STA7734 Project Analysis

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Read data

Check first 6 rows of Data, and missing values

* 32 columns, first two columns are ID and target variable: Diagnosis (B,M).

* No Missing value

```
## # A tibble: 6 x 32
##   ID    Diagnosis radius texture perimeter  area smoothness compactness
##   <chr> <chr>      <dbl>   <dbl>     <dbl> <dbl>      <dbl>       <dbl>
## 1 8423~ M           18.0    10.4     123.  1001      0.118       0.278
## 2 8425~ M           20.6    17.8     133.  1326      0.0847      0.0786
## 3 8430~ M           19.7    21.2     130   1203      0.110       0.160
## 4 8434~ M           11.4    20.4      77.6  386.     0.142       0.284
## 5 8435~ M           20.3    14.3     135.  1297      0.100       0.133
## 6 8437~ M           12.4    15.7      82.6  477.     0.128       0.17
## # ... with 24 more variables: concavity <dbl>, concave_points <dbl>,
## #   symmetry <dbl>, fractal_dimension <dbl>, radiusSE <dbl>,
## #   textureSE <dbl>, perimeterSE <dbl>, areaSE <dbl>, smoothnessSE <dbl>,
## #   compactnessSE <dbl>, concavitySE <dbl>, concave_pointsSE <dbl>,
## #   symmetrySE <dbl>, fractal_dimensionSE <dbl>, radiusW <dbl>,
## #   textureW <dbl>, perimeterW <dbl>, areaW <dbl>, smoothnessW <dbl>,
## #   compactnessW <dbl>, concavityW <dbl>, concave_pointsW <dbl>,
## #   symmetryW <dbl>, fractal_dimensionW <dbl>
```

```
##                 ID           Diagnosis              radius 
##                  0                   0                   0 
##             texture           perimeter                area 
##                  0                   0                   0 
##          smoothness         compactness           concavity 
##                  0                   0                   0 
##      concave_points            symmetry   fractal_dimension 
##                  0                   0                   0 
##            radiusSE           textureSE         perimeterSE 
##                  0                   0                   0 
##              areaSE        smoothnessSE       compactnessSE 
##                  0                   0                   0 
##         concavitySE    concave_pointsSE          symmetrySE 
##                  0                   0                   0 
## fractal_dimensionSE             radiusW            textureW 
##                  0                   0                   0 
##          perimeterW               areaW         smoothnessW 
##                  0                   0                   0 
##        compactnessW          concavityW     concave_pointsW 
##                  0                   0                   0 
##           symmetryW  fractal_dimensionW                     
##                  0                   0
```

Descriptive Statistics on numeric variables and target variable: Diagnosis

```
##                     vars   n   mean     sd median trimmed    mad    min
## Diagnosis*             1 569    NaN     NA     NA     NaN     NA    Inf
## radius                 2 569  14.13   3.52  13.37   13.82   2.82   6.98
## texture                3 569  19.29   4.30  18.84   19.04   4.17   9.71
## perimeter              4 569  91.97  24.30  86.24   89.74  18.84  43.79
## area                   5 569 654.89 351.91 551.10  606.13 227.28 143.50
## smoothness             6 569   0.10   0.01   0.10    0.10   0.01   0.05
## compactness            7 569   0.10   0.05   0.09    0.10   0.05   0.02
## concavity              8 569   0.09   0.08   0.06    0.08   0.06   0.00
## concave_points         9 569   0.05   0.04   0.03    0.04   0.03   0.00
## symmetry              10 569   0.18   0.03   0.18    0.18   0.03   0.11
## fractal_dimension     11 569   0.06   0.01   0.06    0.06   0.01   0.05
## radiusSE              12 569   0.41   0.28   0.32    0.36   0.16   0.11
## textureSE             13 569   1.22   0.55   1.11    1.16   0.47   0.36
## perimeterSE           14 569   2.87   2.02   2.29    2.51   1.14   0.76
## areaSE                15 569  40.34  45.49  24.53   31.69  13.63   6.80
## smoothnessSE          16 569   0.01   0.00   0.01    0.01   0.00   0.00
## compactnessSE         17 569   0.03   0.02   0.02    0.02   0.01   0.00
## concavitySE           18 569   0.03   0.03   0.03    0.03   0.02   0.00
## concave_pointsSE      19 569   0.01   0.01   0.01    0.01   0.01   0.00
## symmetrySE            20 569   0.02   0.01   0.02    0.02   0.01   0.01
## fractal_dimensionSE   21 569   0.00   0.00   0.00    0.00   0.00   0.00
## radiusW               22 569  16.27   4.83  14.97   15.73   3.65   7.93
## textureW              23 569  25.68   6.15  25.41   25.39   6.42  12.02
## perimeterW            24 569 107.26  33.60  97.66  103.42  25.01  50.41
## areaW                 25 569 880.58 569.36 686.50  788.02 319.65 185.20
## smoothnessW           26 569   0.13   0.02   0.13    0.13   0.02   0.07
## compactnessW          27 569   0.25   0.16   0.21    0.23   0.13   0.03
## concavityW            28 569   0.27   0.21   0.23    0.25   0.20   0.00
## concave_pointsW       29 569   0.11   0.07   0.10    0.11   0.07   0.00
## symmetryW             30 569   0.29   0.06   0.28    0.28   0.05   0.16
## fractal_dimensionW    31 569   0.08   0.02   0.08    0.08   0.01   0.06
##                        max   range skew kurtosis    se
## Diagnosis*            -Inf    -Inf   NA       NA    NA
## radius               28.11   21.13 0.94     0.81  0.15
## texture              39.28   29.57 0.65     0.73  0.18
## perimeter           188.50  144.71 0.99     0.94  1.02
## area               2501.00 2357.50 1.64     3.59 14.75
## smoothness            0.16    0.11 0.45     0.82  0.00
## compactness           0.35    0.33 1.18     1.61  0.00
## concavity             0.43    0.43 1.39     1.95  0.00
## concave_points        0.20    0.20 1.17     1.03  0.00
## symmetry              0.30    0.20 0.72     1.25  0.00
## fractal_dimension     0.10    0.05 1.30     2.95  0.00
## radiusSE              2.87    2.76 3.07    17.45  0.01
## textureSE             4.88    4.52 1.64     5.26  0.02
## perimeterSE          21.98   21.22 3.43    21.12  0.08
## areaSE              542.20  535.40 5.42    48.59  1.91
## smoothnessSE          0.03    0.03 2.30    10.32  0.00
## compactnessSE         0.14    0.13 1.89     5.02  0.00
## concavitySE           0.40    0.40 5.08    48.24  0.00
## concave_pointsSE      0.05    0.05 1.44     5.04  0.00
## symmetrySE            0.08    0.07 2.18     7.78  0.00
```

```
## fractal_dimensionSE    0.03    0.03 3.90    25.94  0.00
## radiusW               36.04   28.11 1.10     0.91  0.20
## textureW              49.54   37.52 0.50     0.20  0.26
## perimeterW           251.20  200.79 1.12     1.04  1.41
## areaW               4254.00 4068.80 1.85     4.32 23.87
## smoothnessW            0.22    0.15 0.41     0.49  0.00
## compactnessW           1.06    1.03 1.47     2.98  0.01
## concavityW             1.25    1.25 1.14     1.57  0.01
## concave_pointsW        0.29    0.29 0.49    -0.55  0.00
## symmetryW              0.66    0.51 1.43     4.37  0.00
## fractal_dimensionW     0.21    0.15 1.65     5.16  0.00
```

```
##   B   M
## 357 212
```

Data visiualization

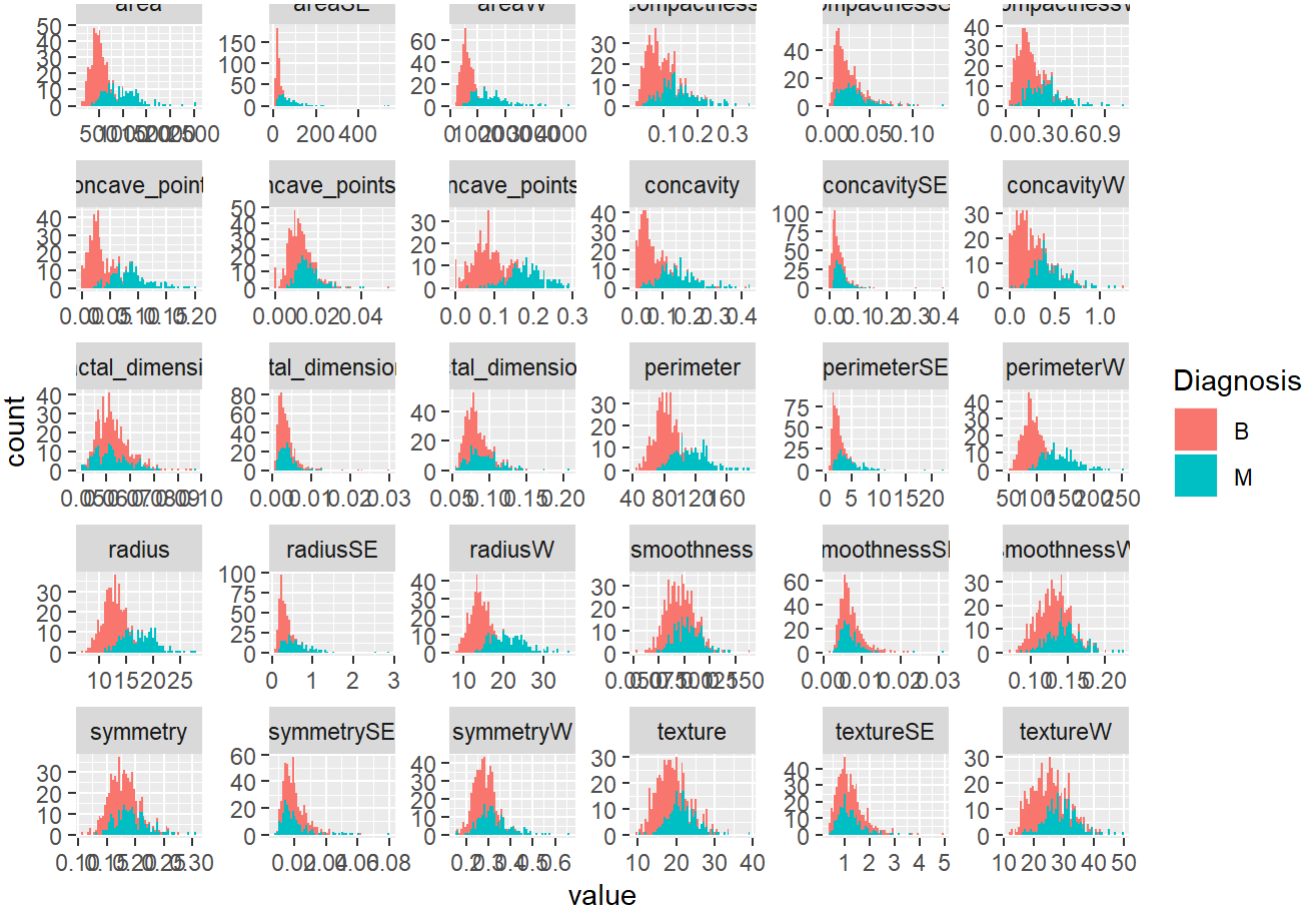
* Plot Diagnosis;

