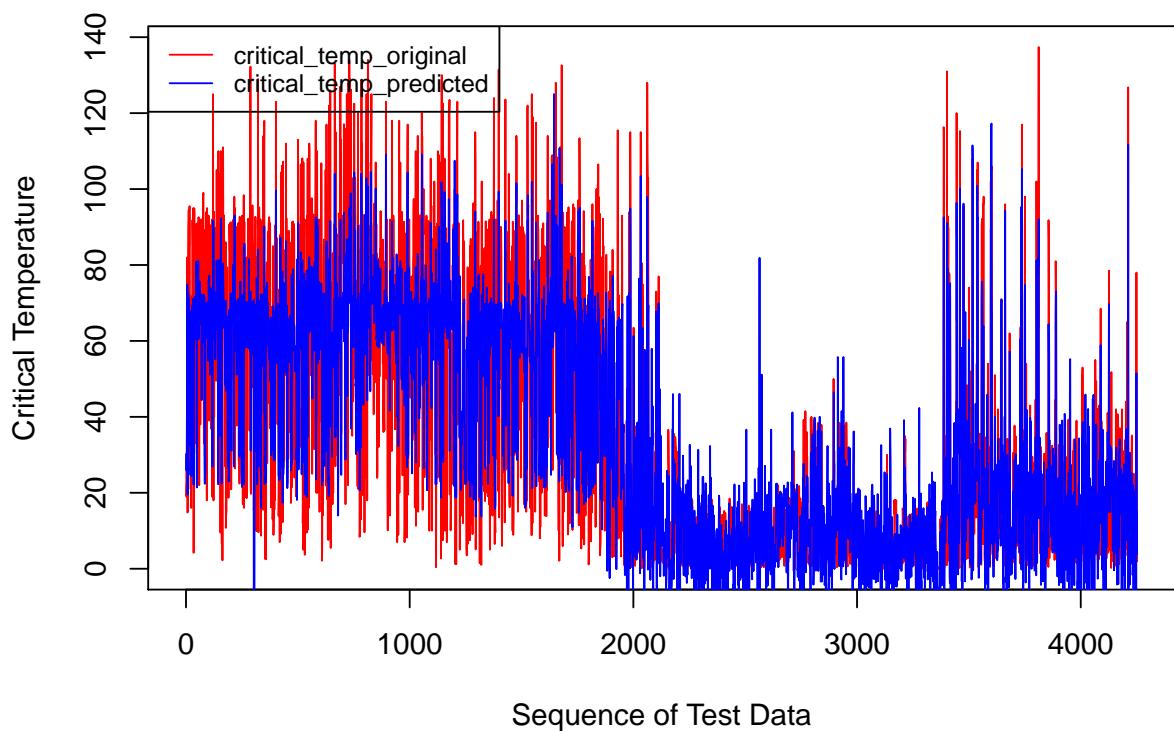


Figure 105: Sequence of Prediction vs Real Values with Linear Regression Model 2 Trans

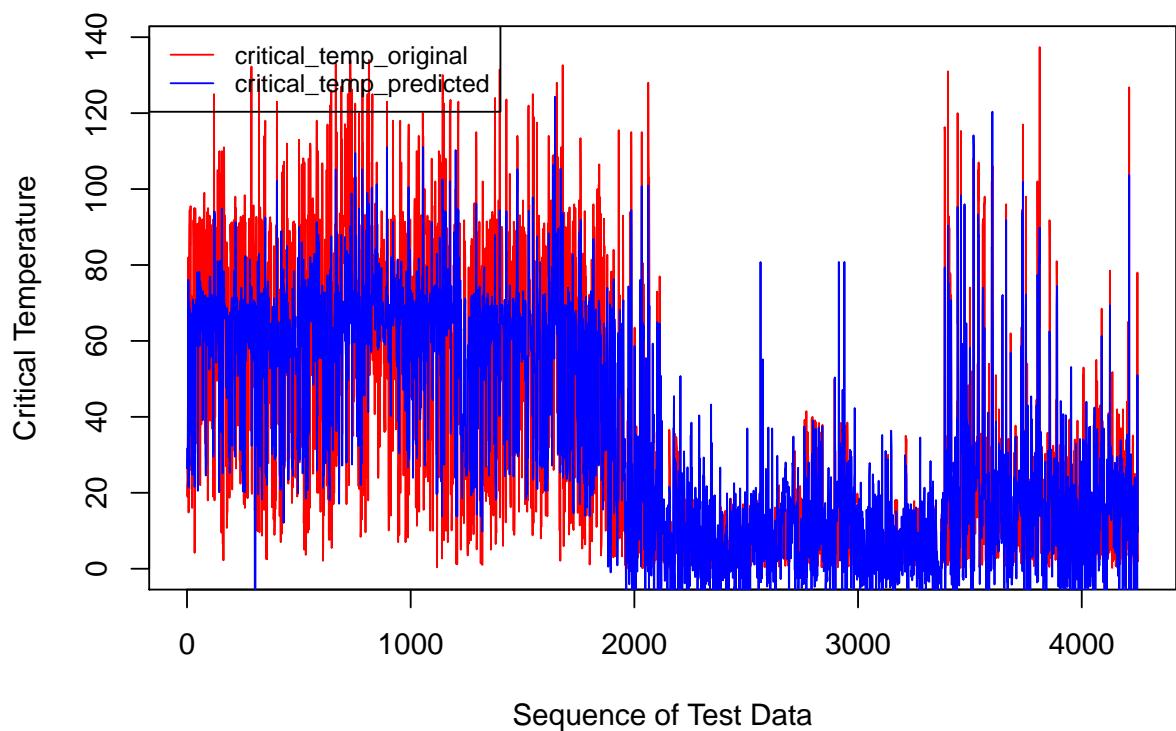


Figure 106: Sequence of Prediction vs Real Values with Linear regression Model 3 Trans

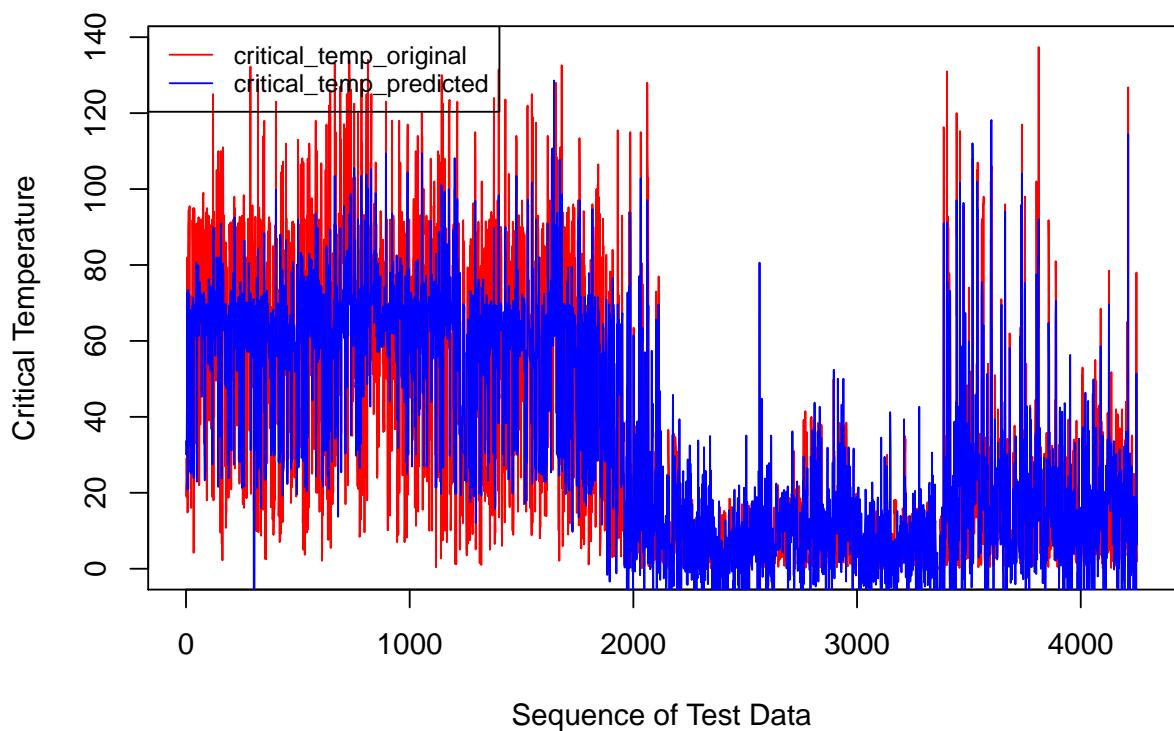


Figure 107: Sequence of Prediction vs Real Values with Linear Regression Backward Selection Trans

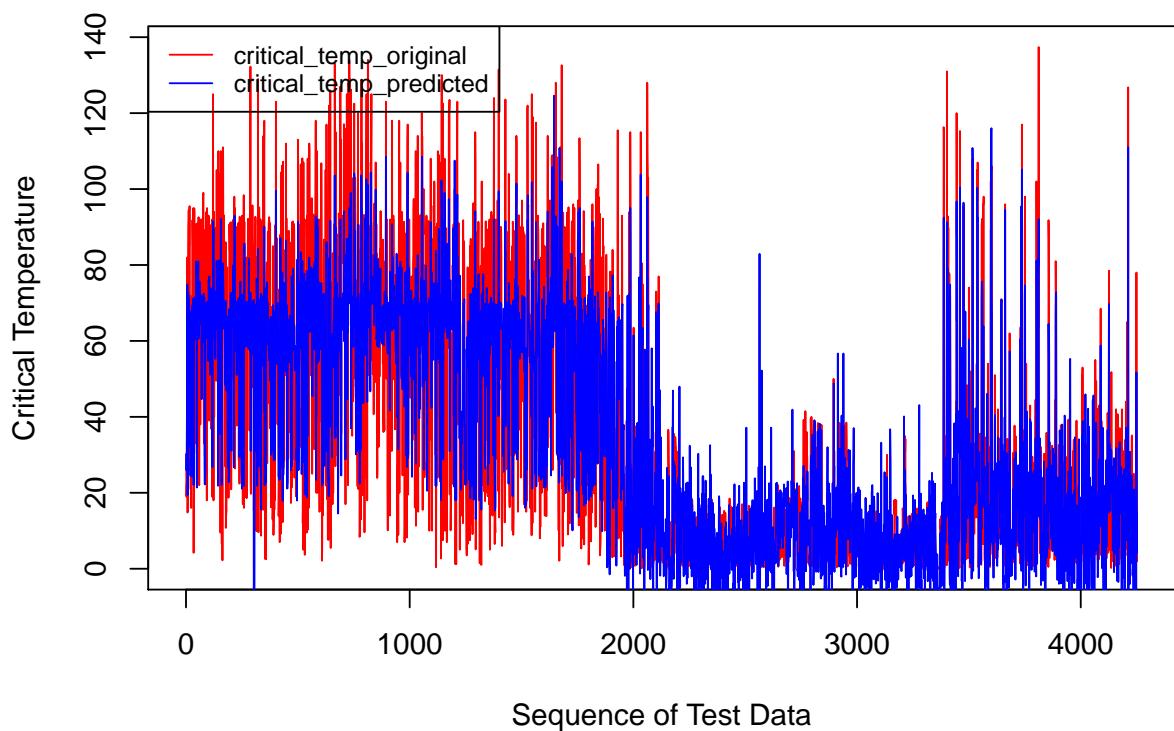


Figure 108: Sequence of Prediction vs Real Values with Linear Regression Forward Selection Trans

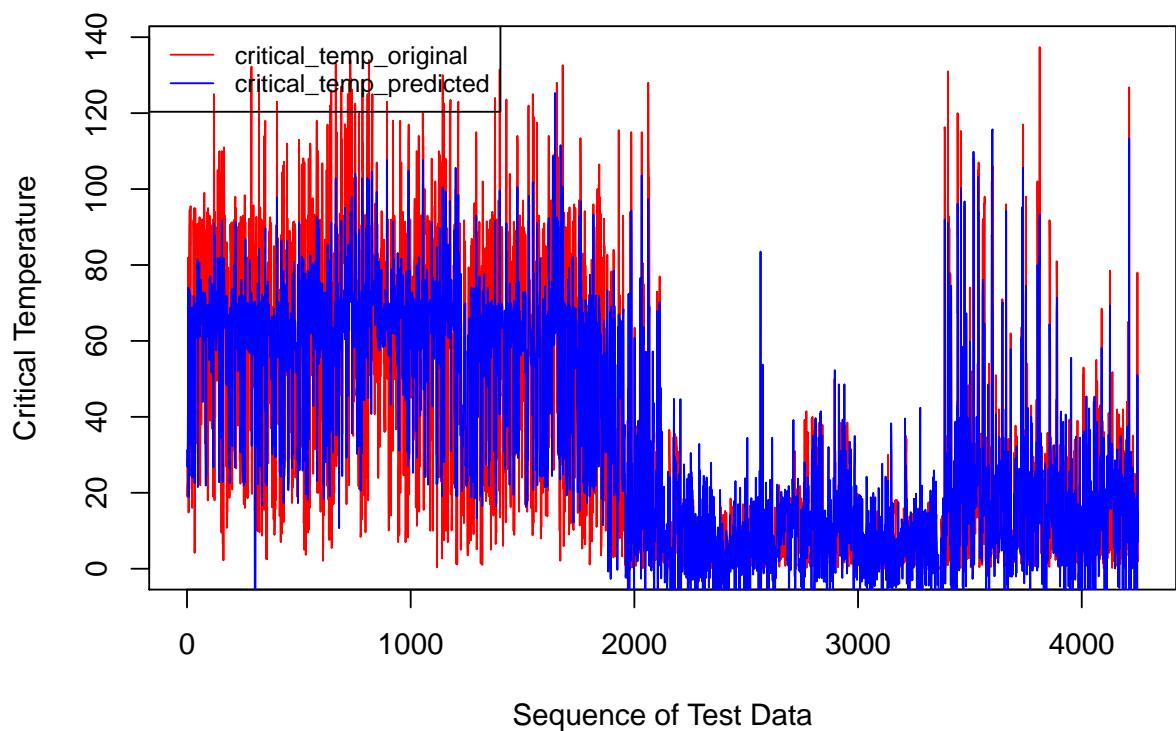


Figure 109: Sequence of Prediction vs Real Values with Linear Regression Stepwise Selection Trans

