(UBIT) DEPARTMENT OF COMPUTER SCIENCE

Critical Temperature of Superconductivity

MCS – Batch 2020-2021

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Superconductors

Introduction:

Superconductivity is a set of physical properties observed in certain materials where electrical resistance vanishes and magnetic flux fields are expelled from the material. Any material exhibiting these properties is a **superconductor**. Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. An electric current through a loop of superconducting wire can persist indefinitely with no power source temperatures

Problem Statement:

There are a number of superconducting materials which have critical temperatures on which they behave as superconductors. In order to understand the factors that affect these critical temperatures we use data mining techniques based on features of atoms and molecules in each superconducting material.

List of main features:

- **atomic_mass**, total proton and neutron rest masses, in Atomic Mass Units (AMU).
- **fie**, First Ionization Energy, energy required to remove a valence electron, in kilo-Joules per mole (kJ/mol).
- **atomic_radius**, calculated atomic radius, in picometer (pm).
- **density**, density at standard temperature and pressure, in kilograms per meters cubed (kg/m3).
- **electron_affinity**, energy required to add an electron to a neutral atom, in kilo-Joules per mole (kJ/mol).
- **fusion_heat**, energy to change from solid to liquid without temperature change, in kilo-Joules per mole (kJ/mol).
- **thermal_conductivity**, thermal conductivity coefficient k, in watts per meter-kelvin (W/(m ?? K)).
- **valence**, typical number of chemical bonds formed by the element, no units.
- **critical_temp**, superconductor critical temperature, in Kelvin.

R Markdown

This is an R Markdown document. Markdown is a simple formatting syntax for authoring HTML, PDF, and MS Word documents. For more details on using R Markdown see http://rmarkdown.rstudio.com.

When you click the Knit button a document will be generated that includes both content as well as the output of any embedded R code chunks within the document. You can embed an R code chunk like this:

```
summary(train4)
```

Including Plots

Heat Map and data loading

The heat map shows the correlation among each feature and show how much one feature is correlated to the other. This will help us to use most correlated features in our data mining models. The correlation is among 40 x 40 features. This is done by dividing the data into two halves as row and column of features in corrplot or heatmap.

```
library(readxl)
```

```
## Warning: package 'readxl' was built under R version 4.1.2
```

```
train4 <- read_excel("train4.xlsx")
View(train4)
library("corrplot")
```

```
## Warning: package 'corrplot' was built under R version 4.1.2
```

```
## corrplot 0.92 loaded
```

```
corr_matrix <- cor(train4)
```

```
# create a new df and order columns alphabetically
train4_new <- train4[, order(colnames(train4))]
```

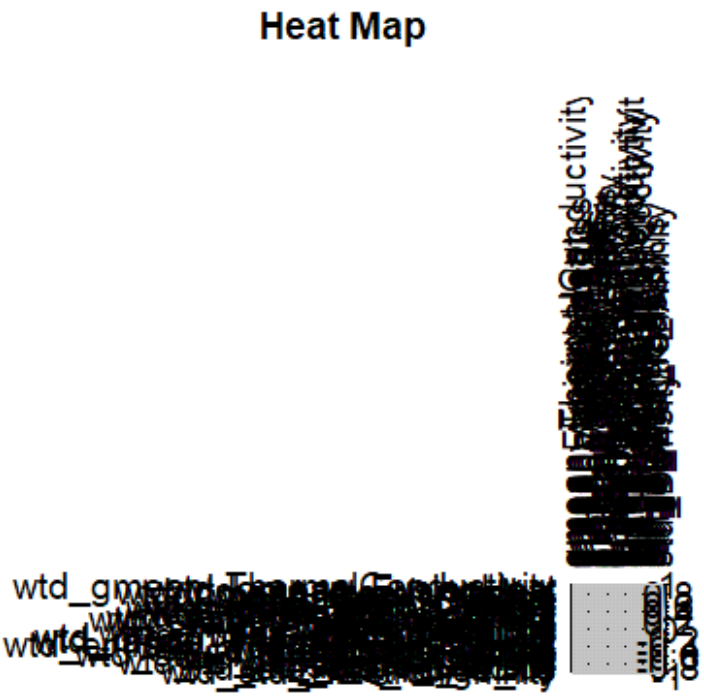
```
# correlation
train4_new.mat <- cor(train4_new)
```

```
# remove unwanted rows and columns from the correlation matrix
train4_new_mat <- train4_new.mat[42:82, 1:41] #41 x 41 square correlation
```

```
# run plot
corrplot(
  train4_new_mat,
```

```
  title = "Heat Map",
  method = "circle",
  type = "full",
  tl.col = "black",
  order = "hclust",
  hclust.method = "ward.D2",
  tl.cex = 1.2,
  cl.cex=1.2,
  outline = T,
  mar=c(0,0,4,5),
  sig.level = 0.05,

)
```

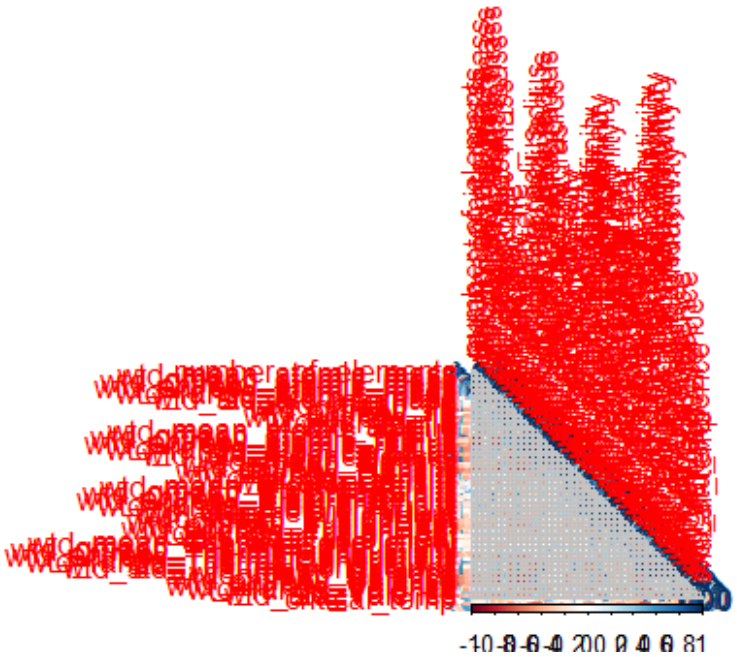
```
## Warning in corrplot(train4_new_mat, title = "Heat Map", method = "circle", :
## Not been able to calculate text margin, please try again with a clean new empty
## window using {plot.new(); dev.off()} or reduce tl.cex
```



Here, 80 x 80 features are used in corrplot as heatmap.

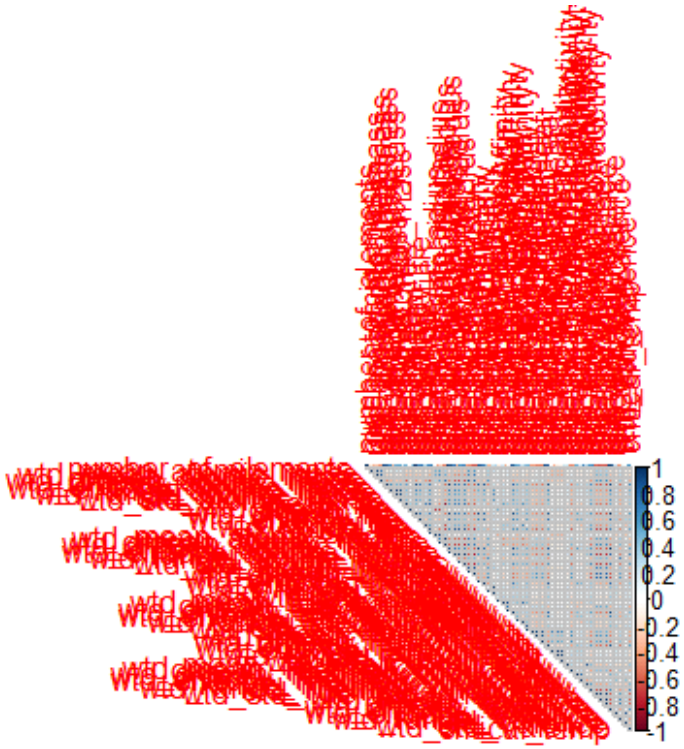
```
# with numbers and lower
corrplot(corr_matrix,
```

```
      method = 'number',
      type = "lower")
```



Here, 80 x 80 corrplot as heatmap

```
library("corrplot")
cr <- cor(train4)
#corrplot(cr)
corrplot(cr, type="upper")
```



Normalization:

