```
In [1]: | # Author: HG
       # Date: 1/22/2021; Last edit dt:4/25/2021
       # Purpose: To Predict the onset of diabetes based on diagnostic measures
       # Problem Statement
       # NIDDK (National Institute of Diabetes and Digestive and Kidney Diseases) research cre
       # The dataset used in this project is originally from NIDDK. The objective is to predic
       # Build a model to accurately predict whether the patients in the dataset have diabetes
       # Load Packages
       # install.packages("SmartEDA")
       #.libPaths("C:/Program Files/R/R-4.0.4/Library")
       # .libPaths()
       library(tidyverse)
       library(SmartEDA)
       library(kableExtra)
       library(IRdisplay)
       # install.packages("SmartEDA")
       # install.packages("kableExtra")
       # install.packages("IRdisplay")
        -- Attaching packages ----- tidyverse 1.3.1 --
       v ggplot2 3.3.3 v purrr 0.3.4
v tibble 3.1.0 v dplyr 1.0.5
       -- Conflicts ------ tidyverse_conflicts() --
       x dplyr::filter() masks stats::filter()
       x dplyr::lag() masks stats::lag()
       Warning message:
       "package 'SmartEDA' was built under R version 4.0.5"
       Registered S3 method overwritten by 'GGally':
         method from
         +.gg ggplot2
       Attaching package: 'kableExtra'
       The following object is masked from 'package:dplyr':
           group_rows
```

1. Perform descriptive analysis. Understand the variables and their corresponding values

```
In [2]: #-----
       #setwd("I:/DSforR/capstone/")
        #getwd()
        # Lets create any new data frame object as df with a sequence # as suffix and
        # any additional relevant text post that
        ds1 diabds <- read csv("I:/DSforR/capstone/Project2/Healthcare-Diabetes/health care dia
        #First step is understanding the overview of the given data -(1)
        #Understanding the dimensions of the dataset, variable names, overall missing summary d
        str(ds1_diabds)
        #Overview of the data - Type = 1
        kable(SmartEDA::ExpData(data=ds1_diabds,type=1), format = "html") %>%
        toString() %>%
        display_html()
        #Structure of the data - Type = 2
        kable(ExpData(data=ds1_diabds,type=2)) %>% toString() %>%
        display_html()
        #Summary of all numeric variables
        kableExtra::kable(ExpNumStat(ds1_diabds,gp="Outcome",Qnt=seq(0,1,0.1),MesofShape=2,Outl
        toString() %>%
        display_html()
        count((ds1_diabds %>% mutate(GlucoseGRP = ifelse(Glucose==0,"==0",">0"),
                                         BPGRP = ifelse(BloodPressure==0,"==0",">0"),
                                     SkinThGRP = ifelse(SkinThickness==0,"==0",">0"),
                                    InsulinGRP = ifelse(Insulin==0,"==0",">0"),
                                        BMIGRP = ifelse(BMI==0,"==0",">0"))),
             GlucoseGRP,
             BPGRP,
             SkinThGRP,
             InsulinGRP,
             BMIGRP)
        #On the columns above, a value of zero does not make sense and thus indicates missing \sqrt{ }
        # Skin Thickness and Insulin are almost 30-50% missing
        -- Column specification -------
        cols(
          Pregnancies = col_double(),
          Glucose = col_double(),
          BloodPressure = col_double(),
          SkinThickness = col_double(),
          Insulin = col_double(),
          BMI = col_double(),
         DiabetesPedigreeFunction = col_double(),
         Age = col_double(),
          Outcome = col_double()
```

113 165 03 5760 03 763 113 167113 16711371 1 6 1

On the columns above, a value of zero (except but for Pregnancies column), does not make sense and thus indicates missing value:

## Skin Thickness and Insulin are almost 30-50% missing

Since our goal is to predict diabetes and Insulin is a key variable related to diabetes, we can't drop this variable. Instead of dropping this variable and skin thickness, we can use the median value to replace missing values, along with the other independent variabe's missing values (over here depicted by 0) replaced by their medians. There is a lot of Standard deviation in the insulin's value and the mean vs median are distinctly different, indicating there are significant outliers (# count of 34 from the above table) and hence we are resorting to using median to replace the missing values, as it is a better central tendency.

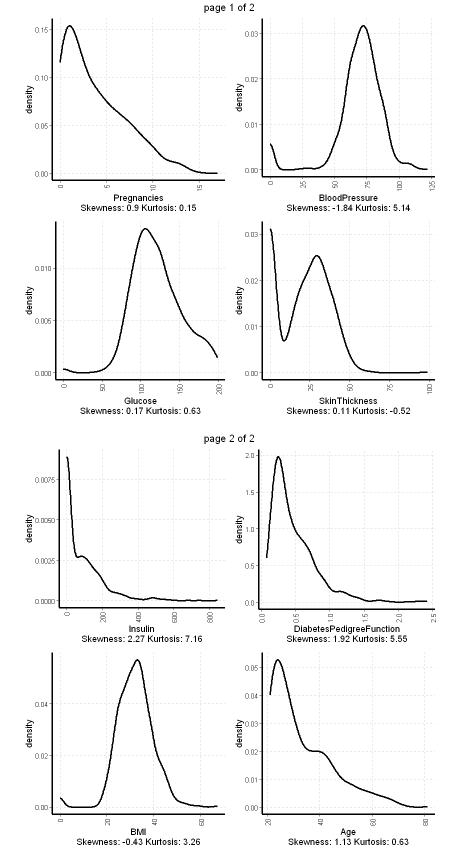
There are 768 observations with 9 main variables. Independent variables ~ Pregnancies , Glucose, Blood Pressure, Skin Thickness, Insulin, BMI , DiabetesPedigree Function , Age ; Dependent Variable = Outcome. Median age of patients is 29 with minimum being 21 and maximum 81. Median value of the other independent variables ~ BMI = 32 , BP = 72, DPF = 0.37, Glucose = 117, Insulin = 30.5, Preg = 3 , ST = 23 ;

Note: 1) For pregnancies, I am not planning to change the 0 value with the median as it is possible for some people not to have been pregnant at all 2) R is weakly typed and has only numeric and character types as opposed to the full fledged data types in Python. So based on the questions for week 1 all the data types are numeric as per this dataset and the counts are 768 for each variable

```
# Distributions of numerical variables
# Graphical representation of all numeric features
# Density plot (Univariate)
# Note: Variable excluded (if unique value of variable which is less
# than or eaual to 10 [nlim=10])
plot1 <- ExpNumViz(ds1_diabds,target=NULL,nlim=10,Page=c(2,2),sample=8)</pre>
plot1
# Next we are going to explore the Outcome variable with regards to other continuous vo
plot2 <- ExpNumViz(ds1_diabds, target="Outcome", type=1, nlim=3, fname=NULL, col=c("darkgree")</pre>
plot2
#Information Value
# ExpCatStat(ds1_diabds, Target="Outcome", result = "IV", clim=10,
#
             nlim=5,bins=10,Pclass="Yes",plot=FALSE,top=20,Round=2)
# ExpCatStat(ds1_diabds, Target="Outcome", result = "IV", clim=10,
             nlim=5, bins=5, Pclass="Yes", plot=FALSE, top=20, Round=2)
#
# # Statistical test
# et4 <- ExpCatStat(ds1_diabds, Target="Outcome", result = "Stat",</pre>
                     clim=10,nlim=5,bins=10,Pclass="Yes",plot=FALSE,top=20,Round = 2)
#
#
# et4
# Variable importance based on Information value
#
# varimp <- ExpCatStat(ds1_diabds,Target="Outcome",result = "Stat",</pre>
                        clim=10,nlim=5,bins=10,Pclass="Yes",plot=TRUE,top=10,Round = 2)
```