* Histogram for all Variables;

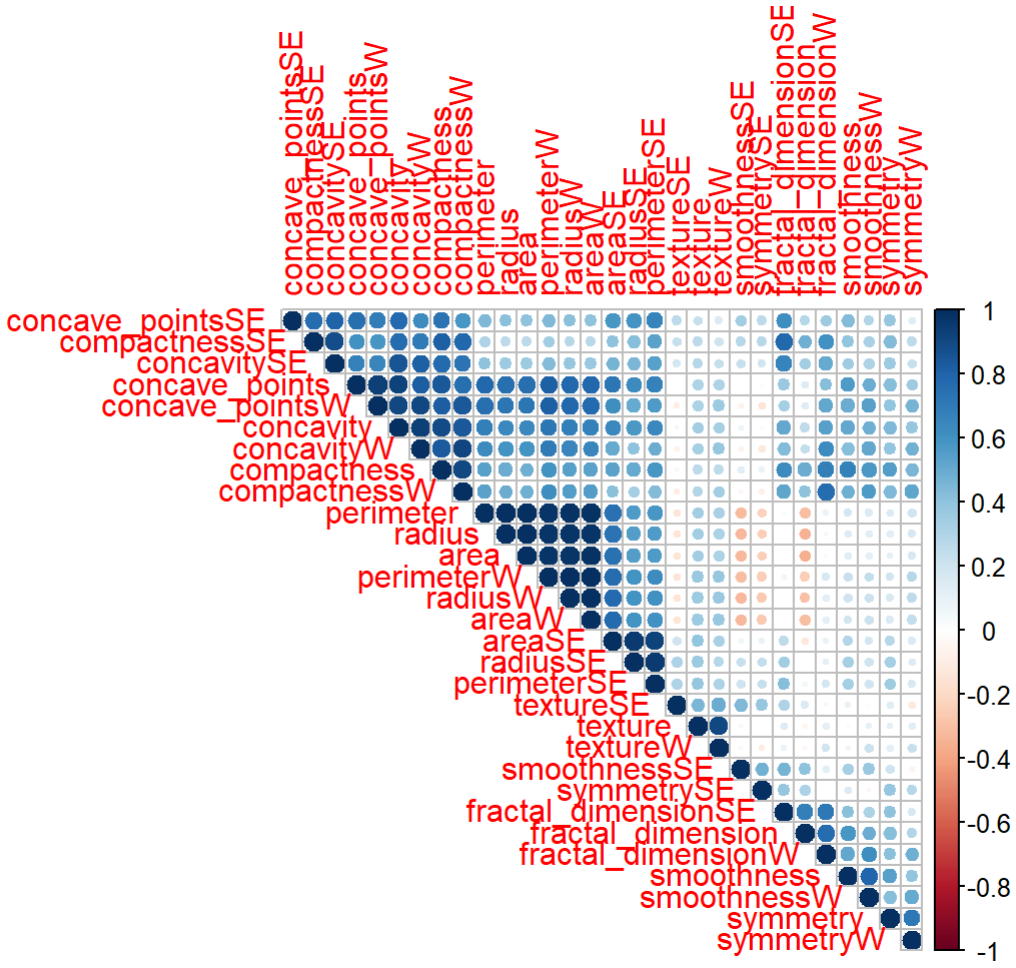
* Histogram for all Variables by Diagnosis.

There are differences between B and M Diagnosis such as area, compactness, perimeter, radius, etc


Diagnosis percentages
Percent
0.6
0.4
0.2
0.0
B
M
Diagnosis
Diagnosis
B
M
area
areaSE
areaW
compactness
compactnessSE
compactnessW
concave_points
concavity
concavitySE
concavityW
perimeter
perimeterSE
perimeterW
radius
radiusSE
radiusW
smoothness
smoothnessSE
smoothnessW
symmetry
symmetrySE
symmetryW
texture
textureSE
textureW
count
value



Correlaion analysis by spearman since most variables are non normal distributed



Drop variables with multicolinearity, where correlation >0.9, and remove the variable with the largest mean absolute correlation

```
## Compare row 7  and column  28 with corr  0.905
##   Means:  0.579 vs 0.417 so flagging column 7
## Compare row 28  and column  8 with corr  0.937
##   Means:  0.557 vs 0.405 so flagging column 28
## Compare row 6  and column  26 with corr  0.901
##   Means:  0.541 vs 0.396 so flagging column 6
## Compare row 27  and column  26 with corr  0.915
##   Means:  0.508 vs 0.385 so flagging column 27
## Compare row 23  and column  21 with corr  0.994
##   Means:  0.497 vs 0.375 so flagging column 23
## Compare row 21  and column  24 with corr  0.999
##   Means:  0.462 vs 0.366 so flagging column 21
## Compare row 24  and column  3 with corr  0.981
##   Means:  0.436 vs 0.359 so flagging column 24
## Compare row 3  and column  1 with corr  0.998
##   Means:  0.401 vs 0.353 so flagging column 3
## Compare row 1  and column  4 with corr  1
##   Means:  0.356 vs 0.35 so flagging column 1
## Compare row 14  and column  13 with corr  0.927
##   Means:  0.385 vs 0.346 so flagging column 14
## Compare row 13  and column  11 with corr  0.958
##   Means:  0.397 vs 0.345 so flagging column 13
## Compare row 22  and column  2 with corr  0.909
##   Means:  0.241 vs 0.346 so flagging column 2
## All correlations <= 0.9
```

Highly correlated variables

```
##  [1] "concavity"       "concave_pointsW" "compactness"
##  [4] "concavityW"      "perimeterW"      "radiusW"
##  [7] "areaW"           "perimeter"       "radius"
## [10] "areaSE"          "perimeterSE"     "texture"
```

Number of features left

```
## [1] 18
```

Data Transformation/ Dimension Reduction by using PCA, after dropping label.