Min-max normalization is done to normalize data from 0-1. This is done because the scale of features is different. Then we found the statistics using summary of the normalized data.

```
min_max <- function(x){
  res <- (x - min(x))/(max(x)-min(x))
  return(res)
}
newd<- as.data.frame(sapply(train4[,1:82],min_max))


summary(newd)
```

```
##  number_of_elements mean_atomic_mass wtd_mean_atomic_mass gmean_atomic_mass
##  Min.   :0.0000     Min.   :0.0000   Min.   :0.0000       Min.   :0.0000
##  1st Qu.:0.2500     1st Qu.:0.3243   1st Qu.:0.2257       1st Qu.:0.2589
##  Median :0.3750     Median :0.3860   Median :0.2679       Median :0.2997
##  Mean   :0.3894     Mean   :0.3990   Mean   :0.3286       Mean   :0.3239
##  3rd Qu.:0.5000     3rd Qu.:0.4626   3rd Qu.:0.3934       3rd Qu.:0.3574
##  Max.   :1.0000     Max.   :1.0000   Max.   :1.0000       Max.   :1.0000
##  wtd_gmean_atomic_mass entropy_atomic_mass wtd_entropy_atomic_mass
##  Min.   :0.0000        Min.   :0.0000      Min.   :0.0000
##  1st Qu.:0.1608        1st Qu.:0.4873      1st Qu.:0.3960
##  Median :0.1834        Median :0.6047      Median :0.5856
##  Mean   :0.2733        Mean   :0.5876      Mean   :0.5433
```

```
##  3rd Qu.:0.3437        3rd Qu.:0.7282      3rd Qu.:0.6942
##  Max.   :1.0000        Max.   :1.0000      Max.   :1.0000
##  range_atomic_mass wtd_range_atomic_mass std_atomic_mass  wtd_std_atomic_mass
##  Min.   :0.0000    Min.   :0.00000       Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.3775    1st Qu.:0.08183       1st Qu.:0.3256   1st Qu.:0.2825
##  Median :0.5910    Median :0.12956       Median :0.4467   Median :0.4384
##  Mean   :0.5558    Mean   :0.16161       Mean   :0.4394   Mean   :0.4103
##  3rd Qu.:0.7411    3rd Qu.:0.18657       3rd Qu.:0.5872   3rd Qu.:0.5309
##  Max.   :1.0000    Max.   :1.00000       Max.   :1.0000   Max.   :1.0000
##     mean_fie       wtd_mean_fie      gmean_fie       wtd_gmean_fie
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.3714   1st Qu.:0.3737   1st Qu.:0.3381   1st Qu.:0.3619
##  Median :0.4153   Median :0.5290   Median :0.3759   Median :0.5049
##  Mean   :0.4203   Mean   :0.5089   Mean   :0.3861   Mean   :0.4803
##  3rd Qu.:0.4488   3rd Qu.:0.6464   3rd Qu.:0.4162   3rd Qu.:0.5904
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000   Max.   :1.0000
##   entropy_fie     wtd_entropy_fie    range_fie      wtd_range_fie
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.5032   1st Qu.:0.3697   1st Qu.:0.2011   1st Qu.:0.2325
##  Median :0.6285   Median :0.4498   Median :0.5857   Median :0.4077
##  Mean   :0.6021   Mean   :0.4546   Mean   :0.4387   Mean   :0.3862
##  3rd Qu.:0.7189   3rd Qu.:0.5208   3rd Qu.:0.6214   3rd Qu.:0.5517
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000   Max.   :1.0000
##     std_fie        wtd_std_fie     mean_atomic_radius wtd_mean_atomic_radius
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000     Min.   :0.0000
##  1st Qu.:0.2284   1st Qu.:0.1941   1st Qu.:0.4053     1st Qu.:0.2565
##  Median :0.5331   Median :0.5394   Median :0.4490     Median :0.3119
##  Mean   :0.4315   Mean   :0.4676   Mean   :0.4399     Mean   :0.3469
##  3rd Qu.:0.5958   3rd Qu.:0.7151   3rd Qu.:0.4874     3rd Qu.:0.4411
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000     Max.   :1.0000
##  gmean_atomic_radius wtd_gmean_atomic_radius entropy_atomic_radius
##  Min.   :0.0000      Min.   :0.0000          Min.   :0.0000
##  1st Qu.:0.3422      1st Qu.:0.1648          1st Qu.:0.4979
##  Median :0.3792      Median :0.2607          Median :0.6213
##  Mean   :0.3858      Mean   :0.2920          Mean   :0.5919
##  3rd Qu.:0.4318      3rd Qu.:0.4120          3rd Qu.:0.7061
##  Max.   :1.0000      Max.   :1.0000          Max.   :1.0000
##  wtd_entropy_atomic_radius range_atomic_radius wtd_range_atomic_radius
##  Min.   :0.0000            Min.   :0.0000      Min.   :0.0000
##  1st Qu.:0.4476            1st Qu.:0.3125      1st Qu.:0.1191
##  Median :0.6529            Median :0.6680      Median :0.1790
##  Mean   :0.5942            Mean   :0.5442      Mean   :0.2139
##  3rd Qu.:0.7489            3rd Qu.:0.8008      3rd Qu.:0.2508
##  Max.   :1.0000            Max.   :1.0000      Max.   :1.0000
##  std_atomic_radius wtd_std_atomic_radius  mean_Density    wtd_mean_Density
##  Min.   :0.0000    Min.   :0.0000        Min.   :0.0000   Min.   :0.0000
```

```
##  1st Qu.:0.3040    1st Qu.:0.3296        1st Qu.:0.1998   1st Qu.:0.1327
##  Median :0.5079    Median :0.6170        Median :0.2359   Median :0.1905
##  Mean   :0.4468    Mean   :0.5388        Mean   :0.2705   Mean   :0.2331
##  3rd Qu.:0.6011    3rd Qu.:0.7595        3rd Qu.:0.2978   3rd Qu.:0.2840
##  Max.   :1.0000    Max.   :1.0000        Max.   :1.0000   Max.   :1.0000
##  gmean_Density     wtd_gmean_Density  entropy_Density  wtd_entropy_Density
##  Min.   :0.00000   Min.   :0.000000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.03903   1st Qu.:0.002924   1st Qu.:0.4677   1st Qu.:0.4043
##  Median :0.05926   Median :0.067053   Median :0.5581   Median :0.5182
##  Mean   :0.15314   Mean   :0.137966   Mean   :0.5488   Mean   :0.5025
##  3rd Qu.:0.25648   3rd Qu.:0.255224   3rd Qu.:0.6774   3rd Qu.:0.6346
##  Max.   :1.00000   Max.   :1.000000   Max.   :1.0000   Max.   :1.0000
##  range_Density    wtd_range_Density  std_Density     wtd_std_Density
##  Min.   :0.0000   Min.   :0.00000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.2943   1st Qu.:0.07385   1st Qu.:0.2629   1st Qu.:0.2463
##  Median :0.3966   Median :0.09285   Median :0.3079   Median :0.3483
##  Mean   :0.3836   Mean   :0.12939   Mean   :0.3186   Mean   :0.3188
##  3rd Qu.:0.4329   3rd Qu.:0.15196   3rd Qu.:0.3734   3rd Qu.:0.3803
##  Max.   :1.0000   Max.   :1.00000   Max.   :1.0000   Max.   :1.0000
##  mean_ElectronAffinity wtd_mean_ElectronAffinity gmean_ElectronAffinity
##  Min.   :0.0000        Min.   :0.0000            Min.   :0.0000
##  1st Qu.:0.1867        1st Qu.:0.2213            1st Qu.:0.0992
##  Median :0.2206        Median :0.3123            Median :0.1539
##  Mean   :0.2322        Mean   :0.2810            Mean   :0.1628
##  3rd Qu.:0.2588        3rd Qu.:0.3365            3rd Qu.:0.2033
##  Max.   :1.0000        Max.   :1.0000            Max.   :1.0000
##  wtd_gmean_ElectronAffinity entropy_ElectronAffinity
##  Min.   :0.0000             Min.   :0.0000
##  1st Qu.:0.1518             1st Qu.:0.5038
##  Median :0.2208             Median :0.6439
##  Mean   :0.2185             Mean   :0.6054
##  3rd Qu.:0.2726             3rd Qu.:0.7614
##  Max.   :1.0000             Max.   :1.0000
##  wtd_entropy_ElectronAffinity range_ElectronAffinity wtd_range_ElectronAffinity
##  Min.   :0.0000               Min.   :0.0000         Min.   :0.0000
##  1st Qu.:0.3943               1st Qu.:0.2484         1st Qu.:0.1556
##  Median :0.4663               Median :0.3640         Median :0.3254
##  Mean   :0.4600               Mean   :0.3459         Mean   :0.2713
##  3rd Qu.:0.5238               3rd Qu.:0.3972         3rd Qu.:0.3507
##  Max.   :1.0000               Max.   :1.0000         Max.   :1.0000
##  std_ElectronAffinity wtd_std_ElectronAffinity mean_FusionHeat
##  Min.   :0.0000       Min.   :0.0000           Min.   :0.00000
##  1st Qu.:0.2356       1st Qu.:0.1978           1st Qu.:0.07031
##  Median :0.3139       Median :0.2841           Median :0.08668
##  Mean   :0.3003       Mean   :0.2627           Mean   :0.13432
##  3rd Qu.:0.3451       3rd Qu.:0.3154           3rd Qu.:0.16122
```

```
##  Max.   :1.0000       Max.   :1.0000          Max.   :1.00000
##  wtd_mean_FusionHeat gmean_FusionHeat  wtd_gmean_FusionHeat entropy_FusionHeat
##  Min.   :0.00000     Min.   :0.00000   Min.   :0.00000      Min.   :0.0000
##  1st Qu.:0.04592     1st Qu.:0.03711   1st Qu.:0.01050      1st Qu.:0.4096
##  Median :0.07739     Median :0.04802   Median :0.04493      Median :0.5466
##  Mean   :0.13005     Mean   :0.09463   Mean   :0.09467      Mean   :0.5374
##  3rd Qu.:0.17458     3rd Qu.:0.12768   3rd Qu.:0.15468      3rd Qu.:0.6774
##  Max.   :1.00000     Max.   :1.00000   Max.   :1.00000      Max.   :1.0000
##  wtd_entropy_FusionHeat range_FusionHeat wtd_range_FusionHeat std_FusionHeat
##  Min.   :0.0000         Min.   :0.0000   Min.   :0.00000      Min.   :0.00000
##  1st Qu.:0.3850         1st Qu.:0.1229   1st Qu.:0.02269      1st Qu.:0.08253
##  Median :0.5695         Median :0.1229   Median :0.03347      Median :0.09583
##  Mean   :0.5232         Mean   :0.2018   Mean   :0.08004      Mean   :0.16120
##  3rd Qu.:0.6624         3rd Qu.:0.2214   3rd Qu.:0.10225      3rd Qu.:0.17510
##  Max.   :1.0000         Max.   :1.0000   Max.   :1.00000      Max.   :1.00000
##  wtd_std_FusionHeat mean_ThermalConductivity wtd_mean_ThermalConductivity
##  Min.   :0.00000    Min.   :0.0000          Min.   :0.0000
##  1st Qu.:0.08908    1st Qu.:0.1834          1st Qu.:0.1331
##  Median :0.10644    Median :0.2902          Median :0.1801
##  Mean   :0.14933    Mean   :0.2697          Mean   :0.2003
##  3rd Qu.:0.15514    3rd Qu.:0.3338          3rd Qu.:0.2434
##  Max.   :1.00000    Max.   :1.0000          Max.   :1.0000
##  gmean_ThermalConductivity wtd_gmean_ThermalConductivity
##  Min.   :0.00000           Min.   :0.000000
##  1st Qu.:0.02615           1st Qu.:0.002831
##  Median :0.04487           Median :0.016152
##  Mean   :0.09380           Mean   :0.072565
##  3rd Qu.:0.13322           3rd Qu.:0.125755
##  Max.   :1.00000           Max.   :1.000000
##  entropy_ThermalConductivity wtd_entropy_ThermalConductivity
##  Min.   :0.0000              Min.   :0.0000
##  1st Qu.:0.2802              1st Qu.:0.1554
##  Median :0.4521              Median :0.3384
##  Mean   :0.4453              Mean   :0.3348
##  3rd Qu.:0.5889              3rd Qu.:0.4819
##  Max.   :1.0000              Max.   :1.0000
##  range_ThermalConductivity wtd_range_ThermalConductivity
##  Min.   :0.0000            Min.   :0.00000
##  1st Qu.:0.2009            1st Qu.:0.07311
##  Median :0.9298            Median :0.14088
##  Mean   :0.5835            Mean   :0.15453
##  3rd Qu.:0.9302            3rd Qu.:0.22885
##  Max.   :1.0000            Max.   :1.00000
##  std_ThermalConductivity wtd_std_ThermalConductivity  mean_Valence
##  Min.   :0.0000          Min.   :0.0000               Min.   :0.0000
##  1st Qu.:0.1764          1st Qu.:0.1500               1st Qu.:0.2222
```

```
##  Median :0.6315         Median :0.5324            Median :0.3056
##  Mean   :0.4602         Mean   :0.4512            Mean   :0.3664
##  3rd Qu.:0.7154         3rd Qu.:0.7628            3rd Qu.:0.5000
##  Max.   :1.0000         Max.   :1.0000            Max.   :1.0000
##  wtd_mean_Valence gmean_Valence    wtd_gmean_Valence entropy_Valence
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000    Min.   :0.0000
##  1st Qu.:0.1861   1st Qu.:0.2133   1st Qu.:0.1819    1st Qu.:0.4953
##  Median :0.2697   Median :0.2692   Median :0.2390    Median :0.6391
##  Mean   :0.3589   Mean   :0.3428   Mean   :0.3426    Mean   :0.6049
##  3rd Qu.:0.5044   3rd Qu.:0.4547   3rd Qu.:0.4858    3rd Qu.:0.7419
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000    Max.   :1.0000
##  wtd_entropy_Valence range_Valence    wtd_range_Valence  std_Valence
##  Min.   :0.0000      Min.   :0.0000   Min.   :0.0000    Min.   :0.0000
##  1st Qu.:0.3978      1st Qu.:0.1667   1st Qu.:0.1318    1st Qu.:0.1506
##  Median :0.5983      Median :0.3333   Median :0.1520    Median :0.2667
##  Mean   :0.5400      Mean   :0.3402   Mean   :0.2121    Mean   :0.2798
##  3rd Qu.:0.6826      3rd Qu.:0.5000   3rd Qu.:0.2744    3rd Qu.:0.4000
##  Max.   :1.0000      Max.   :1.0000   Max.   :1.0000    Max.   :1.0000
##  wtd_std_Valence  critical_temp
##  Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.1023   1st Qu.:0.0290
##  Median :0.1667   Median :0.1081
##  Mean   :0.2247   Mean   :0.1861
##  3rd Qu.:0.3401   3rd Qu.:0.3405
##  Max.   :1.0000   Max.   :1.0000
```

Principal Component Analysis(PCA):

The features are too many causing too much problems without having importance. So those features that contribute least are removed using a dimensionality reduction technique called Principal Component Analysis. In this technique, Components are made on projections of the features from the original data points resulting in components. These components tell us how much does a particular feature contributes in obtaining the target or dependent variable outcome. These components are in dimensions where each feature represent single dimension. The first principal component is the projection of data points projecting most of the information then the second principal component has the second most information as projection of data points. Here the value of 5.6156 shows that PC1 has the most standard deviation covering the data points. Proportion is there of each component and cumulative proportion is telling that how much components from PC1 till the specific PC contributes in projecting information to produce data points. Here PC17 has cumulative proportion 0.94810. which means 94.810% informations has been projected by PC1 to PC17.

```
library("factoextra")
```

```
## Warning: package 'factoextra' was built under R version 4.1.2
```

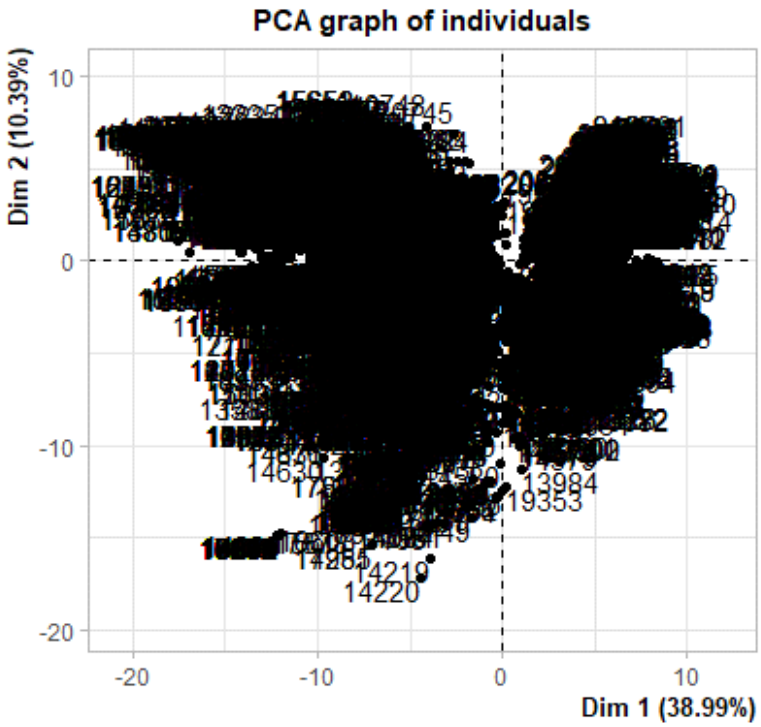
```
## Loading required package: ggplot2
```