In [3]:





Outcome

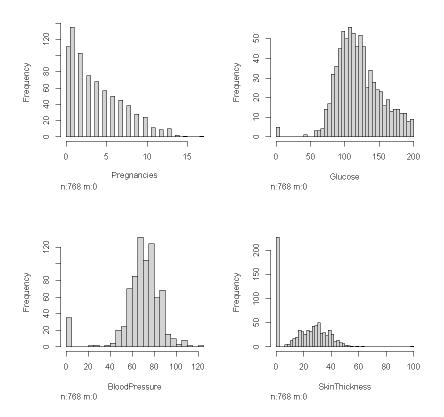
20 -

Outcome

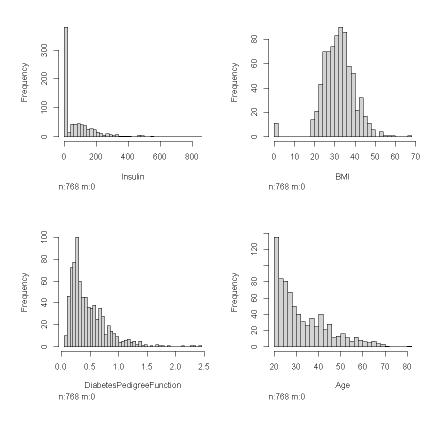
Joining, by = "SNO"

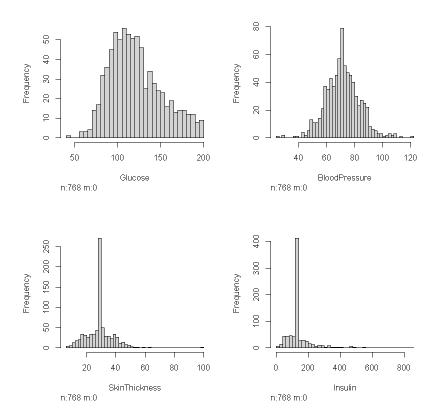
```
Glucose
                  BloodPressure
                                   SkinThickness
                                                       Insulin
Min.
       : 44.00
                 Min.
                        : 24.00
                                   Min.
                                           : 7.00
                                                    Min.
                                                            : 14.0
1st Qu.: 99.75
                  1st Qu.: 64.00
                                   1st Qu.:25.00
                                                    1st Qu.:121.5
Median :117.00
                 Median : 72.00
                                   Median :29.00
                                                    Median :125.0
Mean
                         : 72.39
                                   Mean
                                           :29.11
       :121.66
                 Mean
                                                    Mean
                                                            :140.7
3rd Qu.:140.25
                  3rd Qu.: 80.00
                                   3rd Qu.:32.00
                                                    3rd Qu.:127.2
Max.
       :199.00
                         :122.00
                                   Max.
                                           :99.00
                                                            :846.0
                                                    Max.
     BMI
                DiabetesPedigreeFunction
                                                                 SNO
                                                Age
Min.
       :18.20
                Min.
                        :0.0780
                                           Min.
                                                  :21.00
                                                            Min.
                                                                   : 1.0
1st Qu.:27.50
                1st Qu.:0.2437
                                           1st Qu.:24.00
                                                            1st Qu.:192.8
Median :32.30
                Median :0.3725
                                           Median :29.00
                                                            Median :384.5
Mean
       :32.46
                Mean
                        :0.4719
                                           Mean
                                                  :33.24
                                                            Mean
                                                                   :384.5
                 3rd Qu.:0.6262
3rd Qu.:36.60
                                           3rd Qu.:41.00
                                                            3rd Qu.:576.2
Max.
       :67.10
                Max.
                                                            Max.
                        :2.4200
                                           Max.
                                                  :81.00
                                                                   :768.0
 Pregnancies
                     Outcome
Min.
       : 0.000
                 Min.
                         :0.000
1st Qu.: 1.000
                  1st Qu.:0.000
Median : 3.000
                 Median :0.000
Mean
       : 3.845
                 Mean
                         :0.349
3rd Qu.: 6.000
                  3rd Qu.:1.000
       :17.000
Max.
                 Max.
                         :1.000
```

In [6]: # install.packages("Hmisc")
# Histogram of the dependent variables before changing the 0 values to median <Week 1 (
# the values at 0 act as outliers before replacing them by medians for all of these exc
Hmisc::hist.data.frame(ds1\_diabds %>% select(1:4))

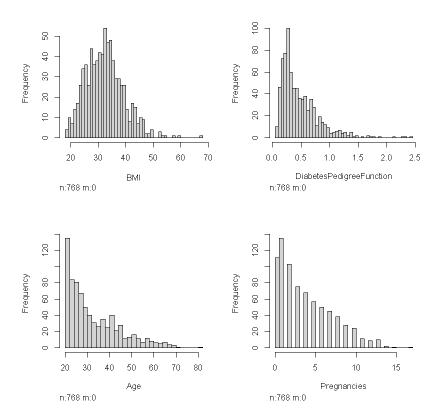


In [7]: Hmisc::hist.data.frame(ds1\_diabds %>% select(5:8))





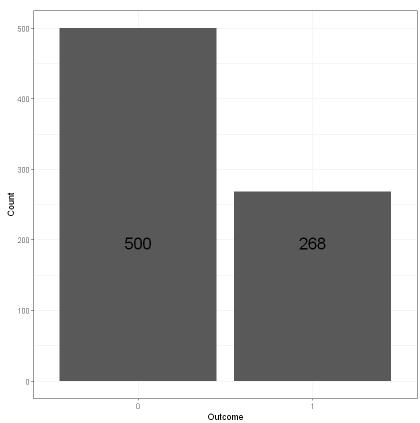
In [9]: # Histogram of the dependent variables after changing the 0 values to median <Week 1 Q2
Hmisc::hist.data.frame(ds1\_diabds\_mod %>% select(5:7,9))



---- ## Week 2 analysis checkpoint starts here ----

- 1. Check the balance of the data by plotting the count of outcomes by their value. Describe your findings and plan future course of action.
- 2. Create scatter charts between the pair of variables to understand the relationships. Describe your findings.
- 3. Perform correlation analysis. Visually explore it using a heat map.

```
In [10]: ggplot(data = ds1_diabds_mod, aes(x=factor(Outcome))) +
    geom_bar()+ theme_bw()+ xlab("Outcome") + ylab("Count") +
    geom_text(aes(label = ..count..), stat = "count", position = "fill", vjust = -10.5, siz
```



## There is a very high difference between the count of outcome values 1 (Minority~ 35% or n=268) and 0 (Majority ~ 65% or n=500). ## Hence we can say our dataset is Imbalanced Dataset.