PCA components summary for raw data

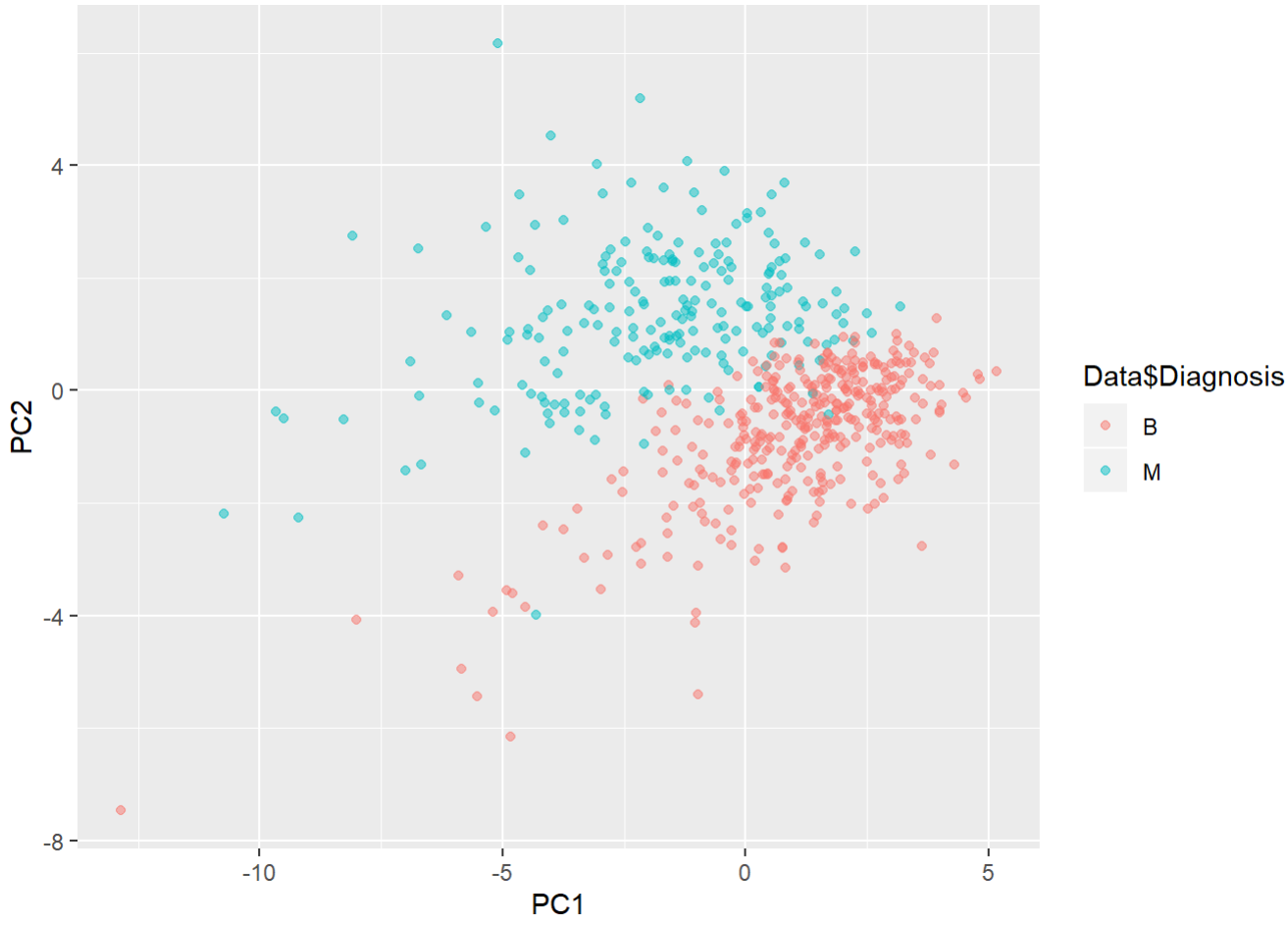
```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6
## Standard deviation     3.6444 2.3857 1.67867 1.40735 1.28403 1.09880
## Proportion of Variance 0.4427 0.1897 0.09393 0.06602 0.05496 0.04025
## Cumulative Proportion  0.4427 0.6324 0.72636 0.79239 0.84734 0.88759
##                            PC7     PC8    PC9    PC10   PC11    PC12
## Standard deviation     0.82172 0.69037 0.6457 0.59219 0.5421 0.51104
## Proportion of Variance 0.02251 0.01589 0.0139 0.01169 0.0098 0.00871
## Cumulative Proportion  0.91010 0.92598 0.9399 0.95157 0.9614 0.97007
##                           PC13    PC14    PC15    PC16    PC17    PC18
## Standard deviation     0.49128 0.39624 0.30681 0.28260 0.24372 0.22939
## Proportion of Variance 0.00805 0.00523 0.00314 0.00266 0.00198 0.00175
## Cumulative Proportion  0.97812 0.98335 0.98649 0.98915 0.99113 0.99288
##                           PC19    PC20   PC21    PC22    PC23   PC24
## Standard deviation     0.22244 0.17652 0.1731 0.16565 0.15602 0.1344
## Proportion of Variance 0.00165 0.00104 0.0010 0.00091 0.00081 0.0006
## Cumulative Proportion  0.99453 0.99557 0.9966 0.99749 0.99830 0.9989
##                           PC25    PC26    PC27    PC28    PC29    PC30
## Standard deviation     0.12442 0.09043 0.08307 0.03987 0.02736 0.01153
## Proportion of Variance 0.00052 0.00027 0.00023 0.00005 0.00002 0.00000
## Cumulative Proportion  0.99942 0.99969 0.99992 0.99997 1.00000 1.00000
```

PCA without highly correlated variables

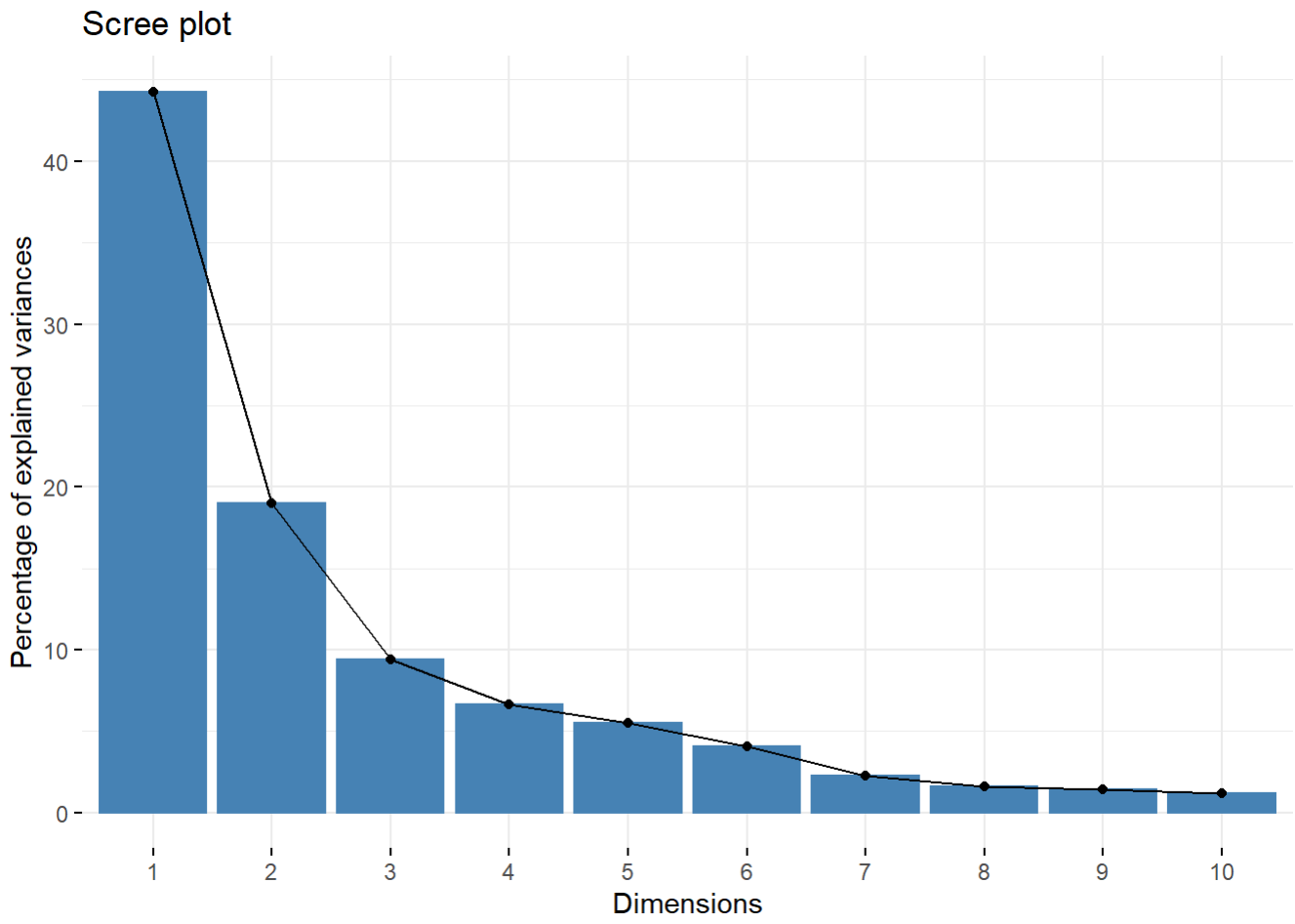
```
## Importance of components:
##                           PC1    PC2    PC3     PC4     PC5     PC6
## Standard deviation     2.6151 1.6197 1.5256 1.21914 1.12496 1.09311
## Proportion of Variance 0.3799 0.1457 0.1293 0.08257 0.07031 0.06638
## Cumulative Proportion  0.3799 0.5257 0.6550 0.73756 0.80787 0.87425
##                            PC7     PC8     PC9    PC10    PC11    PC12
## Standard deviation     0.68529 0.66200 0.56110 0.49260 0.42947 0.40531
## Proportion of Variance 0.02609 0.02435 0.01749 0.01348 0.01025 0.00913
## Cumulative Proportion  0.90034 0.92469 0.94218 0.95566 0.96591 0.97503
##                           PC13   PC14    PC15   PC16   PC17    PC18
## Standard deviation     0.3698 0.3576 0.25151 0.2326 0.2079 0.15547
## Proportion of Variance 0.0076 0.0071 0.00351 0.0030 0.0024 0.00134
## Cumulative Proportion  0.9826 0.9897 0.99325 0.9962 0.9987 1.00000
```