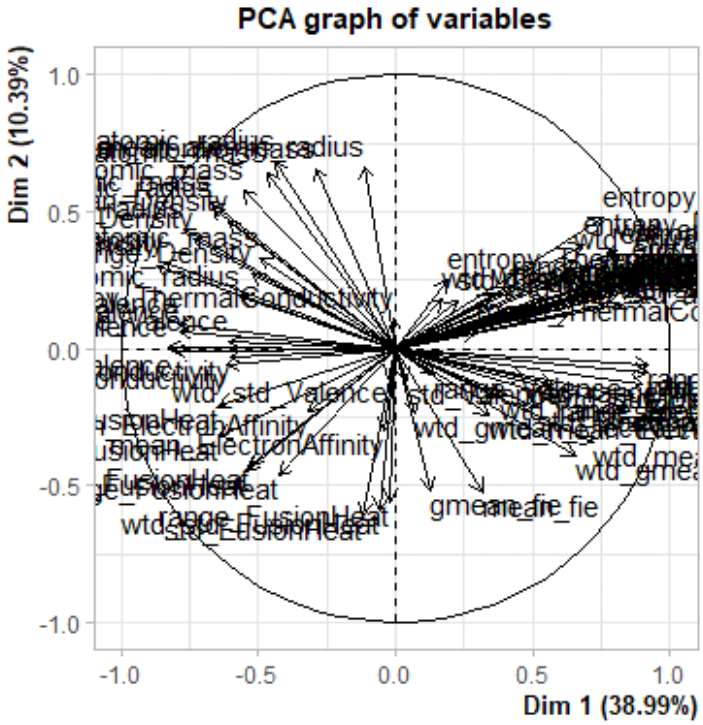
```
## Warning: package 'ggplot2' was built under R version 4.1.2

## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa

library("FactoMineR")

## Warning: package 'FactoMineR' was built under R version 4.1.2

# before the PCA analysis
res.pca <- prcomp(train4[,c(1:81)],  scale = TRUE)
summary(res.pca)

## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6     PC7
## Standard deviation     5.6156 2.9139 2.77708 2.53086 2.18279 1.75174 1.71290
## Proportion of Variance 0.3893 0.1048 0.09521 0.07908 0.05882 0.03788 0.03622
## Cumulative Proportion  0.3893 0.4941 0.58935 0.66843 0.72725 0.76513 0.80136
##                            PC8     PC9    PC10    PC11    PC12    PC13    PC14
## Standard deviation     1.58643 1.38293 1.26573 1.21695 1.08695 0.97701 0.89935
## Proportion of Variance 0.03107 0.02361 0.01978 0.01828 0.01459 0.01178 0.00999
## Cumulative Proportion  0.83243 0.85604 0.87582 0.89410 0.90869 0.92047 0.93046
##                           PC15    PC16    PC17    PC18    PC19    PC20    PC21
## Standard deviation     0.89208 0.79563 0.76303 0.66348 0.62570 0.55602 0.49481
## Proportion of Variance 0.00982 0.00782 0.00719 0.00543 0.00483 0.00382 0.00302
## Cumulative Proportion  0.94028 0.94810 0.95529 0.96072 0.96555 0.96937 0.97239
##                           PC22    PC23    PC24    PC25    PC26   PC27    PC28
## Standard deviation     0.48177 0.45580 0.40959 0.39968 0.38845 0.3711 0.33985
## Proportion of Variance 0.00287 0.00256 0.00207 0.00197 0.00186 0.0017 0.00143
## Cumulative Proportion  0.97526 0.97782 0.97989 0.98187 0.98373 0.9854 0.98686
##                           PC29    PC30    PC31    PC32    PC33    PC34    PC35
## Standard deviation     0.31984 0.30537 0.28801 0.27892 0.27287 0.24129 0.23554
## Proportion of Variance 0.00126 0.00115 0.00102 0.00096 0.00092 0.00072 0.00068
## Cumulative Proportion  0.98812 0.98927 0.99029 0.99125 0.99217 0.99289 0.99358
##                           PC36    PC37    PC38    PC39    PC40    PC41    PC42
## Standard deviation     0.22426 0.21502 0.19983 0.18811 0.18503 0.16253 0.15744
## Proportion of Variance 0.00062 0.00057 0.00049 0.00044 0.00042 0.00033 0.00031
## Cumulative Proportion  0.99420 0.99477 0.99526 0.99570 0.99612 0.99645 0.99675
##                           PC43    PC44    PC45    PC46   PC47    PC48    PC49
## Standard deviation     0.14428 0.13868 0.13456 0.13208 0.1262 0.12326 0.12100
## Proportion of Variance 0.00026 0.00024 0.00022 0.00022 0.0002 0.00019 0.00018
## Cumulative Proportion  0.99701 0.99725 0.99747 0.99769 0.9979 0.99807 0.99825
##                           PC50    PC51    PC52    PC53    PC54    PC55    PC56
## Standard deviation     0.11914 0.11255 0.11162 0.10131 0.09863 0.09771 0.09242
## Proportion of Variance 0.00018 0.00016 0.00015 0.00013 0.00012 0.00012 0.00011
## Cumulative Proportion  0.99843 0.99858 0.99874 0.99886 0.99898 0.99910 0.99921
##                           PC57    PC58    PC59    PC60    PC61    PC62    PC63
## Standard deviation     0.08503 0.08118 0.08045 0.07627 0.07243 0.06789 0.05995
## Proportion of Variance 0.00009 0.00008 0.00008 0.00007 0.00006 0.00006 0.00004
```

```
## Cumulative Proportion  0.99930 0.99938 0.99946 0.99953 0.99959 0.99965 0.99970
##                        PC64    PC65    PC66    PC67    PC68    PC69    PC70
## Standard deviation     0.05968 0.05650 0.05349 0.05107 0.04773 0.04298 0.04084
## Proportion of Variance 0.00004 0.00004 0.00004 0.00003 0.00003 0.00002 0.00002
## Cumulative Proportion  0.99974 0.99978 0.99981 0.99985 0.99988 0.99990 0.99992
##                        PC71    PC72    PC73    PC74    PC75    PC76    PC77
## Standard deviation     0.03832 0.03676 0.03457 0.02734 0.02483 0.02113 0.01819
## Proportion of Variance 0.00002 0.00002 0.00001 0.00001 0.00001 0.00001 0.00000
## Cumulative Proportion  0.99994 0.99995 0.99997 0.99998 0.99999 0.99999 0.99999
##                        PC78    PC79     PC80     PC81
## Standard deviation     0.01366 0.01096 0.008603 0.007042
## Proportion of Variance 0.00000 0.00000 0.000000 0.000000
## Cumulative Proportion  1.00000 1.00000 1.000000 1.000000
```

```
# Extract the  eigenvalues/variances

res.pca<-prcomp(train4,scale. = TRUE)

pca <- PCA(train4, scale.unit=TRUE, ncp=5, graph=T)
```

The below PCA graph represent what data points are represented by which component or dimension the most.


PCA graph of individuals
Dim 2 (10.39%)
Dim 1 (38.99%)
10
0
-10
-20
-20
-10
0
10
13984
19353
14219
14220


PCA graph of variables
Dim 2 (10.39%)
Dim 1 (38.99%)
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0
entropy
wtd_std_Valence
ElectronAffinity
gmean_fie
wtd_gmea

