# SMU Data Science
# Statistics 6372
# Sec. 402 (2019 Spr)
# Final Project

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# Contents

# Introduction

Data science plays an increasing role for organizations to manage their info and contribute to their processes. Statistical science forms a crucial backbone—it spans real world considerations and provides a framework to any object of study, providing characterization, modeling, and ultimately prediction.

In this statistics project we have two primary objectives. The first objective is to demonstrate exploratory data analysis and building a logistic regression model.
With the logistic regression model as the base, the second objective is to create competing models to contrast and enhance the prediction performance metrics.
We considered data from multiple data sources and selected a cancer diagnostic set from an academic setting. The project was an exercise in working and refining models for explanatory and predictive analysis.

# Data Description

## Overview of the Data Set

The data is a collection of the Breast Cancer Diagnostic Data Set collected by the University of Wisconsin-Madison. 569 observations were taken using digitized imaging of breast mass biopsy samples taken between 1989 and 1991. Biopsies were acquired using FNA, Fine Needle Aspiration.

The data set was taken from UC Irvine's Machine Learning repository.
https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Diagnostic%29

Below is a description of the data set:

DEPENDENT VARIABLE
Diagnosis: Binomial – B [benign] or M [malignant]

INDEPENDENT VARIABLES
Ten real-valued features are computed for each cell nucleus:

a) radius (distance from center to points on the perimeter)
b) texture (standard deviation of gray-scale values)
c) perimeter
d) area
e) smoothness (local variation in radius lengths)
f) compactness (perimeter^2 / area - 1.0)
g) concavity (severity of concave portions of the contour)

h) concave points (number of concave portions of the contour)
i) symmetry
j) fractal dimension ("coastline approximation" - 1)

For each of these metrics the data set included

- Mean
- Standard Error
- Worst [for asymmetrical masses, this is the “longest” or “largest” value]

## Exploratory Data Analysis

First, we validate assumptions of the data, then we apply visual analysis aided by a PCA to identify the influential parameters.

### Data Assumption Checks

**Sample Size**: The sample size is moderately sized with over 500 observations. Approximately 37.3% were Malignant and 62.7% were Benign.

**Independence**: Specific details as to patient selection were not available, so we will assume that independence is maintained. Points of possible concern would be that it is a sample without proper diversity to represent the true population.

**Normality**: Normality assumptions were for the most part met. In cases where skew exists, the Central Limit Theorem applied.

Figures A-1: Assumption Checks

### Analysis of Data Correlation

**Radius, Perimeter, Area**

These are obviously highly correlated since they are all a function of the radius and Pi. This is confirmed with a visual examination via scatter plot that shows a strong positive correlation present between size-based measurements of the tumorous mass and the "malignant" vs "benign" diagnosis.

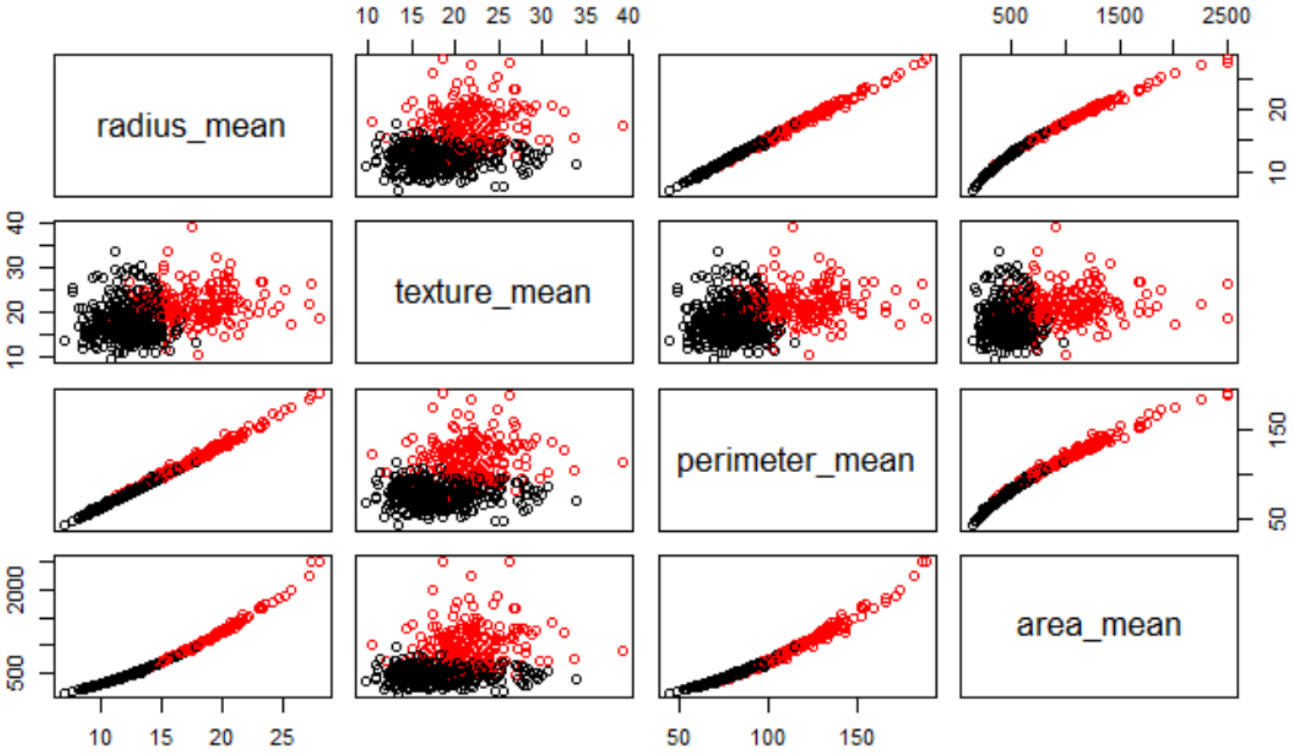
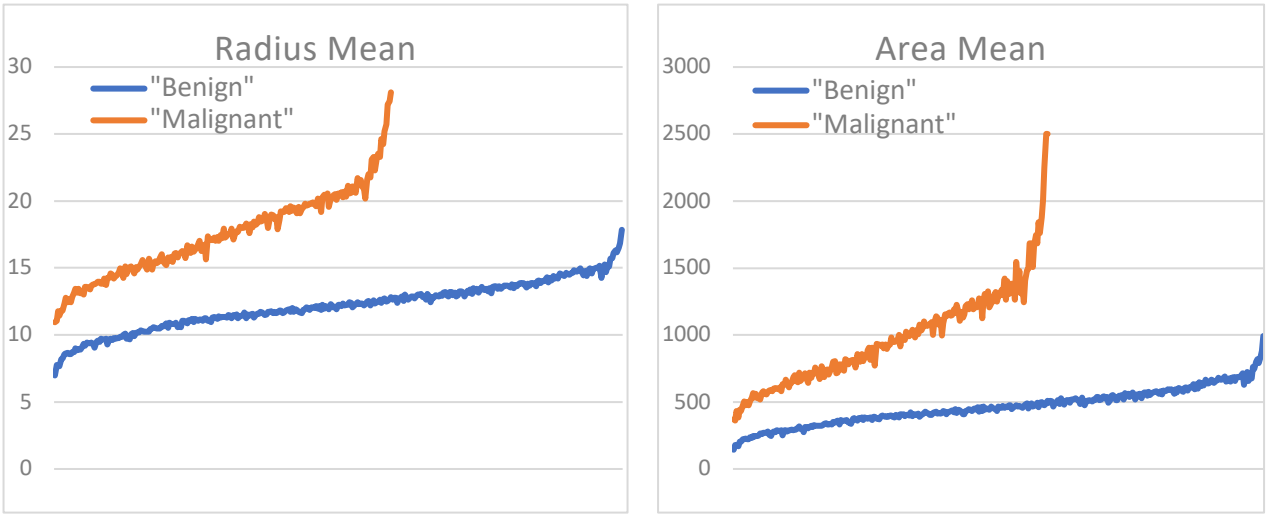
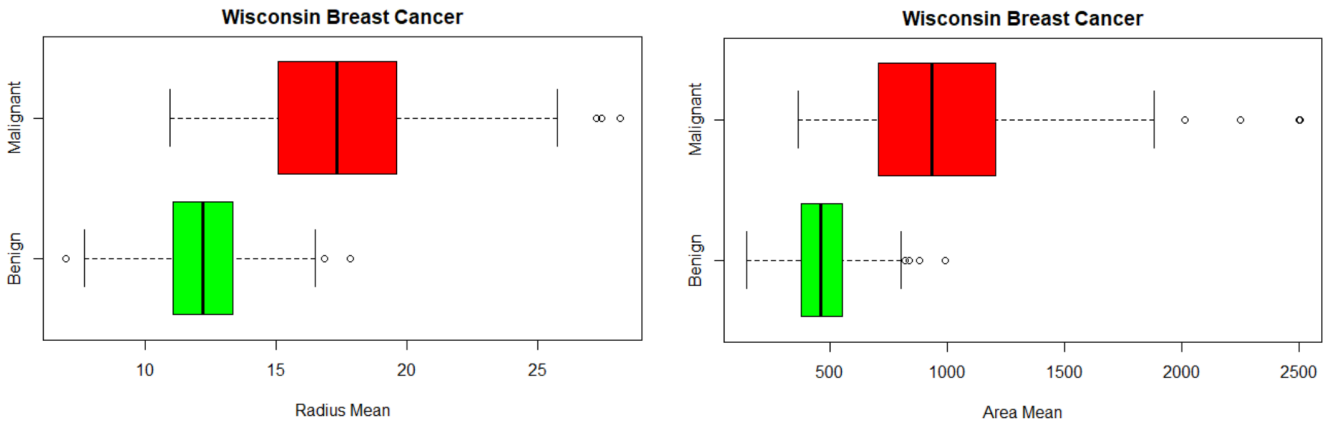