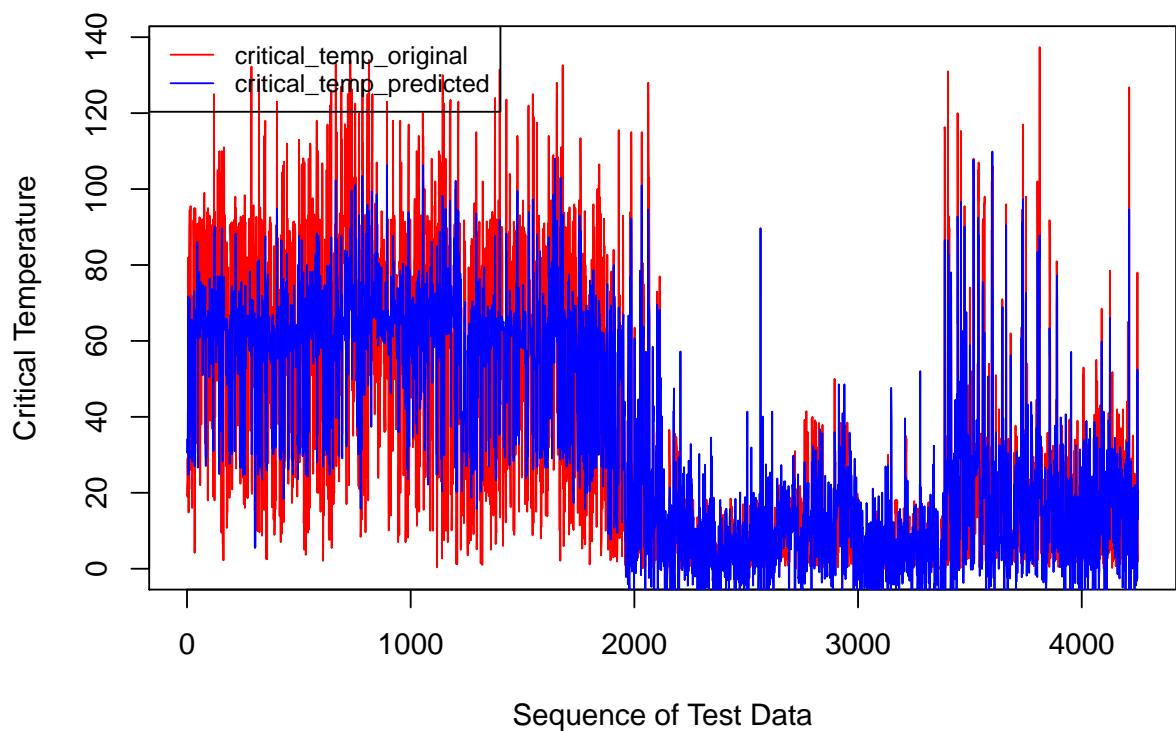


Figure 110: Sequence of Prediction vs Real Values with Ridge Regression Trans

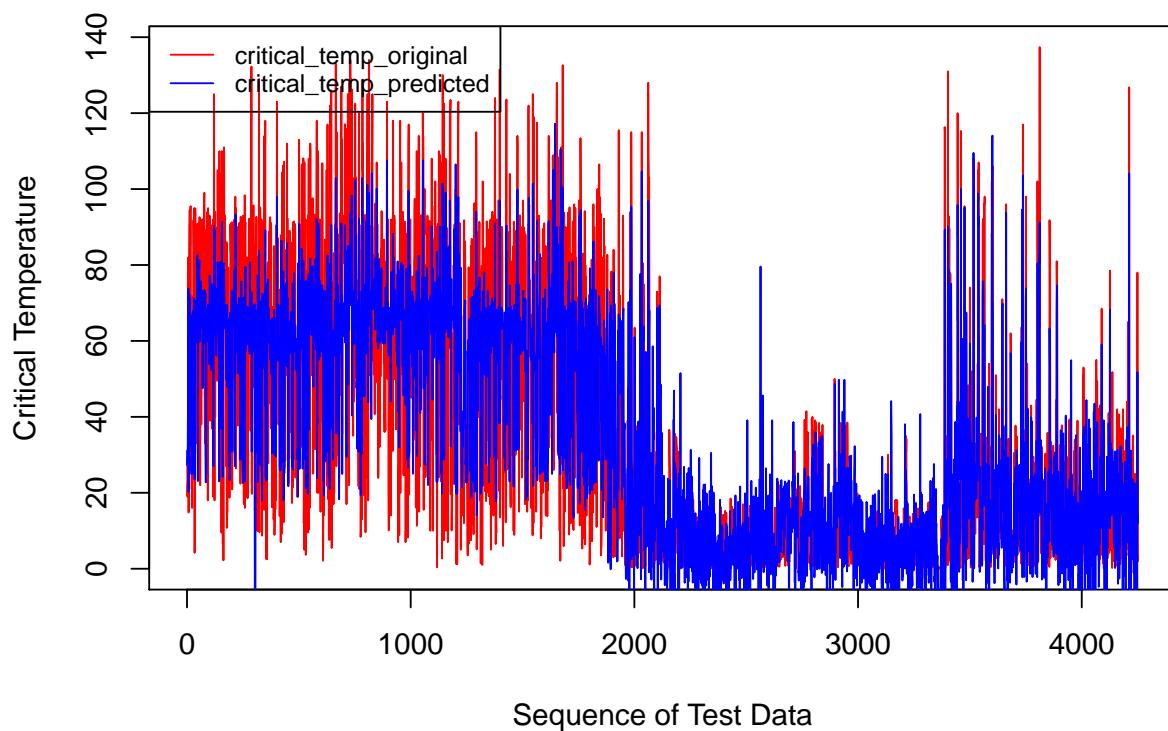


Figure 111: Sequence of Prediction vs Real Values with Lasso Regression Trans

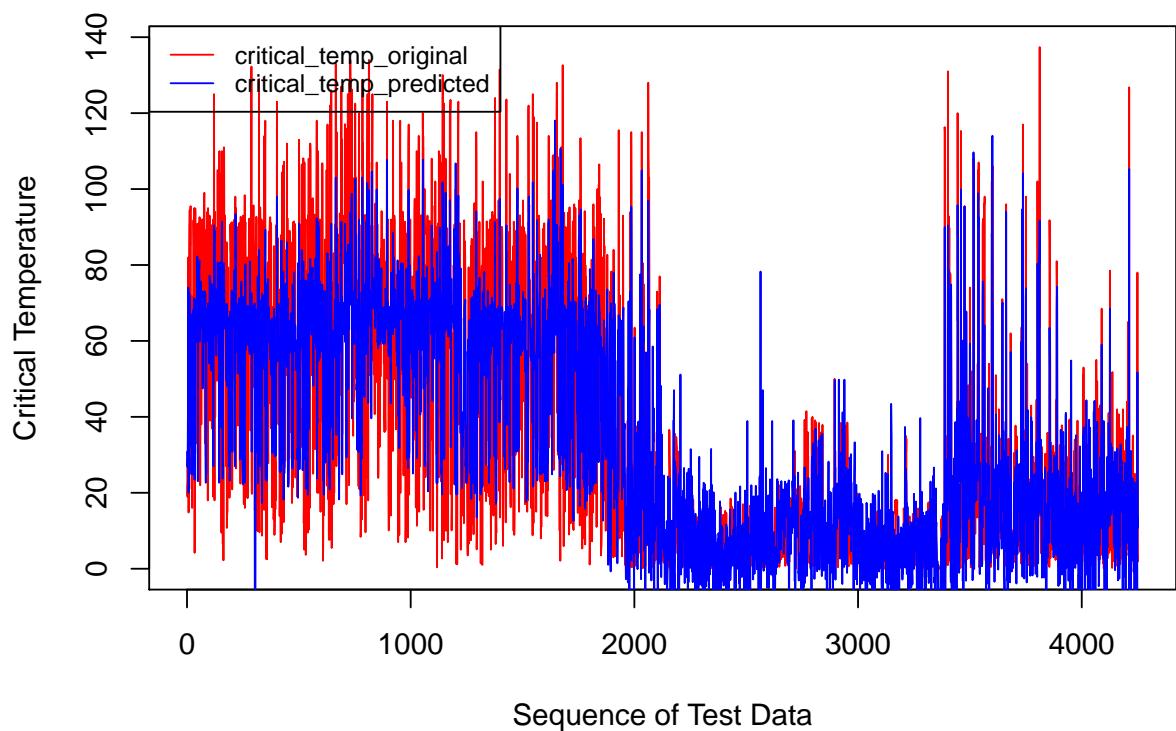


Figure 112: Sequence of Prediction vs Real Values with Elastic Net Trans

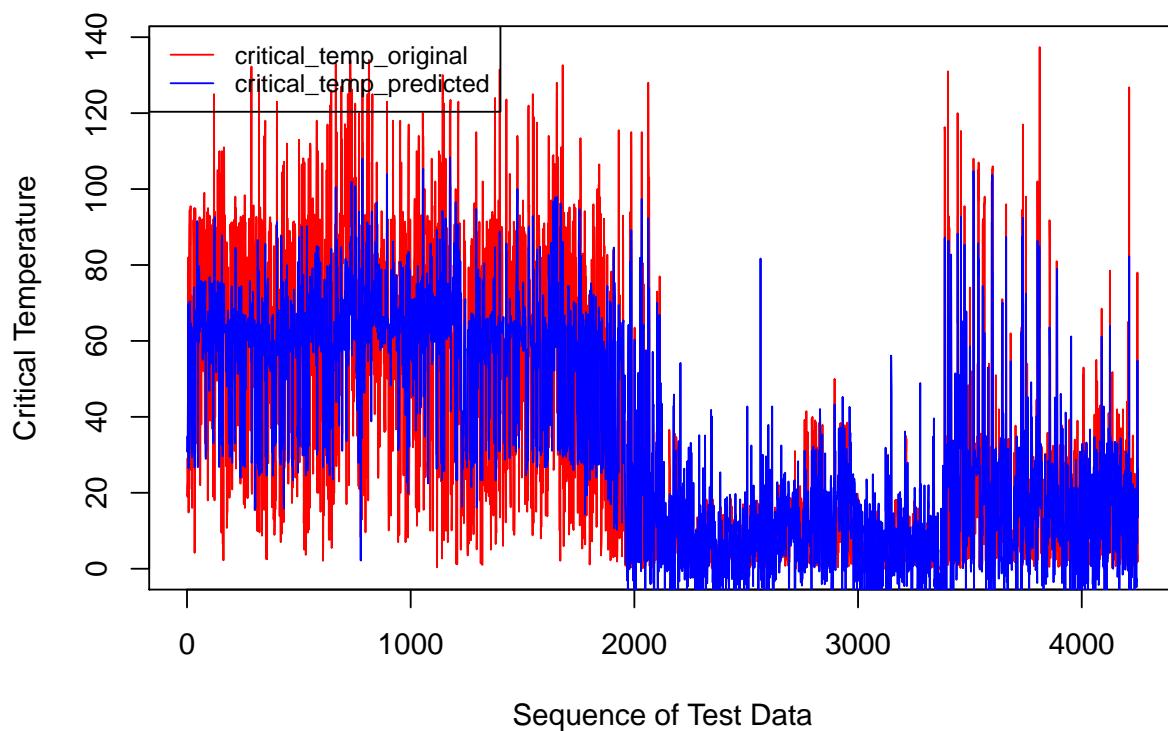


Figure 113: Sequence of Prediction vs Real Values with Principal Component Regression Trans

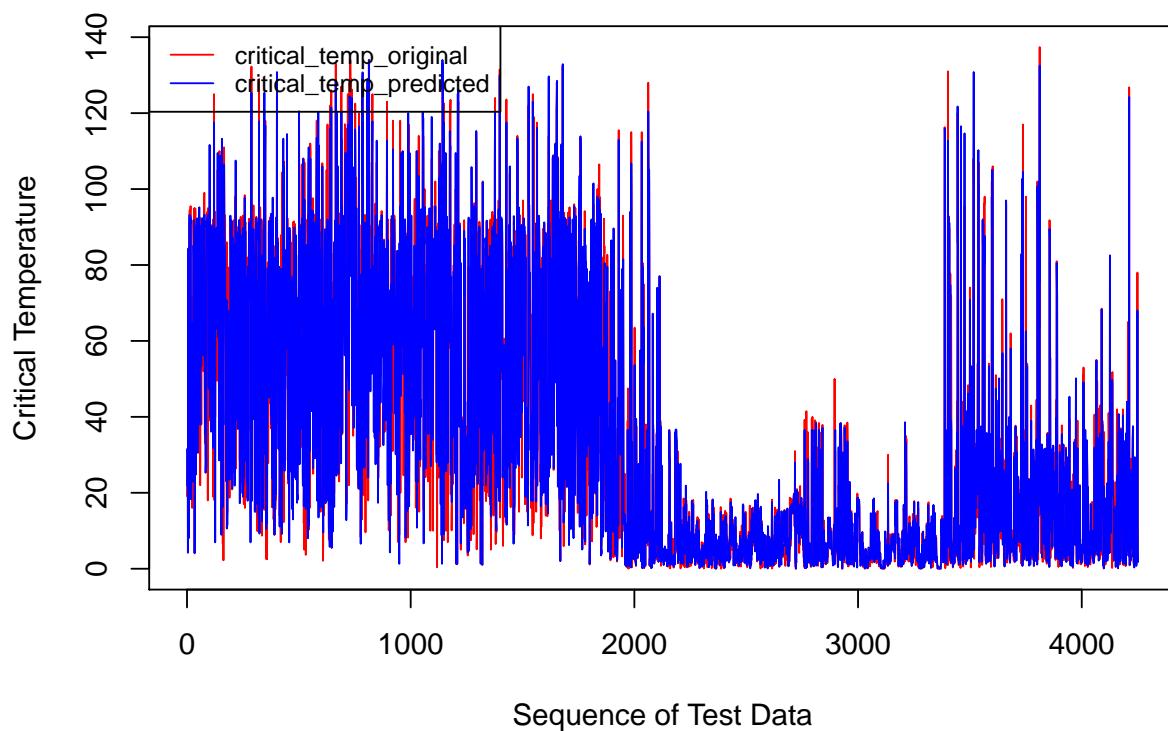


Figure 114: Sequence of Prediction vs Real Values with K-Nearest Neighbor Regression Trans

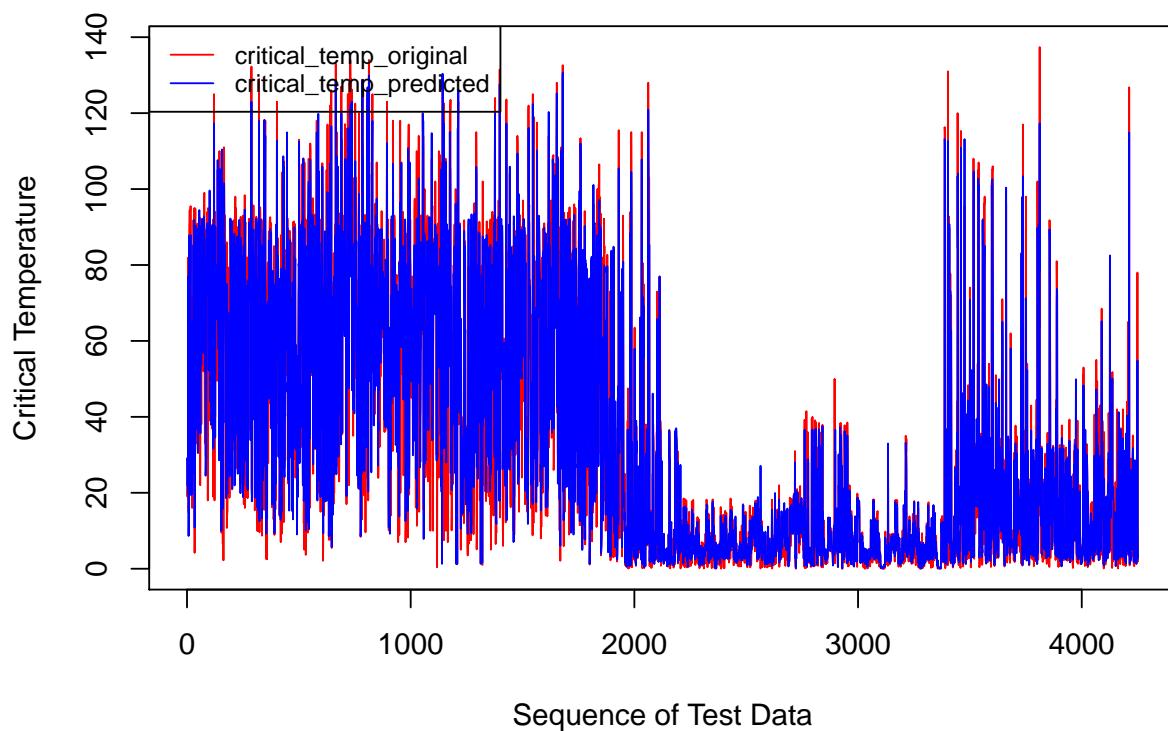


Figure 115: Sequence of Prediction vs Real Values with Random Forest Trans

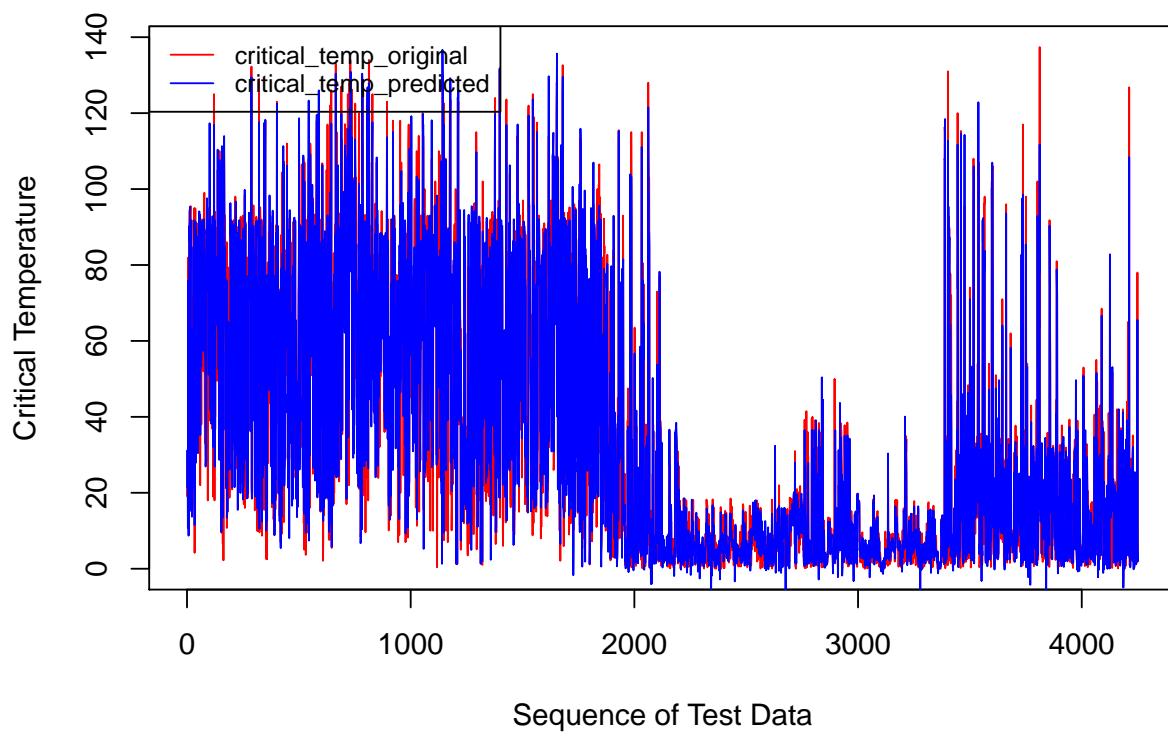


Figure 116: Sequence of Prediction vs Real Values with Gradient Boosting Machine Trans