Techniques to Convert Imbalanced Dataset into Balanced Dataset

- 1) Using the right evaluation metrics (either of these can be used):
- a) Confusion Matrix: a table showing correct predictions and types of incorrect predictions.
- b) Precision: the number of true positives divided by all positive predictions. Precision is also called Positive Predictive Value. It is a measure of a classifier's exactness. Low precision indicates a high number of false positives.
- c) Recall: the number of true positives divided by the number of positive values in the test data. Recall is also called Sensitivity or the True Positive Rate. It is a measure of a classifier's completeness. Low recall indicates a high number of false negatives.
- d) F1-Score: the weighted average of precision and recall.
- 2) We can also do Feature selection identify the significant features from each class based on information gain, odds ratio or correlation coefficient.
- 3) Another possible solution is using Ensemble Learning Techniques (Bagging, Boosting, etc.)- combining the result or performance of several classifiers to improve the performance of single classifier.

4) We can also do Upsampling (over sampling) and/or Downsampling (under sampling) to treat imbalanced dataset - For the 1's which is insufficient, the oversampling method tries to balance the dataset by incrementing the size of rare samples (1) or . Under-sampling, on contrary , aims to reduce the number of majority samples (0) to balance the Outcome class distribution. But the issue with using either of these to counter imbalanced dataset is that we may encounter over-fitting (in upsampling) or loss of important/useful information (in downsampling).

The course of action which we are going to see in this project is first looking for correlated variables and remove redundant features if very strong correlation is found, apply some automated feature selection technique provided by caret package and then use the above evaluation metrics and also look at ROC curves etc eventually.

We can rank the Features by Importance and also perform feature selection using Caret R Package .The automatic method for feature selection provided by the caret R package is called Recursive Feature Elimination or RFE.

```
In [35]: library(gridExtra)
         #scatter plots below - there are a few tha are positively correlated (we can see the cd
         # BloodPressure SkinThickness Insulin BMI DiabetesPedigreeFunction
         Preg1_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=Glucose)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg2_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=BloodPressure)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg3_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=SkinThickness)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg4_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=Insulin)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg5_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=BMI)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg6_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=DiabetesPedigreeFunctid</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         Preg7_scat <- ggplot(data = ds1_diabds_mod, aes(y=Pregnancies,x=Age)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI1_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=Glucose)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI2_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=BloodPressure)) +</pre>
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI3_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=SkinThickness)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI4_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=Insulin)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI5_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=DiabetesPedigreeFunction)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BMI6_scat <- ggplot(data = ds1_diabds_mod, aes(y=BMI,x=Age)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BP1_scat <- ggplot(data = ds1_diabds_mod, aes(y=BloodPressure,x=Glucose)) +
         geom_point()+ theme_bw()+
         geom_smooth(se=FALSE, method="loess")
         BP2_scat <- ggplot(data = ds1_diabds_mod, aes(y=BloodPressure,x=SkinThickness)) +</pre>
         geom_point()+ theme_bw()+
```

```
geom_smooth(se=FALSE, method="loess")
BP3_scat <- ggplot(data = ds1_diabds_mod, aes(y=BloodPressure,x=Insulin)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
BP4_scat <- ggplot(data = ds1_diabds_mod, aes(y=BloodPressure,x=DiabetesPedigreeFunctid
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
BP5_scat <- ggplot(data = ds1_diabds_mod, aes(y=BloodPressure,x=Age)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
ST1_scat <- ggplot(data = ds1_diabds_mod, aes(y=SkinThickness,x=Glucose)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
ST2_scat <- ggplot(data = ds1_diabds_mod, aes(y=SkinThickness,x=Age)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
ST3_scat <- ggplot(data = ds1_diabds_mod, aes(y=SkinThickness,x=Insulin)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
ST4_scat <- ggplot(data = ds1_diabds_mod, aes(y=SkinThickness,x=DiabetesPedigreeFunctid
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Insulin1_scat <- ggplot(data = ds1_diabds_mod, aes(y=Insulin,x=Glucose)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Insulin2_scat <- ggplot(data = ds1_diabds_mod, aes(y=Insulin,x=Age)) +</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Insulin3_scat <- ggplot(data = ds1_diabds_mod, aes(y=Insulin,x=DiabetesPedigreeFunction</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Age1_scat <- ggplot(data = ds1_diabds_mod, aes(y=Age,x=Glucose)) +
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Age2_scat <- ggplot(data = ds1_diabds_mod, aes(y=Age,x=DiabetesPedigreeFunction)) +
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
Gluc2_scat <- ggplot(data = ds1_diabds_mod, aes(y=Glucose,x=DiabetesPedigreeFunction))</pre>
geom_point()+ theme_bw()+
geom_smooth(se=FALSE, method="loess")
grid.arrange(Preg1_scat,Preg2_scat,Preg3_scat,Preg4_scat,Preg5_scat,Preg6_scat,Preg7_sd
grid.arrange(BMI1_scat,BMI2_scat,BMI3_scat,BMI4_scat,BMI5_scat,BMI6_scat)
grid.arrange(BP1_scat,BP2_scat,BP3_scat,BP4_scat,BP5_scat)
grid.arrange(ST1_scat,ST2_scat,ST3_scat,ST4_scat)
grid.arrange(Insulin1_scat,Insulin2_scat,Insulin3_scat)
grid.arrange(Age1_scat,Age2_scat)
grid.arrange(Gluc2_scat)
```

```
`geom_smooth()` using formula 'y ~ x'

'geom_smooth()` using formula 'y ~ x'

In [13]: # calculate correlation matrix

correlationMatrix <- cor((ds1_diabds_mod %>% select(-SNO))[,c(1:9)])

#ds1_diabds_mod
```

#### In [14]: correlationMatrix

A matrix: 9 × 9 of type dbl

	Glucose	BloodPressure	SkinThickness	Insulin	ВМІ	DiabetesPedigreeF
Glucose	1.0000000	0.218937186	0.19261490	0.41945051	0.23104855	0.137
BloodPressure	0.2189372	1.000000000	0.19189239	0.04536330	0.28125656	-0.002
SkinThickness	0.1926149	0.191892388	1.00000000	0.15561028	0.54320507	0.102
Insulin	0.4194505	0.045363305	0.15561028	1.00000000	0.18024114	0.126
ВМІ	0.2310486	0.281256564	0.54320507	0.18024114	1.00000000	0.153
DiabetesPedigreeFunction	0.1373269	-0.002378336	0.10218827	0.12650309	0.15343767	1.000
Age	0.2669092	0.324915391	0.12610719	0.09710125	0.02559691	0.033
Pregnancies	0.1282130	0.208615412	0.08176982	0.02504748	0.02155873	-0.033
Outcome	0.4927824	0.165722913	0.21487322	0.20379034	0.31203834	0.173