The command below prints the dimensions which have features and each dimension shows the features it represents. This is shown by correlation on each dimension of a particular feature.

```
dimdesc(pca, proba = 0.05)[1:3]
```

```
## $Dim.1
## $quanti
##                              correlation       p.value
## range_fie                     0.92046417  0.000000e+00
## range_atomic_radius           0.91904268  0.000000e+00
## wtd_entropy_atomic_radius     0.91778556  0.000000e+00
## wtd_std_fie                   0.91748375  0.000000e+00
## wtd_std_atomic_radius         0.90113776  0.000000e+00
## entropy_Valence               0.89176439  0.000000e+00
## wtd_entropy_atomic_mass       0.87973401  0.000000e+00
## entropy_fie                   0.87923400  0.000000e+00
## wtd_entropy_Valence           0.87629309  0.000000e+00
## number_of_elements            0.87535434  0.000000e+00
## std_fie                       0.87131505  0.000000e+00
## entropy_atomic_radius         0.86123082  0.000000e+00
## std_atomic_radius             0.84056075  0.000000e+00
## entropy_atomic_mass           0.82243946  0.000000e+00
## range_ThermalConductivity     0.80867436  0.000000e+00
## wtd_entropy_FusionHeat        0.80430780  0.000000e+00
## entropy_ElectronAffinity      0.78446897  0.000000e+00
## wtd_std_ThermalConductivity   0.78436087  0.000000e+00
```

```
## std_ThermalConductivity        0.75894547  0.000000e+00
## entropy_FusionHeat             0.75441643  0.000000e+00
## wtd_mean_fie                   0.72227709  0.000000e+00
## range_atomic_mass              0.69955467  0.000000e+00
## entropy_Density                0.68480768  0.000000e+00
## critical_temp                  0.66902484  0.000000e+00
## wtd_gmean_fie                  0.65693036  0.000000e+00
## wtd_entropy_Density            0.65074563  0.000000e+00
## wtd_std_atomic_mass            0.63176259  0.000000e+00
## wtd_entropy_fie                0.61762155  0.000000e+00
## range_ElectronAffinity         0.58416110  0.000000e+00
## wtd_std_ElectronAffinity       0.57589779  0.000000e+00
## std_atomic_mass                0.55321568  0.000000e+00
## wtd_entropy_ElectronAffinity   0.53933799  0.000000e+00
## std_ElectronAffinity           0.51424829  0.000000e+00
## wtd_range_fie                  0.47779881  0.000000e+00
## range_Density                  0.42402538  0.000000e+00
## wtd_std_Density                0.40022557  0.000000e+00
## wtd_range_ElectronAffinity     0.38367867  0.000000e+00
## wtd_range_ThermalConductivity  0.34996606  0.000000e+00
## wtd_mean_ElectronAffinity      0.33809853  0.000000e+00
## mean_fie                       0.31701654  0.000000e+00
## mean_ThermalConductivity       0.29620194  0.000000e+00
## std_Density                    0.22826110 2.178196e-249
## entropy_ThermalConductivity    0.18940244 6.279825e-171
## wtd_mean_ThermalConductivity   0.17076247 7.570906e-139
## range_Valence                  0.14129766  3.023857e-95
## gmean_fie                      0.12860001  4.338743e-79
## wtd_gmean_ElectronAffinity     0.06980364  2.186663e-24
## std_Valence                    0.04090541  2.417922e-09
## range_FusionHeat              -0.02055268  2.725618e-03
## wtd_std_Valence               -0.02747752  6.143021e-05
## mean_ElectronAffinity         -0.04129886  1.697919e-09
## wtd_std_FusionHeat            -0.06075596  7.513841e-19
## mean_atomic_radius            -0.11342657  7.926033e-62
## std_FusionHeat                -0.11765823  2.030178e-66
## mean_atomic_mass              -0.28868269  0.000000e+00
## gmean_ElectronAffinity        -0.31767723  0.000000e+00
## wtd_range_FusionHeat          -0.42532385  0.000000e+00
## gmean_atomic_radius           -0.43730065  0.000000e+00
## gmean_atomic_mass             -0.46554120  0.000000e+00
## wtd_range_atomic_mass         -0.49355092  0.000000e+00
## wtd_range_Density             -0.52343837  0.000000e+00
## mean_FusionHeat               -0.52899113  0.000000e+00
## wtd_mean_FusionHeat           -0.54398504  0.000000e+00
## wtd_mean_atomic_mass          -0.55531207  0.000000e+00
```

```
## wtd_range_atomic_radius       -0.56486605  0.000000e+00
## wtd_gmean_ThermalConductivity -0.60308214  0.000000e+00
## wtd_range_Valence             -0.60708527  0.000000e+00
## mean_Density                  -0.61054661  0.000000e+00
## gmean_ThermalConductivity     -0.61551155  0.000000e+00
## wtd_gmean_FusionHeat          -0.64409026  0.000000e+00
## gmean_FusionHeat              -0.64829636  0.000000e+00
## wtd_mean_atomic_radius        -0.66938644  0.000000e+00
## wtd_gmean_atomic_mass         -0.67216169  0.000000e+00
## wtd_mean_Density              -0.73433523  0.000000e+00
## wtd_gmean_atomic_radius       -0.77268185  0.000000e+00
## mean_Valence                  -0.78662037  0.000000e+00
## gmean_Valence                 -0.79361492  0.000000e+00
## wtd_mean_Valence              -0.81445591  0.000000e+00
## wtd_gmean_Valence             -0.82539165  0.000000e+00
## gmean_Density                 -0.84446153  0.000000e+00
## wtd_gmean_Density             -0.87301402  0.000000e+00
##
## attr(,"class")
## [1] "condes" "list"
##
## $Dim.2
## $quanti
##                               correlation       p.value
## gmean_atomic_radius            0.68167713  0.000000e+00
## mean_atomic_radius             0.66504058  0.000000e+00
## mean_atomic_mass               0.65644178  0.000000e+00
## gmean_atomic_mass              0.63929439  0.000000e+00
## wtd_mean_atomic_mass           0.57529754  0.000000e+00
## wtd_gmean_atomic_mass          0.53587674  0.000000e+00
## wtd_mean_atomic_radius         0.51633720  0.000000e+00
## entropy_FusionHeat             0.47673743  0.000000e+00
## mean_Density                   0.46398703  0.000000e+00
## wtd_gmean_atomic_radius        0.43750465  0.000000e+00
## wtd_mean_Density               0.40344396  0.000000e+00
## entropy_Density                0.38191494  0.000000e+00
## wtd_entropy_FusionHeat         0.36005144  0.000000e+00
## entropy_atomic_mass            0.34484284  0.000000e+00
## wtd_range_atomic_mass          0.33231029  0.000000e+00
## wtd_entropy_Density            0.32310756  0.000000e+00
## gmean_Density                  0.31649483  0.000000e+00
## wtd_gmean_Density              0.29871581  0.000000e+00
## entropy_atomic_radius          0.28634199  0.000000e+00
## wtd_range_Density              0.26996354  0.000000e+00
## number_of_elements             0.25460952 8.013862e-312
## entropy_ElectronAffinity       0.25206096 1.899392e-305
```

```
## entropy_Valence                0.25103947 6.505063e-303
## entropy_ThermalConductivity    0.24904279 5.420126e-298
## entropy_fie                    0.24348872 1.544223e-284
## wtd_entropy_atomic_mass        0.23132177 2.993597e-256
## range_Density                  0.22192520 1.666650e-235
## wtd_entropy_Valence            0.21726943 1.411601e-225
## wtd_std_ThermalConductivity    0.21319731 4.404216e-217
## range_atomic_mass              0.20607990 1.173004e-202
## wtd_entropy_fie                0.20530750 4.006428e-201
## range_ThermalConductivity      0.19517664 1.377324e-181
## wtd_range_ThermalConductivity  0.19479479 7.153866e-181
## wtd_entropy_ElectronAffinity   0.19077407 1.982001e-173
## wtd_range_atomic_radius        0.18899701 3.415364e-170
## critical_temp                  0.18711175 8.538577e-167
## wtd_entropy_atomic_radius      0.18283110 3.247462e-159
## wtd_mean_ThermalConductivity   0.17936794 3.215705e-153
## std_Density                    0.17330578 5.122922e-143
## std_atomic_mass                0.16591035 4.502477e-131
## std_ThermalConductivity        0.15904763 1.765521e-120
## wtd_std_Density                0.14830786 7.688343e-105
## wtd_std_atomic_mass            0.12588009  7.848046e-76
## wtd_entropy_ThermalConductivity  0.11141295  1.056165e-59
## gmean_Valence                  0.08941303  5.324612e-39
## mean_Valence                   0.06219686  1.108918e-19
## mean_ThermalConductivity       0.06037699  1.233762e-18
## wtd_range_Valence              0.02332677  6.695946e-04
## wtd_gmean_ThermalConductivity  -0.03475167  4.006161e-07
## gmean_ThermalConductivity      -0.05864941  1.138246e-17
## range_atomic_radius            -0.06176945  1.965100e-19
## range_fie                      -0.08570388  5.839791e-36
## wtd_std_fie                    -0.09058521  5.478348e-40
## range_Valence                  -0.09275429  7.532435e-42
## wtd_range_fie                  -0.10904607  2.962440e-57
## wtd_std_Valence                -0.11033541  1.395723e-58
## std_Valence                    -0.11799068  8.700596e-67
## wtd_std_atomic_radius          -0.13096386  5.600872e-82
## wtd_std_ElectronAffinity       -0.13130401  2.128488e-82
## wtd_range_ElectronAffinity     -0.17236895 1.790575e-141
## range_ElectronAffinity         -0.17939302 2.912712e-153
## std_fie                        -0.18091637 6.943638e-156
## gmean_FusionHeat               -0.20667041 7.811820e-204
## std_atomic_radius              -0.21271336 4.381935e-216
## std_ElectronAffinity           -0.21438203 1.551538e-219
## gmean_ElectronAffinity         -0.23137046 2.323850e-256
## wtd_gmean_ElectronAffinity     -0.23833055 2.393993e-272
## wtd_mean_ElectronAffinity      -0.24087723 2.495171e-278
```

```
## mean_ElectronAffinity          -0.30386218  0.000000e+00
## wtd_gmean_FusionHeat           -0.32428766  0.000000e+00
## wtd_mean_fie                   -0.34592732  0.000000e+00
## wtd_gmean_fie                  -0.39372832  0.000000e+00
## mean_FusionHeat                -0.42535096  0.000000e+00
## wtd_mean_FusionHeat            -0.44636614  0.000000e+00
## wtd_range_FusionHeat           -0.46339928  0.000000e+00
## gmean_fie                      -0.51908230  0.000000e+00
## mean_fie                       -0.52408945  0.000000e+00
## range_FusionHeat               -0.56051346  0.000000e+00
## wtd_std_FusionHeat             -0.59069348  0.000000e+00
## std_FusionHeat                 -0.61134638  0.000000e+00
##
## attr(,"class")
## [1] "condes" "list"
##
## $Dim.3
## $quanti
##                                 correlation       p.value
## wtd_entropy_ThermalConductivity  0.68321723  0.000000e+00
## wtd_std_Valence                  0.64580114  0.000000e+00
## range_Valence                    0.63133780  0.000000e+00
## std_Valence                      0.58536906  0.000000e+00
## wtd_entropy_fie                  0.58200794  0.000000e+00
## entropy_ThermalConductivity      0.57343410  0.000000e+00
## wtd_entropy_ElectronAffinity     0.54880498  0.000000e+00
## range_FusionHeat                 0.47445960  0.000000e+00
## wtd_std_FusionHeat               0.46712185  0.000000e+00
## std_Density                      0.44986330  0.000000e+00
## std_FusionHeat                   0.44016177  0.000000e+00
## wtd_entropy_Density              0.42136393  0.000000e+00
## range_Density                    0.41615003  0.000000e+00
## range_ElectronAffinity           0.40041365  0.000000e+00
## wtd_std_Density                  0.37209554  0.000000e+00
## mean_FusionHeat                  0.36381373  0.000000e+00
## std_ElectronAffinity             0.36302687  0.000000e+00
## wtd_std_ElectronAffinity         0.35406723  0.000000e+00
## wtd_mean_Valence                 0.35025512  0.000000e+00
## wtd_mean_FusionHeat              0.34661815  0.000000e+00
## mean_Valence                     0.34157900  0.000000e+00
## gmean_fie                        0.33900866  0.000000e+00
## mean_ElectronAffinity            0.33585141  0.000000e+00
## std_atomic_mass                  0.33498785  0.000000e+00
## range_atomic_mass                0.30696842  0.000000e+00
## wtd_gmean_Valence                0.30195072  0.000000e+00
## wtd_entropy_Valence              0.30191882  0.000000e+00
```

```
## wtd_gmean_FusionHeat            0.29789638  0.000000e+00
## wtd_std_atomic_mass             0.29338235  0.000000e+00
## gmean_FusionHeat                0.28887915  0.000000e+00
## wtd_mean_Density                0.28687515  0.000000e+00
## mean_fie                        0.28250884  0.000000e+00
## entropy_fie                     0.27933930  0.000000e+00
## entropy_atomic_radius           0.27573143  0.000000e+00
## gmean_Valence                   0.27392631  0.000000e+00
## entropy_ElectronAffinity        0.27274639  0.000000e+00
## entropy_Density                 0.24890423 1.185366e-297
## wtd_entropy_FusionHeat          0.23744745 2.734582e-270
## wtd_range_FusionHeat            0.23162605 6.144149e-257
## mean_Density                    0.22689063 2.386834e-246
## number_of_elements              0.22335091 1.365638e-238
## wtd_entropy_atomic_radius       0.22119393 6.259242e-234
## gmean_ElectronAffinity          0.22060879 1.128279e-232
## entropy_Valence                 0.21270633 4.530384e-216
## wtd_gmean_atomic_radius         0.19422870 8.175360e-180
## wtd_gmean_Density               0.19253300 1.152796e-176
## entropy_atomic_mass             0.18581969 1.734197e-164
## wtd_range_Density               0.18299026 1.710200e-159
## wtd_mean_atomic_mass            0.18078365 1.177680e-155
## entropy_FusionHeat              0.17742541 6.561092e-150
## wtd_gmean_ThermalConductivity   0.17241498 1.504371e-141
## wtd_mean_atomic_radius          0.17026823 4.806763e-138
## gmean_Density                   0.16331523 5.183589e-127
## wtd_range_atomic_mass           0.15842074 1.552969e-119
## wtd_entropy_atomic_mass         0.15019643 1.653360e-107
## gmean_ThermalConductivity       0.12945478  3.971103e-80
## wtd_range_Valence               0.12738383  1.266825e-77
## wtd_gmean_atomic_mass           0.10370126  6.355040e-52
## mean_atomic_mass                0.05446844  1.896493e-15
## wtd_range_atomic_radius         0.03674694  8.327960e-08
## wtd_mean_ElectronAffinity       0.02758685  5.741283e-05
## range_fie                       0.01558255  2.307284e-02
## std_fie                        -0.02126057  1.932922e-03
## gmean_atomic_mass              -0.03798606  3.011970e-08
## range_atomic_radius            -0.04130919  1.682152e-09
## std_atomic_radius              -0.04469708  7.005865e-11
## wtd_mean_ThermalConductivity   -0.05505559  9.454669e-16
## wtd_gmean_ElectronAffinity     -0.06788064  3.800818e-23
## wtd_std_atomic_radius          -0.08810064  6.557393e-38
## wtd_range_ElectronAffinity     -0.13351733  3.685527e-85
## wtd_std_fie                    -0.13800671  6.588525e-91
## wtd_gmean_fie                  -0.16612006 2.100548e-131
## gmean_atomic_radius            -0.17605024 1.370420e-147
```

```
## wtd_mean_fie                  -0.19096452 8.878314e-174
## mean_ThermalConductivity      -0.19512477 1.723152e-181
## critical_temp                 -0.19900969 7.464744e-189
## wtd_range_ThermalConductivity -0.20451624 1.469433e-199
## mean_atomic_radius            -0.26974046  0.000000e+00
## range_ThermalConductivity     -0.27440666  0.000000e+00
## wtd_std_ThermalConductivity   -0.29175148  0.000000e+00
## std_ThermalConductivity       -0.32058964  0.000000e+00
## wtd_range_fie                 -0.40641062  0.000000e+00
##
## attr(,"class")
## [1] "condes" "list"
```

A new dataframe has been created based on the most contributing features by checking the above PCA analysis.

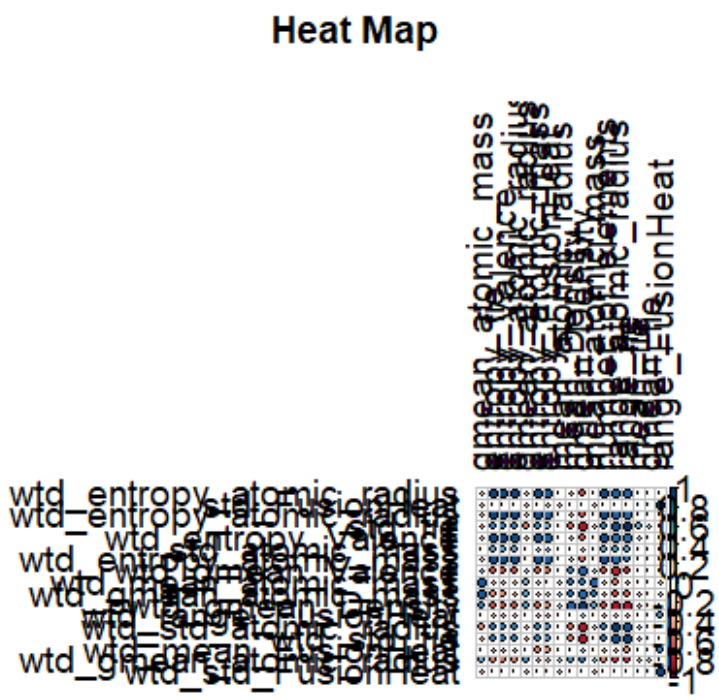
```
# creating new df with reduced features
dfnew = data.frame()
dfnew <- train4[,c("range_fie" , "range_atomic_radius" , "wtd_entropy_atomic_radius" , "wtd_std_fie"
          , "wtd_std_atomic_radius" , "entropy_Valence" , "wtd_entropy_atomic_mass" , "entropy_fie"
          , "wtd_entropy_Valence"
          , "number_of_elements" , "wtd_gmean_Density" , "std_fie" , "entropy_atomic_radius" , "gmean_Density"
          , "std_atomic_mass" , "wtd_gmean_Valence" , "entropy_atomic_mass" , "mean_atomic_radius"
          , "gmean_atomic_radius"
          , "mean_atomic_mass" , "gmean_atomic_mass" , "std_FusionHeat" , "wtd_std_FusionHeat"
          , "wtd_mean_atomic_mass"
          , "range_FusionHeat" , "wtd_gmean_atomic_mass" , "mean_fie" , "gmean_fie" , "wtd_entropy_atomic_radius"
          , "entropy_FusionHeat" , "mean_Density" , "wtd_range_FusionHeat" , "wtd_mean_FusionHeat"
          , "wtd_gmean_atomic_radius")]
head(dfnew)
```

```
## # A tibble: 6 x 34
##   range_fie range_atomic_radius wtd_entropy_atomi~ wtd_std_fie wtd_std_atomic_r~
##       <dbl>              <dbl>              <dbl>       <dbl>            <dbl>
## 1      811.                205               1.21        356.             69.2
## 2      811.                205               1.20        355.             68.0
## 3      811.                205               1.13        355.             67.8
## 4      811.                205               1.17        355.             68.5
## 5      811.                205               1.26        356.             70.6
```

```
## 6      811.              205             1.33       358.            73.3
## # ... with 29 more variables: entropy_Valence <dbl>,
## #   wtd_entropy_atomic_mass <dbl>, entropy_fie <dbl>,
## #   wtd_entropy_Valence <dbl>, number_of_elements <dbl>,
## #   wtd_gmean_Density <dbl>, std_fie <dbl>, entropy_atomic_radius <dbl>,
## #   gmean_Density <dbl>, std_atomic_mass <dbl>, wtd_gmean_Valence <dbl>,
## #   entropy_atomic_mass <dbl>, mean_atomic_radius <dbl>,
## #   gmean_atomic_radius <dbl>, mean_atomic_mass <dbl>, ...
```