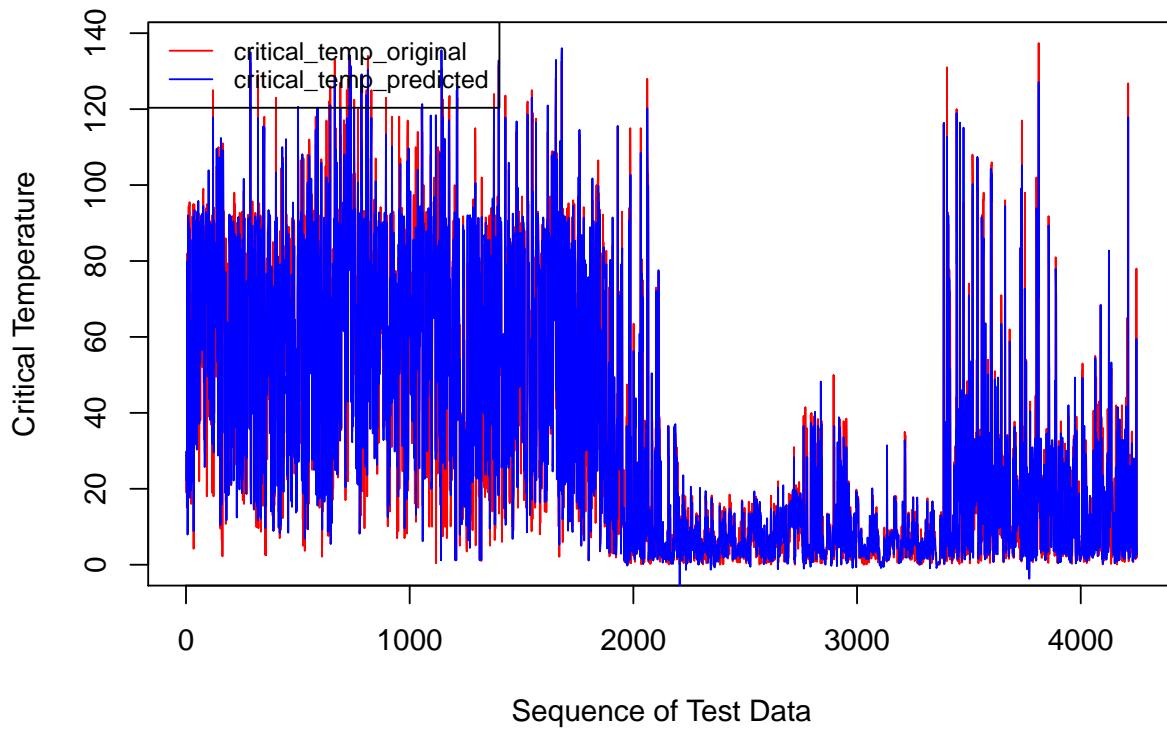


Figure 117: Sequence of Prediction vs Real Values with XG-Boost Regression Trans

Next, we will visualise scatter plot of the real critical temperature compared to the predicted critical temperature. As shown below, the better model has a more linear relationship between the real critical temperature and the predicted value.

```
# Visualise the Scatter Plot of Prediction vs Real Value
for(label in models.label){
  plot(test.data$critical_temp, pred.data[,label], col="red", ylab = paste0("Prediction with ", label),
       xlab = "Real Value")
  grid()
  abline(0, 1, col = "blue", lwd = 2)
  cat('\n\n')
}
```

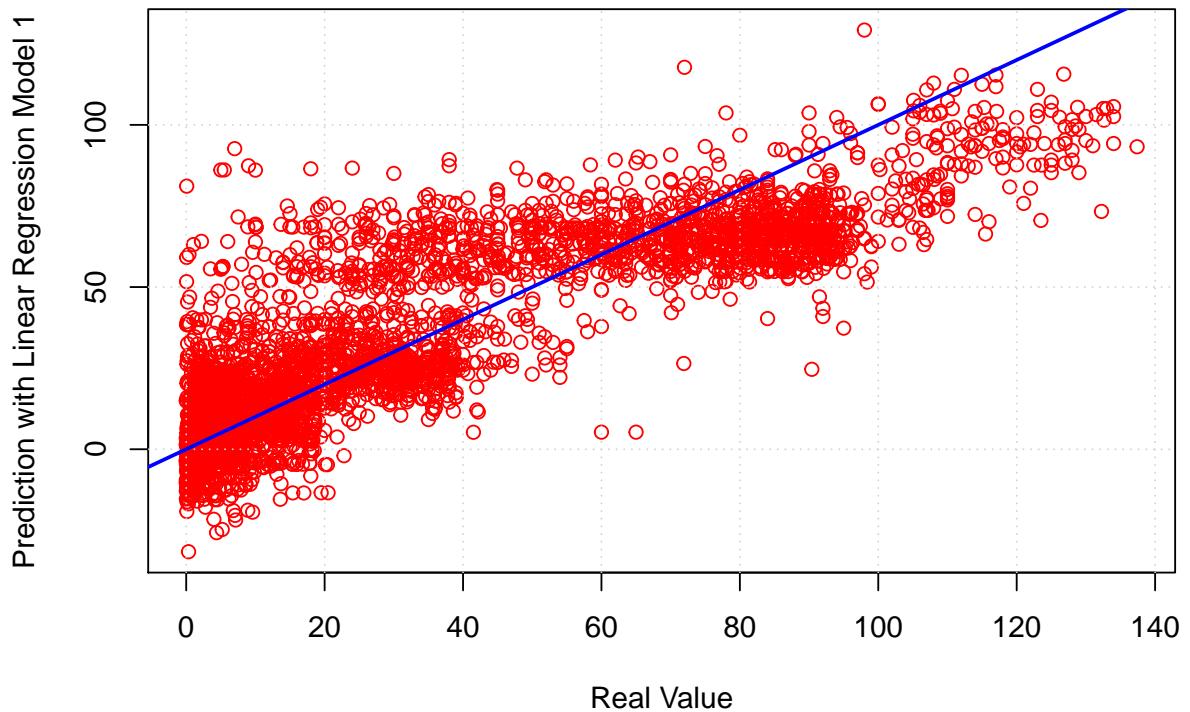


Figure 118: Scatter Plot of Prediction vs Real Values with Linear Regression Model 1

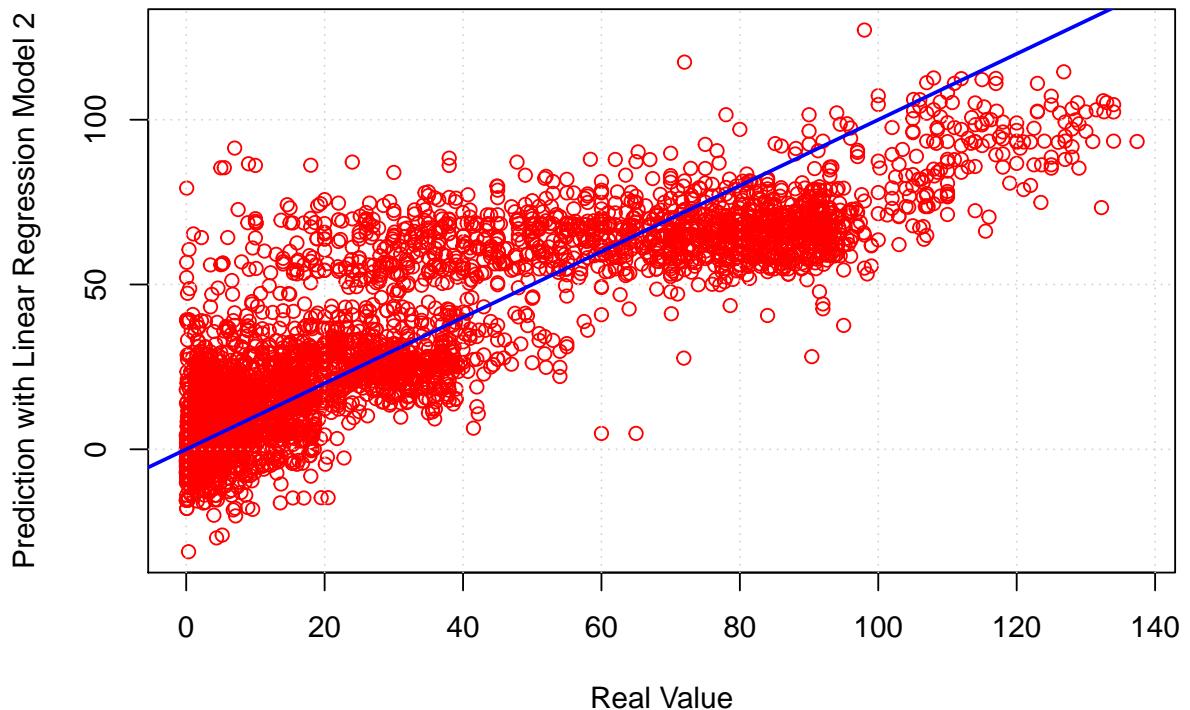


Figure 119: Scatter Plot of Prediction vs Real Values with Linear Regression Model 2

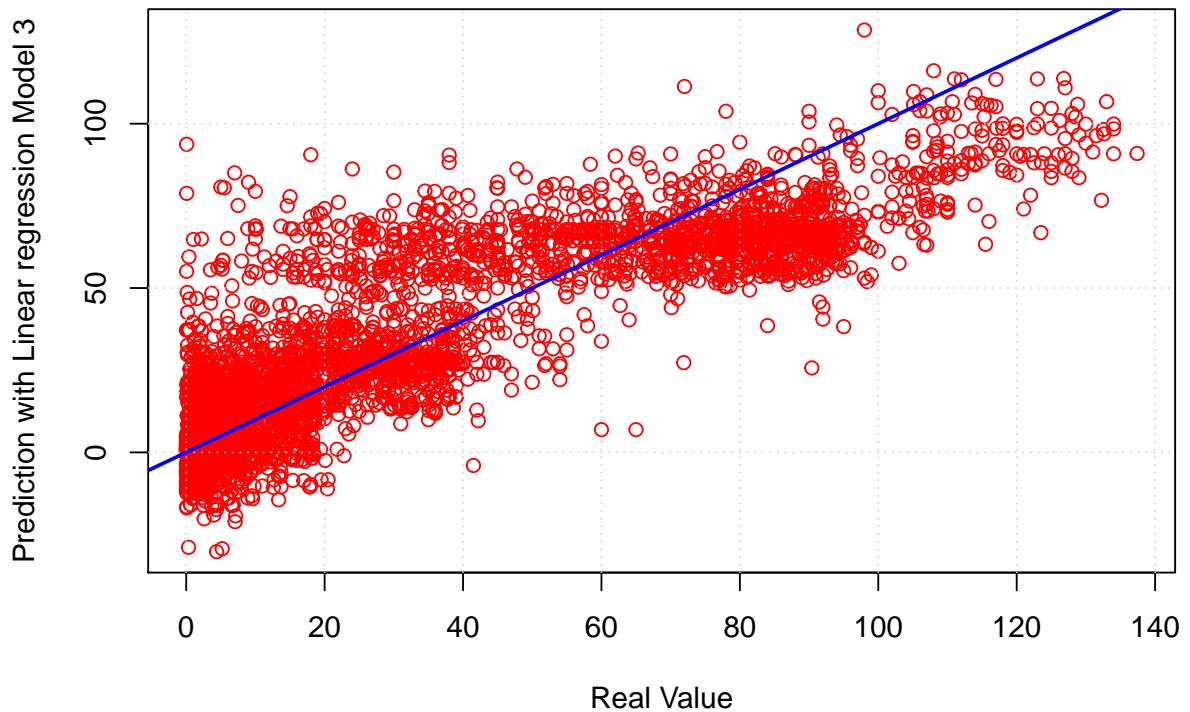


Figure 120: Scatter Plot of Prediction vs Real Values with Linear regression Model 3

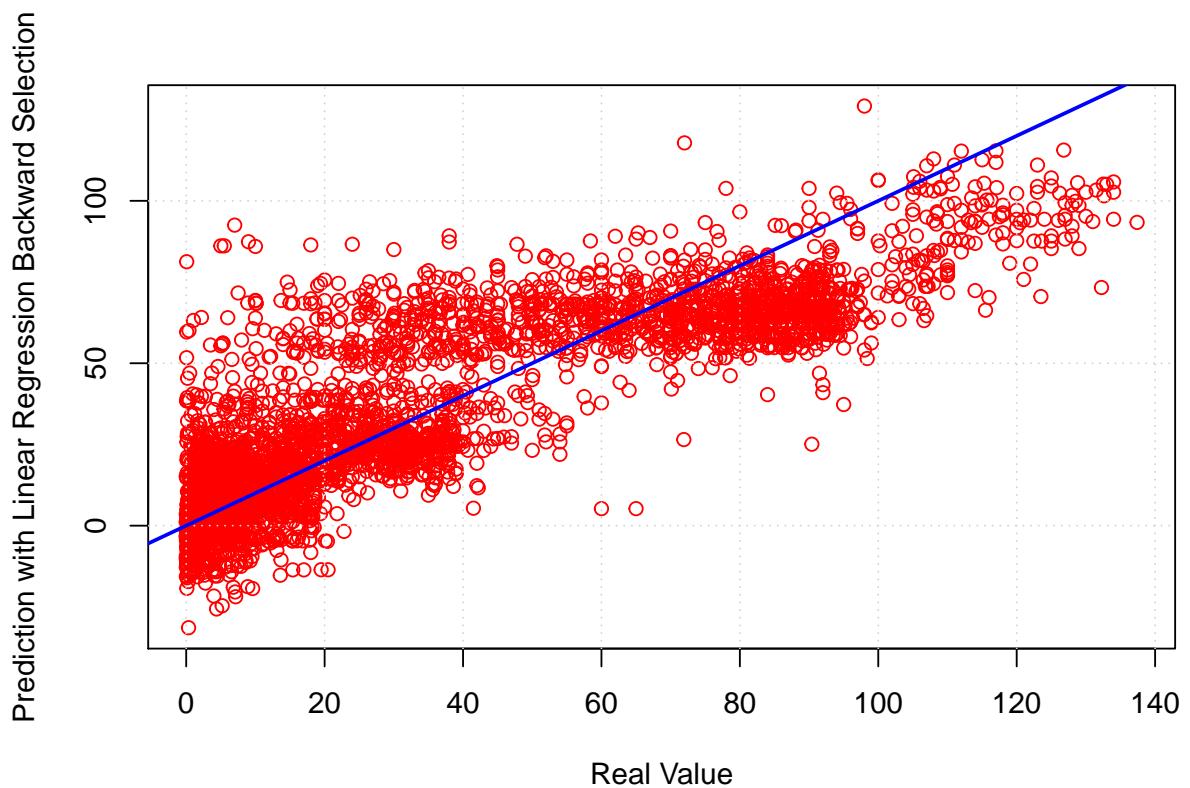


Figure 121: Scatter Plot of Prediction vs Real Values with Linear Regression Backward Selection

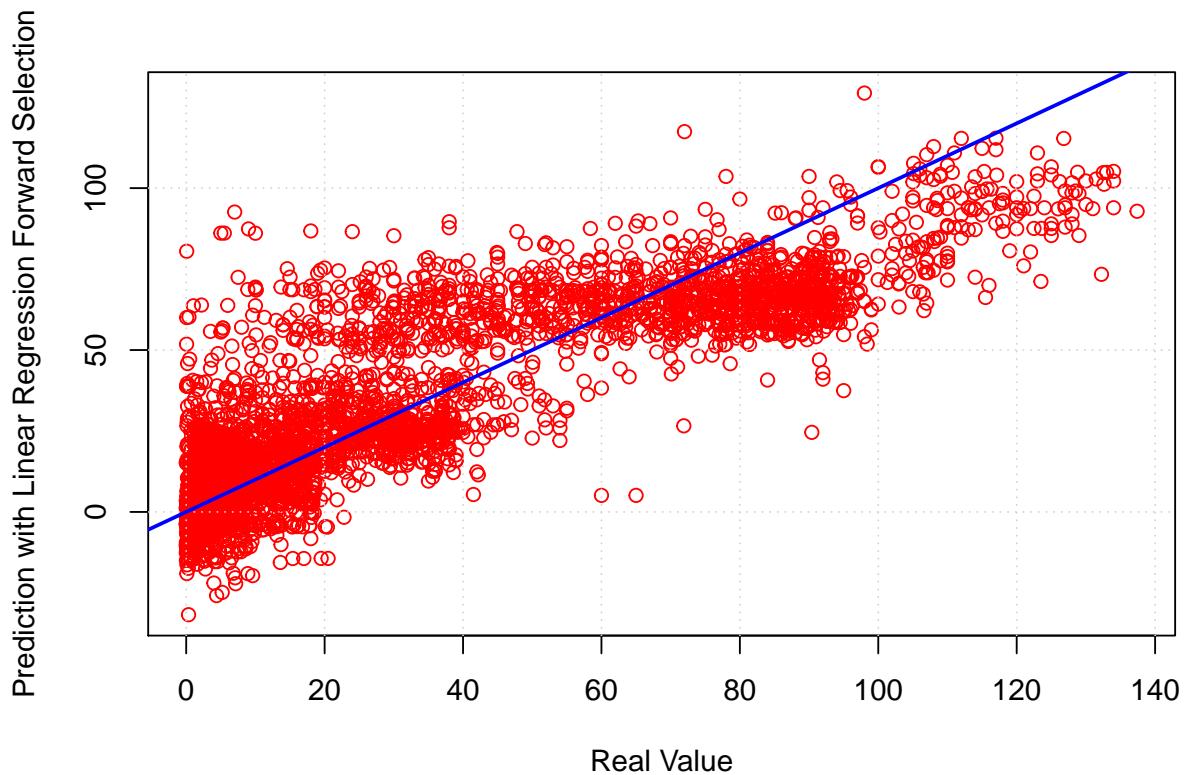


Figure 122: Scatter Plot of Prediction vs Real Values with Linear Regression Forward Selection