Figure A-2: Correlations

The line chart below shows the progression of measurements, from smallest to largest, for both radius and area, separated by diagnosis. Overall the malignant biopsies appear to be larger.



Figures A-3: Comparison of Benign & Malignant
A box plot comparison also validates this initial observation.




Figures A-4: Boxplots of Benign vs. Malignant

## Overall Sample Behavior

Looking at the dashboard below, it's apparent that despite the majority of samples taken being benign, the malignant samples overall make up more than half the area, and the variance of the malignant samples is almost 7 times higher.

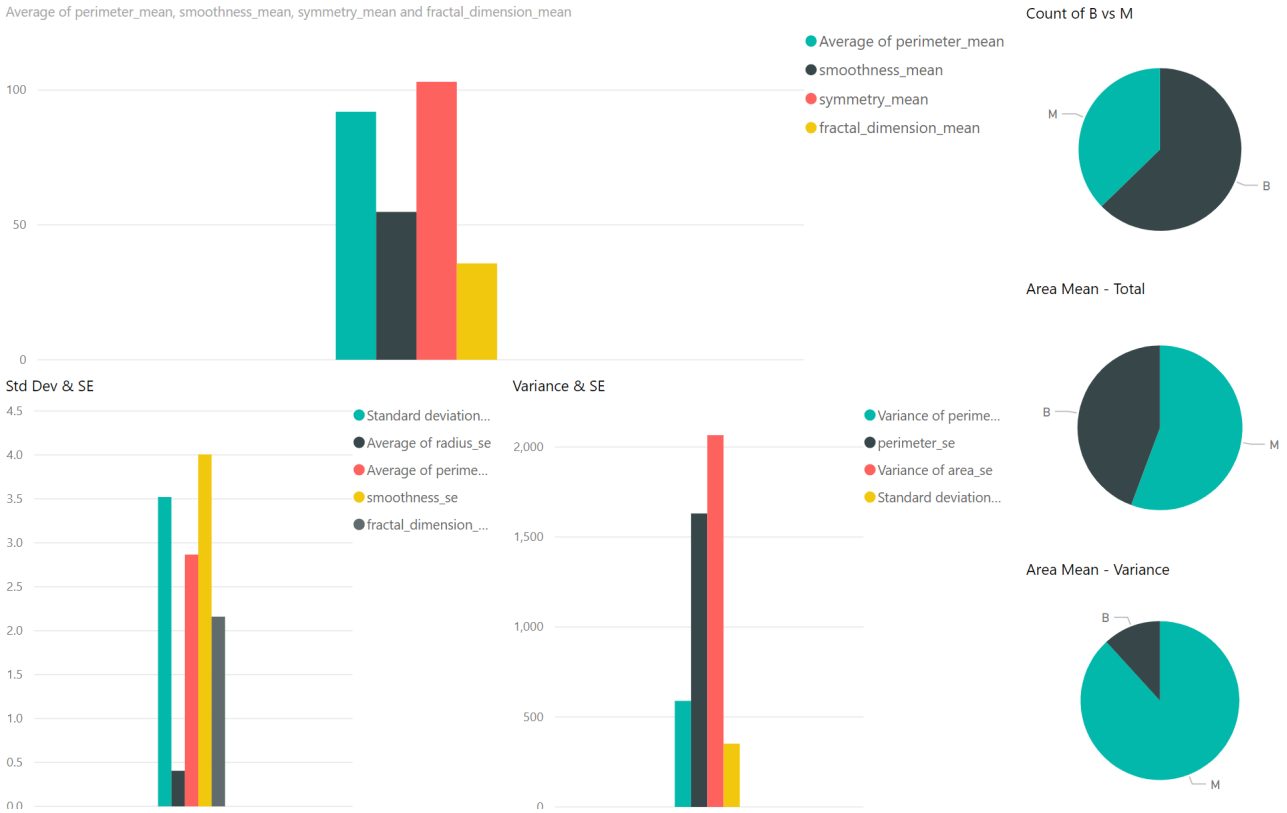


Figure A-5: Variance

When we select just the Benign subset, we can see across all measurements of variance, standard deviation, and standard error for measurements of the samples size [i.e. radius, perimeter, and area], that these are lower across the board.