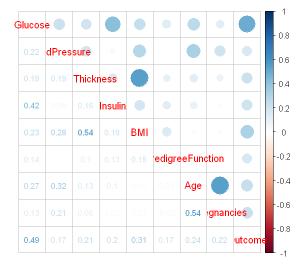
```
In [15]: # install.packages("caret")
         library(caret)
         highlyCorrelated <- findCorrelation(correlationMatrix, cutoff=0.5)</pre>
         highlyCorrelated # indexes of highly correlated attributes
         # Sys.which("make")
         #install.packages("usethis")
         ##library(usethis)
         #install.packages("devtools")
         #devtools::install_github("taiyun/corrplot", build_vignettes = TRUE)
         #install.packages("corrplot")
         library(corrplot)
         # Heatmap of the correlation plot
         corrplot.mixed(correlationMatrix,number.cex= 7/ncol(ds1_diabds))
         Warning message:
         "package 'caret' was built under R version 4.0.5"
         Loading required package: lattice
         Attaching package: 'caret'
         The following object is masked from 'package:purrr':
             lift
```

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Warning message:

corrplot 0.84 loaded

"package 'corrplot' was built under R version 4.0.5"

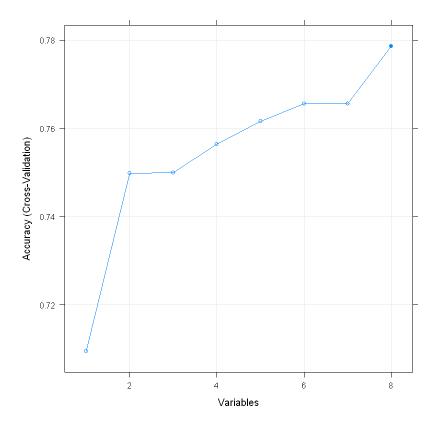


Technically we would want to remove the highly correlated terms with correlation greater than 0.7 or 0.75 but in this dataset we have two columns with moderate/marginal value i.e 0.54 as the correlation which is the max value of correlated terms between the independent variables. BMI is relatively highly correlated with Skin Thickness and Age with Pregnancies; So using one of these correlated terms in the model may mostly suffice. We could use either of the two correlated interchangably as they are confounded but which actually makes more clinical relevance needs to be figured. Since some diabetes actually involves due to pregnancies, we can choose to drop age feature from analysis and pregnancies will be more apt for analysis clinically. But lets try using the automatic feature selection by caretmethod instead of manually dropping the variable manually. Had it had a very strong correlation, we could have dropped one of the columns manually even before using the automatic feature selection. A popular automatic method for feature selection provided by the caret R package is called Recursive Feature Elimination or RFE.

Cross Validation - A technique for evaluating ML models by training several models on subsets of data. It is used to prevent over-fitting.

Recursive Feature Elimination is a backward selection of predictors; It begins by building a model on the entire set of predictors and computing an importance score for each predictor. The least important predictors are removed and model is rebuilt and importance scores are computed again. Hence, it is recursive.

```
In [16]: set.seed(123)
         # load the library
         library(mlbench)
         library(caret)
         #install.packages("e1071")
         library(e1071)
         #install.packages("randomForest")
         #library(randomForest)
         control <- rfeControl(functions=rfFuncs, method="cv", number=10) # defining the control
         arg1 <- as.data.frame((ds1_diabds_mod %>% select(-SNO))[,(1:8)])
         arg2 <- as.data.frame(ds1_diabds_mod %>% select(10))
         names(arg2) = "Outcome"
         arg2 <- arg2 %>% mutate(Outcome = factor(Outcome))
         results <- rfe(arg1,
                        arg2[,1], #without calling arg2[,1] we can encounter err: there should b
                        sizes=c(1:8), rfeControl=control) # run the RFE algorithm
         results
         predictors(results) # chosen features list
         plot(results, type = c("g","o"))
         Warning message:
         "package 'mlbench' was built under R version 4.0.5"
         Warning message:
         "package 'e1071' was built under R version 4.0.5"
         Recursive feature selection
         Outer resampling method: Cross-Validated (10 fold)
         Resampling performance over subset size:
          Variables Accuracy Kappa AccuracySD KappaSD Selected
                  1
                     0.7096 0.3011 0.04224 0.10808
                  2
                     0.7498 0.4310 0.03898 0.08681
                  3 0.7500 0.4419 0.03480 0.06941
                     0.7564 0.4566 0.04584 0.09664
                  4
                     0.7616 0.4670 0.03566 0.07491
                  5
                      0.7656 0.4702 0.02383 0.06186
                  6
                  7
                      0.7656 0.4704 0.02090 0.05413
                      0.7786 0.4966 0.02825 0.08080
         The top 5 variables (out of 8):
            Glucose, BMI, Age, Insulin, Pregnancies
         'Glucose' 'BMl' 'Age' 'Insulin' 'Pregnancies' 'DiabetesPedigreeFunction' 'SkinThickness'
         'BloodPressure'
```



## From the above plot we see that we can perhaps choose all 8 variables as the accuracy is close to max using all variables.

#####1. Devise strategies for model building. It is important to decide the right validation framework. Express your thought process.

#####2. Apply an appropriate classification algorithm to build a model. Compare various models with the results from KNN algorithm.

We will be overestimating the model performance if we assess the performance of a model using the same dataset that was used to fit the model. So we need to split the data and use one part to fit the model and the other one to test it. In ML, the data used to fit the model is the training data and the data that is used to assess the model performance is the test data. We will be using K-fold cross-validation as mentioned above to avoid over-fitting. It is one of the model validation techniques. In k-fold cross-validation, the data is divided into k folds. The model is trained on k-1 folds with one fold used for testing. The process is repeated to ensure each fold of the dataset gets the chance to be the test set. Once the process is completed, we can summarize the evaluation metric using the mean/median and/or the standard deviation. If we just split the data into one train and test set, the presence of an outlier can change vastly an out of sample RMSE (root mean sq error). So a better approach is using multiple train test splits and averaging out of sample error using CV. But over here, we take a step further and develop train and test sets and then on top do the cross validation in the training set to reduce further error.

Having a lower K means less variance and thus, more bias, while having a higher K means more variance and thus, and lower bias.

Also, we should keep in mind the computational costs for the different values. High K means more folds, thus higher computational time and vice versa. So, we need to find an optimal spot between those by doing a hyperparameter tuning analysis. There is an automatic hyperparameter tuning provided by caret package for random forest algorithm. There are many classification algorithms such as logistic regression, support vector machine, naive Bayes classifier, decision trees and Random Forest. Since caret package handles automatic hyperparameter tuning, lets focus on Random Forest first.