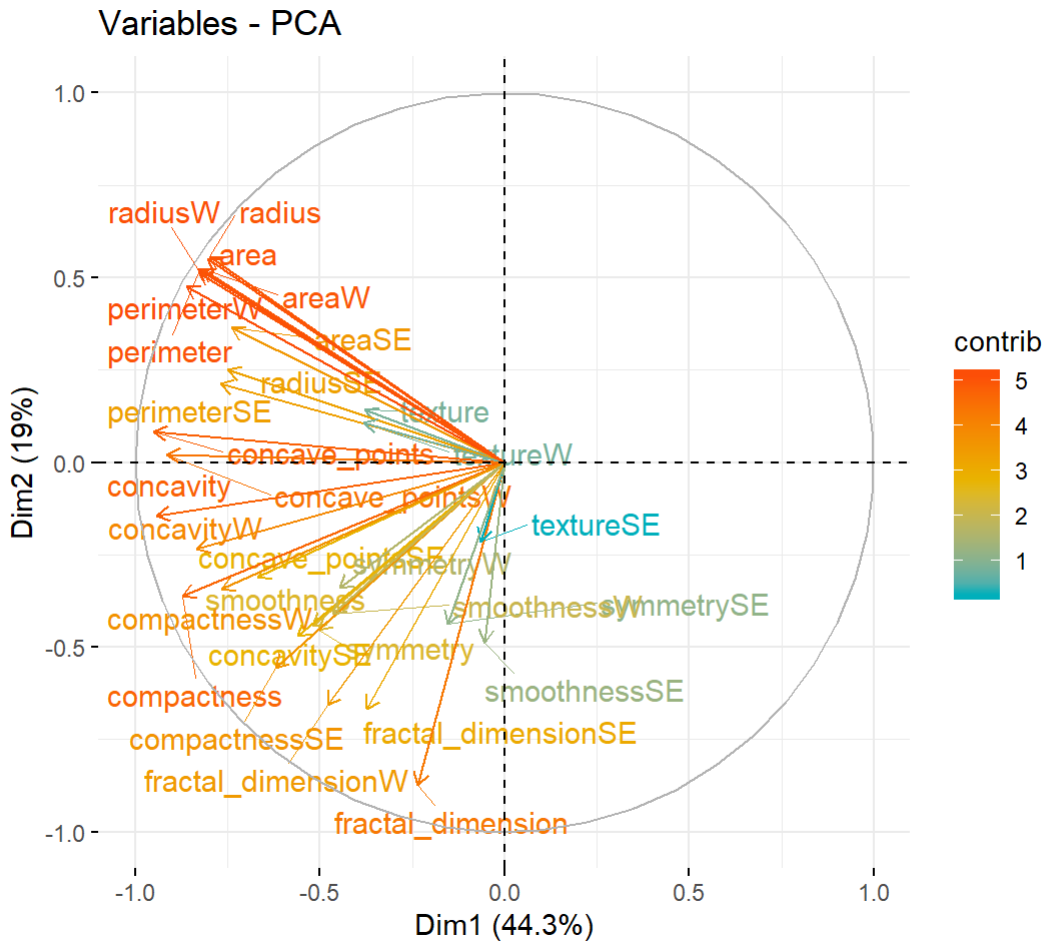
Plot first 2 PCA components

Plot PCA without highly correlated variables on the first 2 components

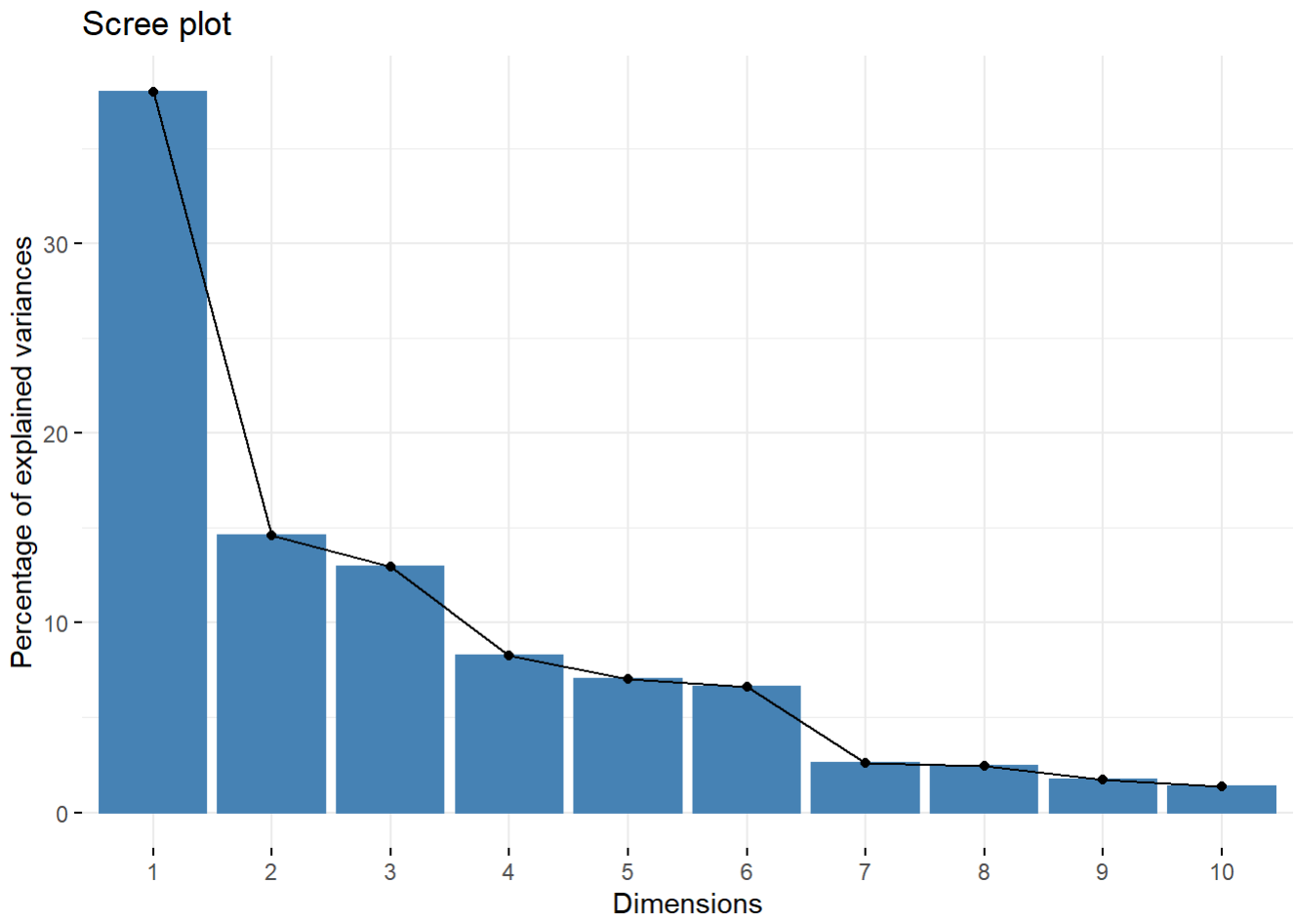


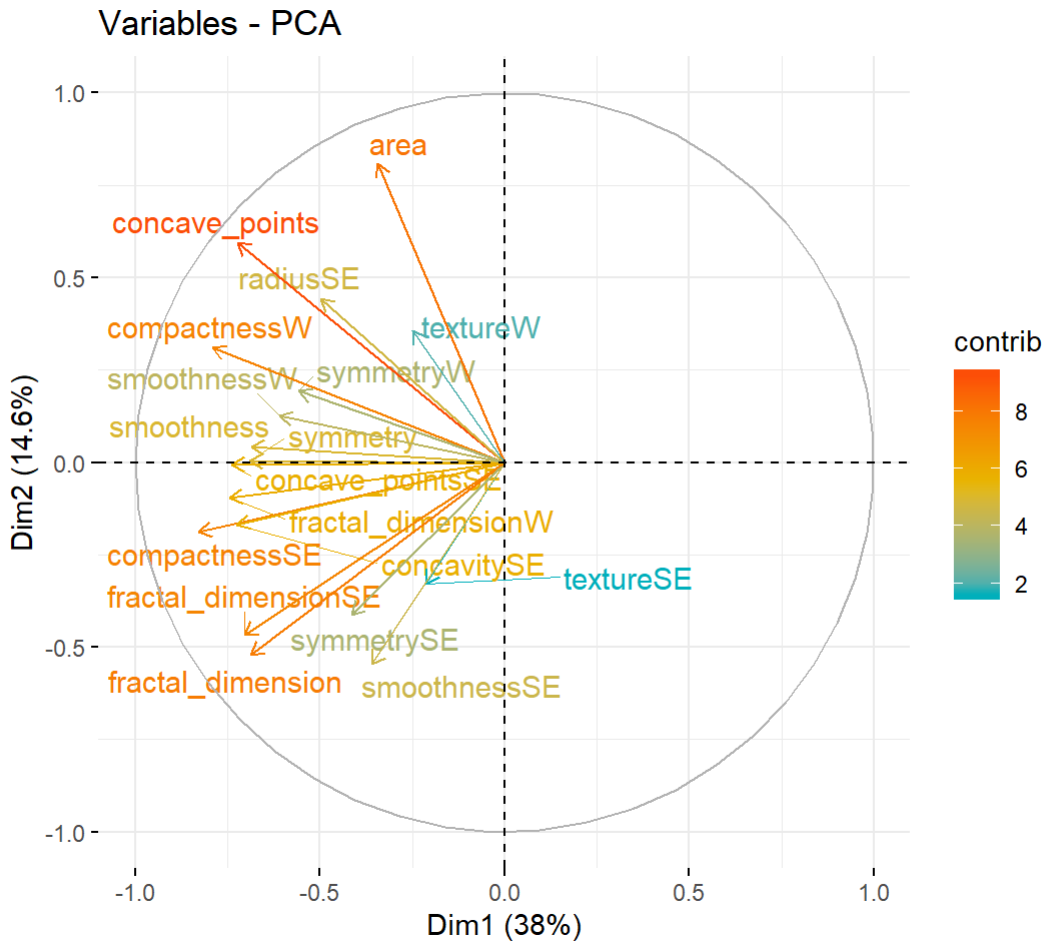
Visualize which variables are the most influential. Individuals with a similar profile are grouped together


Scree plot
Percentage of explained variances
Dimensions
0
10
20
30
40
1
2
3
4
5
6
7
8
9
10


Variables - PCA
Dim2 (19%)
Dim1 (44.3%)
contrib
5
4
3
2
1
radiusW
radius
area
areaW
perimeterW
areaSE
perimeter
radiusSE
perimeterSE
texture
concave_points
concavity
concave_pointsW
concavityW
textureSE
concave_pointsSE
symmetryW
smoothness
smoothnessW
symmetrySE
compactnessW
concavitySE
symmetry
smoothnessSE
compactness
compactnessSE
fractal_dimensionSE
fractal_dimensionW
fractal_dimension

After correlated variables were dropped


Scree plot
Percentage of explained variances
30
20
10
0
1
2
3
4
5
6
7
8
9
10
Dimensions