Figure A-6: Variance, Benign

When selecting the Malignant sample, again, the mean, standard error, and variance of size-related measurements go higher than the overall average of those categories.

Other qualities like smoothness, symmetry, and fractal do not appear to favor either Malignant or Benign diagnoses. (see below highlighted Figure A-7).

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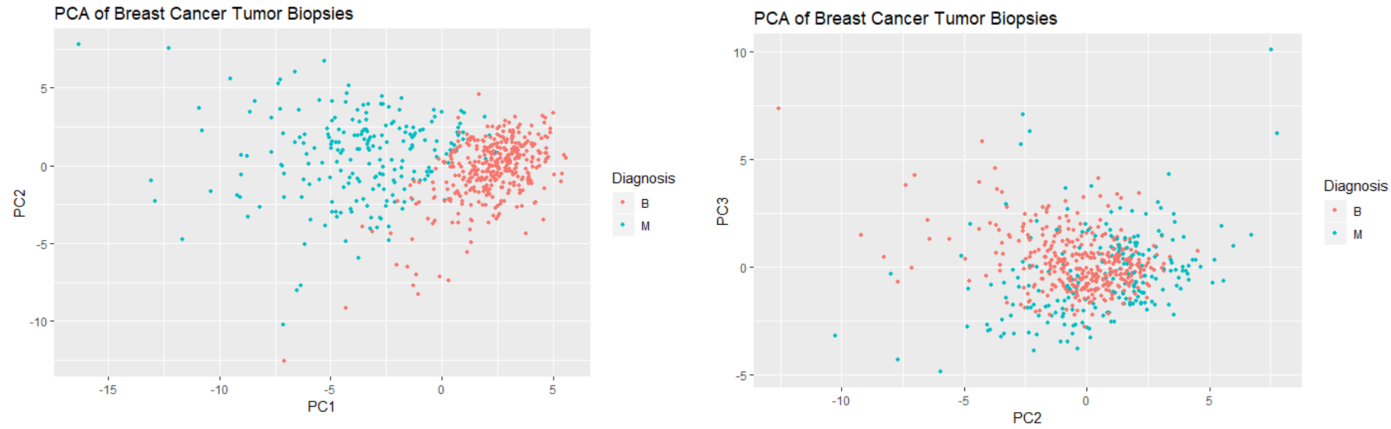
Figure A-7: Variance, Malignant

## Principal Components Analysis

Below we will conduct PCA on the predictors and plot the first few Principal Components [PC's] against each other and examine what level of separation they provide. The number of PCs to explore can be dictated by the scree plot. As part of the initial exploratory data analysis, this will allow us to see if there are clear patterns that emerge in the data.




Figures A-8: PCA Scree plots

We can see in the first graphic that a clear separation exists between malignant and benign, which complements our initial visual examinations above. Because this clear separation exists in the PC's, this implies that a predictive model will probably do well.

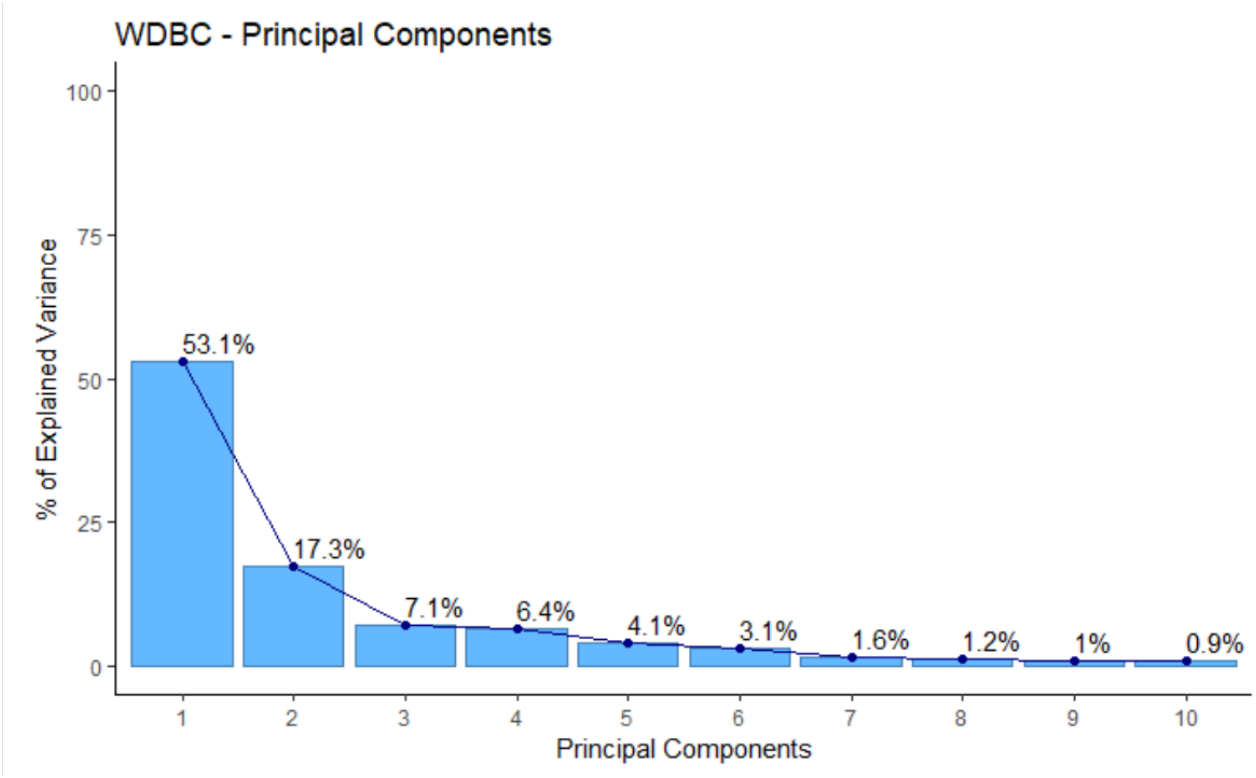



Figure A-9: % of Explained Variance vs. Principal Components

```
Importance of components:
                          Comp.1    Comp.2     Comp.3     Comp.4     Comp.5     Comp.6     Comp.7
Standard deviation     0.5751101 0.3281171 0.21051526 0.19984110 0.15953874 0.13832097 0.09923315
Proportion of Variance 0.5309769 0.1728349 0.07114442 0.06411259 0.04086072 0.03071494 0.01580837
Cumulative Proportion  0.5309769 0.7038118 0.77495621 0.83906880 0.87992952 0.91064446 0.92645284
```

Looking at the performance of the PC's, we can see that 70% of the variance is explained by the first 2 components, and improvement significantly tapers off following that. This is further emphasized by the two scatterplots above showing significantly poorer separation using PC2 x PC2 compared to PC1 x PC2. We can see from this pairs plot of just the first few variables, that the malignant and benign groups are pretty well separated.