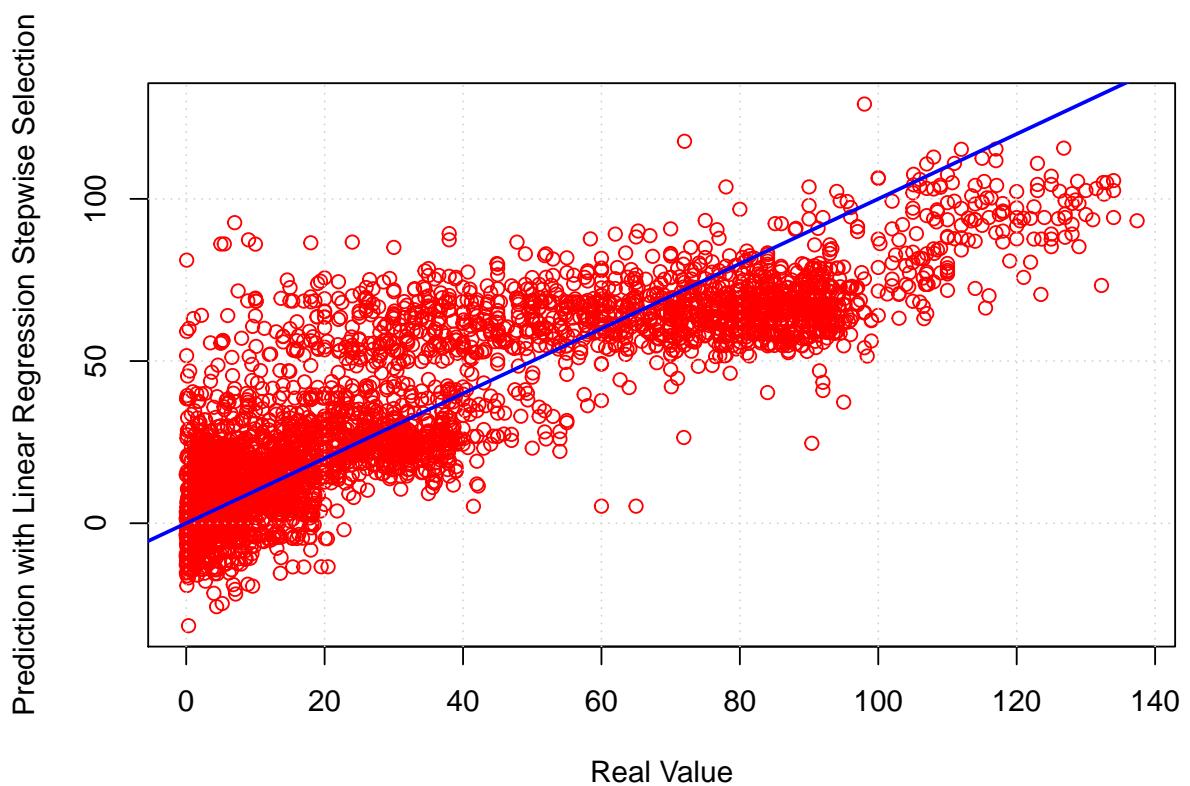


Figure 123: Scatter Plot of Prediction vs Real Values with Linear Regression Stepwise Selection

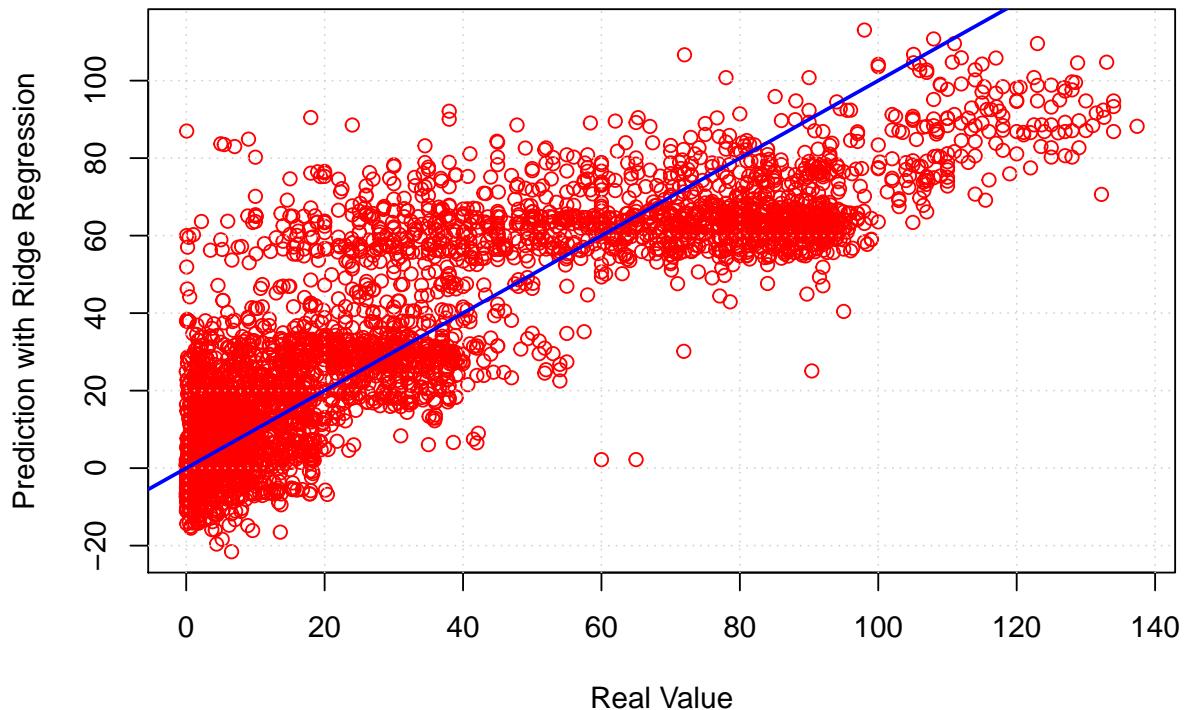


Figure 124: Scatter Plot of Prediction vs Real Values with Ridge Regression

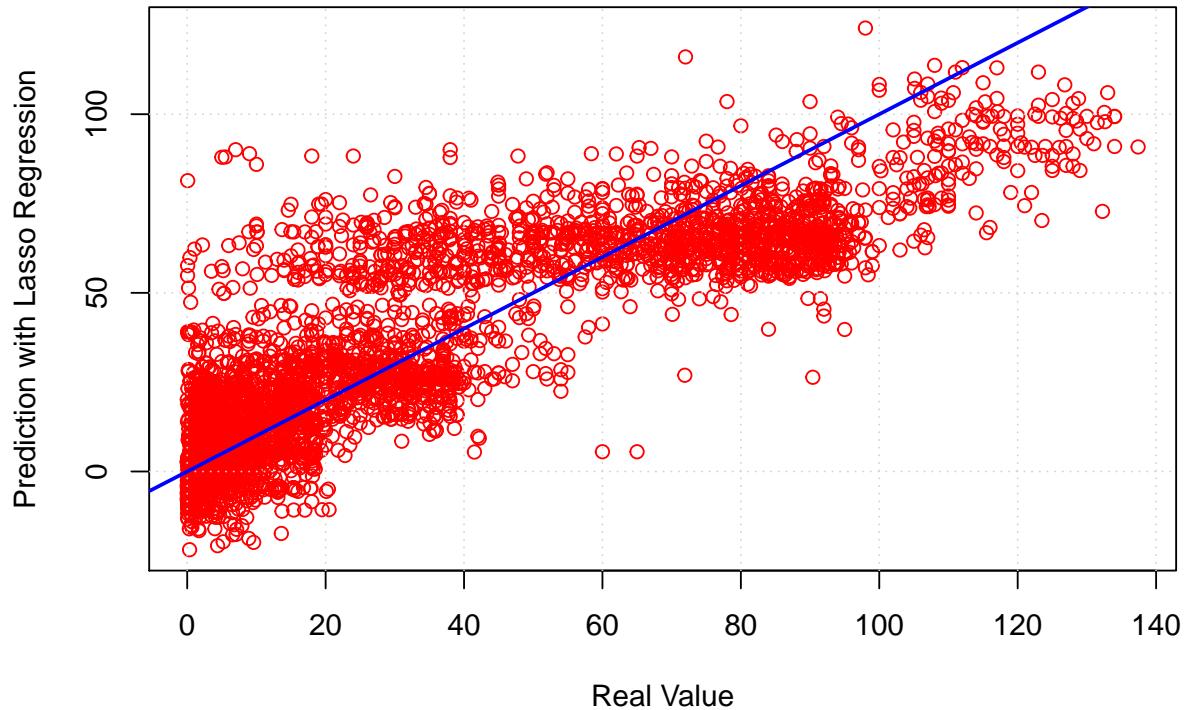


Figure 125: Scatter Plot of Prediction vs Real Values with Lasso Regression

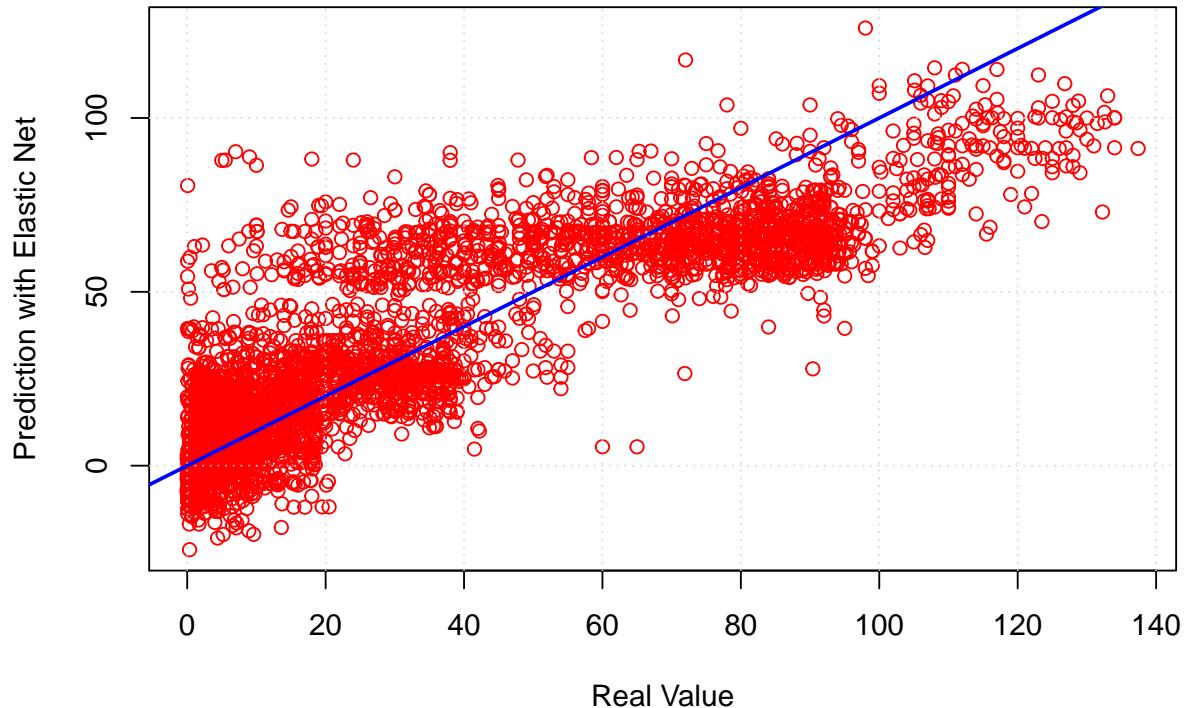


Figure 126: Scatter Plot of Prediction vs Real Values with Elastic Net

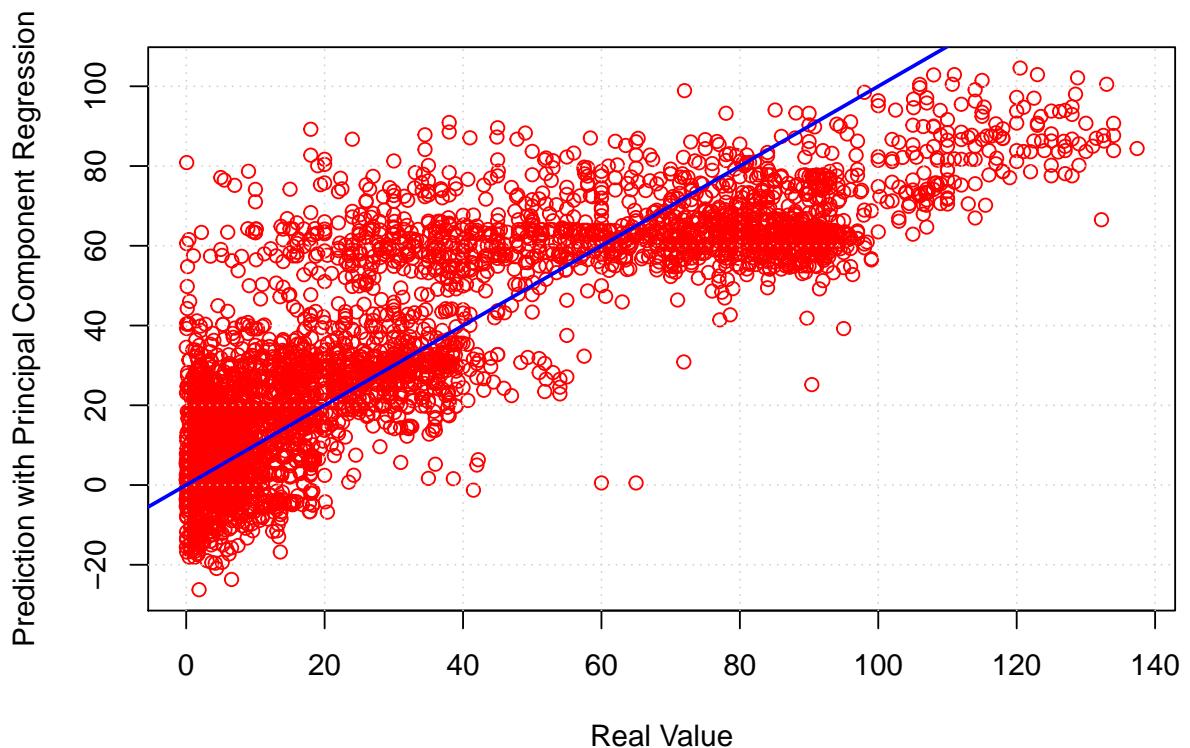


Figure 127: Scatter Plot of Prediction vs Real Values with Principal Component Regression

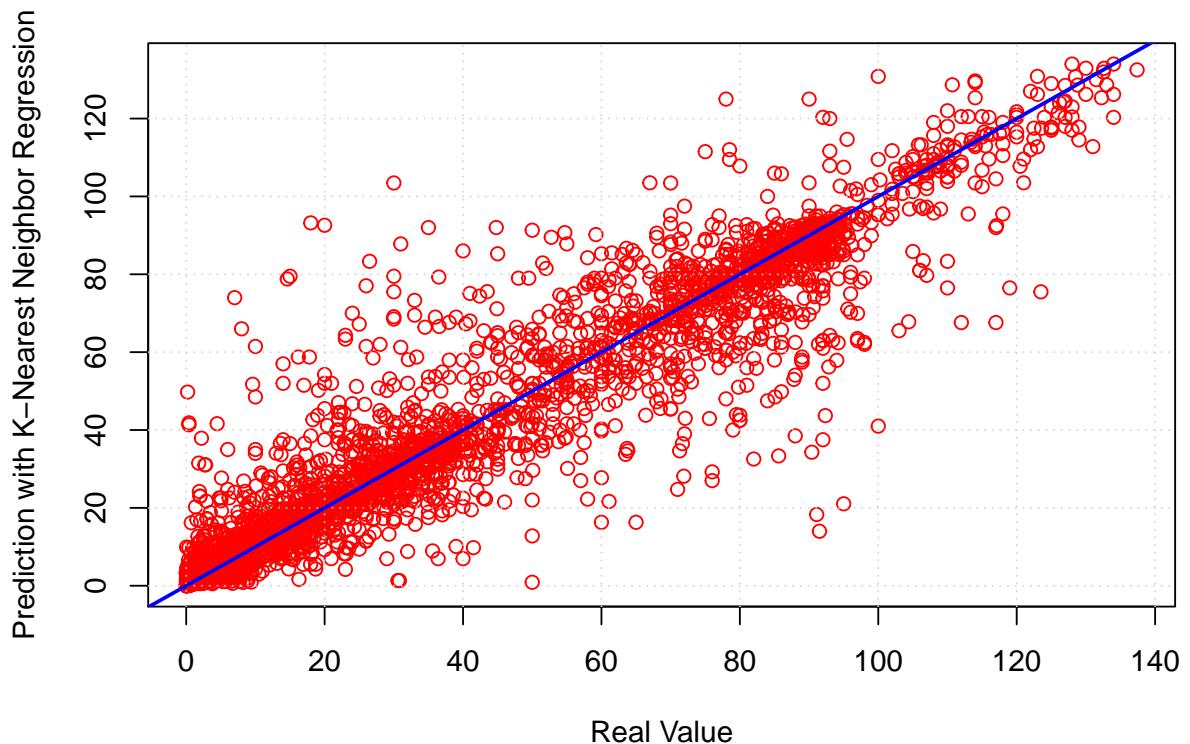


Figure 128: Scatter Plot of Prediction vs Real Values with K-Nearest Neighbor Regression