Random Forest - The random forest is a classification algorithm consisting of many decisions trees. It uses bagging and feature randomness when building each individual tree to try to create an uncorrelated forest of trees whose prediction by the group of trees is more accurate than that of any individual tree.

```
In [17]: ds1_diabds_mod2 <- ds1_diabds_mod %>% mutate(Outcome = as.factor(Outcome))
    table(ds1_diabds_mod2$Outcome)

levels(ds1_diabds_mod2$Outcome) <- c("No","Yes")

table(ds1_diabds_mod2$Outcome)

set.seed(123456)
partitionRule = createDataPartition(ds1_diabds_mod2$Outcome, p= 0.7, list=F) #70 percer
    trainingSet <-ds1_diabds_mod2[partitionRule,]

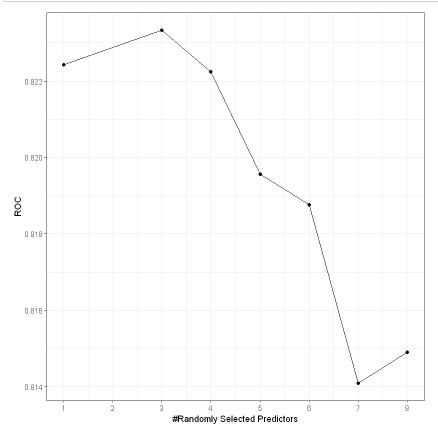
testSet <- ds1_diabds_mod2[-partitionRule,]

str(trainingSet)
str(testSet)</pre>
```

```
1
  0
500 268
No Yes
500 268
tibble[,10] [538 x 10] (S3: tbl_df/tbl/data.frame)
 $ Glucose
                           : num [1:538] 85 89 116 78 125 110 168 139 189 166 ...
 $ BloodPressure
                          : num [1:538] 66 66 74 50 96 92 74 80 60 72 ...
 $ SkinThickness
                          : num [1:538] 29 23 29 32 29 29 29 29 23 19 ...
                           : num [1:538] 125 94 125 88 125 125 125 125 846 175 ...
 $ Insulin
$ BMI
                           : num [1:538] 26.6 28.1 25.6 31 32.3 37.6 38 27.1 30.1 25.
 $ DiabetesPedigreeFunction: num [1:538] 0.351 0.167 0.201 0.248 0.232 ...
                           : num [1:538] 31 21 30 26 54 30 34 57 59 51 ...
 $ Age
 $ SNO
                           : int [1:538] 2 4 6 7 10 11 12 13 14 15 ...
                           : num [1:538] 1 1 5 3 8 4 10 10 1 5 ...
 $ Pregnancies
                           : Factor w/ 2 levels "No", "Yes": 1 1 1 2 2 1 2 1 2 2 ...
 $ Outcome
tibble[,10] [230 x 10] (S3: tbl_df/tbl/data.frame)
                           : num [1:230] 148 183 137 115 197 147 88 92 138 180 ...
 $ Glucose
 $ BloodPressure
                          : num [1:230] 72 64 40 72 70 76 58 92 76 64 ...
 $ SkinThickness
                          : num [1:230] 35 29 35 29 45 29 11 29 29 25 ...
                           : num [1:230] 125 125 168 125 543 125 54 125 125 70 ...
 $ Insulin
 $ BMI
                           : num [1:230] 33.6 23.3 43.1 35.3 30.5 39.4 24.8 19.9 33.2
34 ...
 $ DiabetesPedigreeFunction: num [1:230] 0.627 0.672 2.288 0.134 0.158 ...
                           : num [1:230] 50 32 33 29 53 43 22 28 35 26 ...
 $ Age
 $ SNO
                           : int [1:230] 1 3 5 8 9 27 33 34 37 41 ...
 $ Pregnancies
                           : num [1:230] 6 8 0 10 2 7 3 6 11 3 ...
                           : Factor w/ 2 levels "No", "Yes": 2 2 2 1 2 2 1 1 1 1 ...
 $ Outcome
```

```
In [18]:
         # K-fold cross-validation
         # setting seed to generate a
         # reproducible random sampling
         set.seed(125)
         # defining training control
         # as cross-validation and
         # value of K equal to 10
         train_control <- trainControl(method = "repeatedcv",</pre>
                                        number = 10, search ="random", repeats =3,
                                        savePredictions=T,classProbs = TRUE,
           summaryFunction = twoClassSummary,
                       verboseIter = TRUE)
         # in order to use the ROC metric, we have to add summary Function = twoClassSummary
         set.seed(125)
         # training the model by assigning Output column
         # as target variable and rest other column
         # as independent varaible
         rfmodel <- train(Outcome ~.-SNO, data = trainingSet ,</pre>
                        method = "rf",
                        trControl = train_control,
                         preProc = c("center", "scale"),
                        ntree = 500, tuneLength =10,
                       metric="ROC")
         # printing model performance metrics
         # along with other details
         print(rfmodel)
         + Fold01.Rep1: mtry=7
         - Fold01.Rep1: mtry=7
         + Fold01.Rep1: mtry=8
         - Fold01.Rep1: mtry=8
         + Fold01.Rep1: mtry=3
         - Fold01.Rep1: mtry=3
         + Fold01.Rep1: mtry=1
         - Fold01.Rep1: mtry=1
         + Fold01.Rep1: mtry=4
         - Fold01.Rep1: mtry=4
         + Fold01.Rep1: mtry=6
         - Fold01.Rep1: mtry=6
         + Fold01.Rep1: mtry=5
         - Fold01.Rep1: mtry=5
         + Fold02.Rep1: mtry=7
```

- Fold02.Rep1: mtry=7
+ Fold02.Rep1: mtry=8
- Fold02.Rep1: mtry=8
+ Fold02.Rep1: mtry=3



```
In [20]: rfOutcome <- predict(rfmodel, newdata = testSet)
    str(rfOutcome)
    rfProbs <- predict(rfmodel, newdata = testSet, type = "prob")
    head(rfProbs)
    confusionMatrix(data = rfOutcome, testSet$Outcome)

Factor w/ 2 levels "No", "Yes": 2 2 2 2 2 1 1 2 2 ...</pre>
```

A data.frame: 6 × 2

	No	Yes		
	<dbl></dbl>	<dbl></dbl>		
1	0.416	0.584		
2	0.428	0.572		

3 0.362 0.6384 0.478 0.522

**5** 0.306 0.694

**6** 0.256 0.744

Confusion Matrix and Statistics

Reference Prediction No Yes No 128 29 Yes 22 51

Accuracy : 0.7783

95% CI: (0.719, 0.8302)

No Information Rate : 0.6522 P-Value [Acc > NIR] : 2.232e-05

Kappa : 0.5011

Mcnemar's Test P-Value: 0.4008

Sensitivity: 0.8533 Specificity: 0.6375 Pos Pred Value: 0.8153 Neg Pred Value: 0.6986 Prevalence: 0.6522