Given the above, we suspect an LDA analysis is appropriate to determine if the quantitative measurement parameters can be used to determine binomial categorical diagnosis response. However, we will do multiple analysis models and compare the results.

## Objective 1 – Explanatory Analysis: Logistic Regression

Our initial model will be a logistic regression without modeling in the variable interactions. However, the immediate concern is the covariance between multiple parameters. Running the full model through a VIF analysis shows significant covariance, with most of the scores having VIF values well above 10.

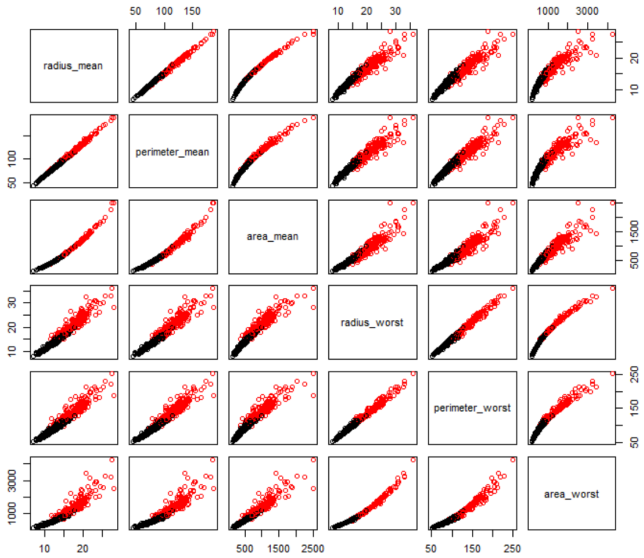
| | | | | |
|---|---|---|---|---|
| radius_mean | texture_mean | perimeter_mean | area_mean | smoothness_mean |
| 3806.115296 | 11.884048 | 3786.400419 | 347.878657 | 8.194282 |
| compactness_mean | concavity_mean | concave_points_mean | symmetry_mean | fractal_dimension_mean |
| 50.505168 | 70.767720 | 60.041733 | 4.220656 | 15.756977 |
| radius_se | texture_se | perimeter_se | area_se | smoothness_se |
| 75.462027 | 4.205423 | 70.359695 | 41.163091 | 4.027923 |
| compactness_se | concavity_se | concave_points_se | symmetry_se | fractal_dimension_se |
| 15.366324 | 15.694833 | 11.520796 | 5.175426 | 9.717987 |
| radius_worst | texture_worst | perimeter_worst | area_worst | smoothness_worst |
| 799.105946 | 18.569966 | 405.023336 | 337.221924 | 10.923061 |
| compactness_worst | concavity_worst | concave_points_worst | symmetry_worst | fractal_dimension_worst |
| 36.982755 | 31.970723 | 36.763714 | 9.520570 | 18.861533 |

This is not entirely surprising because:

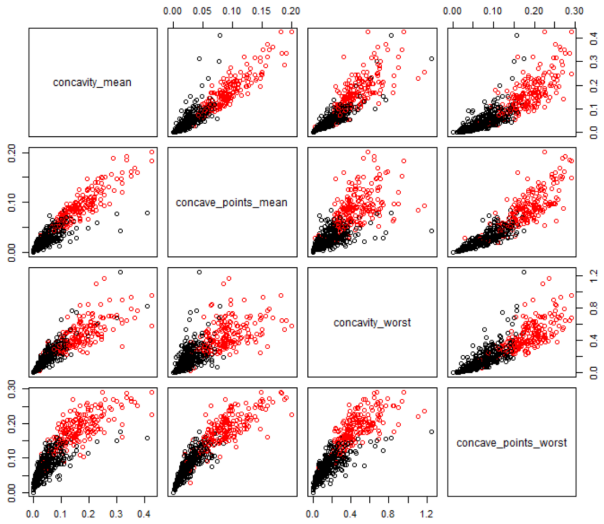
1. Perimeter, Radius, and Area are all of a function of each other with respect to Pi.
2. The other category of measurements is simply the standard error [i.e. variance] or the worst single measurement used to derive this.

Visually inspecting this correlation also verifies this assumption as well.