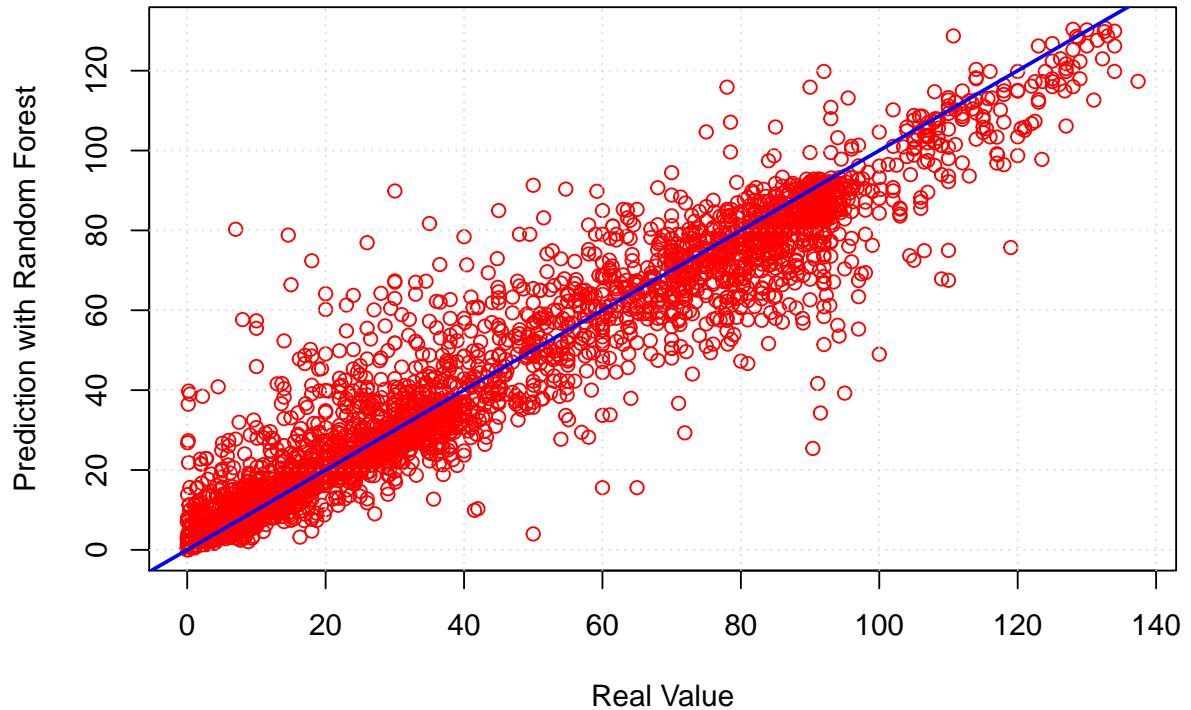


Figure 129: Scatter Plot of Prediction vs Real Values with Random Forest

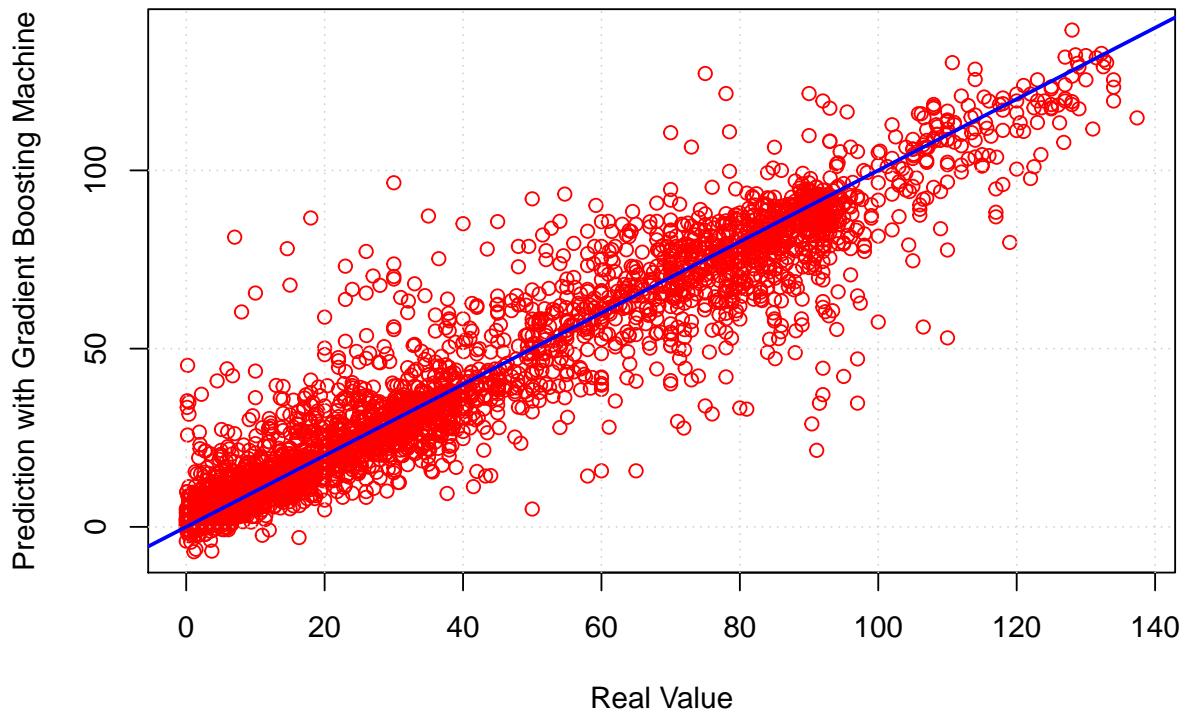


Figure 130: Scatter Plot of Prediction vs Real Values with Gradient Boosting Machine

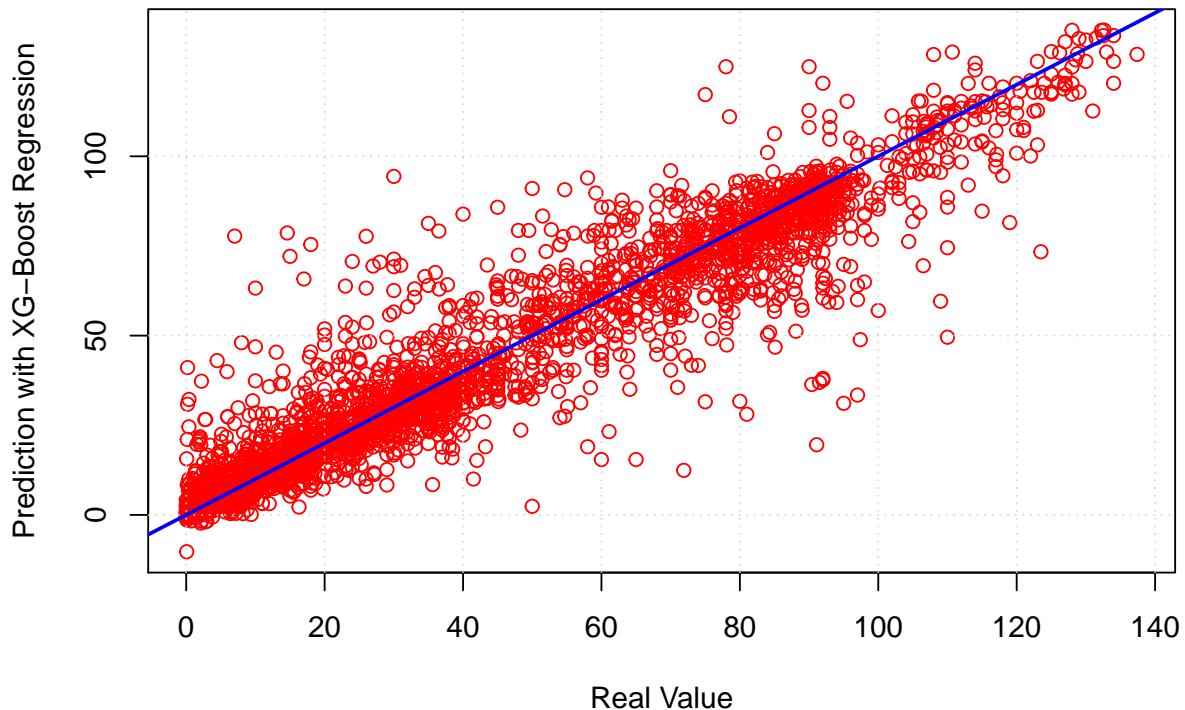


Figure 131: Scatter Plot of Prediction vs Real Values with XG-Boost Regression

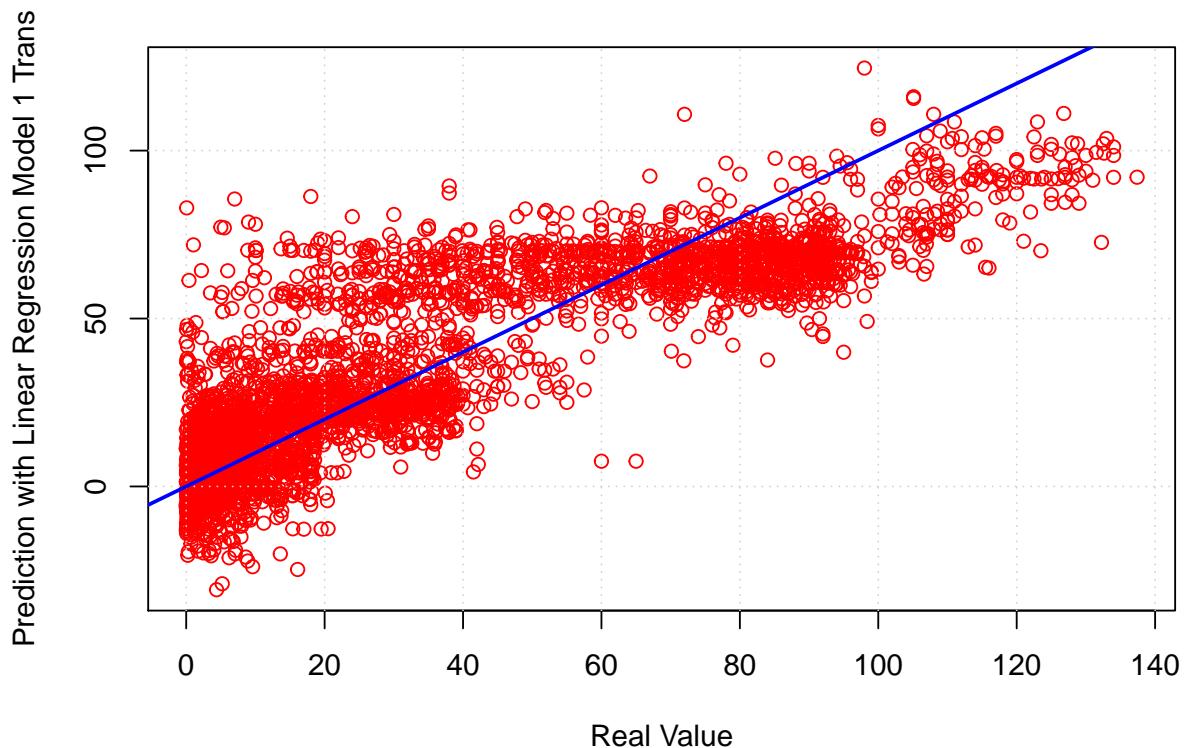


Figure 132: Scatter Plot of Prediction vs Real Values with Linear Regression Model 1 Trans

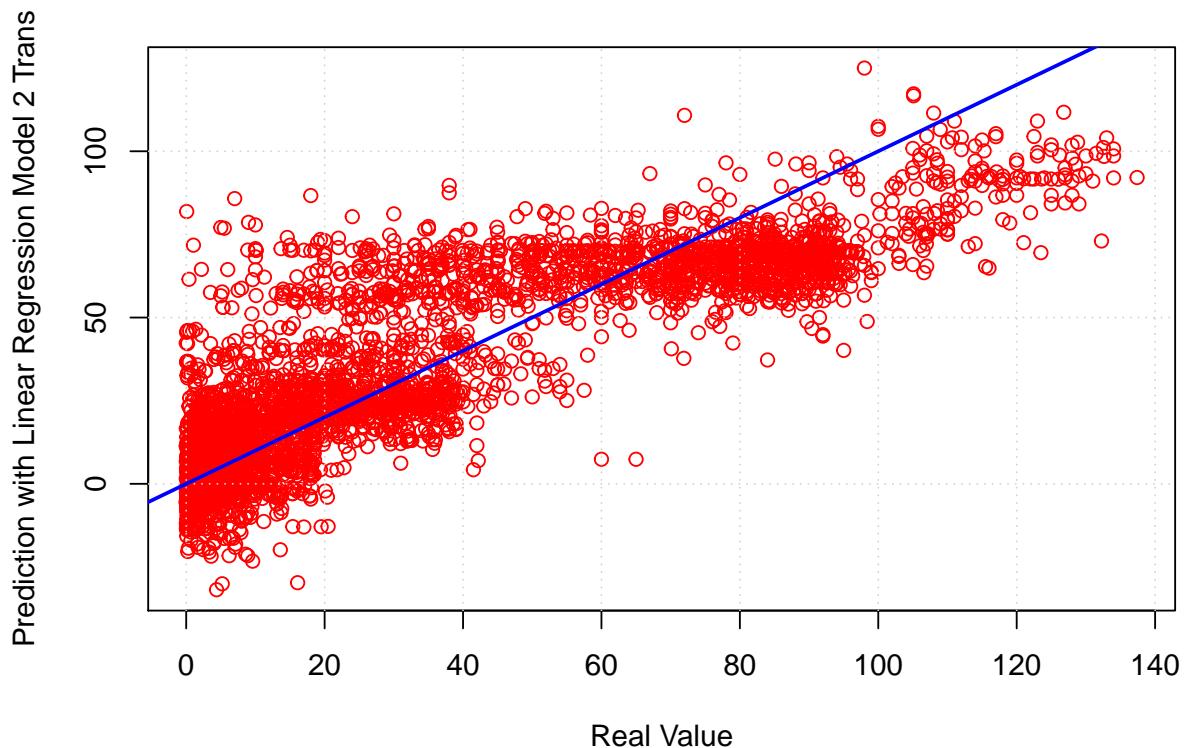


Figure 133: Scatter Plot of Prediction vs Real Values with Linear Regression Model 2 Trans

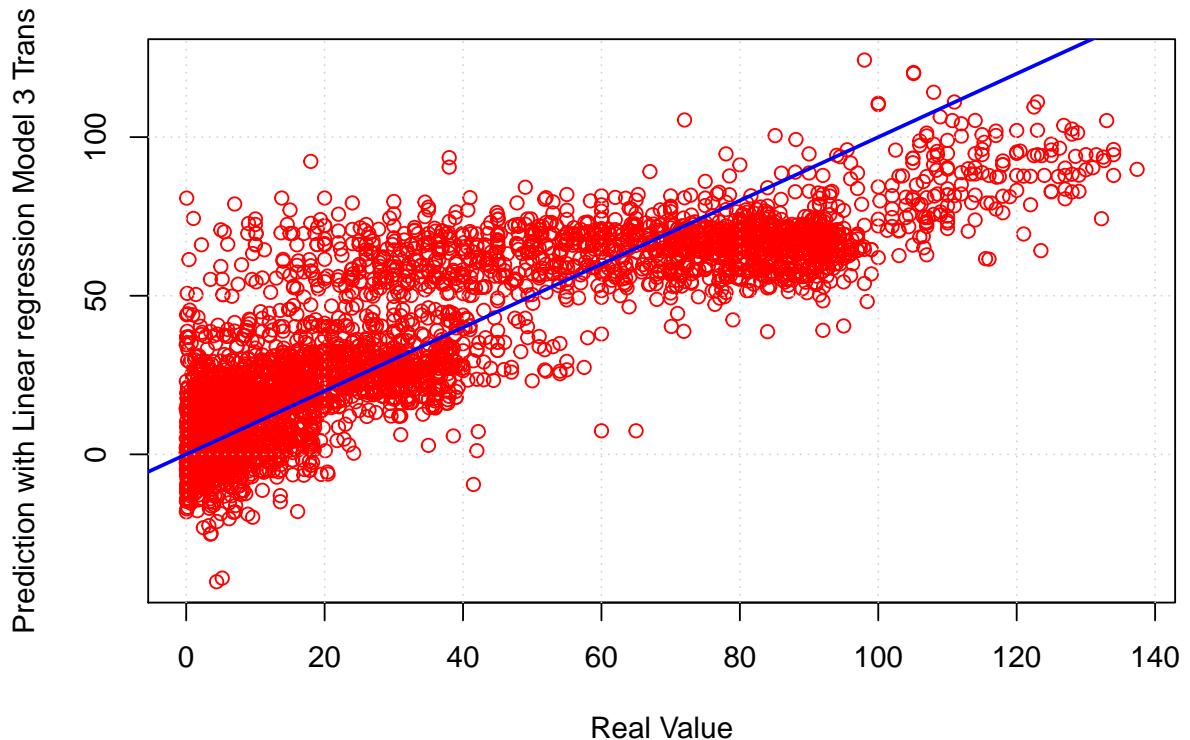


Figure 134: Scatter Plot of Prediction vs Real Values with Linear regression Model 3 Trans