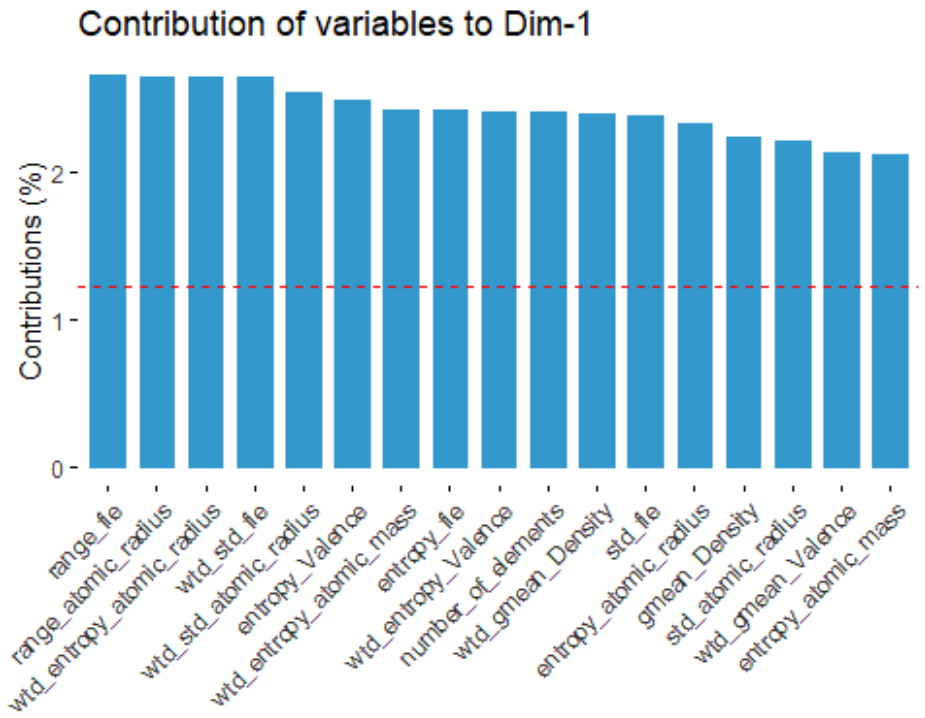
A new corrplot has been constructed based on the new dataset.

```
dfnew_matrix <- cor(dfnew)
dfnew_new <- dfnew[, order(colnames(dfnew))]

# correlation
dfnew_new.mat <- cor(dfnew_new)

# remove unwanted rows and columns from the correlation matrix
dfnew_new_mat <- dfnew_new.mat[18:34, 1:17] #41 x 41 square correlation

# run plot
corrplot(
  dfnew_new_mat,
  title = "Heat Map",
  method = "circle",
  type = "full",
  tl.col = "black",
  order = "hclust",
  hclust.method = "ward.D2",
  tl.cex = 1.2,
  cl.cex=1.2,
  outline = T,
  mar=c(0,0,4,5),
  sig.level = 0.05,

)
```

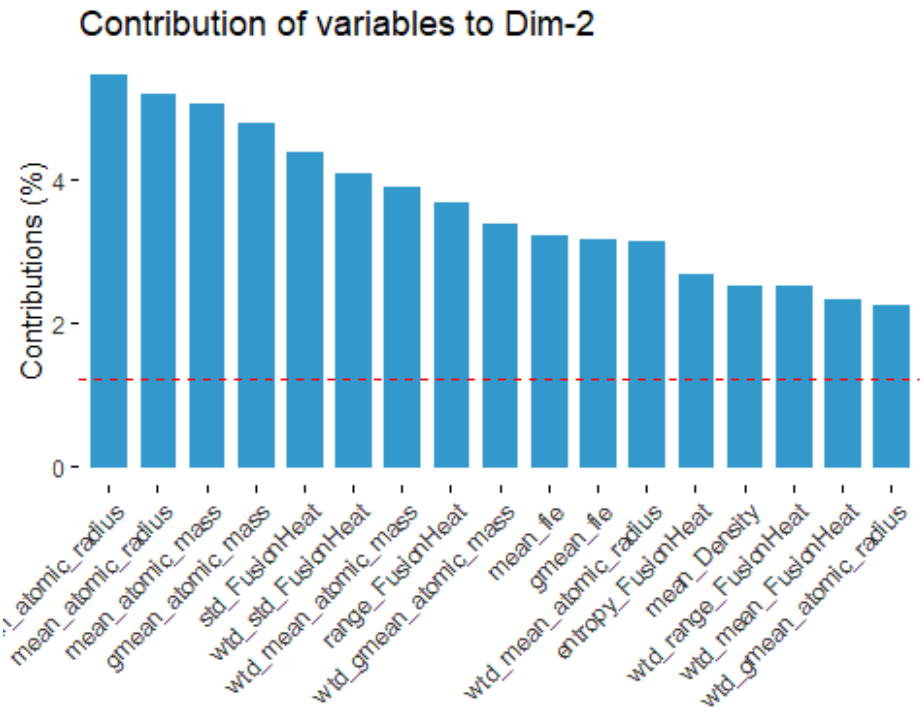


The below barplot shows the contribution by percentage of each component.

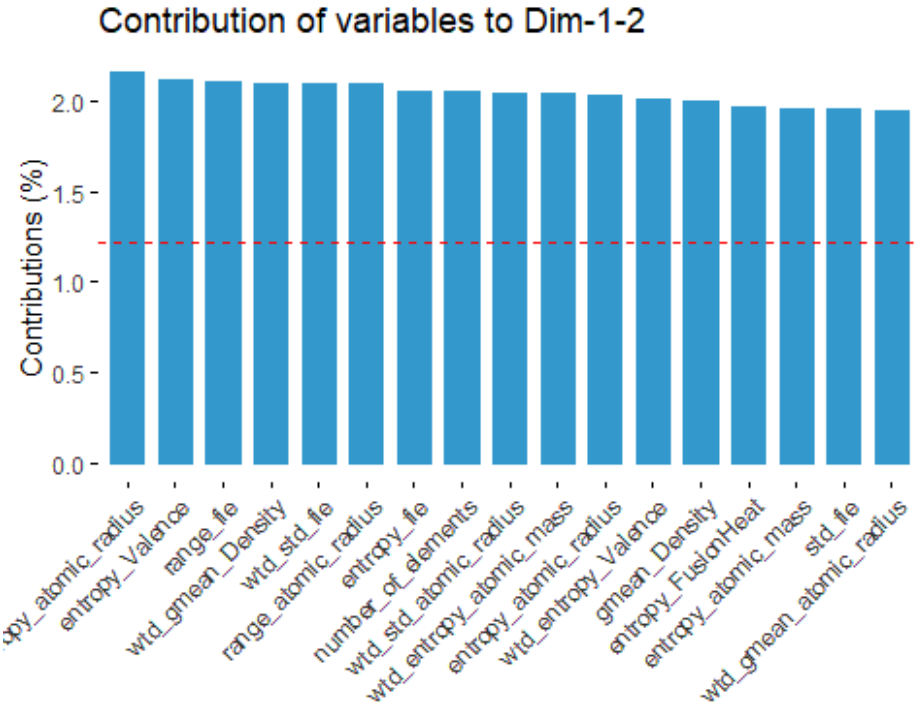
```
fviz_contrib(res.pca, choice = "var", axes = 1, top = 17)
```



```
# Contributions of variables to PC2
fviz_contrib(res.pca, choice = "var", axes = 2, top = 17)
```

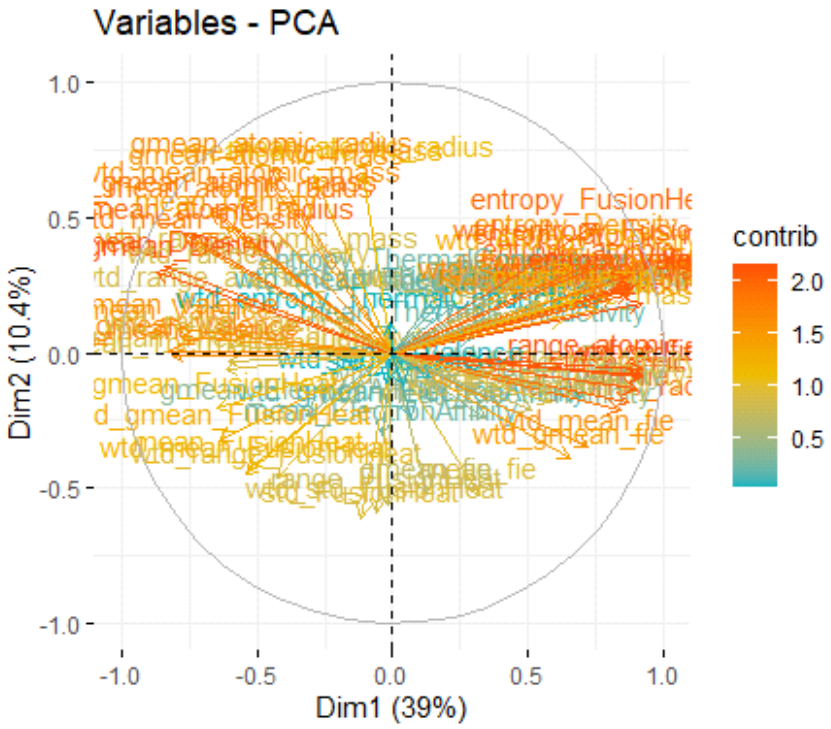



```
fviz_contrib(res.pca, choice = "var", axes = 1:2, top = 17)
```



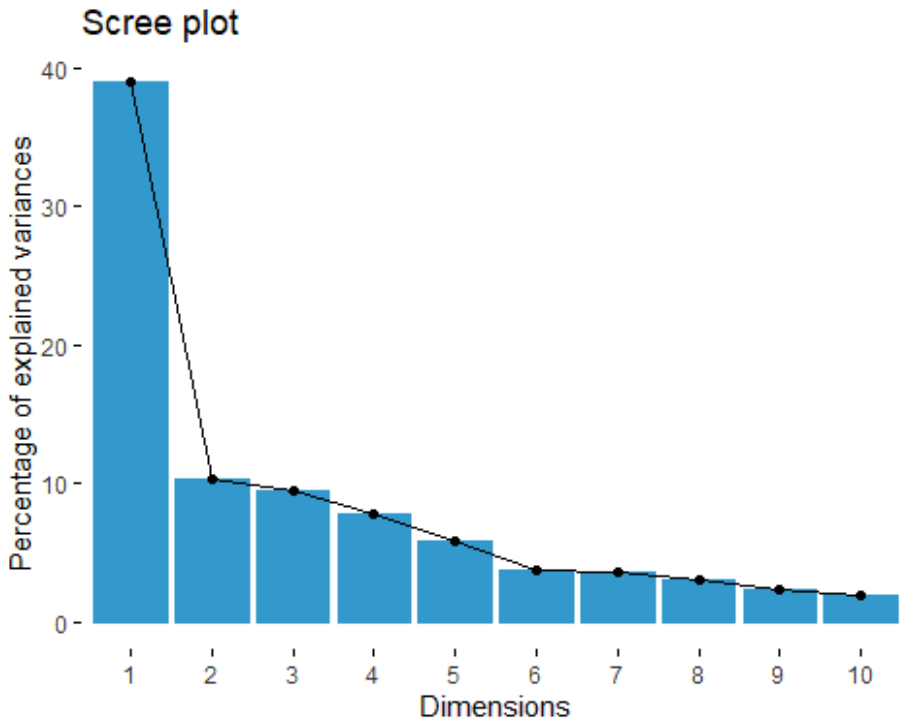
The below graph shows the factor plot which represent each feature as vector in 2 dimensions of principal component. The larger the vector, the more it contributes in particular dimension.

```
fviz_pca_var(res.pca, col.var = "contrib",
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07")
             )
```



Next is scree plot. The screeplot shows the explained variances vs each dimension taken in explaining it.

```
library("factoextra")
fviz_eig(res.pca)
```




```
get_eig(res.pca)
```

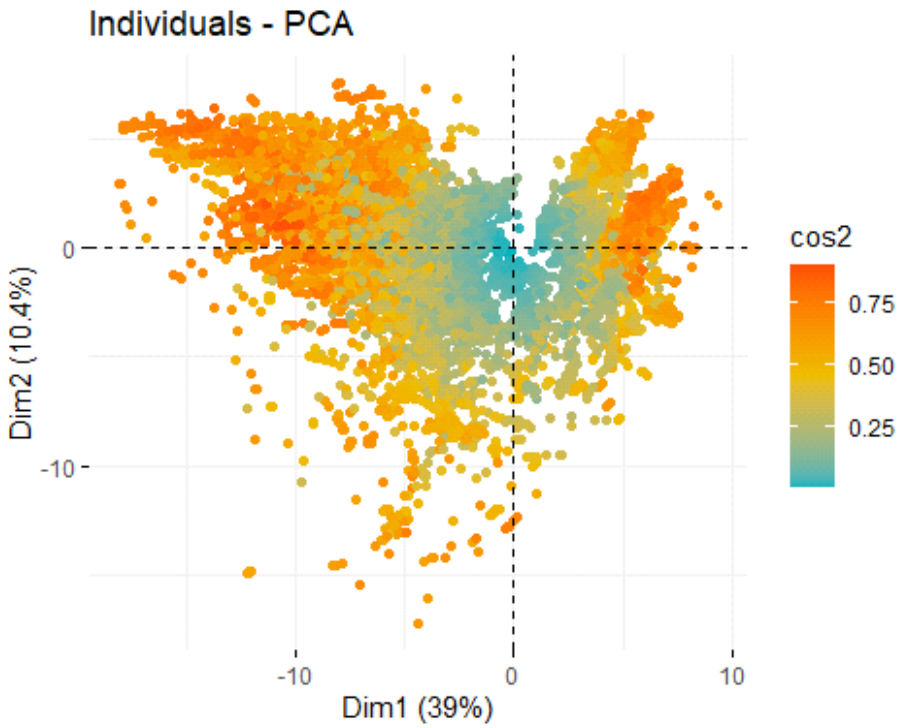
```
##          eigenvalue variance.percent cumulative.variance.percent
## Dim.1  3.197402e+01     3.899271e+01                      38.99271
## Dim.2  8.522273e+00     1.039302e+01                      49.38573
## Dim.3  7.750981e+00     9.452416e+00                      58.83814
## Dim.4  6.414113e+00     7.822089e+00                      66.66023
## Dim.5  4.793358e+00     5.845559e+00                      72.50579
## Dim.6  3.103236e+00     3.784435e+00                      76.29022
## Dim.7  2.935335e+00     3.579677e+00                      79.86990
## Dim.8  2.517540e+00     3.070171e+00                      82.94007
## Dim.9  1.919869e+00     2.341304e+00                      85.28138
## Dim.10 1.602099e+00     1.953779e+00                      87.23516
## Dim.11 1.496689e+00     1.825231e+00                      89.06039
## Dim.12 1.186767e+00     1.447277e+00                      90.50766
## Dim.13 9.562231e-01     1.166126e+00                      91.67379
## Dim.14 8.168746e-01     9.961886e-01                      92.66998
## Dim.15 8.081725e-01     9.855762e-01                      93.65555
## Dim.16 6.331548e-01     7.721400e-01                      94.42769
## Dim.17 5.823045e-01     7.101274e-01                      95.13782
## Dim.18 4.948232e-01     6.034430e-01                      95.74126
## Dim.19 4.083654e-01     4.980066e-01                      96.23927
## Dim.20 3.772613e-01     4.600747e-01                      96.69935
## Dim.21 2.821501e-01     3.440855e-01                      97.04343
## Dim.22 2.432141e-01     2.966026e-01                      97.34003
## Dim.23 2.313789e-01     2.821694e-01                      97.62220
```