**Radius, Perimeter, Area - Mean vs Worst**

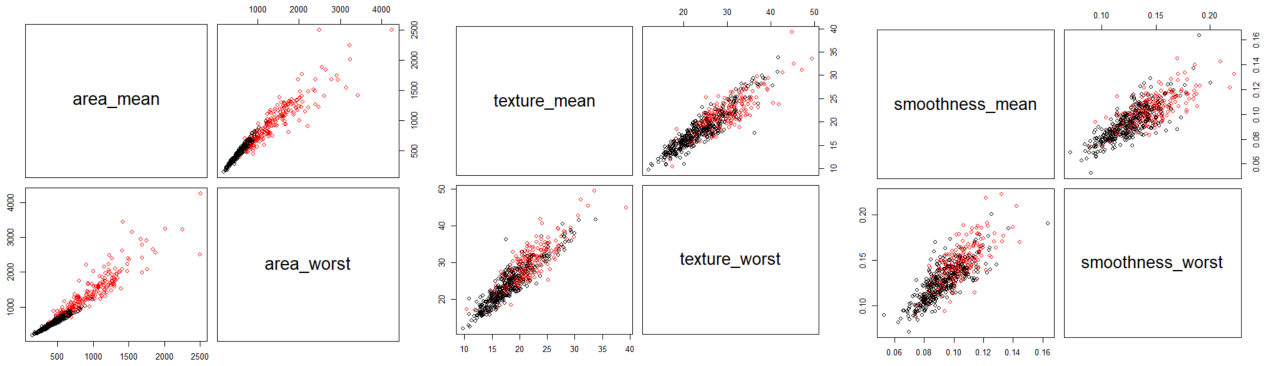



**Concavity & Concavity Point: Mean vs**




Figures A-10: Correlations, Mean vs. Worst

**Area: Mean vs Worst** **Texture: Mean vs Worst** **Smoothness: Mean vs Worst**




Figures A-11: Correlations, Mean vs. Worst

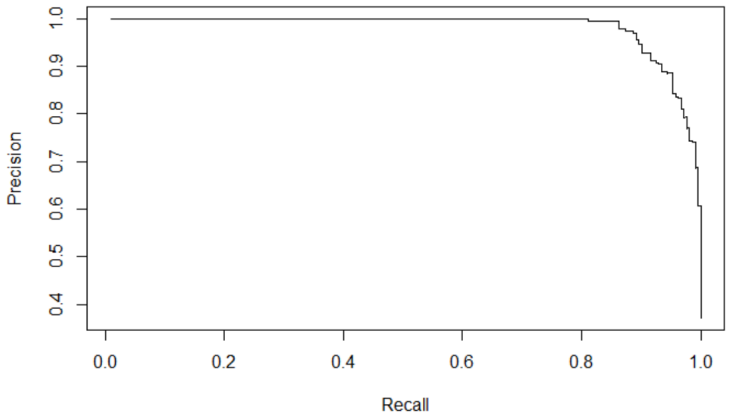
By simplifying the model to only use the Area measurements to represent the tumor size [which overall had the lower comparative VIF values than respective Radius and Perimeter measurements], and only keep the "mean" category of measurements, we were able to reduce the parameter VIF's to values less than 10 across the board.

| | | | | |
|---|---|---|---|---|
| texture_mean | area_mean | smoothness_mean | compactness_mean | concavity_mean |
| 1.764829 | 3.250272 | 4.288467 | 5.763065 | 4.987014 |
| concave_points_mean | symmetry_mean | fractal_dimension_mean | | |
| 5.744502 | 1.823926 | 8.311224 | | |

When comparing the two logistic regression models, the "full" model had a significantly worse AIC score than the simplified one.

**ROC Curve for Reduced Logistic Model**

We can see significant lift on the reduced model that accounts for Area mean, texture mean, smoothness mean, and concave points mean.




Figures A-12: ROC Curve for Reduced Logistic Model

## Comparison of outputs for different logistic models:

In the following section, we are comparing different logistic models.

### OUTPUT FOR FULL LOGISTIC MODEL:

```
glm(formula = diagnosis  ~ ., family = binomial(link = "logit"),
    data = bc.boolean, control = list(maxit = 50))

Deviance Residuals:
   Min      1Q  Median      3Q     Max
 -8.49    0.00    0.00    0.00    8.49

Coefficients:
                          Estimate Std. Error    z value Pr(>|z|)
(Intercept)             -1.704e+16  1.216e+08 -140095174   <2e-16 ***
radius_mean             -4.508e+15  4.930e+07  -91446497   <2e-16 ***
texture_mean            -2.681e+13  2.257e+06  -11879545   <2e-16 ***
perimeter_mean           5.592e+14  7.131e+06   78428443   <2e-16 ***
area_mean                6.374e+12  1.492e+05   42711010   <2e-16 ***
smoothness_mean          4.804e+16  5.731e+08   83827859   <2e-16 ***
compactness_mean        -2.931e+16  3.789e+08  -77357485   <2e-16 ***
concavity_mean           3.110e+14  2.971e+08    1046677   <2e-16 ***
concave_points_mean      8.171e+15  5.623e+08   14531119   <2e-16 ***
symmetry_mean           -8.564e+15  2.110e+08  -40582198   <2e-16 ***
fractal_dimension_mean  -1.030e+16  1.583e+09   -6507058   <2e-16 ***
radius_se                8.161e+15  8.821e+07   92524229   <2e-16 ***
texture_se              -4.617e+14  1.047e+07  -44105313   <2e-16 ***
perimeter_se            -8.989e+14  1.168e+07  -76951480   <2e-16 ***
area_se                  6.591e+12  3.971e+05   16595576   <2e-16 ***
smoothness_se           -1.037e+16  1.882e+09   -5509676   <2e-16 ***
compactness_se           4.729e+16  6.164e+08   76728075   <2e-16 ***
concavity_se            -2.689e+16  3.696e+08  -72764771   <2e-16 ***
concave_points_se        1.993e+17  1.549e+09  128680606   <2e-16 ***
symmetry_se             -4.806e+16  7.749e+08  -62015895   <2e-16 ***
fractal_dimension_se    -4.364e+17  3.317e+09 -131546226   <2e-16 ***
radius_worst             1.102e+15  1.647e+07   66911477   <2e-16 ***
texture_worst            1.390e+14  1.974e+06   70396825   <2e-16 ***
perimeter_worst          6.421e+13  1.686e+06   38076691   <2e-16 ***
area_worst              -9.950e+12  9.082e+04 -109559685   <2e-16 ***
smoothness_worst        -6.379e+15  4.076e+08  -15649766   <2e-16 ***
compactness_worst       -7.493e+15  1.088e+08  -68848424   <2e-16 ***
concavity_worst          6.282e+15  7.632e+07   82312806   <2e-16 ***
concave_points_worst    -7.308e+15  2.597e+08  -28137342   <2e-16 ***
symmetry_worst           1.098e+16  1.404e+08   78221084   <2e-16 ***
fractal_dimension_worst  4.755e+16  6.771e+08   70226947   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 751.44  on 568  degrees of freedom
Residual deviance: 792.96  on 538  degrees of freedom
AIC: 854.96
```

The AIC for Full Logistic is 854.96.

### OUTPUT FOR LASSO MODEL

```
> summary(main.lasso.glm)

Call:
glm(formula = diagnosis ~ concavity_mean + concave_points_mean +
    fractal_dimension_mean + radius_se + smoothness_se + compactness_se +
    symmetry_se + fractal_dimension_se + radius_worst + texture_worst +
    smoothness_worst + concavity_worst + concave_points_worst +
    symmetry_worst, family = binomial(link = "logit"), data = bc.clean)
```

```
Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.6432  -0.0231  -0.0011   0.0001   3.4988

Coefficients:
                         Estimate Std. Error z value Pr(>|z|)
(Intercept)             -49.94186   14.89788  -3.352 0.000801 ***
concavity_mean           12.70977   38.43786   0.331 0.740903
concave_points_mean      26.32819   70.41186   0.374 0.708466
fractal_dimension_mean  -44.16790  144.43201  -0.306 0.759754
radius_se                15.63875    4.93316   3.170 0.001524 **
smoothness_se           273.77291  203.10733   1.348 0.177683
compactness_se          -95.33134   60.50492  -1.576 0.115119
symmetry_se             -73.18646  122.55678  -0.597 0.550398
fractal_dimension_se   -270.98565  545.40470  -0.497 0.619293
radius_worst              1.25629    0.42384   2.964 0.003036 **
texture_worst             0.37798    0.08829   4.281 1.86e-05 ***
smoothness_worst         31.84886   36.50939   0.872 0.383019
concavity_worst           8.12142   10.47793   0.775 0.438282
concave_points_worst     30.35111   27.64683   1.098 0.272285
symmetry_worst           23.54037   15.20640   1.548 0.121609
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 751.440  on 568  degrees of freedom
Residual deviance:  55.675  on 554  degrees of freedom
AIC: 85.675

Number of Fisher Scoring iterations: 10
```

The AIC for Lasso is 85.675.