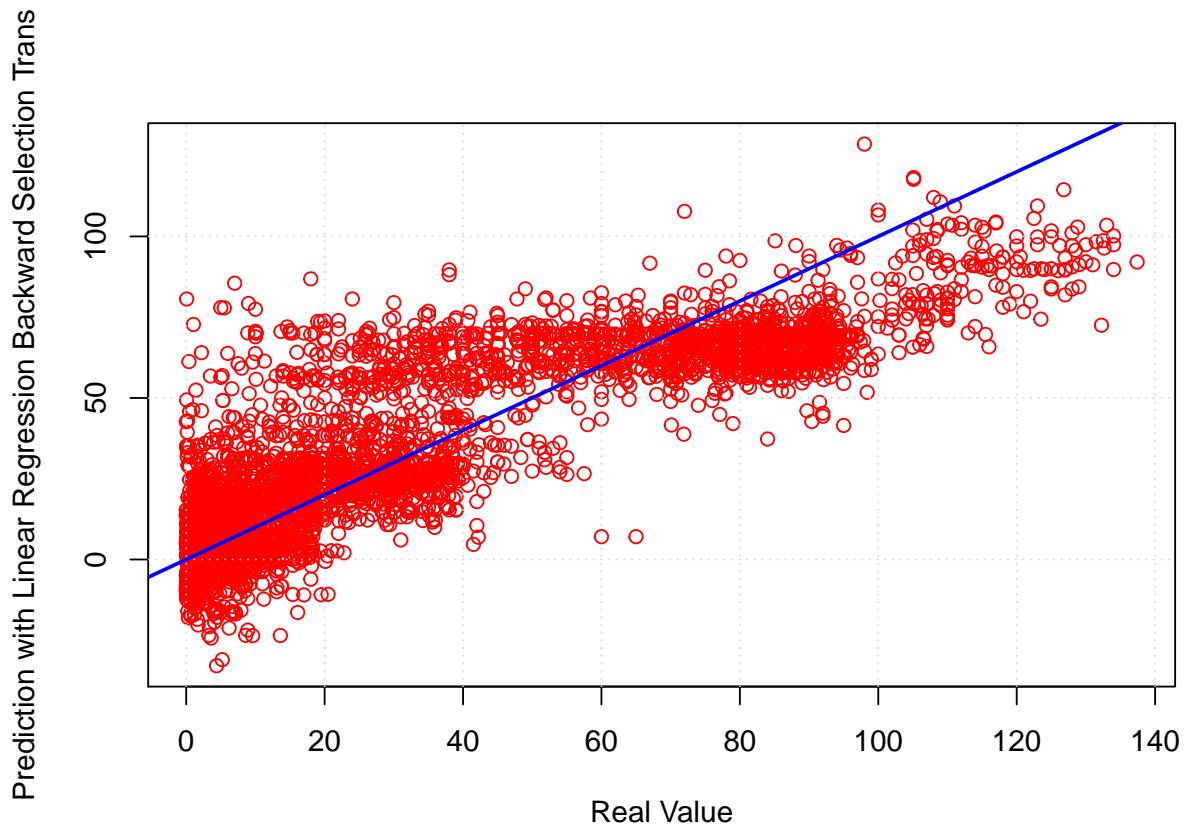


Figure 135: Scatter Plot of Prediction vs Real Values with Linear Regression Backward Selection Trans

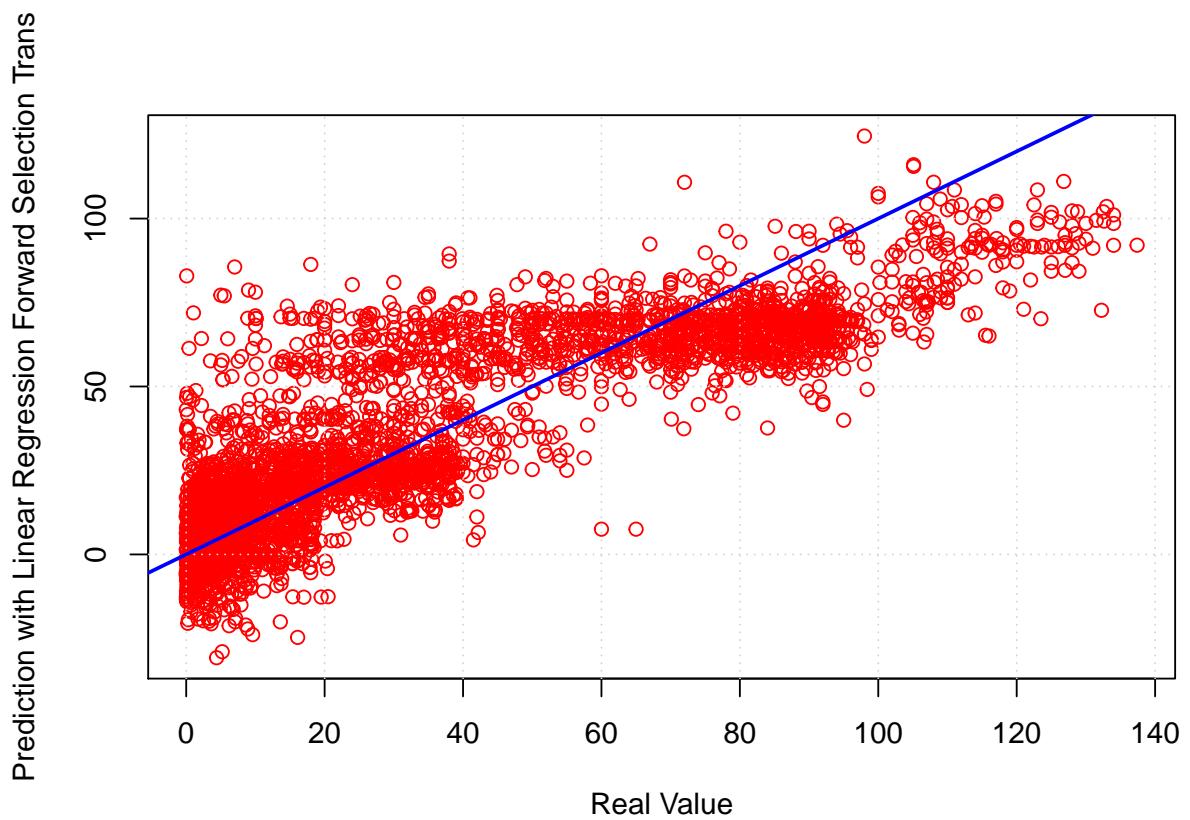


Figure 136: Scatter Plot of Prediction vs Real Values with Linear Regression Forward Selection Trans

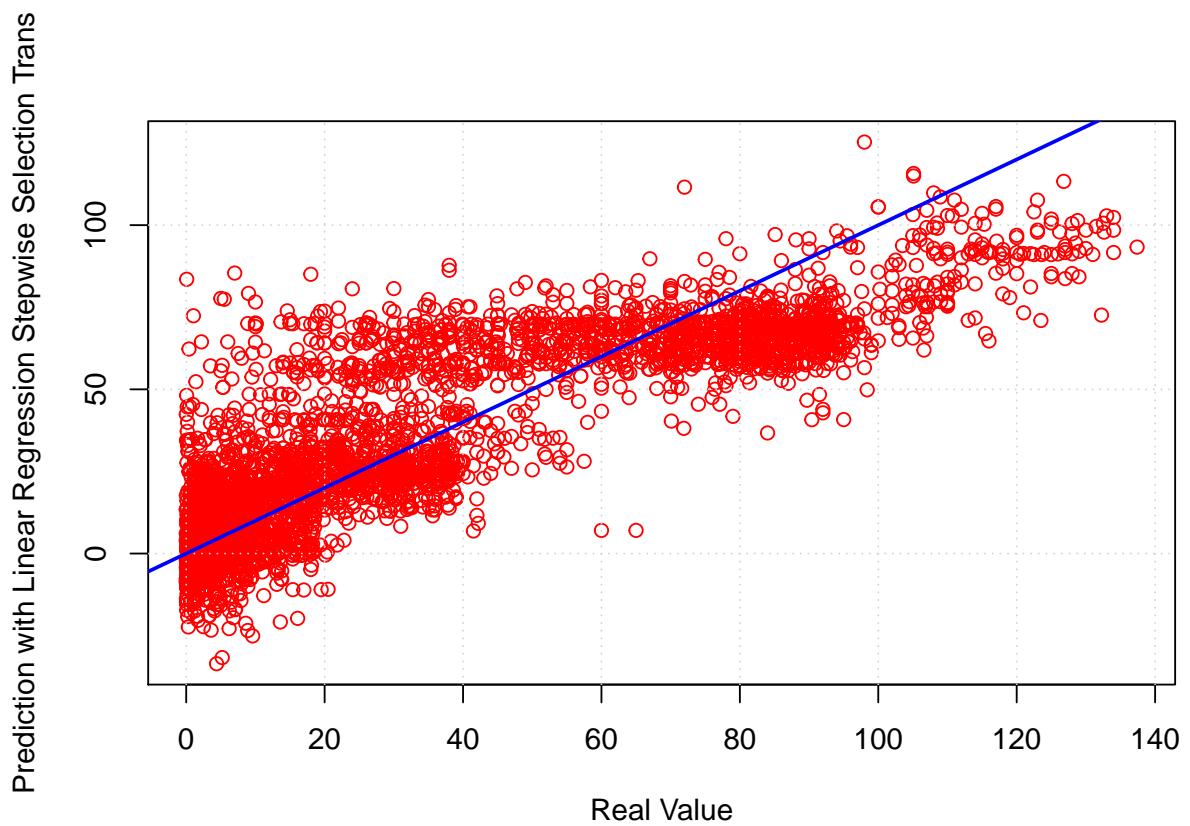


Figure 137: Scatter Plot of Prediction vs Real Values with Linear Regression Stepwise Selection Trans

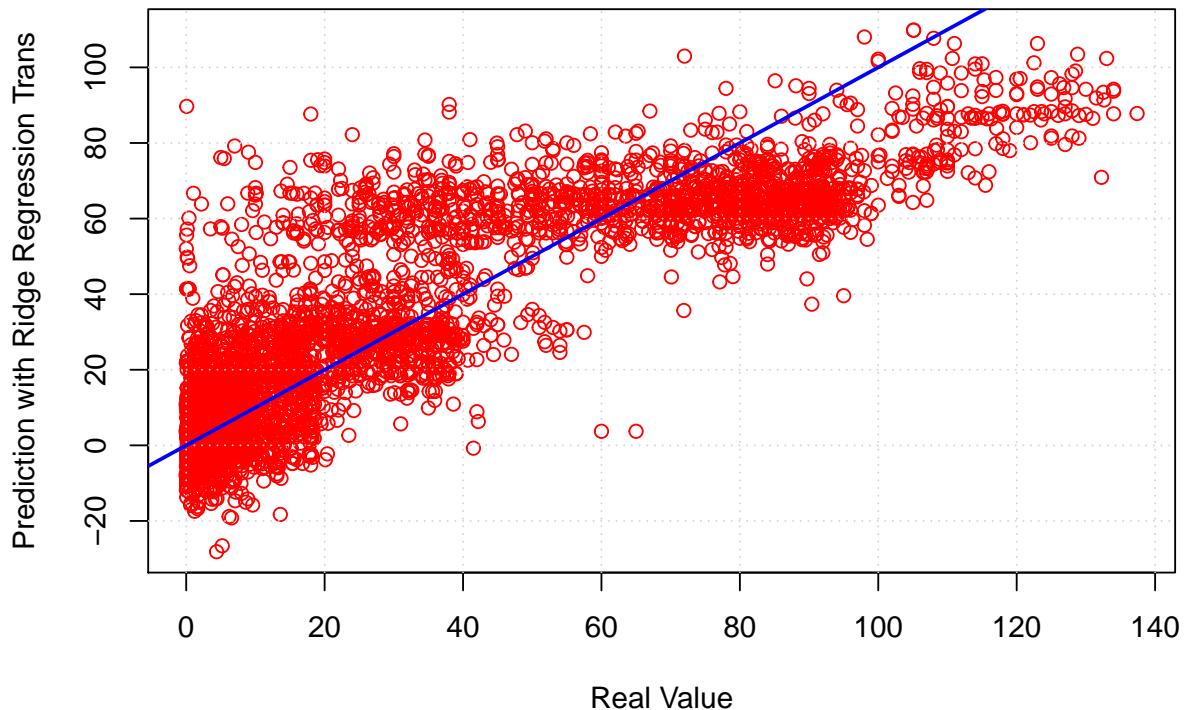


Figure 138: Scatter Plot of Prediction vs Real Values with Ridge Regression Trans

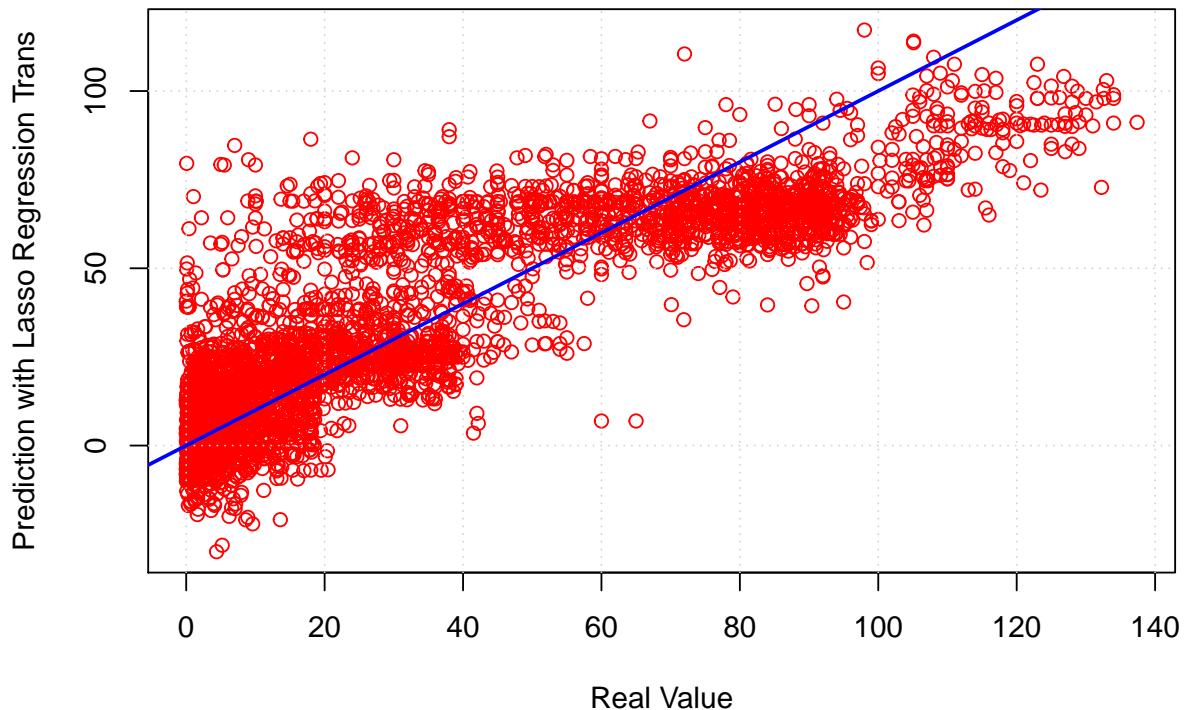


Figure 139: Scatter Plot of Prediction vs Real Values with Lasso Regression Trans

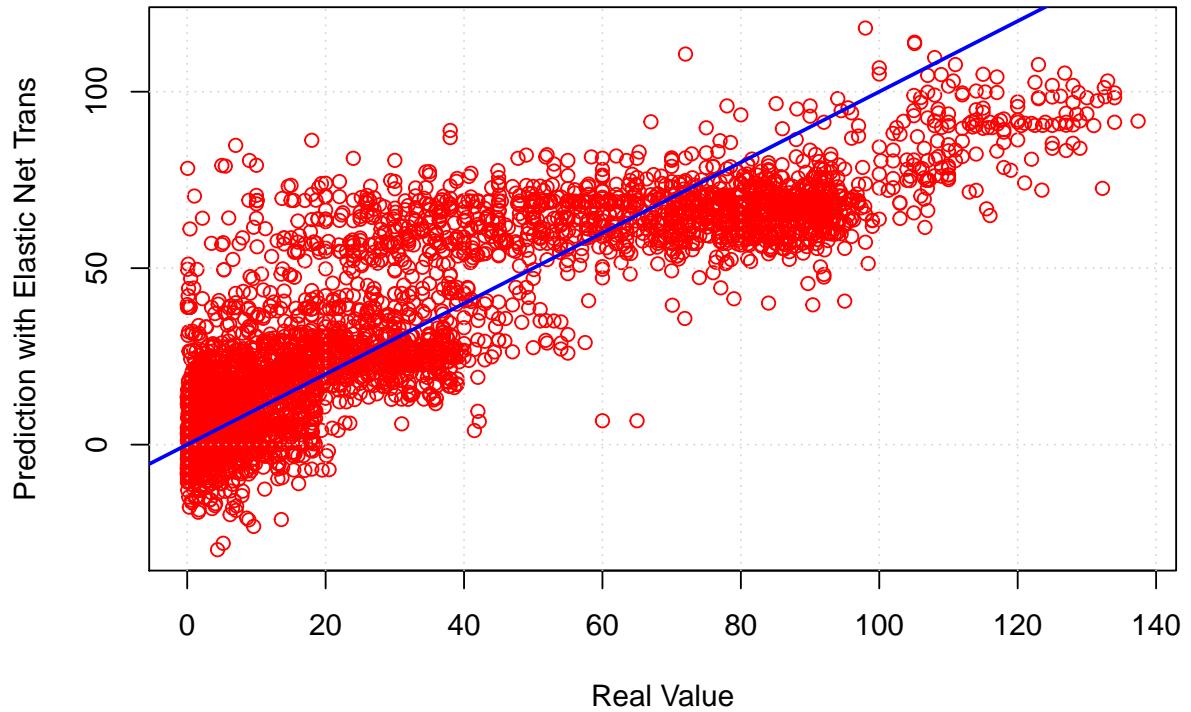


Figure 140: Scatter Plot of Prediction vs Real Values with Elastic Net Trans

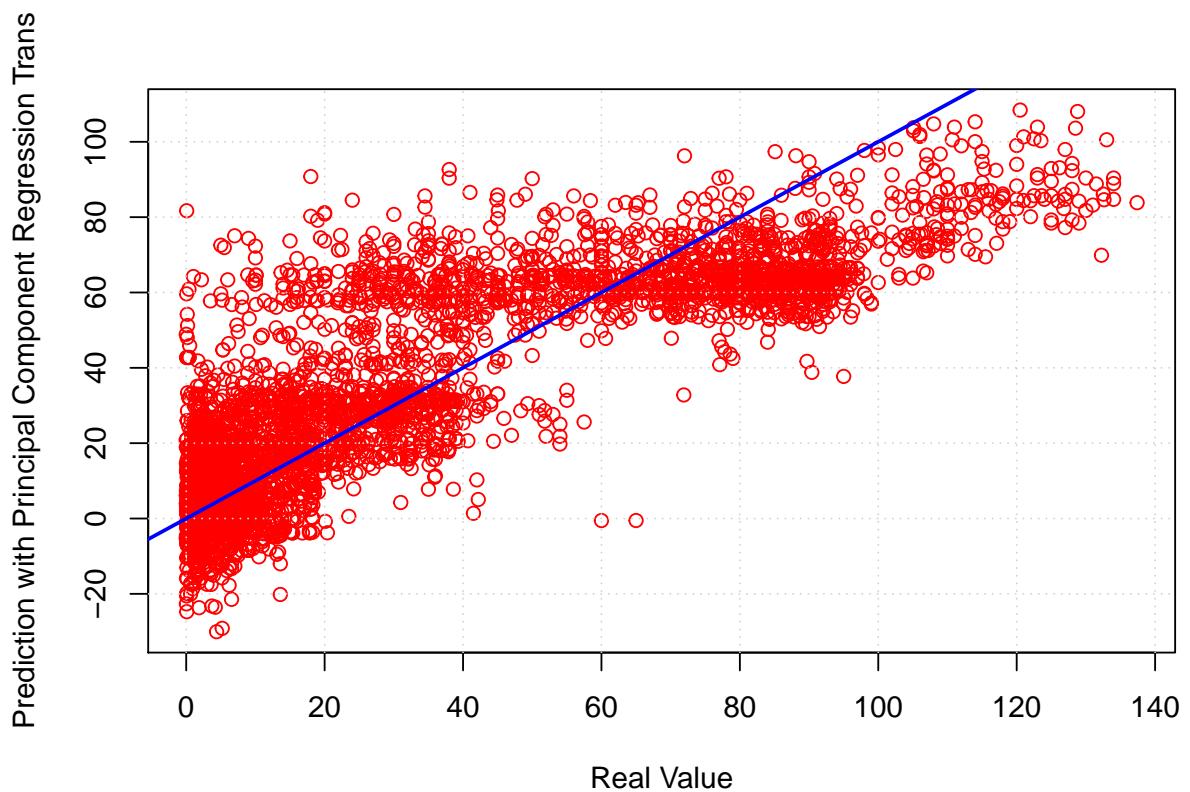


Figure 141: Scatter Plot of Prediction vs Real Values with Principal Component Regression Trans