Variables - PCA
1.0
0.5
0.0
-0.5
-1.0
Dim2 (14.6%)
area
concave_points
radiusSE
compactnessW
textureW
smoothnessW
symmetryW
smoothness
symmetry
concave_pointsSE
fractal_dimensionW
compactnessSE
concavitySE
textureSE
fractal_dimensionSE
symmetrySE
fractal_dimension
smoothnessSE
-1.0
-0.5
0.0
0.5
1.0
Dim1 (38%)
contrib
8
6
4
2

Correlated variables such as area, perimeters, radius are grouped together and they are important contributers

Model Training

Split data into training and test

split data into training and test after dropping correlated variables

Svm with original data by Using library(e1071), data is not scaled;

* Default parameters: Cost =1, gamma = 1/(data dimension)

first gamma:

```
## [1] 0.03333333
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71 42
##          M  0  0
##
##                Accuracy : 0.6283
##                  95% CI : (0.5324, 0.7174)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : 0.542
##
##                   Kappa : 0
##
##  Mcnemar's Test P-Value : 2.509e-10
##
##             Sensitivity : 0.0000
##             Specificity : 1.0000
##          Pos Pred Value :    NaN
##          Neg Pred Value : 0.6283
##              Prevalence : 0.3717
##          Detection Rate : 0.0000
##    Detection Prevalence : 0.0000
##       Balanced Accuracy : 0.5000
##
##        'Positive' Class : M
##
```

Svm with after droped correlated variables with default setting by using library(e1071)

second gamma:

```
## [1] 0.05555556
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 68 15
##          M  3 27
##
##                Accuracy : 0.8407
##                  95% CI : (0.76, 0.9028)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : 6.001e-07
##
##                   Kappa : 0.6378
##
##  Mcnemar's Test P-Value : 0.009522
##
##             Sensitivity : 0.6429
##             Specificity : 0.9577
##          Pos Pred Value : 0.9000
##          Neg Pred Value : 0.8193
##              Prevalence : 0.3717
##          Detection Rate : 0.2389
##    Detection Prevalence : 0.2655
##       Balanced Accuracy : 0.8003
##
##        'Positive' Class : M
##
```

Use caret package to fit models with default parameter tuning with 5 fold cross validation, repeated 5 times; Caret “svmRadial” model uses kernlab package; No data scaling.

* $C = 2^{((1{:}len)-3)}$ (C=0.25)

* Sigma is defined by Kernlab package’s sigest function, sigest estimates are based upon the 0.1 and 0.9 quantile of $||x - x'||^2$. Basically any value in between those two bounds will produce good results. A vector of length 3 defining the range (0.1 quantile, median and 0.9 quantile) of the sigma hyperparameter.

```
## Support Vector Machine object of class "ksvm"
##
## SV type: C-svc  (classification)
##  parameter : cost C = 1
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  0.0445118095276661
##
## Number of Support Vectors : 121
##
## Objective Function Value : -50.3072
## Training error : 0.013158
## Probability model included.
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71  3
##          M  0 39
##
##                Accuracy : 0.9735
##                  95% CI : (0.9244, 0.9945)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9423
##
##  Mcnemar's Test P-Value : 0.2482
##
##             Sensitivity : 0.9286
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9595
##              Prevalence : 0.3717
##          Detection Rate : 0.3451
##    Detection Prevalence : 0.3451
##       Balanced Accuracy : 0.9643
##
##        'Positive' Class : M
##
```

Use caret package to fit models after droped correlated variables with default parameter tuning with 5 fold cross validation, repeated 5 times; No data scaling.

It’s not as good as the previous model with all features but it’s less sensitive on negative predicting.

```
## Support Vector Machine object of class "ksvm"
##
## SV type: C-svc  (classification)
##  parameter : cost C = 1
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  0.0642190212977282
##
## Number of Support Vectors : 130
##
## Objective Function Value : -62.7148
## Training error : 0.013158
## Probability model included.
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 70  3
##          M  1 39
##
##                Accuracy : 0.9646
##                  95% CI : (0.9118, 0.9903)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9235
##
##  Mcnemar's Test P-Value : 0.6171
##
##             Sensitivity : 0.9286
##             Specificity : 0.9859
##          Pos Pred Value : 0.9750
##          Neg Pred Value : 0.9589
##              Prevalence : 0.3717
##          Detection Rate : 0.3451
##    Detection Prevalence : 0.3540
##       Balanced Accuracy : 0.9572
##
##        'Positive' Class : M
##
```

Scale variables and cross validation

```
## Support Vector Machine object of class "ksvm"
##
## SV type: C-svc  (classification)
##  parameter : cost C = 1
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  0.0445118095276661
##
## Number of Support Vectors : 121
##
## Objective Function Value : -50.3072
## Training error : 0.013158
## Probability model included.
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71  3
##          M  0 39
##
##                Accuracy : 0.9735
##                  95% CI : (0.9244, 0.9945)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9423
##
##  Mcnemar's Test P-Value : 0.2482
##
##             Sensitivity : 0.9286
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9595
##              Prevalence : 0.3717
##          Detection Rate : 0.3451
##    Detection Prevalence : 0.3451
##       Balanced Accuracy : 0.9643
##
##        'Positive' Class : M
##
```

Scale variables with pca thresdhold = 0.8. 0.8 is the sweet spot.

```
## Support Vector Machine object of class "ksvm"
##
## SV type: C-svc  (classification)
##  parameter : cost C = 1
##
## Gaussian Radial Basis kernel function.
##  Hyperparameter : sigma =  0.285658961570517
##
## Number of Support Vectors : 128
##
## Objective Function Value : -64.8713
## Training error : 0.02193
## Probability model included.
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 70  1
##          M  1 41
##
##                Accuracy : 0.9823
##                  95% CI : (0.9375, 0.9978)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9621
##
##  Mcnemar's Test P-Value : 1
##
##             Sensitivity : 0.9762
##             Specificity : 0.9859
##          Pos Pred Value : 0.9762
##          Neg Pred Value : 0.9859
##              Prevalence : 0.3717
##          Detection Rate : 0.3628
##    Detection Prevalence : 0.3717
##       Balanced Accuracy : 0.9811
##
##        'Positive' Class : M
##
```

Scale variables with dropped variables and with pca = 0.95;

The results doesn’t improve much anymore, with increasing threshold of pca, the performance increases on the 4th digit and it’s more stable

```
## Support Vector Machines with Radial Basis Function Kernel
##
## 456 samples
##  18 predictor
##   2 classes: 'B', 'M'
##
## Pre-processing: centered (18), scaled (18), principal component
##  signal extraction (18)
## Resampling: Cross-Validated (5 fold, repeated 5 times)
## Summary of sample sizes: 365, 365, 364, 365, 365, 365, ...
## Resampling results across tuning parameters:
##
##   C     ROC        Sens       Spec
##   0.25  0.9911843  0.9656866  0.9482353
##   0.50  0.9919437  0.9705989  0.9494118
##   1.00  0.9928896  0.9706110  0.9482353
##
## Tuning parameter 'sigma' was held constant at a value of 0.09535176
## ROC was used to select the optimal model using the largest value.
## The final values used for the model were sigma = 0.09535176 and C = 1.
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   B   M
##          B 285   7
##          M   1 163
##
##                Accuracy : 0.9825
##                  95% CI : (0.9657, 0.9924)
##     No Information Rate : 0.6272
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9622
##
##  Mcnemar's Test P-Value : 0.0771
##
##             Sensitivity : 0.9588
##             Specificity : 0.9965
##          Pos Pred Value : 0.9939
##          Neg Pred Value : 0.9760
##              Prevalence : 0.3728
##          Detection Rate : 0.3575
##    Detection Prevalence : 0.3596
##       Balanced Accuracy : 0.9777
##
##        'Positive' Class : M
##
```