## Dim.24	1.840713e-01	2.244772e-01	97.84668
## Dim.25	1.676687e-01	2.044740e-01	98.05115
## Dim.26	1.522261e-01	1.856416e-01	98.23680
## Dim.27	1.377349e-01	1.679694e-01	98.40477
## Dim.28	1.337016e-01	1.630507e-01	98.56782
## Dim.29	1.152702e-01	1.405734e-01	98.70839
## Dim.30	1.022925e-01	1.247469e-01	98.83314
## Dim.31	9.281349e-02	1.131872e-01	98.94632
## Dim.32	8.073964e-02	9.846298e-02	99.04479
## Dim.33	7.778120e-02	9.485513e-02	99.13964
## Dim.34	7.414602e-02	9.042198e-02	99.23006
## Dim.35	5.813544e-02	7.089688e-02	99.30096
## Dim.36	5.540346e-02	6.756520e-02	99.36853
## Dim.37	4.931143e-02	6.013589e-02	99.42866
## Dim.38	4.619792e-02	5.633893e-02	99.48500
## Dim.39	3.990563e-02	4.866540e-02	99.53367
## Dim.40	3.538367e-02	4.315082e-02	99.57682
## Dim.41	3.423373e-02	4.174845e-02	99.61857
## Dim.42	2.605810e-02	3.177817e-02	99.65034
## Dim.43	2.476183e-02	3.019736e-02	99.68054
## Dim.44	2.057096e-02	2.508653e-02	99.70563
## Dim.45	1.918792e-02	2.339990e-02	99.72903
## Dim.46	1.810256e-02	2.207629e-02	99.75110
## Dim.47	1.739759e-02	2.121657e-02	99.77232
## Dim.48	1.591674e-02	1.941066e-02	99.79173
## Dim.49	1.516501e-02	1.849391e-02	99.81022
## Dim.50	1.463569e-02	1.784841e-02	99.82807
## Dim.51	1.418925e-02	1.730396e-02	99.84538
## Dim.52	1.266441e-02	1.544440e-02	99.86082
## Dim.53	1.245629e-02	1.519060e-02	99.87601
## Dim.54	1.026163e-02	1.251419e-02	99.88853
## Dim.55	9.551321e-03	1.164795e-02	99.90017
## Dim.56	9.534663e-03	1.162764e-02	99.91180
## Dim.57	8.529773e-03	1.040216e-02	99.92220
## Dim.58	7.219275e-03	8.803994e-03	99.93101
## Dim.59	6.588780e-03	8.035097e-03	99.93904
## Dim.60	6.348146e-03	7.741642e-03	99.94678
## Dim.61	5.704030e-03	6.956134e-03	99.95374
## Dim.62	5.244311e-03	6.395501e-03	99.96014
## Dim.63	4.600197e-03	5.609996e-03	99.96575
## Dim.64	3.579661e-03	4.365440e-03	99.97011
## Dim.65	3.561120e-03	4.342829e-03	99.97445
## Dim.66	3.186982e-03	3.886563e-03	99.97834
## Dim.67	2.848705e-03	3.474031e-03	99.98181
## Dim.68	2.582506e-03	3.149397e-03	99.98496
## Dim.69	2.249312e-03	2.743064e-03	99.98771

```
## Dim.70 1.843828e-03  2.248571e-03  99.98996
## Dim.71 1.657275e-03  2.021067e-03  99.99198
## Dim.72 1.467499e-03  1.789633e-03  99.99377
## Dim.73 1.350994e-03  1.647553e-03  99.99541
## Dim.74 1.191890e-03  1.453524e-03  99.99687
## Dim.75 7.460413e-04  9.098065e-04  99.99778
## Dim.76 6.161272e-04  7.513747e-04  99.99853
## Dim.77 4.455887e-04  5.434008e-04  99.99907
## Dim.78 3.309852e-04  4.036405e-04  99.99948
## Dim.79 1.866172e-04  2.275820e-04  99.99970
## Dim.80 1.195923e-04  1.458443e-04  99.99985
## Dim.81 7.397678e-05  9.021558e-05  99.99994
## Dim.82 4.949803e-05  6.036345e-05 100.00000
```

```
fviz_pca_ind(res.pca,
             col.ind = "cos2", # Color by the quality of representation
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE  # Avoid text overlapping
)
```

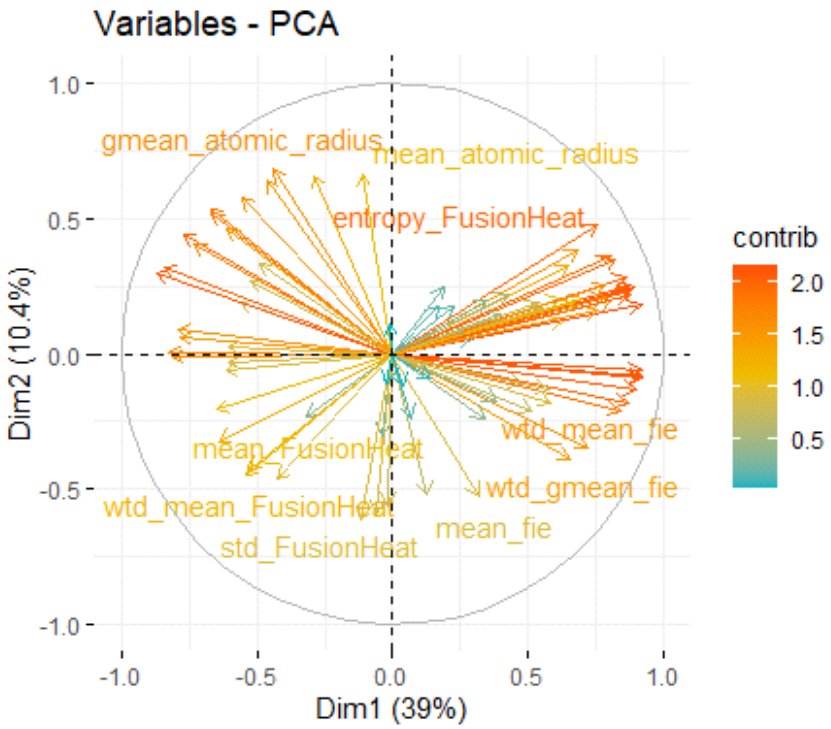
```
## Warning: ggrepel: 21263 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```



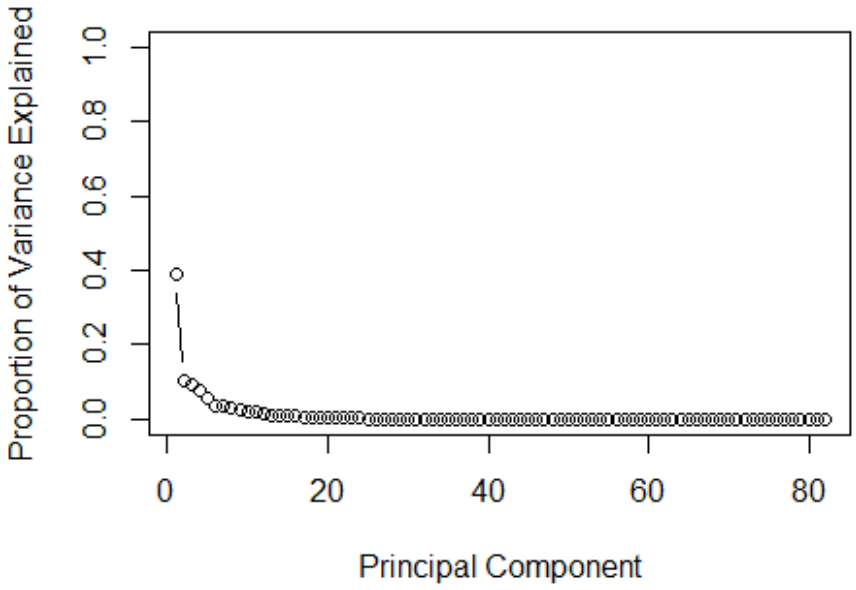

```
fviz_pca_var(res.pca,
             col.var = "contrib", # Color by contributions to the PC
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
```

```
          repel = TRUE   # Avoid text overlapping
)
```

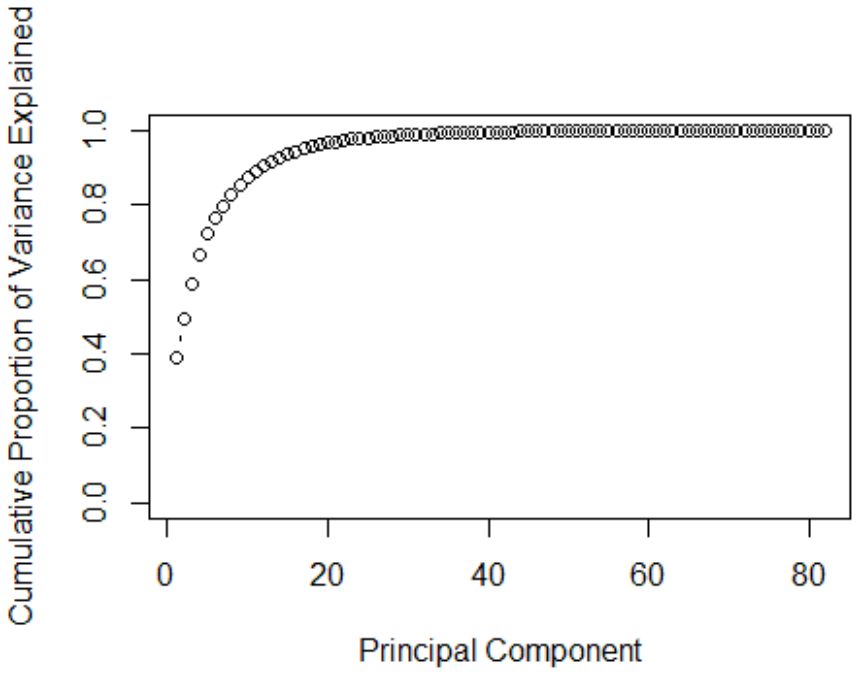
```
## Warning: ggrepel: 73 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```




```
pr_var <-  res.pca$sdev ^ 2
pve <- pr_var / sum(pr_var)
plot(pve, xlab = "Principal Component", ylab = "Proportion of Variance Explained", ylim =
c(0,1), type = 'b')
```

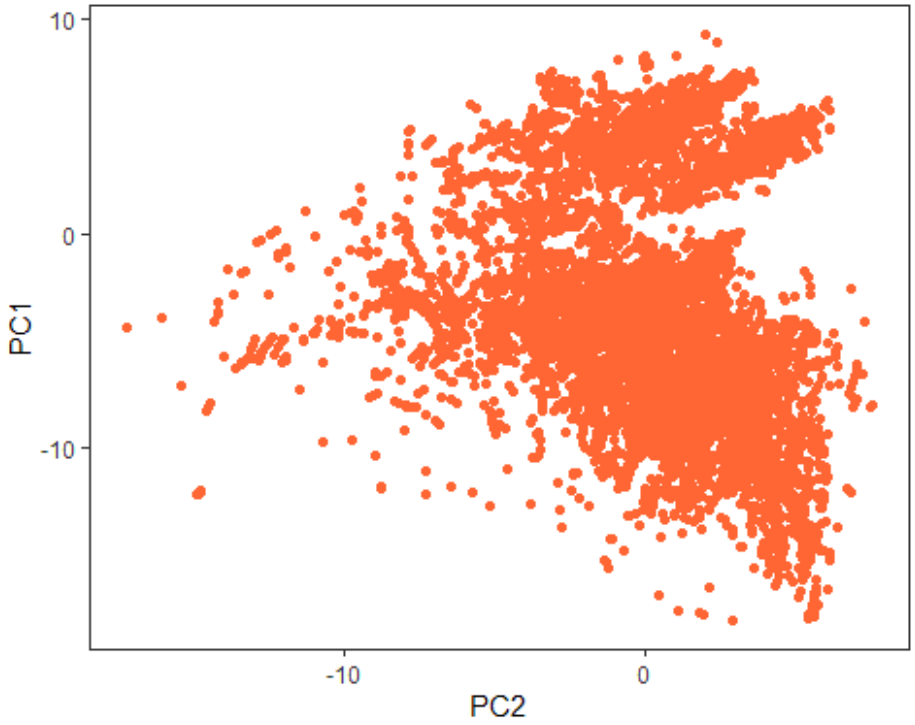



```
# Cumulative PVE plot
plot(cumsum(pve), xlab = "Principal Component", ylab = "Cumulative Proportion of Variance Explained", ylim =c(0,1), type = 'b')
```