## OUTPUT FOR STEPWISE SELECTION MODEL

```
> summary(main.glm.step)

Call:
glm(formula = diagnosis ~ radius_mean + texture_mean + area_mean +
    smoothness_mean + compactness_mean + concavity_mean + concave_points_mean +
    symmetry_mean + fractal_dimension_mean + perimeter_se + area_se +
    smoothness_se + compactness_se + concavity_se + concave_points_se +
    symmetry_se + fractal_dimension_se + radius_worst + texture_worst +
    perimeter_worst + area_worst + concavity_worst + symmetry_worst +
    fractal_dimension_worst, family = binomial(link = "logit"),
    data = bc.clean)

Deviance Residuals:
      Min         1Q     Median         3Q        Max
-0.003832   0.000000   0.000000   0.000000   0.004291

Coefficients:
                         Estimate Std. Error z value Pr(>|z|)
(Intercept)            -5.914e+03  2.619e+05  -0.023    0.982
radius_mean            -6.630e+03  1.150e+05  -0.058    0.954
texture_mean            1.913e+02  1.345e+03   0.142    0.887
area_mean               6.077e+01  1.079e+03   0.056    0.955
smoothness_mean         3.914e+04  2.517e+05   0.155    0.876
compactness_mean       -8.621e+04  9.326e+05  -0.092    0.926
concavity_mean          2.852e+04  2.402e+05   0.119    0.905
concave_points_mean     5.886e+04  1.544e+06   0.038    0.970
symmetry_mean          -1.964e+04  1.347e+05  -0.146    0.884
fractal_dimension_mean  1.626e+05  1.120e+06   0.145    0.885
perimeter_se           -1.253e+03  1.822e+04  -0.069    0.945
area_se                 1.562e+02  2.259e+03   0.069    0.945
smoothness_se          -9.793e+04  1.472e+06  -0.067    0.947
compactness_se          9.217e+04  7.142e+05   0.129    0.897
concavity_se           -8.131e+04  1.097e+06  -0.074    0.941
concave_points_se       4.398e+05  6.736e+06   0.065    0.948
symmetry_se            -1.038e+05  2.160e+06  -0.048    0.962
fractal_dimension_se   -1.092e+06  1.065e+07  -0.103    0.918
radius_worst            2.226e+03  2.134e+04   0.104    0.917
texture_worst           7.269e+01  3.150e+03   0.023    0.982
perimeter_worst         1.267e+02  1.355e+03   0.093    0.926
area_worst             -1.626e+01  1.165e+02  -0.140    0.889
concavity_worst         6.737e+03  1.051e+05   0.064    0.949
```

```
symmetry_worst           2.201e+04  3.283e+05   0.067    0.947
fractal_dimension_worst  5.899e+04  1.032e+06   0.057    0.954

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 7.5144e+02  on 568  degrees of freedom
Residual deviance: 1.6713e-04  on 544  degrees of freedom
AIC: 50

Number of Fisher Scoring iterations: 25
```

The AIC for the Stepwise Selection Model is 50.

## OUTPUT FOR SIMPLIFIED LOGISTIC MODEL

```
glm(formula = diagnosis ~ texture_mean + area_mean + smoothness_mean +
    compactness_mean + concavity_mean + concave_points_mean +
    symmetry_mean + fractal_dimension_mean, family = binomial(link = "logit"),
    data = bc.boolean, control = list(maxit = 50))


Deviance Residuals:
     Min        1Q    Median        3Q       Max
-2.02338  -0.14079  -0.03572   0.01120   3.00158

Coefficients:
                          Estimate Std. Error z value Pr(>|z|)
(Intercept)             -27.253090   6.400270  -4.258 2.06e-05 ***
texture_mean              0.384407   0.063485   6.055 1.40e-09 ***
area_mean                 0.011787   0.002728   4.320 1.56e-05 ***
smoothness_mean          79.598004  32.979533   2.414   0.0158 *
compactness_mean        -13.731887  12.700676  -1.081   0.2796
concavity_mean           13.249936   8.090709   1.638   0.1015
concave_points_mean      57.230227  28.042055   2.041   0.0413 *
symmetry_mean            17.779963  10.854712   1.638   0.1014
fractal_dimension_mean -26.454327  82.469431  -0.321   0.7484
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 751.44  on 568  degrees of freedom
Residual deviance: 149.01  on 560  degrees of freedom
AIC: 167.01
```

The AIC for Simplified Logistic is 167.01.

## CONFIDENCE INTERVALS FOR PARAMETERS OF REDUCED MODEL

```
                              2.5 %       97.5 %
(Intercept)             -4.053919e+01 -15.31563155
texture_mean             2.674975e-01   0.51837370
area_mean                6.757782e-03   0.01749949
smoothness_mean          1.771586e+01 147.27093557
compactness_mean        -3.951821e+01  11.10875994
concavity_mean          -2.529860e+00  29.24616163
concave_points_mean      3.911450e+00 114.21970795
symmetry_mean           -3.644306e+00  39.25139134
fractal_dimension_mean -1.925487e+02 132.60062490
```

## Interpretation for Objective 1 Logistic Regression

The significant parameters to the model were:
area_mean [p-value < 0.001], texture_mean [p-value < 0.001],
smoothness_mean [p-value 0.0158], and concave_points_mean [p-value 0.0413].

area_mean $e^{0.011787} =\sim 1.012$
Texture_mean $e^{0.384407} =\sim 1.469$
smoothness_mean $e^{79.598004} =\sim 3.706 * 10^{34}$
concave_points_mean $e^{57.230227} = 7.158 * 10^{24}$

For Area, holding all other parameters constant, the 1 unit is $[e^{0.011787 * 1 \text{ unit}}] = 1.012$ times more likely to be Malignant than Benign, and
the 5 units is $[e^{0.011787 * 5 \text{ units}}] = 1.061$ times more likely to be Malignant than Benign.