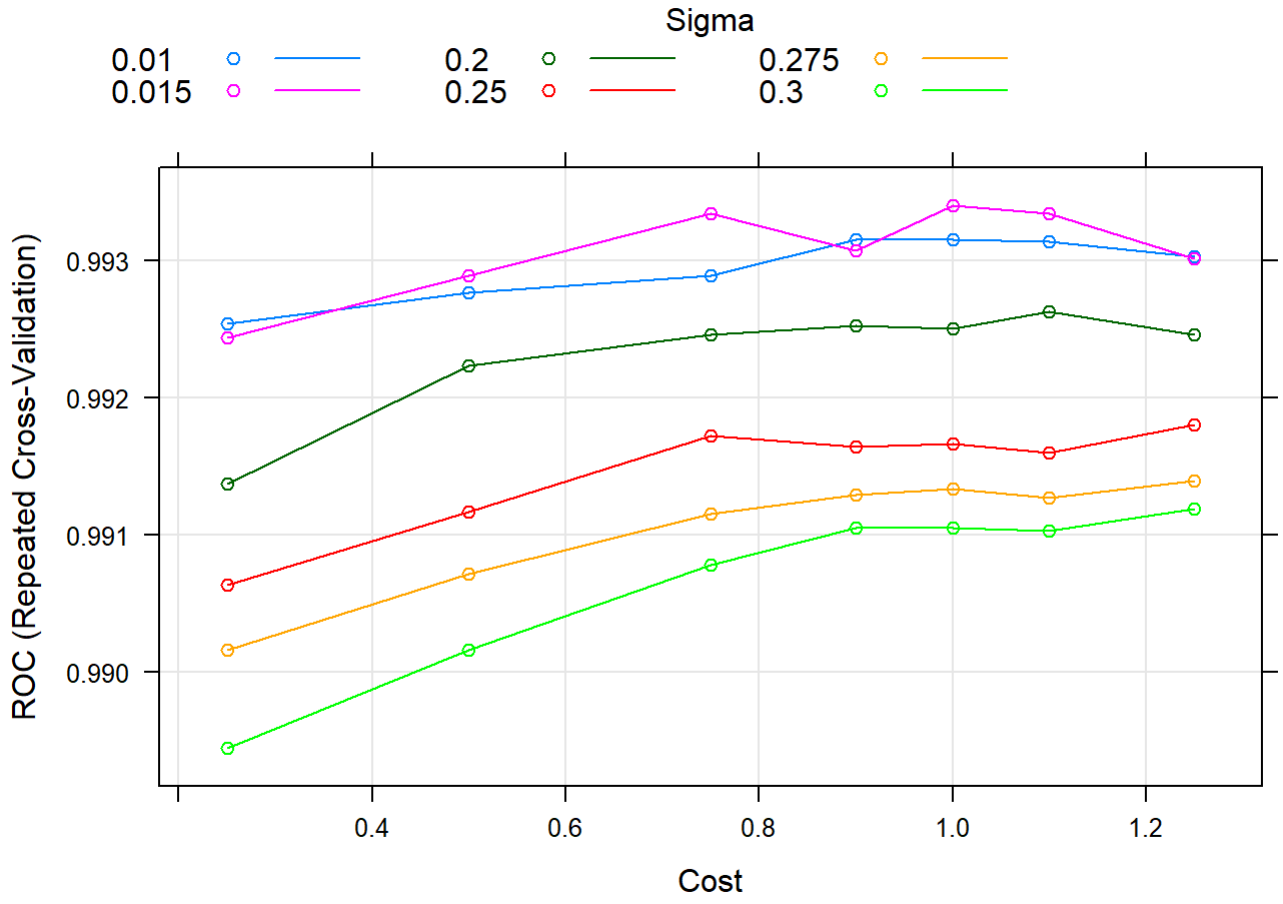
Tune SVM parameters by grid search, total 42 pairs

```
svmGrid <-  expand.grid(sigma = c(.01, .015, 0.2,0.25, 0.275,0.3),
                    C = c(0.25, 0.5, 0.75, 0.9, 1, 1.1, 1.25))

nrow(svmGrid)
```

```
## [1] 42
```

Plot the results on the feature selected data with pca, by grid search



Performance on test data with the best parameters

```
pred_svm_tune <- predict(svm_tune, train_drop_raw)
cm_svm_tune <- confusionMatrix(pred_svm_tune, as.factor(train_drop_raw$Diagnosis), positive =
"M")
cm_svm_tune
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   B   M
##          B 279   9
##          M   7 161
##
##                Accuracy : 0.9649
##                  95% CI : (0.9436, 0.9798)
##     No Information Rate : 0.6272
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9248
##
##  Mcnemar's Test P-Value : 0.8026
##
##             Sensitivity : 0.9471
##             Specificity : 0.9755
##          Pos Pred Value : 0.9583
##          Neg Pred Value : 0.9688
##              Prevalence : 0.3728
##          Detection Rate : 0.3531
##    Detection Prevalence : 0.3684
##       Balanced Accuracy : 0.9613
##
##        'Positive' Class : M
##
```

```
#Plotting the Resampling Profile: Examine the relationship between the estimates of performance
 and the tuning parameters
```

The best parameters on training data doesn't guarentee the best performance on the test data. It could be easily overfitting. The final values used for the model were sigma = 0.015 and C = 1.

Instead of just doing grid search, could we add another regulization papameter to reduce over fitting, or

instead of choosing the best pair of parameters (C, sigma), allow more errors and use another algorithm, for example, select top 3 pairs on test dataset to find the best pair of parameters?

Neural network

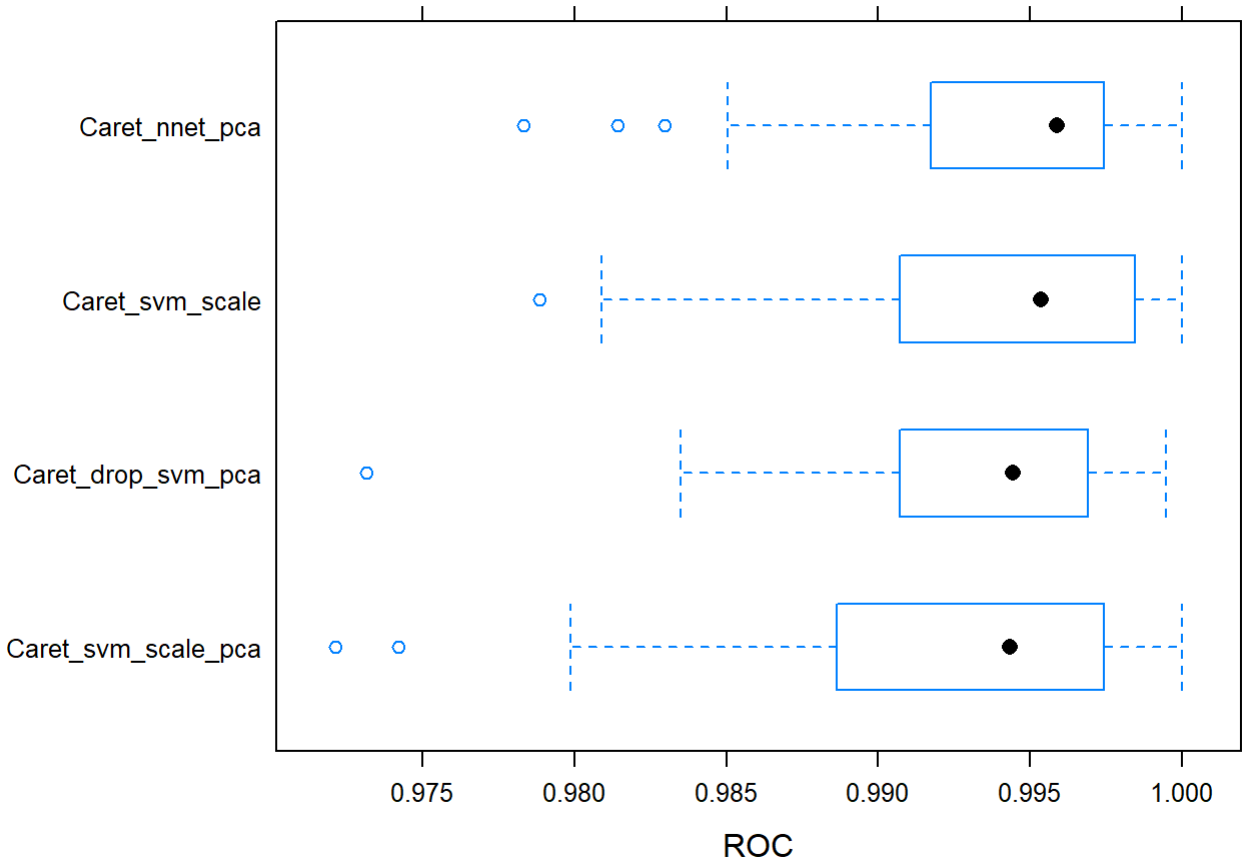
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71  4
##          M  0 38
##
##                Accuracy : 0.9646
##                  95% CI : (0.9118, 0.9903)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9227
##
##  Mcnemar's Test P-Value : 0.1336
##
##             Sensitivity : 0.9048
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9467
##              Prevalence : 0.3717
##          Detection Rate : 0.3363
##    Detection Prevalence : 0.3363
##       Balanced Accuracy : 0.9524
##
##        'Positive' Class : M
##
```

Neural network with pca

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71  3
##          M  0 39
##
##                Accuracy : 0.9735
##                  95% CI : (0.9244, 0.9945)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9423
##
##  Mcnemar's Test P-Value : 0.2482
##
##             Sensitivity : 0.9286
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9595
##              Prevalence : 0.3717
##          Detection Rate : 0.3451
##    Detection Prevalence : 0.3451
##       Balanced Accuracy : 0.9643
##
##        'Positive' Class : M
##
```