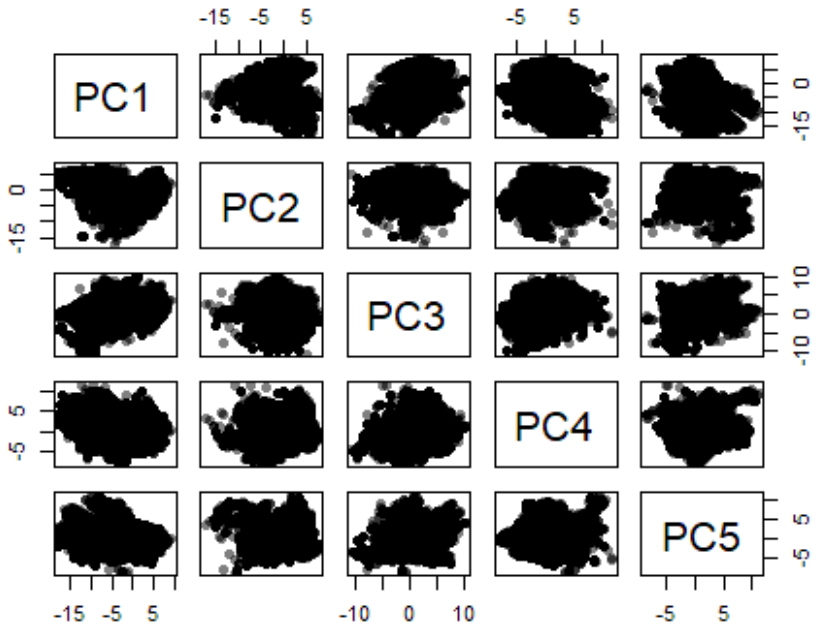



```
# Rotate loadings
```

```
library(ggplot2)
theme_set(theme_bw())

homes.pca <- data.frame(res.pca$x[, 1:2]) # we only need the first two principal components
ggplot(homes.pca, aes(y = PC1, x = PC2)) + geom_point(col = 'tomato2')
```



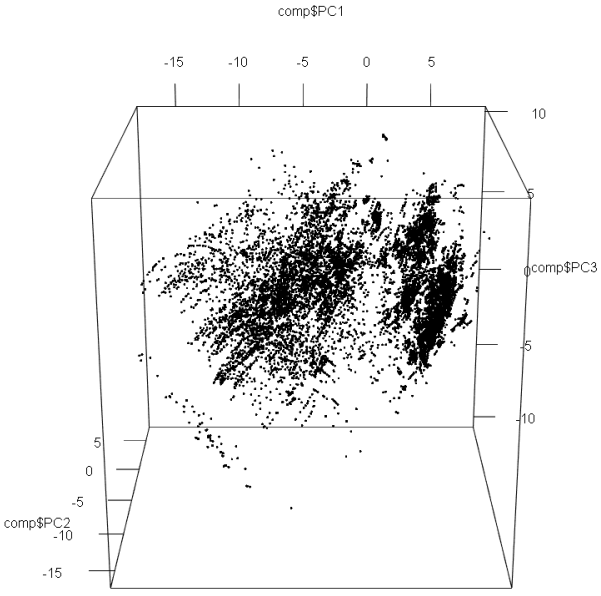

```
comp <- data.frame(res.pca$x[,1:5])
# Plot
plot(comp, pch=16, col=rgb(0,0,0,0.5))
```



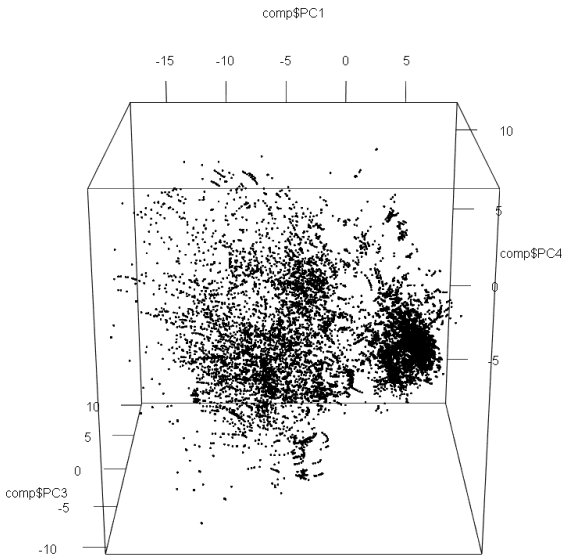

```
library(rgl)
```

```
## Warning: package 'rgl' was built under R version 4.1.2
```

```
# Multi 3D plot
plot3d(comp$PC1, comp$PC2, comp$PC3)
```



```
plot3d(comp$PC1, comp$PC3, comp$PC4)
```



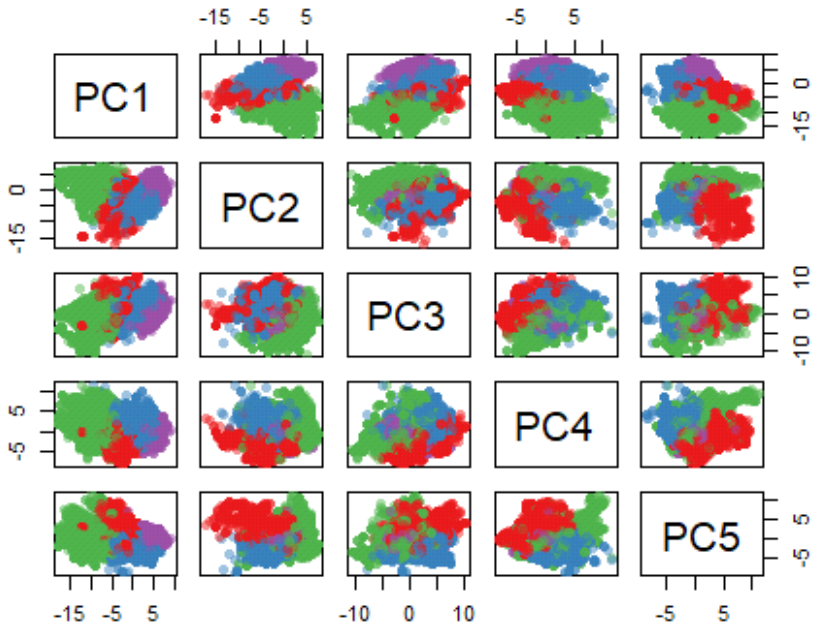
K-Means Clustering:

In k-means clustering the mean is used to calculate the centroid of each cluster. First random points are taken according to the number of k values entered. In our case we have used k=4 forming 4 clusters. Distances between random points selected as centroids and the data points will be taken, the data point nearer to the random point will be taken into the cluster of that centroid/random point. Then means are taken between the each random point and all the datapoints. This will result into a new centroid. Then in the next iteration the same procedure will repeat. And finally when no further data points will change their cluster, the algorithm will stop forming 4 cluster each having different data points.

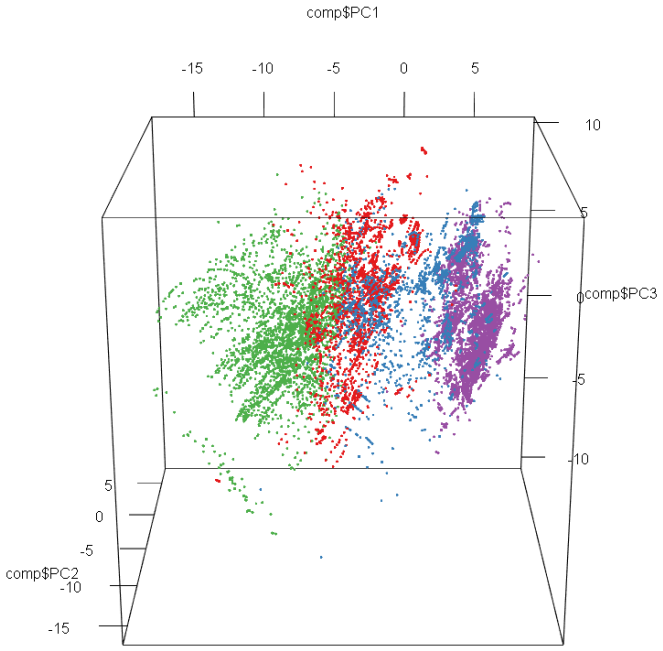
```
# From scree plot elbow occurs at k = 4
# Apply k-means with k=4
k <- kmeans(comp, 4, nstart=25, iter.max=1000)
library(RColorBrewer)
library(scales)
```

```
## Warning: package 'scales' was built under R version 4.1.2
```

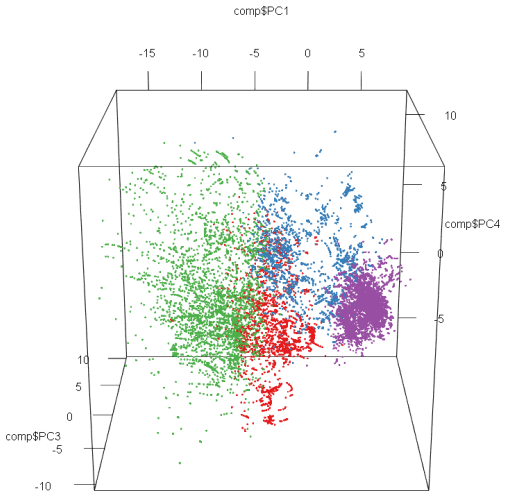
```
palette(alpha(brewer.pal(9,'Set1'), 0.5))
plot(comp, col=k$clust, pch=16)
```




```
# 3D plot
plot3d(comp$PC1, comp$PC2, comp$PC3, col=k$clust)
```




```
plot3d(comp$PC1, comp$PC3, comp$PC4, col=k$clust)
```

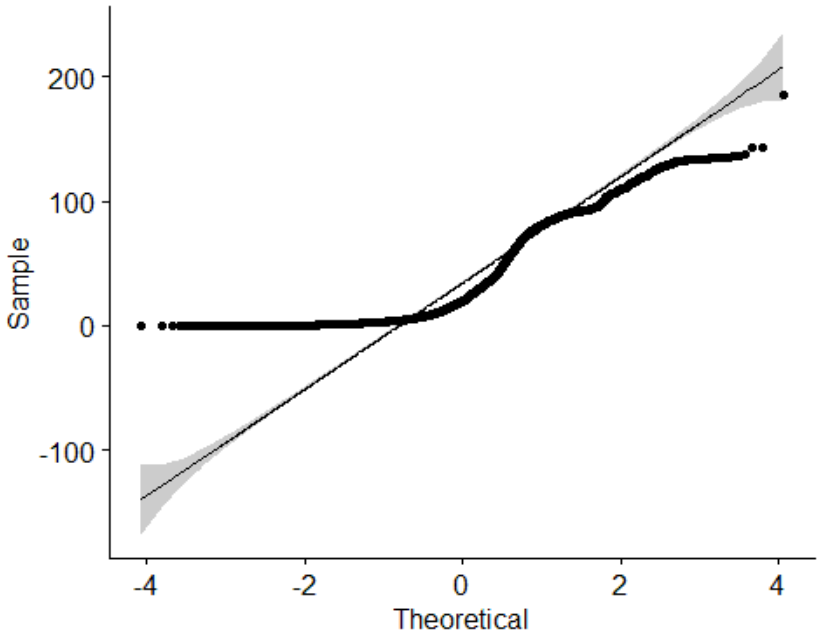


The normality test is done to check whether linear regression would be applicable or not. The test below showed that the data is not nomally skewed on qqplot. Therefore, results of multiple linear regression will not be accurate.

```
library(ggpubr)
```

```
## Warning: package 'ggpubr' was built under R version 4.1.2
```

```
ggqqplot(train4$critical_temp)
```