For Texture, holding all other parameters constant, 1 unit is $[e^{0.384407 * 1 \text{ unit}}] = 1.469$ times more likely to be Malignant than Benign, and
the 5 units is $[e^{0.384407 * 5 \text{ units}}] = 6.835$ times more likely to be Malignant than Benign.

For Smoothness, holding all other parameters constant, 1 unit is $[e^{79.598004 * 1 \text{ unit}}] =$ 3.706 * 10^34 times more likely to be Malignant than Benign, and the
5 units is $[e^{79.598004 * 5 \text{ units}}] = 6.996 * 10^{172}$ times more likely to be Malignant than Benign.

For Concave points, holding all other parameters constant, the 1 unit is $[e^{57.230227 * 1 \text{ unit}}] =$ 7.158 *10^24 times more likely to be Malignant than Benign, and
the 5 units $[e^{57.230227 * 5 \text{ units}}] = 1.879 * 10^{124}$ times more likely to be Malignant than Benign.

## Conclusion:

Model-building and effectiveness depends highly upon the particular area, scope of study, and the nature of data available. Different models will vary in applicability and desirability of metrics, especially in the overall interpretability and predictive ability. In this case, the AIC metric is improved, going from a full to a reduced logistic model. The AIC is further improved with a LASSO, and is best when applying stepwise selection. Despite the Stepwise Feature Selection having a lower AIC score of 50, when looking at the practical significance in light of the parameter estimates, it likely overfits this data set, and will perform poorly for additional observations in the same or similar studies.

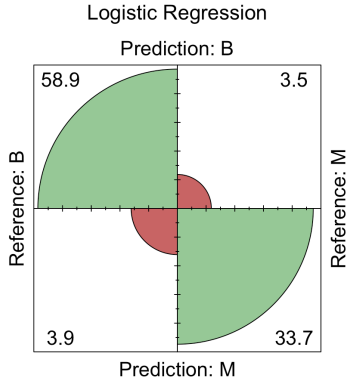
# Objective 2 – Model Creation & Comparison

We have selected 5-fold cross-validation for the models, given the relatively small sample size of the dataset. Also, from page 184 of book "An Introduction to Statistical Learning, 2013".

> *To summarize, there is a bias-variance trade-off associated with the choice of k in k-fold cross-validation. Typically, given these considerations, one performs k-fold cross-validation using k = 5 or k = 10, as these values have been shown empirically to yield test error rate estimates that suffer neither from excessively high bias nor from very high variance.*

## Logistic Regression:

From the confusion matrix and model metrics, it can be observed that the logistic regression model has a prediction accuracy of 92.6%, recall of 90.5%, and F-Score of 90.14%.

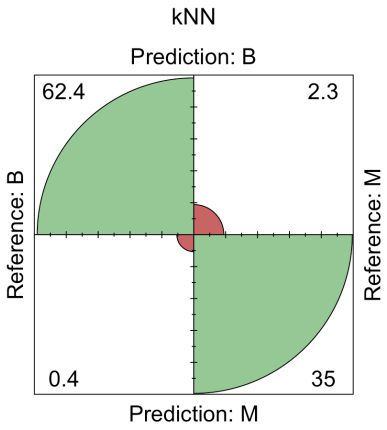



```
##                 Model  Accuracy    Recall Precision        FNR    Fscore
## 1 Logistic Regression 0.9261863 0.9056604 0.8971963 0.09433962 0.9014085
```

Figure B-1: Logistic Regression

## k-Nearest Neighbours:

From the confusion matrix and model metrics, it can be observed that the kNN model has a prediction accuracy of 97.3%, recall of 93.86%, and F-score of 96.36%.

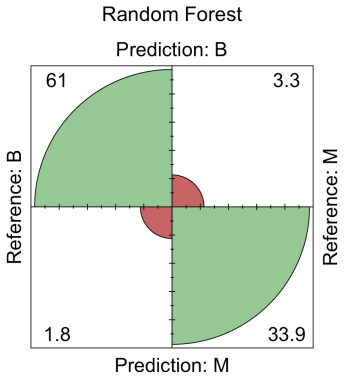



```
##   Model Accuracy    Recall Precision        FNR    Fscore
## 1  k-NN 0.973638 0.9386792 0.9900498 0.06132075 0.9636804
```

Figure B-2: kNN

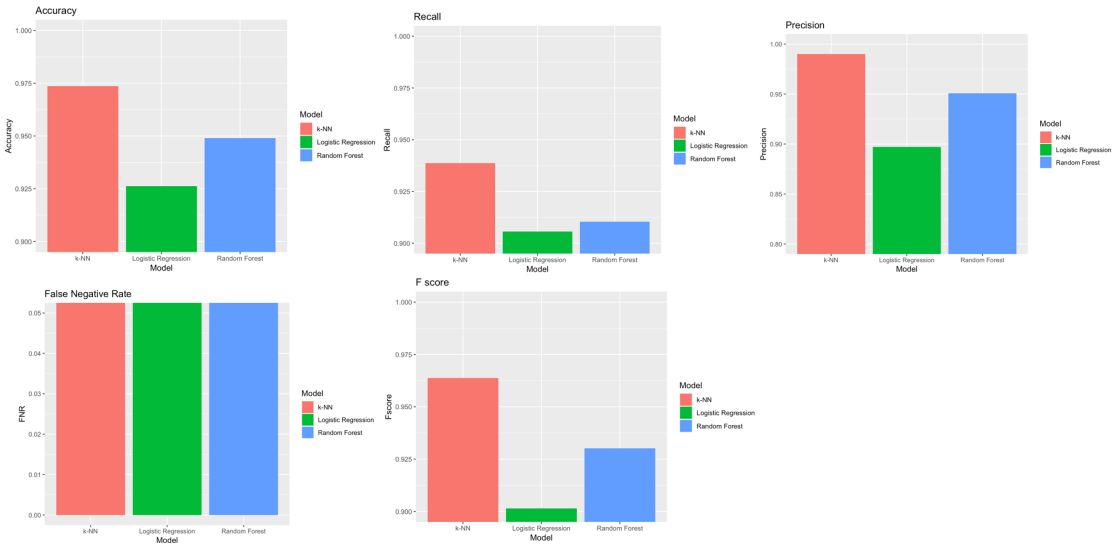
## Random Forest:

From the confusion matrix and model metrics, it can be observed that the Random Forest model has a prediction accuracy of 94.9%, recall of 91.03%, and F-score of 93.01%.




```
##           Model  Accuracy    Recall Precision        FNR    Fscore
## 1 Random Forest 0.9490334 0.9103774 0.9507389 0.08962264 0.9301205
```

Figure B-3: Random Forest




Figures B-4: Model performance metrics

## Results:

As discussed in Objective 1, the explained variance percentage plot (Figure A-9) for PCA analysis showed that the first 10 components account for approximately 95.8% of the variance in the data. We chose to proceed with these components for tuning our models. The tuned models with PCA produced an average CV accuracy of approximately 92.6% for Logistic Regression, 97.3% for kNN, 94.9% for Random Forest.