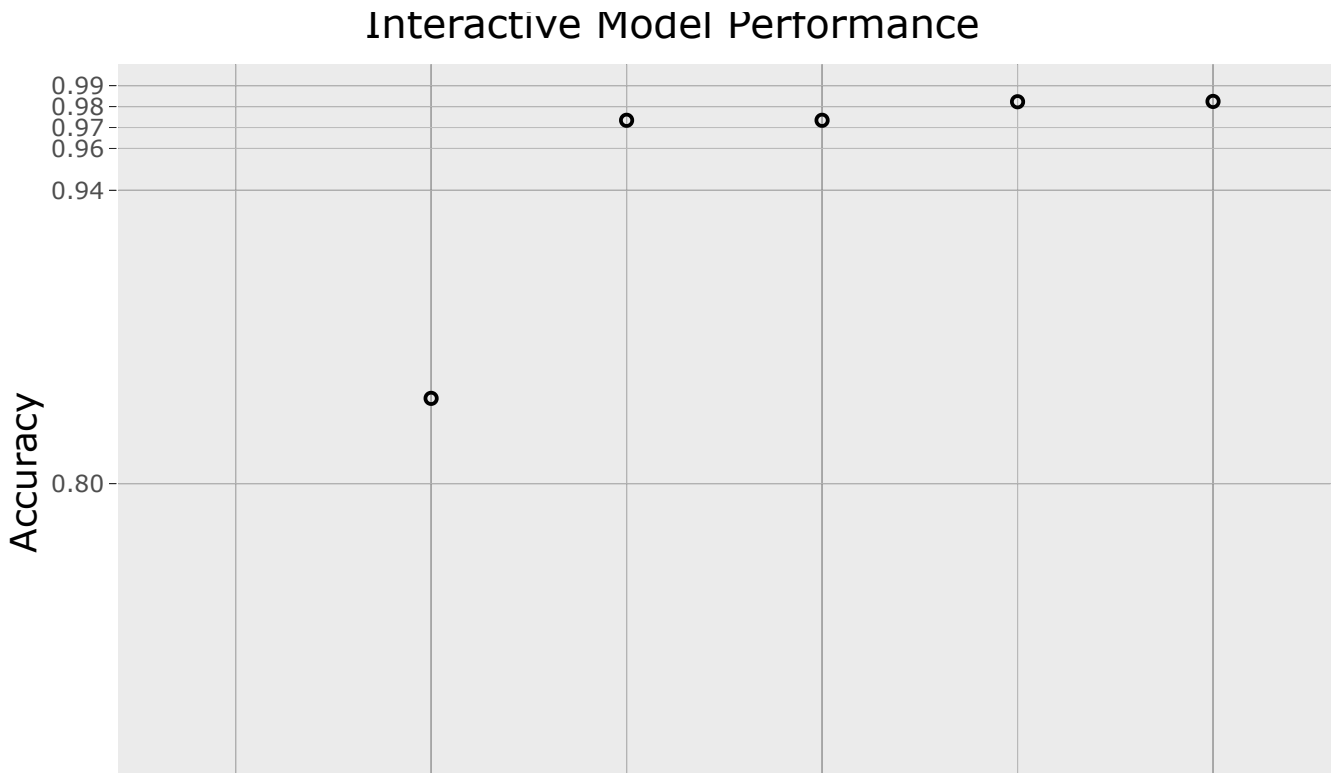
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  B  M
##          B 71  3
##          M  0 39
##
##                Accuracy : 0.9735
##                  95% CI : (0.9244, 0.9945)
##     No Information Rate : 0.6283
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.9423
##
##  Mcnemar's Test P-Value : 0.2482
##
##             Sensitivity : 0.9286
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.9595
##              Prevalence : 0.3717
##          Detection Rate : 0.3451
##    Detection Prevalence : 0.3451
##       Balanced Accuracy : 0.9643
##
##        'Positive' Class : M
##
```

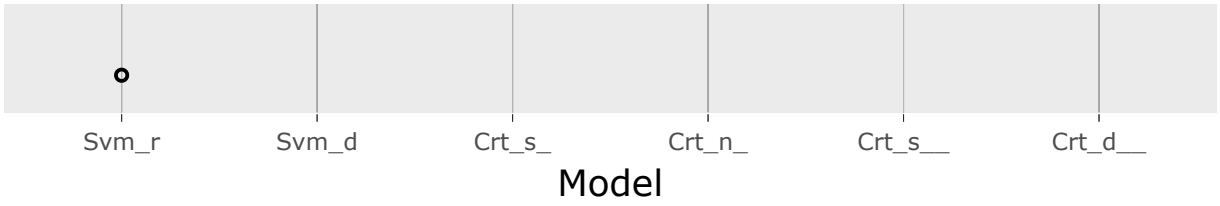
Models evaluation by caret package with cross validation on training model



Overall model evaluation on test data

Final model achieved accuracy of 0.9825.





Takeaways:

1. Scaling variables is very important. and tuning parameters by using resampling technique for example, cross validation is more important.

2. Reduce multicolinearity could stablize the model performance.

3. Dimention deduction (using PCA here) with out feature selection is not robust. It would takes time to find a sweet spot on the optimal PCA value.

4. In another word, with the appropriate feature selection, it reduces the variation of dimention deduction with a stable result.

5. The best tuning parameters on training could be overfitting. Neural network tends to overfit the model.

6. Grid search method could be improved by combing performance on test data instead of sololy relys on training data.

7. A good SVM could perform better than neurual network and could explain important features.

Appendix

```
knitr::opts_chunk$set(echo = TRUE)
library(tidyverse)
library(dplyr)
library(ggplot2)
library(psych)
library(corrplot)
library(e1071)
library(caret)
library(plotly)
library(plyr)

Data <- read_csv("C:/Work/Project/STA7734/SVM-Asymptotic-Normality/Data/data.csv",
                 col_names = T,
                 col_types=cols(ID =col_character(),
                                Diagnosis=col_character(),
                                "3" = col_double(),
                                "4" = col_double(),
                                "5" = col_double(),
                                "6" = col_double(),
                                "7" = col_double(),
                                "8" = col_double(),
                                "9" = col_double(),
                                "10" = col_double(),
                                "11" = col_double(),
                                "12" = col_double(),
                                "13" = col_double(),
                                "14" = col_double(),
                                "15" = col_double(),
                                "16" = col_double(),
                                "17" = col_double(),
                                "18" = col_double(),
                                "19" = col_double(),
                                "20" = col_double(),
                                "21" = col_double(),
                                "22" = col_double(),
                                "23" = col_double(),
                                "24" = col_double(),
                                "25" = col_double(),
                                "26" = col_double(),
                                "27" = col_double(),
                                "28" = col_double(),
                                "29" = col_double(),
                                "30" = col_double(),
                                "31" = col_double(),
                                "32" = col_double()
                                )) %>%
                         dplyr::rename( "radius" = "3",
                                "texture" = "4",
                                "perimeter" = "5",
                                "area" = "6",
                                "smoothness" = "7",
                                "compactness" = "8",
                                "concavity" = "9",
```

```
                                "concave_points" = "10",
                                "symmetry" = "11",
                                "fractal_dimension" = "12",
                                "radiusSE" = "13",
                                "textureSE" = "14",
                                "perimeterSE" = "15",
                                "areaSE" = "16",
                                "smoothnessSE" = "17",
                                "compactnessSE" = "18",
                                "concavitySE" = "19",
                                "concave_pointsSE" = "20",
                                "symmetrySE" = "21",
                                "fractal_dimensionSE" = "22",
                                "radiusW" = "23",
                                "textureW" = "24",
                                "perimeterW" = "25",
                                "areaW" = "26",
                                "smoothnessW" = "27",
                                "compactnessW" = "28",
                                "concavityW" = "29",
                                "concave_pointsW" = "30",
                                "symmetryW" = "31",
                                "fractal_dimensionW" = "32")

#Check specs/data type of the data:
spec(Data)
head(Data)
#tail(Data)
sapply(Data, function(x) sum(is.na(x)))

Data_drop <- Data[,-1] #drop ID
psych::describe(Data_drop) # Describe data
#psych::describeBy(Data_drop,Data_drop$Diagnosis) #Describe data by Diagnosis

Data_drop$Diagnosis <- as.factor(Data_drop$Diagnosis)
summary(Data_drop$Diagnosis)
ggplot(Data,aes(x = Diagnosis) ) +
    geom_bar(aes(y = ..count../sum(..count..), fill = Diagnosis)) +
        ylab("Percent") +
            ggtitle("Diagnosis percentages")


#Plot histogram for all Variables
Data_drop %>%
  keep(is.numeric) %>%
  gather() %>%
  ggplot(aes(value)) +
    geom_histogram() +
    facet_wrap(~key, scales = "free")

#Plot histogram for all Variables by Diagnosis
Data_drop %>%
  gather(key = "Var", value = "value", -Diagnosis) %>%
  ggplot(aes(x=value, fill=Diagnosis)) +
```

```
    geom_histogram(bins = 60) +
    facet_wrap(~Var, scales = "free")
#create correlation matrix
Cor <- Data_drop %>%
       select(-Diagnosis) %>%
       cor(method="spearman")

corrplot(Cor, type="upper", order="hclust")
#Removing all features with a correlation higher than 0.7, keeping the feature with the lower me
an.

highlyCor <- colnames(Data_drop[,-1])[findCorrelation(Cor, cutoff = 0.9, verbose = TRUE)]
highlyCor #highly correlted variables

Data_drop_cor <- Data_drop[, which(!colnames(Data_drop) %in% highlyCor)]#Drop highly correlcted
 variables

ncol(Data_drop_cor)-1
#Drop Diagnosis
Data_pca <- prcomp(Data_drop[,-1], center=TRUE, scale=TRUE)
summary(Data_pca)#need 10 components for variance over 95%
Data_pca_re <- prcomp(Data_drop_cor[,-1], center=TRUE, scale=TRUE)
summary(Data_pca_re)#7 components have variance over 97%
pca_df <- as.data.frame(Data_pca$x)
ggplot(pca_df, aes(x=PC1, y=PC2, col=Data$Diagnosis)) + geom_point(alpha=0.5)
pca_df_re <- as.data.frame(Data_pca_re$x)
ggplot(pca_df_re, aes(x=PC1, y=PC2, col=Data$Diagnosis)) + geom_point(alpha=0.5)
library(factoextra)
fviz_eig(Data_pca)
fviz_pca_var(Data_pca,
             col.var = "contrib", # Color by contributions to the PC
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE     # Avoid text overlapping
             )
fviz_eig(Data_pca_re)
fviz_pca_var(Data_pca_re,
             col.var = "contrib", # Color by contributions to the PC
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE     # Avoid text overlapping
             )


set.seed(1234) # so that the indices will be the same when re-run
trainIndices = createDataPartition(Data_drop$Diagnosis, p=.8, list=F)

train_raw = Data_drop %>%
  slice(trainIndices)

nrow(train_raw)

test_raw = Data_drop %>%
  slice(-trainIndices)
head(test_raw)
```

```
#verify if the randomization process is correct
prop.table(table(train_raw$Diagnosis))
prop.table(table(test_raw$Diagnosis))
#for multicolinearty droped Data_drop_cor
set.seed(1234) # so that the indices will be the same when re-run
trainIndices_drop = createDataPartition(Data_drop_cor$Diagnosis, p=.8, list=F)

train_drop_raw = Data_drop_cor %>%
  slice(trainIndices_drop)

nrow(train_drop_raw)
head(train_drop_raw)

test_drop_raw = Data_drop_cor %>%
  slice(-trainIndices_drop)
head(test_drop_raw)