Detection Rate : 0.5565
Detection Prevalence : 0.6826
Balanced Accuracy : 0.7454

'Positive' Class : No

```
In [21]: |#logistic regression model
         set.seed(125)
         glm_model <-train(Outcome ~.-SNO, data = trainingSet ,</pre>
                        method = "glm",
                        trControl = train_control,
                        preProc = c("center", "scale"),
                        metric="ROC")
         # printing model performance metrics
         # along with other details
         print(glm_model)
         + Fold01.Rep1: parameter=none
         - Fold01.Rep1: parameter=none
         + Fold02.Rep1: parameter=none
         - Fold02.Rep1: parameter=none
         + Fold03.Rep1: parameter=none
         - Fold03.Rep1: parameter=none
         + Fold04.Rep1: parameter=none

    Fold04.Rep1: parameter=none

         + Fold05.Rep1: parameter=none
         - Fold05.Rep1: parameter=none
         + Fold06.Rep1: parameter=none
         - Fold06.Rep1: parameter=none
         + Fold07.Rep1: parameter=none
         Fold07.Rep1: parameter=none
         + Fold08.Rep1: parameter=none
         - Fold08.Rep1: parameter=none
         + Fold09.Rep1: parameter=none
         Fold09.Rep1: parameter=none
         + Fold10.Rep1: parameter=none

    Fold10.Rep1: parameter=none

         + Fold01.Rep2: parameter=none
         - Fold01.Rep2: parameter=none
         + Fold02.Rep2: parameter=none
         Fold02.Rep2: parameter=none
         + Fold03.Rep2: parameter=none
         - Fold03.Rep2: parameter=none
```

+ Fold04.Rep2: parameter=none - Fold04.Rep2: parameter=none + Fold05.Rep2: parameter=none - Fold05.Rep2: parameter=none + Fold06.Rep2: parameter=none Fold06.Rep2: parameter=none + Fold07.Rep2: parameter=none - Fold07.Rep2: parameter=none + Fold08.Rep2: parameter=none Fold08.Rep2: parameter=none + Fold09.Rep2: parameter=none - Fold09.Rep2: parameter=none + Fold10.Rep2: parameter=none - Fold10.Rep2: parameter=none + Fold01.Rep3: parameter=none - Fold01.Rep3: parameter=none + Fold02.Rep3: parameter=none - Fold02.Rep3: parameter=none + Fold03.Rep3: parameter=none - Fold03.Rep3: parameter=none + Fold04.Rep3: parameter=none - Fold04.Rep3: parameter=none + Fold05.Rep3: parameter=none

```
- Fold05.Rep3: parameter=none
+ Fold06.Rep3: parameter=none
- Fold06.Rep3: parameter=none
+ Fold07.Rep3: parameter=none
- Fold07.Rep3: parameter=none
+ Fold08.Rep3: parameter=none
- Fold08.Rep3: parameter=none
+ Fold09.Rep3: parameter=none
- Fold09.Rep3: parameter=none
+ Fold10.Rep3: parameter=none
- Fold10.Rep3: parameter=none
Aggregating results
Fitting final model on full training set
Generalized Linear Model
538 samples
  9 predictor
  2 classes: 'No', 'Yes'
Pre-processing: centered (8), scaled (8)
Resampling: Cross-Validated (10 fold, repeated 3 times)
Summary of sample sizes: 484, 484, 484, 485, 484, 484, ...
Resampling results:
  ROC
                        Spec
             Sens
```

0.8282261 0.8752381 0.558577

 <dbl>
 <dbl>

 1
 0.3045740
 0.6954260

 2
 0.2231260
 0.7768740

 3
 0.1813367
 0.8186633

**4** 0.5676111 0.4323889

**5** 0.3209057 0.6790943

**6** 0.2534184 0.7465816

Confusion Matrix and Statistics

Reference Prediction No Yes No 134 36 Yes 16 44

Accuracy : 0.7739

95% CI: (0.7143, 0.8263)

No Information Rate : 0.6522 P-Value [Acc > NIR] : 4.208e-05

Kappa : 0.4708

Mcnemar's Test P-Value : 0.008418

Sensitivity: 0.8933 Specificity: 0.5500 Pos Pred Value: 0.7882 Neg Pred Value: 0.7333 Prevalence: 0.6522 Detection Rate: 0.5826

Detection Prevalence : 0.7391
Balanced Accuracy : 0.7217

'Positive' Class : No

+ Fold01.Rep1: shrinkage=0.009464, interaction.depth=9, n.minobsinnode=15, n.trees= 4826

Iter	TrainDeviance	ValidDeviance	StepSize	Improve
1	1.2862	nan	0.0095	0.0031
2	1.2790	nan	0.0095	0.0026
3	1.2716	nan	0.0095	0.0026
4	1.2655	nan	0.0095	0.0026
5	1.2591	nan	0.0095	0.0019
6	1.2532	nan	0.0095	0.0023
7	1.2467	nan	0.0095	0.0026
8	1.2403	nan	0.0095	0.0020
9	1.2342	nan	0.0095	0.0024
10	1.2285	nan	0.0095	0.0024
20	1.1735	nan	0.0095	0.0020
40	1.0807	nan	0.0095	0.0013
60	1.0105	nan	0.0095	0.0011
80	0.9535	nan	0.0095	0.0006
100	0.9063	nan	0.0095	0.0003
120	0.8646	nan	0.0095	0.0003
1 10	0.0300		0 0005	0 0000

```
In [25]: # Building the prediction model for DT (Gradient Boosting)
          gbmOutcome <- predict(gbm_model, newdata = testSet)</pre>
          str(gbmOutcome)
          gbmProbs <- predict(gbm_model, newdata = testSet, type = "prob")</pre>
          head(gbmProbs)
          confusionMatrix(data = gbmOutcome, testSet$Outcome)
           Factor w/ 2 levels "No", "Yes": 1 2 2 1 2 2 1 1 1 2 ...
          A data.frame: 6 × 2
                      No
                               Yes
                    <dbl>
                             <dbl>
          1 0.7057127542 0.2942872
           2 0.1694875713 0.8305124
           3 0.1229452619 0.8770547
           4 0.7841698120 0.2158302
```

Confusion Matrix and Statistics

Reference Prediction No Yes No 123 28 Yes 27 52

5 0.0009999095 0.99900016 0.0436698901 0.9563301

Accuracy : 0.7609

95% CI: (0.7004, 0.8145)

No Information Rate : 0.6522 P-Value [Acc > NIR] : 0.000245

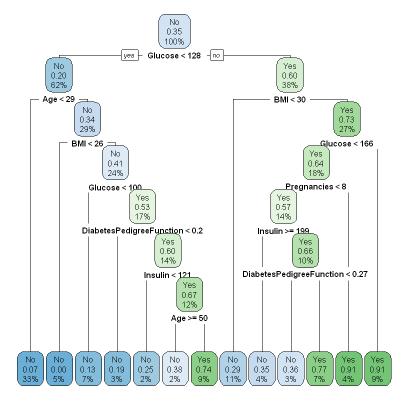
Kappa : 0.4714

Mcnemar's Test P-Value : 1.000000

Sensitivity: 0.8200 Specificity: 0.6500 Pos Pred Value: 0.8146 Neg Pred Value: 0.6582 Prevalence: 0.6522 Detection Rate: 0.5348