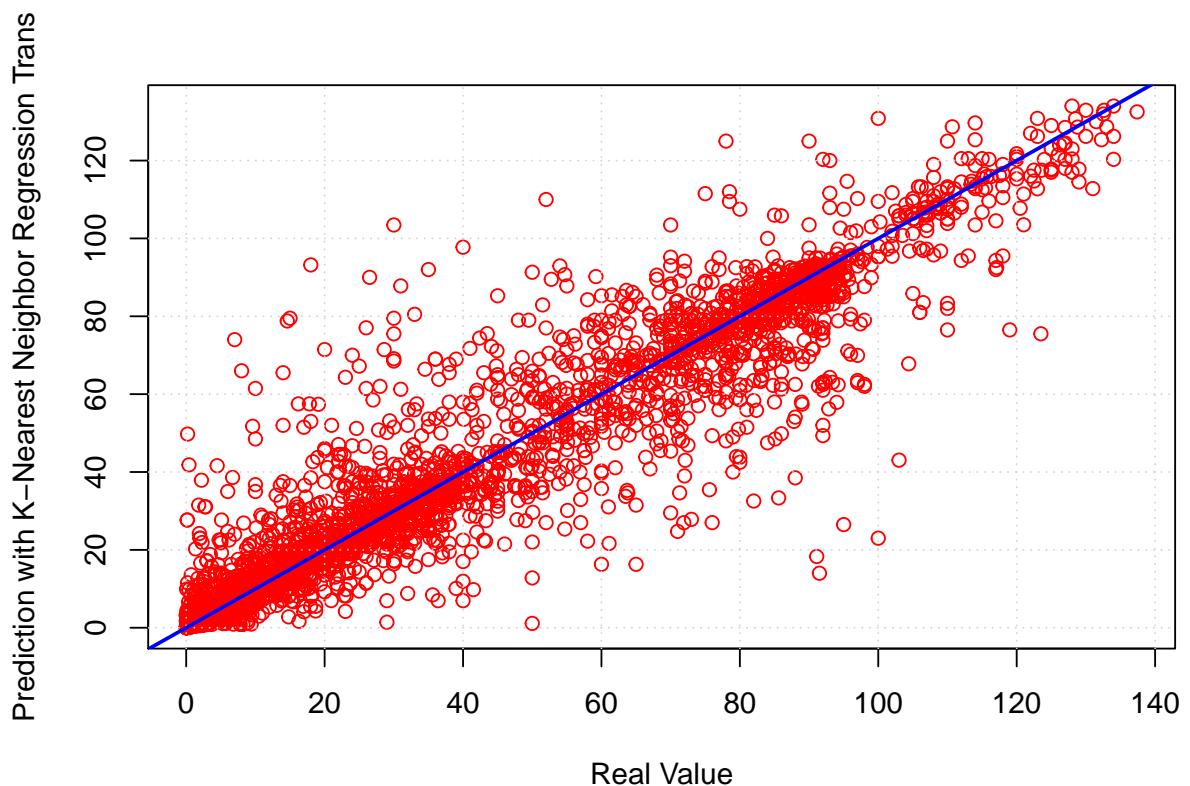


Figure 142: Scatter Plot of Prediction vs Real Values with K-Nearest Neighbor Regression Trans

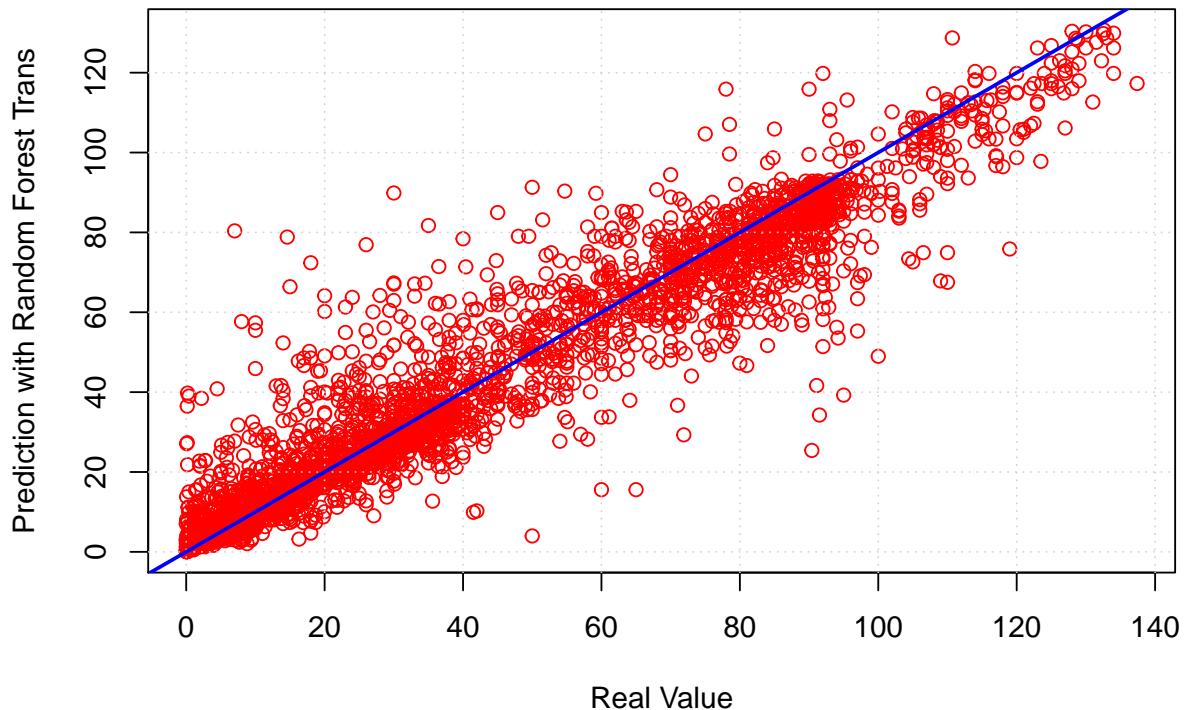


Figure 143: Scatter Plot of Prediction vs Real Values with Random Forest Trans

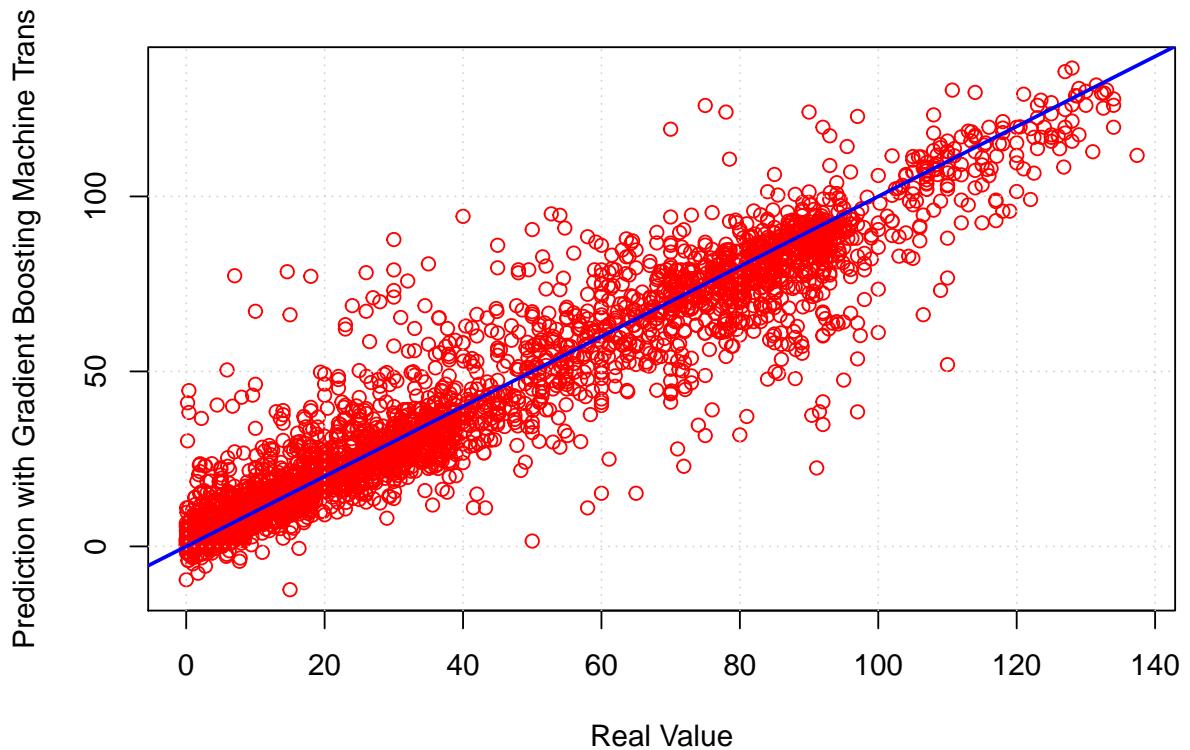


Figure 144: Scatter Plot of Prediction vs Real Values with Gradient Boosting Machine Trans

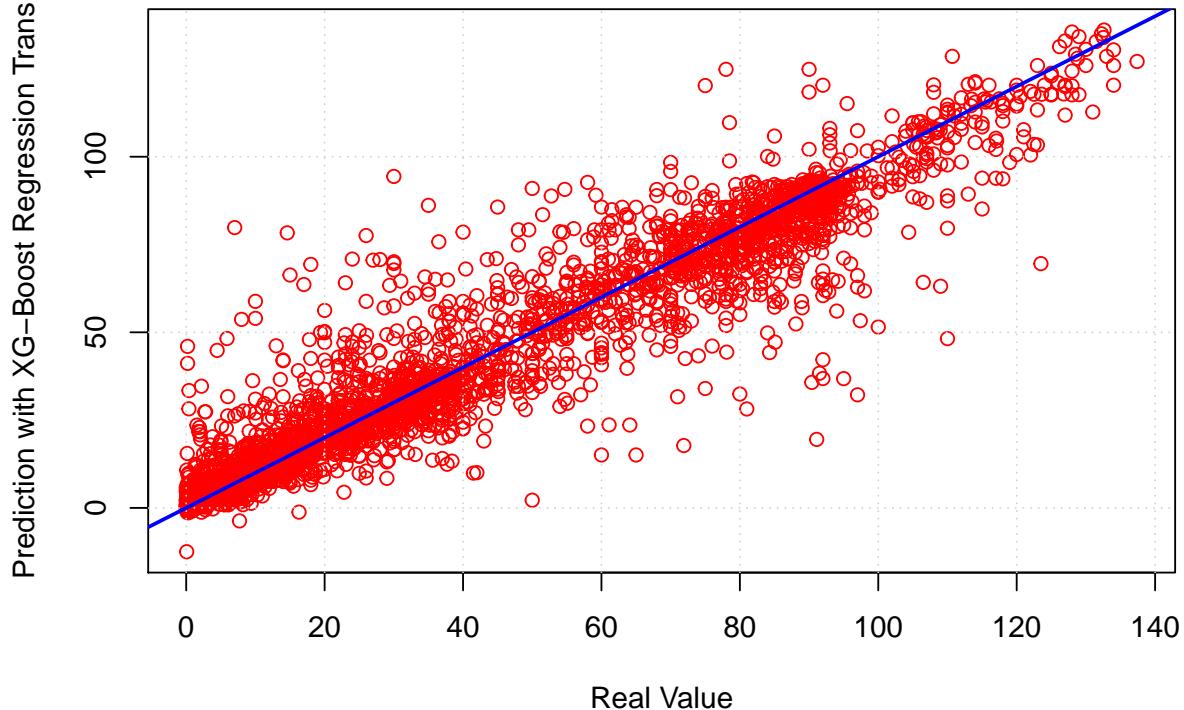


Figure 145: Scatter Plot of Prediction vs Real Values with XG-Boost Regression Trans

We have done the model evaluation, in the next section we will identify the important variable for predicting the critical temperature.

## 5 Variable Identification and Explanation

In this section, we will describe about the variable importance. At the section above, we have show and visualise the variable importance for each model. Here, we will analysis these variables in general. In order to do that, we will store of the variable importance information from each model, then we will do the high level analysis on the data.

```
var.data <- as.data.frame(colnames(train.data[,-82]))
colnames(var.data) <- c("Variables")

i <- 1

# Store the Variables Importance
for(model in models){
  temp <- as.data.frame(varImp(model)$importance)
  temp <- cbind(newColName = rownames(temp), temp)
  rownames(temp) <- 1:nrow(temp)
  temp$Overall <- round(scales::rescale(temp$Overall, to = c(1,100)))
```

```

colnames(temp) <- c("Variables",models.label[i])
var.data <- merge(x = var.data, y = temp, by = "Variables", all.x = TRUE)
i <- i + 1
}
var.data[is.na(var.data)] <- 0
var.data$total <- rowSums(var.data[-1])

var.data.m <- melt(var.data[-30], id = c("Variables"))
var.data.m$Variables <- factor(var.data.m$Variables, levels = unique(colnames(train.data[,-82])))

# Visualise the Variable Importance from All Models
ggplot(var.data.m, aes(x = Variables, y = value, label = value)) +
  geom_boxplot() +
  coord_flip() + theme_bw()

```

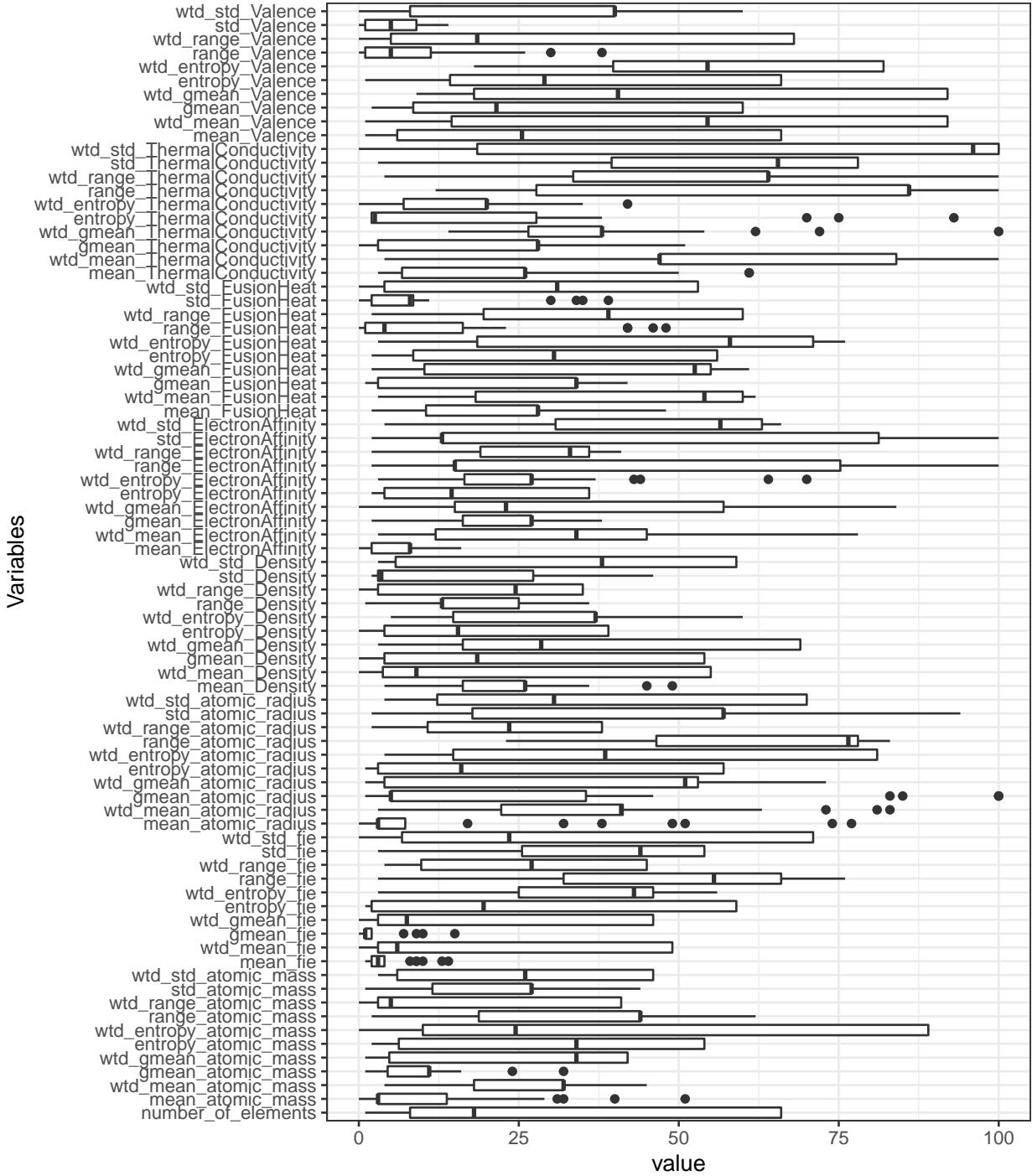


Figure 146: Variables Importance for All Models

Figure 146 shows the variable importance from all models in general. However, different type of models might treat the variable importance differently. Therefore, we will split the variable importance data into 3 parts which are linear models, instance-based models, and ensemble tree-based models as follows.

```
# Visualise the Variable Importance from Linear Models
ggplot(var.data.m[var.data.m$variable %in% linear.models,],
       aes(x = Variables, y = value, label = value)) +
  geom_boxplot() +
  coord_flip() + theme_bw()
```