Although the normality test has been failed but we are applying multiple linear regression model based on the features selected from PCA above. The linear regression model shows coefficients of each feature which represents an increment of 1 unit in that feature will cause and increase with that coefficient in the overall outcome i.e. in our case critical temperature. The R squared value shows the accuracy of the model. Our model has R=0.6344 which means only 63.44% accuracy of our model is there. The adjusted R square shows the R based on removing the extra terms that are very minimal in contributing to the model. R adjusted = 0.6338.

```
lmcriticaltemp = lm(critical_temp~range_fie + range_atomic_radius +
wtd_entropy_atomic_radius + wtd_std_fie
          + wtd_std_atomic_radius + entropy_Valence + wtd_entropy_atomic_mass + entropy_fie
+ wtd_entropy_Valence
          + number_of_elements + wtd_gmean_Density + std_fie + entropy_atomic_radius +
gmean_Density
          + std_atomic_mass + wtd_gmean_Valence + entropy_atomic_mass +
mean_atomic_radius + gmean_atomic_radius
          + mean_atomic_mass + gmean_atomic_mass + std_FusionHeat + wtd_std_FusionHeat +
wtd_mean_atomic_mass
          + range_FusionHeat + wtd_gmean_atomic_mass + mean_fie + gmean_fie +
wtd_entropy_atomic_radius
          + entropy_FusionHeat + mean_Density + wtd_range_FusionHeat +
wtd_mean_FusionHeat
          + wtd_gmean_atomic_radius, data = train4)
summary(lmcriticaltemp)
```

```
##
## Call:
## lm(formula = critical_temp ~ range_fie + range_atomic_radius +
##     wtd_entropy_atomic_radius + wtd_std_fie + wtd_std_atomic_radius +
##     entropy_Valence + wtd_entropy_atomic_mass + entropy_fie +
##     wtd_entropy_Valence + number_of_elements + wtd_gmean_Density +
##     std_fie + entropy_atomic_radius + gmean_Density + std_atomic_mass +
##     wtd_gmean_Valence + entropy_atomic_mass + mean_atomic_radius +
##     gmean_atomic_radius + mean_atomic_mass + gmean_atomic_mass +
##     std_FusionHeat + wtd_std_FusionHeat + wtd_mean_atomic_mass +
##     range_FusionHeat + wtd_gmean_atomic_mass + mean_fie + gmean_fie +
##     wtd_entropy_atomic_radius + entropy_FusionHeat + mean_Density +
##     wtd_range_FusionHeat + wtd_mean_FusionHeat + wtd_gmean_atomic_radius,
##     data = train4)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -79.63 -13.29   0.12  13.09 162.75
##
## Coefficients:
##                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)             -2.673e+01  4.570e+00  -5.850 5.00e-09 ***
```

```
## range_fie                1.144e-01  5.578e-03  20.513  < 2e-16 ***
## range_atomic_radius      2.608e-03  1.597e-02   0.163  0.87030
## wtd_entropy_atomic_radius  6.552e+01  3.605e+00  18.175  < 2e-16 ***
## wtd_std_fie              4.413e-02  8.319e-03   5.305 1.14e-07 ***
## wtd_std_atomic_radius    3.080e-01  3.935e-02   7.828 5.19e-15 ***
## entropy_Valence          1.593e+02  4.295e+00  37.083  < 2e-16 ***
## wtd_entropy_atomic_mass  8.469e+00  3.062e+00   2.766  0.00568 **
## entropy_fie             -4.211e+02  1.539e+01 -27.359  < 2e-16 ***
## wtd_entropy_Valence     -4.740e+01  2.444e+00 -19.397  < 2e-16 ***
## number_of_elements       5.755e+00  6.196e-01   9.289  < 2e-16 ***
## wtd_gmean_Density        1.663e-03  2.182e-04   7.623 2.57e-14 ***
## std_fie                 -3.602e-01  1.619e-02 -22.246  < 2e-16 ***
## entropy_atomic_radius    3.075e+02  1.596e+01  19.267  < 2e-16 ***
## gmean_Density           -2.680e-03  3.049e-04  -8.789  < 2e-16 ***
## std_atomic_mass          1.999e-01  2.283e-02   8.757  < 2e-16 ***
## wtd_gmean_Valence       -8.131e+00  2.779e-01 -29.258  < 2e-16 ***
## entropy_atomic_mass     -7.323e+01  4.331e+00 -16.908  < 2e-16 ***
## mean_atomic_radius       2.684e+00  1.008e-01  26.617  < 2e-16 ***
## gmean_atomic_radius     -3.115e+00  1.100e-01 -28.314  < 2e-16 ***
## mean_atomic_mass         5.459e-03  6.632e-02   0.082  0.93439
## gmean_atomic_mass        9.992e-02  6.828e-02   1.463  0.14341
## std_FusionHeat           2.781e+00  1.930e-01  14.406  < 2e-16 ***
## wtd_std_FusionHeat      -1.498e+00  7.375e-02 -20.318  < 2e-16 ***
## wtd_mean_atomic_mass    -1.215e+00  6.087e-02 -19.965  < 2e-16 ***
## range_FusionHeat        -8.512e-01  7.007e-02 -12.149  < 2e-16 ***
## wtd_gmean_atomic_mass    1.084e+00  5.807e-02  18.661  < 2e-16 ***
## mean_fie                -5.577e-01  4.192e-02 -13.305  < 2e-16 ***
## gmean_fie                6.236e-01  4.194e-02  14.870  < 2e-16 ***
## entropy_FusionHeat      -6.185e+00  2.102e+00  -2.943  0.00325 **
## mean_Density             1.631e-03  2.255e-04   7.233 4.88e-13 ***
## wtd_range_FusionHeat     3.559e-01  3.940e-02   9.033  < 2e-16 ***
## wtd_mean_FusionHeat     -2.487e-01  3.494e-02  -7.116 1.14e-12 ***
## wtd_gmean_atomic_radius  5.227e-01  1.845e-02  28.337  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 20.73 on 21229 degrees of freedom
## Multiple R-squared:  0.6344, Adjusted R-squared:  0.6338
## F-statistic:  1116 on 33 and 21229 DF,  p-value: < 2.2e-16
```

The decision tree is used to split the data based on criteria for each feature splitting. We use regression tree which is used for continuous variable. The data is splitted based on information gain methods such as c4.5,gini index or id3. This will then decide the root and the upper nodes of the tree based on information gain of a feature. Then relational operators are used to split data on each feature. This will produce a tree splitting all data based on features. We used features obtained from PCA.

```
library(rpart)
```

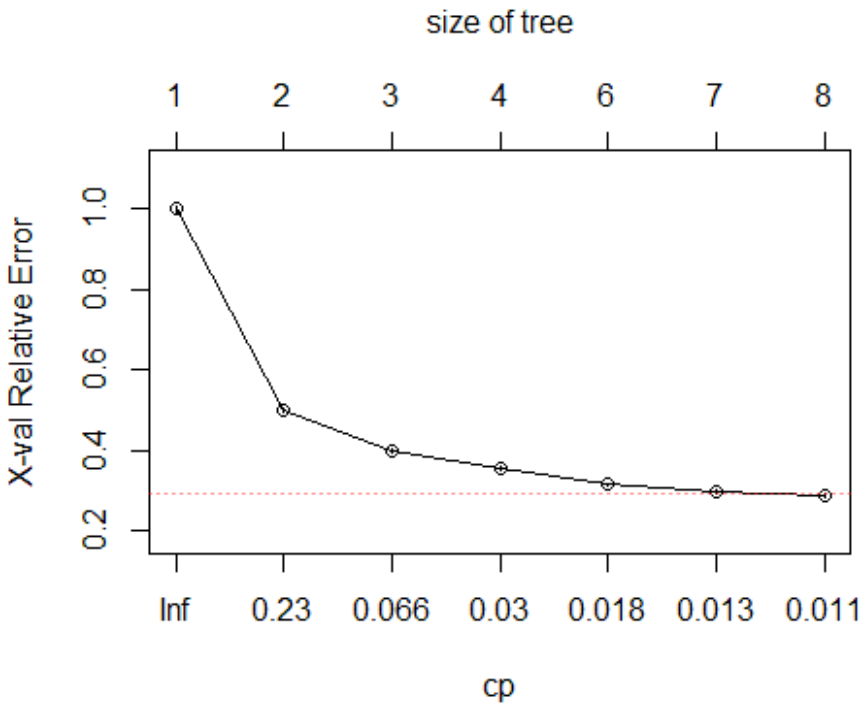
```
## Warning: package 'rpart' was built under R version 4.1.2
```

```
fit <- rpart(critical_temp~range_fie + range_atomic_radius + wtd_entropy_atomic_radius +
wtd_std_fie
             + wtd_std_atomic_radius + entropy_Valence + wtd_entropy_atomic_mass + entropy_fie
+ wtd_entropy_Valence
             + number_of_elements + wtd_gmean_Density + std_fie + entropy_atomic_radius +
gmean_Density
             + std_atomic_mass + wtd_gmean_Valence + entropy_atomic_mass +
mean_atomic_radius + gmean_atomic_radius
             + mean_atomic_mass + gmean_atomic_mass + std_FusionHeat + wtd_std_FusionHeat +
wtd_mean_atomic_mass
             + range_FusionHeat + wtd_gmean_atomic_mass + mean_fie + gmean_fie +
wtd_entropy_atomic_radius
             + entropy_FusionHeat + mean_Density + wtd_range_FusionHeat +
wtd_mean_FusionHeat
             + wtd_gmean_atomic_radius,
             method="anova", data=newd)
printcp(fit)
```

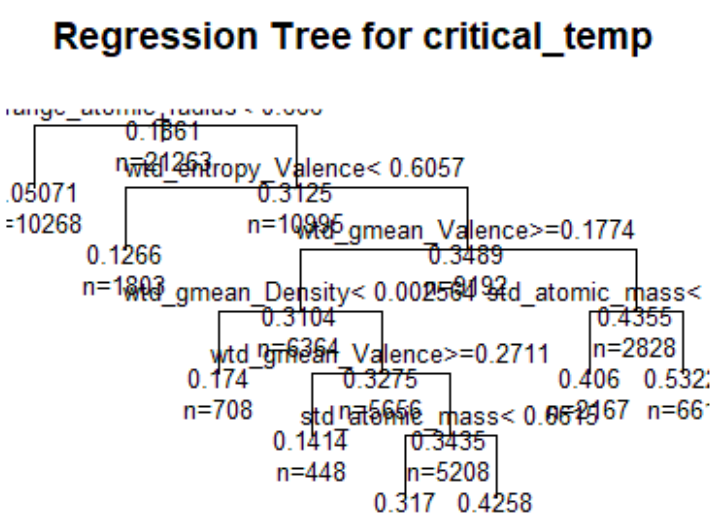
```
##
## Regression tree:
## rpart(formula = critical_temp ~ range_fie + range_atomic_radius +
##     wtd_entropy_atomic_radius + wtd_std_fie + wtd_std_atomic_radius +
##     entropy_Valence + wtd_entropy_atomic_mass + entropy_fie +
##     wtd_entropy_Valence + number_of_elements + wtd_gmean_Density +
##     std_fie + entropy_atomic_radius + gmean_Density + std_atomic_mass +
##     wtd_gmean_Valence + entropy_atomic_mass + mean_atomic_radius +
##     gmean_atomic_radius + mean_atomic_mass + gmean_atomic_mass +
##     std_FusionHeat + wtd_std_FusionHeat + wtd_mean_atomic_mass +
##     range_FusionHeat + wtd_gmean_atomic_mass + mean_fie + gmean_fie +
##     wtd_entropy_atomic_radius + entropy_FusionHeat + mean_Density +
##     wtd_range_FusionHeat + wtd_mean_FusionHeat + wtd_gmean_atomic_radius,
##     data = newd, method = "anova")
##
## Variables actually used in tree construction:
## [1] range_atomic_radius std_atomic_mass     wtd_entropy_Valence
## [4] wtd_gmean_Density   wtd_gmean_Valence
##
## Root node error: 728.94/21263 = 0.034282
##
## n= 21263
##
##         CP nsplit rel error  xerror      xstd
## 1 0.499047      0   1.00000 1.00007 0.0083088
```

```
## 2 0.102224     1  0.50095 0.50109 0.0054271
## 3 0.042031     2  0.39873 0.39930 0.0051075
## 4 0.021732     3  0.35670 0.35752 0.0046578
## 5 0.015561     5  0.31323 0.31543 0.0044826
## 6 0.011056     6  0.29767 0.29918 0.0043998
## 7 0.010000     7  0.28662 0.28769 0.0042865
```

```
plotcp(fit)
```



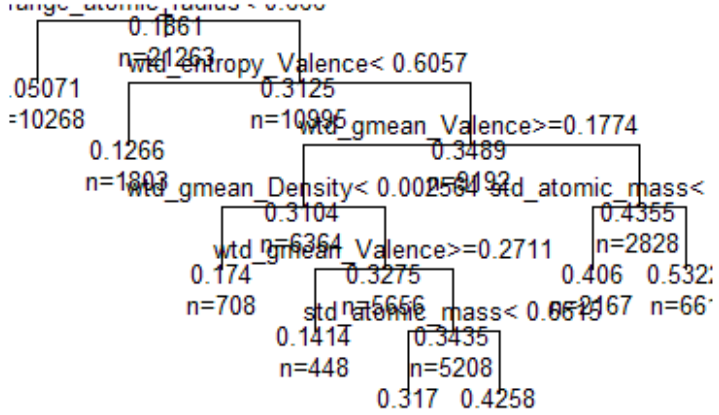

```
plot(fit, uniform=TRUE,
    main="Regression Tree for critical_temp ")
text(fit, use.n=TRUE, all=TRUE, cex=.8)
```



The tree is pruned for irrelevant features which do not provide further splitting. But in our case both trees are same i.e with pruning or without pruning.

```
# prune the tree
pfit<- prune(fit, cp=0.011)
plot(pfit, uniform=TRUE,
    main="Pruned Regression Tree for critical_temp")
text(pfit, use.n=TRUE, all=TRUE, cex=.8)
```

Pruned Regression Tree for critical_temp



-

Conclusion:

Our critical temperature depends upon range_fie , range_atomic_radius , wtd_entropy_atomic_radius , wtd_std_fie , wtd_std_atomic_radius , entropy_Valence wtd_entropy_atomic_mass , entropy_fie , wtd_entropy_Valence , number_of_elements , wtd_gmean_Density , std_fie , entropy_atomic_radius , gmean_Density , std_atomic_mass , wtd_gmean_Valence, entropy_atomic_mass , mean_atomic_radius , gmean_atomic_radius , mean_atomic_mass , gmean_atomic_mass , std_FusionHeat, wtd_std_FusionHeat , wtd_mean_atomic_mass , range_FusionHeat , wtd_gmean_atomic_mass , mean_fie , gmean_fie, wtd_entropy_atomic_radius , entropy_FusionHeat , mean_Density , wtd_range_FusionHeat , wtd_mean_FusionHeat , wtd_gmean_atomic_radius. These factors cause superconductors to behave on critical temperature.