Detection Prevalence : 0.6565
Balanced Accuracy : 0.7350

'Positive' Class : No



Confusion Matrix and Statistics

Reference Prediction No Yes No 126 29 Yes 24 51

Accuracy : 0.7696

95% CI: (0.7097, 0.8224)

No Information Rate : 0.6522 P-Value [Acc > NIR] : 7.748e-05

Kappa: 0.4846

Mcnemar's Test P-Value : 0.5827

Sensitivity : 0.8400 Specificity : 0.6375 Pos Pred Value : 0.8129 Neg Pred Value : 0.6800 Prevalence : 0.6522

Detection Rate : 0.5478
Detection Prevalence : 0.6739
Balanced Accuracy : 0.7388

'Positive' Class : No

```
In [30]: # KNN model - non-parametric classification model
         set.seed(125)
         knn_model <-train(Outcome ~.-SNO, data = trainingSet ,</pre>
                        method = "knn",
                        trControl = train_control,
                         preProc = c("center", "scale"),
                        metric="ROC")
         # printing model performance metrics
         # along with other details
         print(knn_model)
         + Fold01.Rep1: k=125
         - Fold01.Rep1: k=125
         + Fold01.Rep1: k=143
         - Fold01.Rep1: k=143
         + Fold01.Rep1: k= 47
         - Fold01.Rep1: k= 47
         + Fold02.Rep1: k=125
```

- Fold02.Rep1: k=125 + Fold02.Rep1: k=143 - Fold02.Rep1: k=143 + Fold02.Rep1: k= 47 - Fold02.Rep1: k= 47 + Fold03.Rep1: k=125 - Fold03.Rep1: k=125 + Fold03.Rep1: k=143 - Fold03.Rep1: k=44 + Fold03.Rep1: k= 47 - Fold03.Rep1: k= 47 + Fold04.Rep1: k=125

```
In [31]: # Building the prediction model for KNN classifier
          knnOutcome <- predict(knn_model, newdata = testSet)</pre>
          str(knnOutcome)
          knnProbs <- predict(knn_model, newdata = testSet, type = "prob")</pre>
          head(knnProbs)
          confusionMatrix(data = knnOutcome, testSet$Outcome)
          Factor w/ 2 levels "No", "Yes": 2 2 1 1 2 2 1 1 2 1 ...
          A data.frame: 6 × 2
                    Yes
               No
             <dbl> <dbl>
          1 0.432 0.568
          2 0.448 0.552
          3 0.552 0.448
          4 0.648 0.352
          5 0.440 0.560
```

Confusion Matrix and Statistics

Reference Prediction No Yes No 139 47 Yes 11 33

**6** 0.448 0.552

Accuracy : 0.7478

95% CI: (0.6865, 0.8026)

No Information Rate : 0.6522 P-Value [Acc > NIR] : 0.001163

Kappa : 0.379

Mcnemar's Test P-Value : 4.312e-06

Sensitivity: 0.9267
Specificity: 0.4125
Pos Pred Value: 0.7473
Neg Pred Value: 0.7500
Prevalence: 0.6522
Detection Rate: 0.6043
Detection Prevalence: 0.8087

Balanced Accuracy : 0.6696

'Positive' Class : No

```
In [47]: | attributes(rfmodel)
         # the final model from the underlying package used by caret are displayed here
         cat("-----Random Forest Final Model ")
         rfmodel$finalModel
         cat("-----Logistic Regression Final Model \n")
         glm_model$finalModel
         #attributes(glm_model)
         cat("-----Decision Tree (method 1) a.k.a Gradient Boosting Machine Final Model \n")
         gbm_model$finalModel
         cat("-----Decision Tree (method 2)\n")
         DT_fit_method2$finalModel
         cat("----knn classifier Final Model \n")
         knn_model$finalModel
         $names
          'method' 'modellnfo' 'modelType' 'results' 'pred' 'bestTune' 'call' 'dots' 'metric'
          'control' 'finalModel' 'preProcess' 'trainingData' 'resample' 'resampledCM' 'perfNames'
          'maximize' · 'yLimits' · 'times' · 'levels' · 'terms' · 'coefnames' · 'xlevels'
         $class
          'train' · 'train.formula'
         -----Random Forest Final Model
         Call:
          randomForest(x = x, y = y, ntree = 500, mtry = param$mtry)
                        Type of random forest: classification
                              Number of trees: 500
         No. of variables tried at each split: 3
                 OOB estimate of error rate: 25.46%
         Confusion matrix:
              No Yes class.error
         No 290 60 0.1714286
         Yes 77 111 0.4095745
         -----Logistic Regression Final Model
         Call: NULL
         Coefficients:
                                                                         BloodPressure
                      (Intercept)
                                                     Glucose
                          -0.85240
                                                     1.11539
                                                                                0.01300
                    SkinThickness
                                                     Insulin
                                                                                    BMI
```

0.07065 -0.16419 0.64165 DiabetesPedigreeFunction Pregnancies Age 0.25040 0.09927 0.46736 Degrees of Freedom: 537 Total (i.e. Null); 529 Residual Null Deviance: 696.3 Residual Deviance: 505.3 AIC: 523.3 ------Decision Tree (method 1) a.k.a Gradient Boosting Machine Final Model A gradient boosted model with bernoulli loss function. 4826 iterations were performed. There were 8 predictors of which 8 had non-zero influence. -----Decision Tree (method 2) NULL -----knn classifier Final Model 125-nearest neighbor model Training set outcome distribution: No Yes

350 188

```
In [61]: # similar to ROC curve even KS Plot is a good measure to check model's performance
# the cumulative percentage of responders (ones) captured by the model against the expe
# of responders at random (i.e. had there been no model).
# The greater the distance between the random and model cumulatives, the better is the
# to effectively capture the responders (ones).

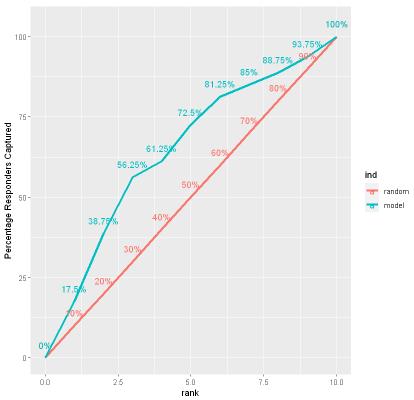
ks_plot(actuals=as.numeric(testSet$Outcome),
predictedScores=as.numeric(glmOutcome)) # the plot is better than random chance - so a

ks_plot(actuals=as.numeric(gbmOutcome)) # the plot is better than random chance - so a

ks_plot(actuals=as.numeric(testSet$Outcome),
predictedScores=as.numeric(testSet$Outcome)) # the plot is better than random chance - so a

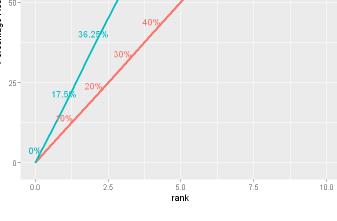
ks_plot(actuals=as.numeric(testSet$Outcome)) # the plot is better than random chance - so a
```