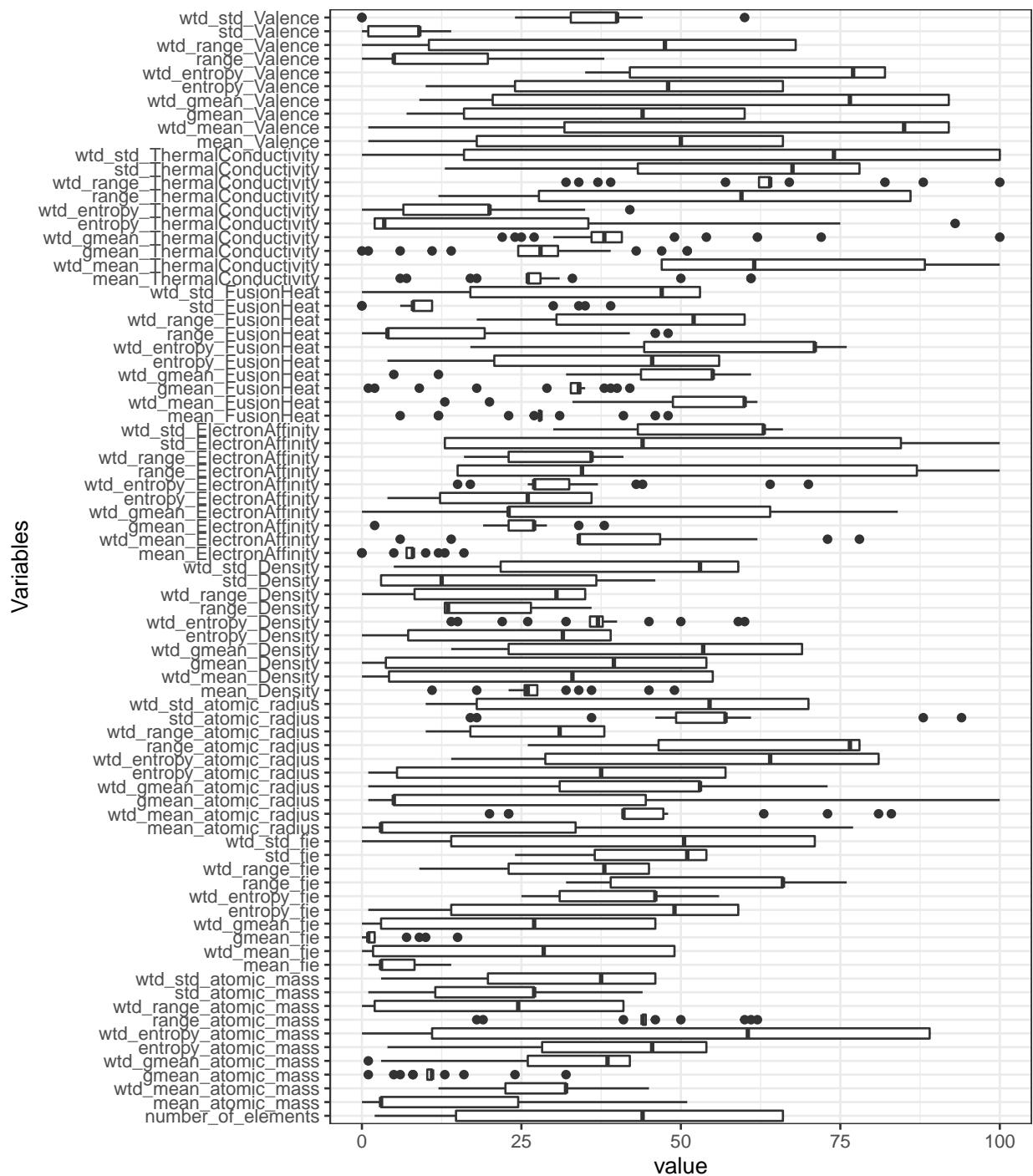


Figure 147: Variables Importance for Linear Models

Figure 147 shows the variable importance from linear related models. If we choose 25 as the threshold, then mean\_atomic\_mass, gmean\_atomic\_mass, mean\_fie, gmean\_fie, std\_Density, mean\_ElectronAffinity, range\_FusionHeat, std\_FusionHeat, wtd\_entropy\_ThermalConductivity, range\_Valence, and std\_Valence are the less important variables. This is inline with our finding from the correlation matrix, all of these variables have no correlation to the response variable. Meanwhile, the top 5 most important variables are wtd\_entropy\_Valence, wtd\_gmean\_Valence, mean\_Valence, wtd\_std\_ThermalConductivity and std\_ThermalConductivity. Therefore, we can conclude that Valence and ThermalConductivity are the two main properties for predicting the critical temperature.

```
# Visualise the Variable Importance from Instance-Based Models
ggplot(var.data.m[var.data.m$variable %in% instance.models],,
       aes(x = Variables, y = value, label = value)) +
  geom_boxplot() +
  coord_flip() + theme_bw()
```

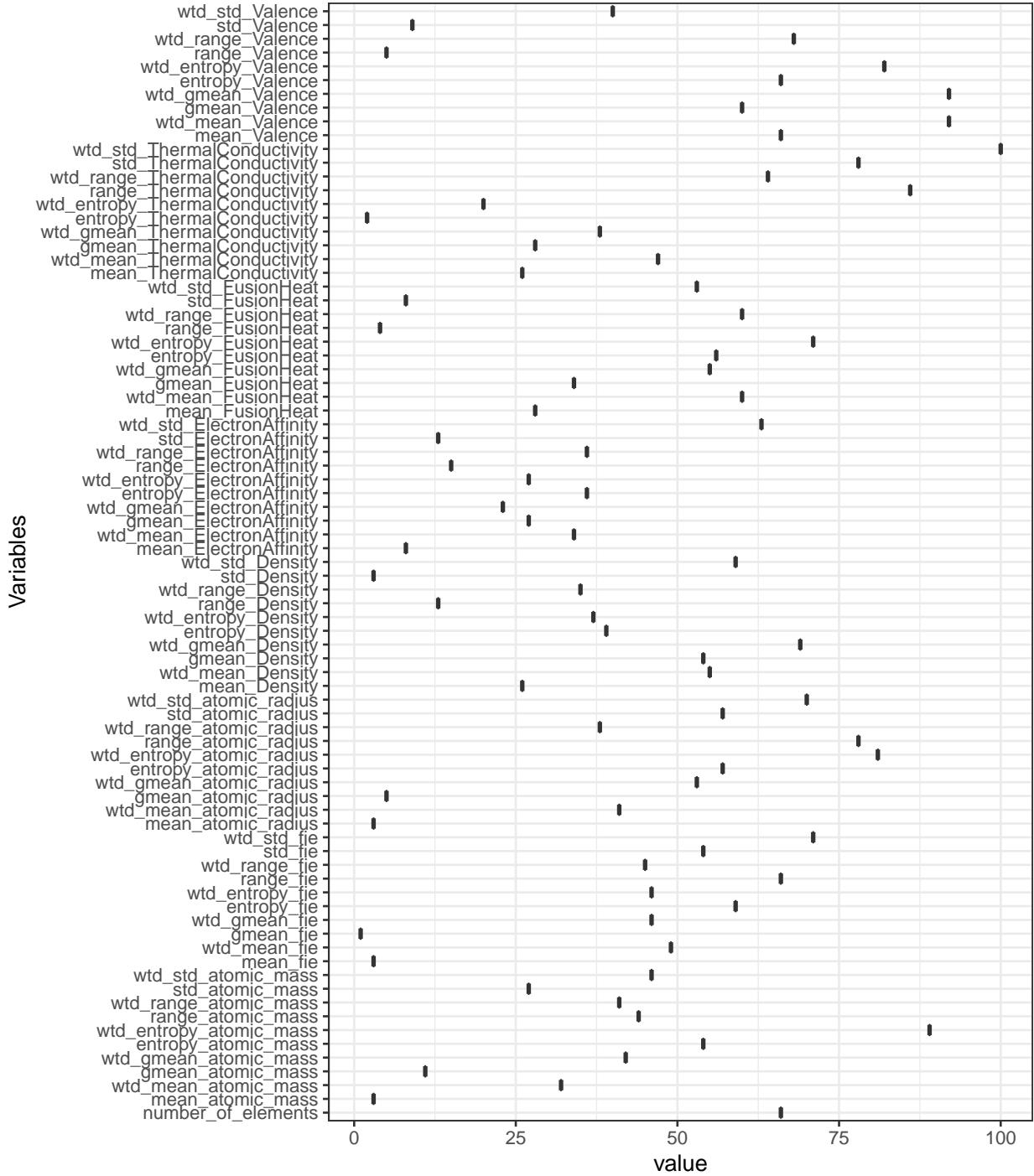


Figure 148: Variables Importance for Instance-Based Models

Figure 148 shows the variable importance from instance-based models. If we choose 25 as the threshold, then `mean_atomic_mass`, `gmean_atomic_mass`, `mean_fie`, `gmean_fie`, `mean_atomic_radius`, `gmean_atomic_radius`, `range_Density`, `std_Density`, `mean_ElectronAffinity`, `wtd_gmean_ElectronAffinity`, `range_ElectronAffinity`, `std_ElectronAffinity`, `range_FusionHeat`, `std_FusionHeat`, `entropy_ThermalConductivity`, `wtd_entropy_ThermalConductivity`, `range_Valence`, and `std_Valance` are the less important variables. Meanwhile, the top 5 most important variables are `wtd_mean_Valence`, `wtd_gmean_Valence`,

wtd\_std\_ThermalConductivity, wtd\_entropy\_atomic\_mass, and range\_ThermalConductivity. Therefore, we can also conclude that Valence and ThermalConductivity are the two main properties for predicting the critical temperature.

```
# Visualise the Variable Importance from Ensemble Tree-Based Models
ggplot(var.data.m[var.data.m$variable %in% treebased.models,],
       aes(x = Variables, y = value, label = value)) +
  geom_boxplot() +
  coord_flip() + theme_bw()
```

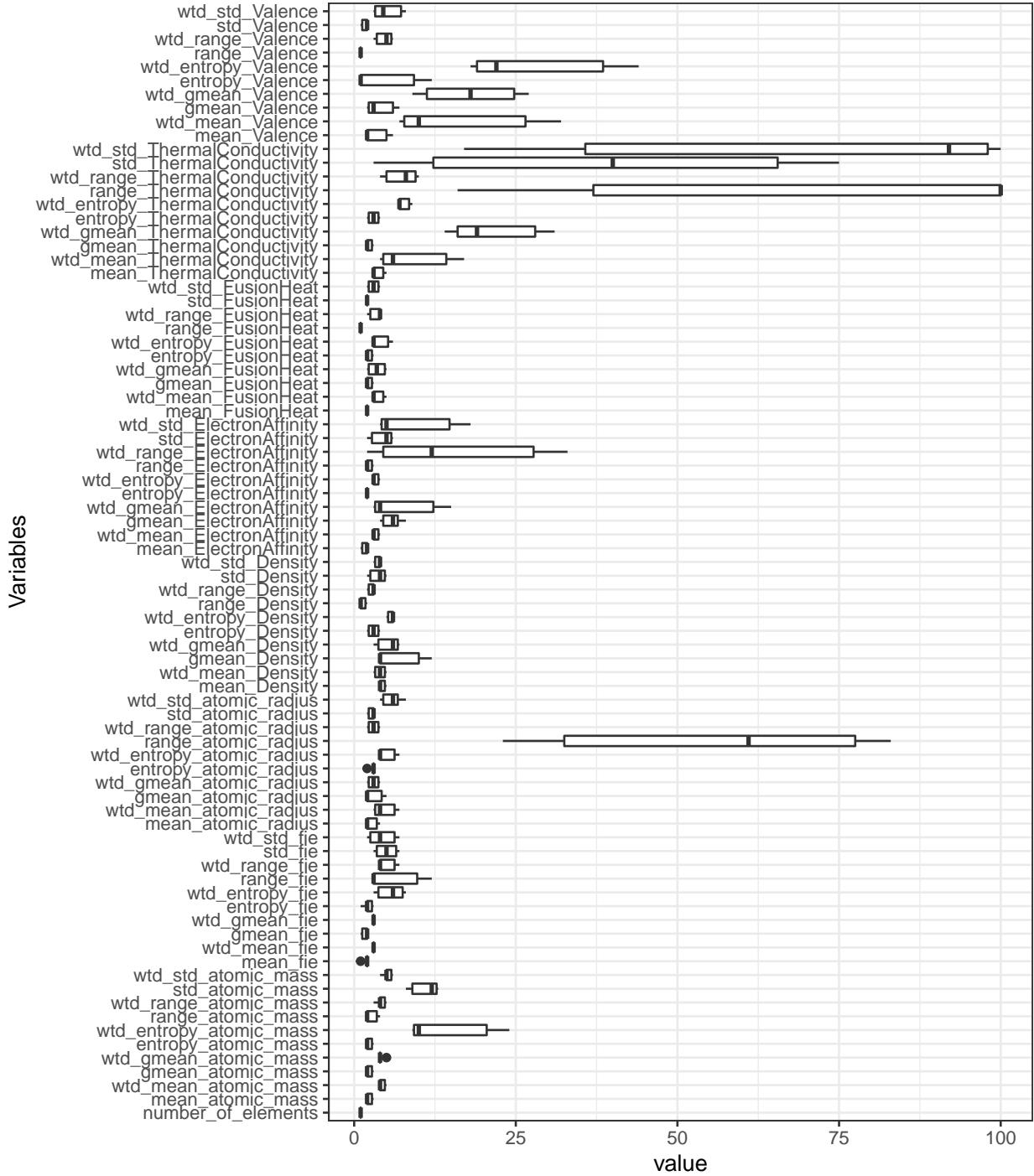


Figure 149: Variables Importance for Ensemble Tree-Based Models

Figure 149 shows the variable importance from instance-based models. If we choose 12.5 as the threshold, then `range_atomic_radius`, `wtd_range_ElectronAffinity`, `wtd_gmean_ThermalConductivity`, `range_ThermalConductivity`, `std_ThermalConductivity`, `wtd_std_ThermalConductivity`, `wtd_gmean_Valence`, `wtd_entropy_Valence` are the most important variables. Therefore, we can also conclude that Valence and ThermalConductivity are the two main properties for predicting the critical temperature.

From the above analysis, we can conclude that in predicting critical temperature of superconductor, Valence and ThermalConductivity are the most important properties.

## 6 Conclusion

The purpose of this assessment is to predict the critical temperature of superconductor materials. In order to achieve this target, Exploratory Data Analysis (EDA) was performed on the dataset to gain the insights and correlations between the variables. Data transformation was one of the main finding during the EDA because most of variables have skewed distribution. In addition, from EDA, we know that most of the variables have no correlation to the response variable. In the model development step, 14 algorithms were applied to original dataset and dataset with BoxCox transformation (28 models in total). Those algorithms consist of regression, regularization, dimensional reduction and ensemble tree-based algorithms.

Meanwhile, in the model evaluation step, the performance of each algorithm was evaluated. The results show that Instance-based and ensemble tree-based algorithm outperformed other linear regression algorithms with R-Squared 0.923 (Random Forest), 0.914 (Gradient Boosting Machine) and 0.918 (XGBoost). This is inline with the early finding that the relation between predictors and response variable is non-linear. Regularization and dimensionality reduction algorithms performed worse compared to original linear regression because there is no significant correlation between predictors.

Finally, in general Valence and ThermalConductivity are the two most important properties in predicting critical temperature of superconductor materials.

## 7 Future Work

To go further with this dataset, one of the promising future works is by applying ensemble learning on top of the models. Ensemble learning is a process by which multiple models are strategically generated and combined to solve particular computational intelligence problem. Besides that, stacking learning might also can enhance the performance of the single algorithm.

Furthermore, in order to increase the accuracy of the model, improving the hyperparameter tuning step will be a choice to go. However, computational cost and time complexity are two main issues that need to be considered for this option.

## References

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