#verify if the randomization process is correct
prop.table(table(train_drop_raw$Diagnosis))
prop.table(table(test_drop_raw$Diagnosis))

svm_raw <- svm(Diagnosis ~ ., data=train_raw, scale = FALSE, kernel =
"radial", type = "C-classification")
#svm_pca <- svm(Diagnosis ~ ., data=Data_pca)
svm_raw$gamma

pred_svm <- predict(svm_raw, test_raw)

cm_svm <- confusionMatrix(pred_svm, as.factor(test_raw$Diagnosis), positive = "M")
cm_svm
#summary(svm_raw)
svm_drop_raw <- svm(Diagnosis ~ ., data=train_drop_raw, scale = FALSE, kernel =
"radial", type = "C-classification")
#svm_pca <- svm(Diagnosis ~ ., data=Data_pca)
svm_drop_raw$gamma

pred_drop_svm <- predict(svm_drop_raw, test_drop_raw)

cm_drop_svm <- confusionMatrix(pred_drop_svm, as.factor(test_drop_raw$Diagnosis), positive = "M"
)
cm_drop_svm
#fitControl <- trainControl(method = "none", classProbs = TRUE)
fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                          repeats =5,
                           preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                           classProbs = TRUE,
                           summaryFunction = twoClassSummary)
set.seed(825)
svm_raw_caret <- train(Diagnosis~.,
                    data = train_raw,
                    method="svmRadial",
                    metric="ROC",
                    trace=FALSE,
```

```
                    trControl=fitControl)
svm_raw_caret$finalModel
pred_svm_caret <- predict(svm_raw_caret, test_raw)
cm_svm_caret <- confusionMatrix(pred_svm_caret, as.factor(test_raw$Diagnosis), positive = "M")
cm_svm_caret

#fitControl <- trainControl(method = "none", classProbs = TRUE)
fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                          repeats =5,
                           preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                           classProbs = TRUE,
                           summaryFunction = twoClassSummary)
set.seed(825)
svm_drop_caret <- train(Diagnosis~.,
                    data = train_drop_raw,
                    method="svmRadial",
                    metric="ROC",
                    trace=FALSE,
                    trControl=fitControl)
svm_drop_caret$finalModel
pred_drop_svm_caret <- predict(svm_drop_caret, test_drop_raw)
cm_drop_svm_caret <- confusionMatrix(pred_drop_svm_caret, as.factor(test_drop_raw$Diagnosis), po
sitive = "M")
cm_drop_svm_caret

fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                          repeats =5,
                           preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                           classProbs = TRUE,
                           summaryFunction = twoClassSummary)
set.seed(825)
svm_scale <- train(Diagnosis~.,
                    data = train_raw,
                    method="svmRadial",
                    metric="ROC",
                    preProcess=c('center', 'scale'),
                    trace=FALSE,
                    trControl=fitControl)
svm_scale$finalModel
pred_svm_scale <- predict(svm_scale, test_raw)
cm_svm_scale <- confusionMatrix(pred_svm_scale, as.factor(test_raw$Diagnosis), positive = "M")
cm_svm_scale


fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                          repeats =5,
                           preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                           classProbs = TRUE,
                           summaryFunction = twoClassSummary)
set.seed(825)
svm_scale_pca <- train(Diagnosis~.,
```

```
                    data = train_raw,
                    method="svmRadial",
                    metric="ROC",
                    preProcess=c('center', 'scale','pca'),
                    trace=FALSE,
                    trControl=fitControl)
svm_scale_pca$finalModel
pred_svm_scale_pca <- predict(svm_scale_pca, test_raw)
cm_svm_scale_pca <- confusionMatrix(pred_svm_scale_pca, as.factor(test_raw$Diagnosis), positive
 = "M")
cm_svm_scale_pca

fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                            repeats =5,
                            preProcOptions = list(thresh = 0.95), # threshold for pca preprocess
                            classProbs = TRUE,
                            summaryFunction = twoClassSummary)
set.seed(825)
svm_drop_pca  <- train(Diagnosis~.,
                    data = train_drop_raw,
                    method="svmRadial",
                    metric="ROC",
                    preProcess=c('center', 'scale','pca'),
                    trace=FALSE,
                    trControl=fitControl
                    #tuneLength = 8
                    )
svm_drop_pca
pred_svmdrop_pca <- predict(svm_drop_pca, train_drop_raw)
cm_svmdrop_pca <- confusionMatrix(pred_svmdrop_pca, as.factor(train_drop_raw$Diagnosis), positiv
e = "M")
cm_svmdrop_pca

svmGrid <-  expand.grid(sigma = c(.01, .015, 0.2,0.25, 0.275,0.3),
                    C = c(0.25, 0.5, 0.75, 0.9, 1, 1.1, 1.25))

nrow(svmGrid)
fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                            repeats =5,
                            preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                            classProbs = TRUE,
                            summaryFunction = twoClassSummary)
set.seed(825)
svm_tune <- train(Diagnosis ~ .,
                  data = train_drop_raw,
                  method="svmRadial",
                  metric="ROC",
                  preProcess=c('center', 'scale','pca'),
                  trace=FALSE,
                  trControl=fitControl,
                  tuneGrid = svmGrid)
#svm_tune
```

```
#ten fold The final values used for the model were sigma = 0.015 and C = 0.9.
#five fold The final values used for the model were sigma = 0.015 and C = 0.75.
#The final values used for the model were sigma = 0.015 and C = 1.

plot(svm_tune)
pred_svm_tune <- predict(svm_tune, train_drop_raw)
cm_svm_tune <- confusionMatrix(pred_svm_tune, as.factor(train_drop_raw$Diagnosis), positive =
"M")
cm_svm_tune

#Plotting the Resampling Profile: Examine the relationship between the estimates of performance
 and the tuning parameters

fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                            repeats =5,
                            classProbs = TRUE,
                            summaryFunction = twoClassSummary)
set.seed(825)
model_nnet <- train(Diagnosis~.,
                    data = train_drop_raw,
                    method="nnet",
                    metric="ROC",
                    preProcess=c('center', 'scale'),
                    trace=FALSE,
                    tuneLength=10,
                    trControl=fitControl)
#model_nnet
pred_nnet <- predict(model_nnet, test_drop_raw)
cm_nnet <- confusionMatrix(pred_nnet, as.factor(test_drop_raw$Diagnosis), positive = "M")

# #grid search for nnet
# nnetGrid <-  expand.grid(size = seq(from = 1, to = 10, by = 1),
#                          decay = seq(from = 0.1, to = 0.5, by = 0.1))
cm_nnet
set.seed(825)
fitControl <- trainControl(method="repeatedcv",
                           number = 5,
                            repeats =5,
                            preProcOptions = list(thresh = 0.8), # threshold for pca preprocess
                            classProbs = TRUE,
                            summaryFunction = twoClassSummary)
nnet_pca <- train(Diagnosis~.,
                  data = train_raw,
                  method = "nnet",
                  metric = "ROC",
                  preProcess=c('center', 'scale','pca'),
                  trace=FALSE,
                  tuneLength=10,
                  trControl = fitControl)
#nnet_pca
pred_nnet_pca <- predict(nnet_pca, test_raw)
cm_nnet_pca <- confusionMatrix(pred_nnet_pca, as.factor(test_raw$Diagnosis), positive = "M")
cm_nnet_pca
```

```
cm_nnet_pca
model_list <- list(Caret_svm_scale= svm_scale, Caret_svm_scale_pca=svm_scale_pca,
                   Caret_drop_svm_pca=svm_drop_pca, Caret_nnet_pca=nnet_pca)
resamples <- resamples(model_list)
bwplot(resamples, metric = "ROC")
overall <- data.frame(model = rep(c("Svm_raw", "Svm_drop","Caret_svm_scale", "Caret_svm_scale_pc
a", "Caret_drop_svm_pca", "Caret_nnet_pca")),
                      rbind(cm_svm$overall,
                            cm_drop_svm$overall,
                            cm_svm_scale$overall,
                            cm_svm_scale_pca$overall,
                            cm_svmdrop_pca$overall,
                            cm_nnet_pca$overall))
#overall
overall_gather <- overall[,1:3] %>%
  gather(measure, value, Accuracy:Kappa)
#overall_gather
byClass <- data.frame(model = rep(c("Svm_raw", "Svm_drop","Caret_svm_scale", "Caret_svm_scale_pc
a", "Caret_drop_svm_pca", "Caret_nnet_pca")),
                      rbind(cm_svm$byClass,
                            cm_drop_svm$byClass,
                            cm_svm_scale$byClass,
                            cm_svm_scale_pca$byClass,
                            cm_svmdrop_pca$byClass,
                            cm_nnet_pca$byClass))
#byClass
byClass_gather <- byClass[,1:3] %>%
  gather(measure, value, Sensitivity:Specificity)
#byClass_gather

overall_byClass_gather <- rbind(overall_gather, byClass_gather)
overall_byClass_gather <- within(overall_byClass_gather, model <- factor(model, levels = c("Svm_
raw", "Svm_drop","Caret_svm_scale", "Caret_nnet_pca", "Caret_svm_scale_pca", "Caret_drop_svm_pc
a")))

#overall_byClass_gather
OV<-overall_byClass_gather %>%
  filter(measure == "Accuracy")  %>%
  arrange(value)

#OV

Per<-ggplot(OV, aes(x = model, y = value)) +
    geom_point(shape=1)  +
    scale_x_discrete(labels = abbreviate) +
    scale_y_continuous(breaks=c(0.6,0.8, 0.94, 0.96,0.97,0.98, 0.99))

Performance <- ggplotly(Per) %>%
  layout(title = 'Interactive Model Performance',
         xaxis = list(title = 'Model'),
         yaxis = list (title = 'Accuracy'))
Performance
```