#### **KS Plot**

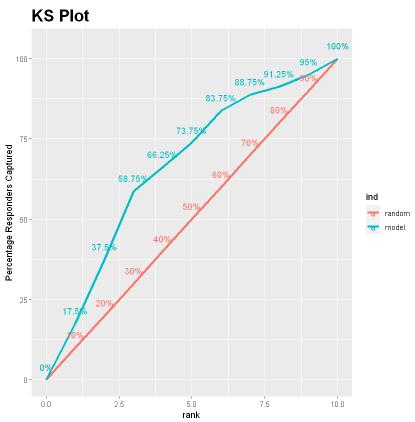


## **KS Plot** 100% 100-95% 88.75% 90% 75 Percentage Responders Captured

ind 💳 random <del>a</del> model







## **KS Plot** 100% 100 76.25% 75 Responders Captured

#### In [51]: # Compare the models (descriptive stats) resamps <- resamples(list(RF=rfmodel, GLM = glm\_model, GBM = gbm\_model, KNN = knn\_model summary(resamps) #attributes(resamps)

💳 random 💳 model

#### Call:

summary.resamples(object = resamps)

Models: RF, GLM, GBM, KNN Number of resamples: 30

#### ROC

Min. 1st Qu. Median Mean 3rd Qu. Max. NA's 0.6210526 0.7787594 0.8368421 0.8233333 0.8771617 0.9240602 GLM 0.6285714 0.7827068 0.8225564 0.8282261 0.8849624 0.9383459 0 GBM 0.5969925 0.7315789 0.7721805 0.7821888 0.8348997 0.9127820 0 KNN 0.6000000 0.7874060 0.8293233 0.8208382 0.8751880 0.9323308 0

#### Sens

Min. 1st Qu. Median Mean 3rd Qu. Max. NA's 0.6285714 0.8000000 0.8571429 0.8409524 0.8857143 0.9714286 0 GLM 0.7428571 0.8285714 0.8857143 0.8752381 0.9142857 0.9714286 0 GBM 0.6571429 0.7714286 0.8142857 0.8085714 0.8500000 0.9714286 0 KNN 0.8285714 0.9142857 0.9428571 0.9409524 0.9714286 1.0000000 0

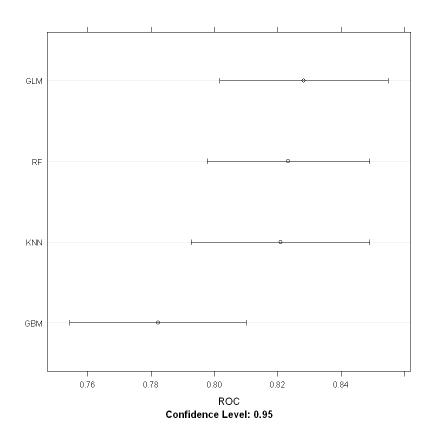
#### Spec

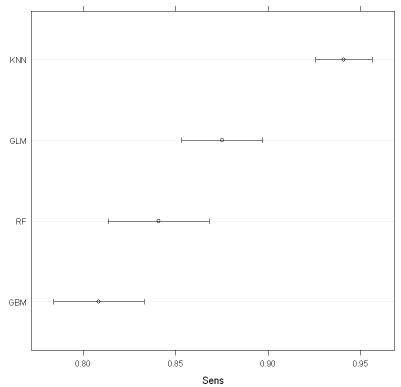
Min. 1st Qu. Median Mean 3rd Qu. Max. NA's 0.3157895 0.5263158 0.5950292 0.5975634 0.6710526 0.7894737 0 GLM 0.3157895 0.4802632 0.5409357 0.5585770 0.6315789 0.7894737 0 GBM 0.3157895 0.4736842 0.5263158 0.5550682 0.6578947 0.7894737 0 KNN 0.1578947 0.3157895 0.4210526 0.4240741 0.5263158 0.6315789 0

```
In [62]: # compare the models visually
    trellis.par.set(caretTheme())
    dotplot(resamps, metric = "ROC") # comparison of ROC metric
    # Logistic Regression performs best among these just based on ROC;
    # but pls note these are based on mean values. when we look at the median above, RF is
    # We should prefer median central tendency over mean because outliers tend to dictate n
    # So RF is the best one based on ROC even if visually it is not the best.

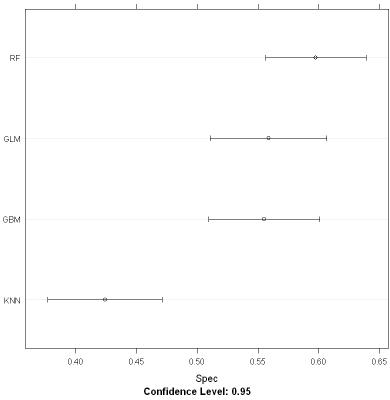
dotplot(resamps, metric = "Sens")
    # KNNN performs best among these just based on Sensitivity

dotplot(resamps, metric = "Spec")
# Random forest performs best among these just based on Specificity
```





Confidence Level: 0.95



Balanced accuracy is a metric that one can use when evaluating how good a binary classifier is. It is especially useful when the classes are imbalanced, i.e. one of the two classes appears a lot more often than the other. This happens often in many settings such as anomaly detection and the presence of a disease.

Balanced accuracy is based on two more commonly used metrics: sensitivity (also known as true positive rate or recall) and specificity (also known as true negative rate, or 1 – false positive rate). Sensitivity answers the question ~ how many of the truly positive cases are found. Specificity answers that same question but for the negative cases.

Since BA metric encompasses both, we are choosing that as our metric for now.

### So depending on what is more important (metric) to us for the biz decision, we can choose that as our model to predict.

If specificity was more important to us we should avoid knn as it produced the worst value (0.42 or 42%) and actually choose RF model with a (0.595 or 59.5% specificity); If sensitivity was more important to us we should choose knn algorithm for this data as it hadthe highest value (0.94 or 94%) among the different models.

# Among all the balanced accuracies, RF model performed best (74.54%), so lets choose as our model for predictions, assuming we wanted a good model for all purposes.

Please note that we didnt tweak much of the hyperparameters. Had we done that the GBM model would have probably given a better metric than the one now.

```
In [63]: # export the dataset for tableau purposes
write_csv(ds1_diabds_mod2,"I:/DSforR/capstone/tableau_hg_input.csv", na='')
```