## Conclusion:

The performance of an algorithm depends greatly upon the data set. A more powerful algorithm might not always outperform a weaker one. All 3 models performed well for classification of breast cancer. However, k-NN slightly outperformed Random Forest and Logistic Regression (in accuracy/recall/f-score). In the health domain, recall and f-score are more informative than just relying on the accuracy metric.

## Future Work:

- Exploring the difference in just using the 10 original features rather than also including the additional correlated attributes as separate features. This would significantly reduce the dimensionality of the dataset.

# APPENDIX

**Code: Loading, Cleaning, & Normalizing Data**

```
bc<-read.table("https://archive.ics.uci.edu/ml/machine-learning-databases/breast-cancer-
wisconsin/wdbc.data",header=F,sep=",")
names(bc)<- c('id_number', 'diagnosis', 'radius_mean',
        'texture_mean', 'perimeter_mean', 'area_mean',
        'smoothness_mean', 'compactness_mean',
        'concavity_mean','concave_points_mean',
        'symmetry_mean', 'fractal_dimension_mean',
        'radius_se', 'texture_se', 'perimeter_se',
        'area_se', 'smoothness_se', 'compactness_se',
        'concavity_se', 'concave_points_se',
        'symmetry_se', 'fractal_dimension_se',
        'radius_worst', 'texture_worst',
        'perimeter_worst', 'area_worst',
        'smoothness_worst', 'compactness_worst',
        'concavity_worst', 'concave_points_worst',
        'symmetry_worst', 'fractal_dimension_worst')
# Data Summary
summary(bc)
# Normalize Data
bc.clean <- bc[,-c(1)]
normalize <- function(x){
  return (( x - min(x))/(max(x) -min(x)))
}
bc.clean.normalized <- as.data.frame(
  lapply(bc.clean[,2:31],normalize)
)
bc.clean.normalized <- cbind(
  bc.clean[,1],
  bc.clean.normalized
)
names(bc.clean.normalized)[1] <- "diagnosis"
summary(bc.clean.normalized)
```

**Code: Box Plot Analysis**

```
#Box Plot: Area Mean
boxplot(area_mean ~ diagnosis,data=wdbc,
horizontal=TRUE,
names=c("Benign","Malignant"),
col=c("green","red"),
xlab="Area Mean", main="Wisconsin Breast Cancer")
```

```
#Box Plot: Radius Mean
boxplot(radius_mean ~ diagnosis,data=wdbc,
horizontal=TRUE,
names=c("Benign","Malignant"),
col=c("green","red"),
xlab="Radius Mean",
main="Wisconsin Breast Cancer")
```

**Code: Principal Component Analysis**

```
pc.bc<-prcomp(bc[,-c(1,2)],scale.=TRUE)
pc.bc.scores<-pc.bc$x
#Adding the response column to the PC's data frame
pc.bc.scores<-data.frame(pc.bc.scores)
pc.bc.scores$Diagnosis<-bc$diagnosis
#Use ggplot2 to plot the first few pc's
library(ggplot2)
ggplot(data = pc.bc.scores, aes(x = PC1, y = PC2)) +
  geom_point(aes(col=Diagnosis), size=1)+
  ggtitle("PCA of Breast Cancer Tumor Biopsies")
ggplot(data = pc.bc.scores, aes(x = PC2, y = PC3)) +
  geom_point(aes(col=Diagnosis), size=1)+
  ggtitle("PCA of Breast Cancer Tumor Biopsies")
```

**Code: Logistic Regression Full & VIF**

```
main.glm <- glm(diagnosis ~ . , data=bc.clean, family = binomial(link = "logit") , control = list(maxit = 50))
summary(main.glm)

# VIF for covariance between Radius, Perimeter, Area
vif(main.glm) -> main.glm.vif
main.glm.vif
```

**Code: Logistic Regression Simplified & VIF**

```
# REDUCED model removing all "SE"" measurements, all "Worst"", and only using "Area" in place of
'perimeter' and 'radius'
redux.glm <- glm(diagnosis ~ texture_mean + area_mean + smoothness_mean + compactness_mean +
concavity_mean + concave_points_mean + symmetry_mean + fractal_dimension_mean , data=bc.clean,
family = binomial(link = "logit") , control = list(maxit = 60))
summary(redux.glm)
```

```
# VIF for covariance between Radius, Perimeter, Area
vif(redux.glm) -> redux.glm.vif
redux.glm.vif

#95% CONFIDENCE INTERVALS
confint(redux.glm, level = 0.95)
```

**Code: ROC Curve for Reduced Logistic Model**

```
#ROC CURVE TO ASSESS

library(ROCR)
bc_lasso_pred <- predict(redux.glm, newx = bc.clean, type = "response")
bc.lasso.pred <- prediction(bc_lasso_pred, bc.clean$diagnosis)
bc.lasso.perf <- performance(bc.lasso.pred, measure = "prec", x.measure = "rec")

plot(bc.lasso.perf)
```

**Code: LASSO Model Selection**

```
library(glmnet)

#NOTE: GLMNET requires dataframe to be converted to matrix
bc_lasso_mat <- model.matrix(diagnosis ~ ., bc.clean)[,-1]
bc.lasso.glm <- glmnet(bc_lasso_mat, bc.clean$diagnosis, family = "binomial" )
bc.lasso.cv <- cv.glmnet(bc_lasso_mat, bc.clean$diagnosis, family = "binomial")

bc_lambda_lasso <- bc.lasso.cv$lambda.min
bc_lambda_lasso

# Output the final coefficients from GLMNET LASSO
predict(bc.lasso.cv, type = "coefficients", s = bc_lambda_lasso )
```

**Code: AIC Stepwise Feature Selection**

```
library(MASS)
main.glm.step <- stepAIC(
        main.glm, trace = 0, family = binomial(link = "logit"), direction = "both", test="Chisq"
)

plot(main.glm.step)
summary(main.glm.step)
```

**Code: Plotting Logistic Regression Simplified Model – Area Mean, Texture Mean, Smoothness Mean**

```
# Area Mean vs Diagnosis
library(popbio)
logi.hist.plot(bc.boolean$radius_mean, bc.boolean$diag_bool, boxp = F, type = "hist")

# Texture Mean vs Diagnosis
library(popbio)
logi.hist.plot(bc.boolean$texture_mean, bc.boolean$diag_bool, boxp = F, type = "hist")

# Smoothness Mean vs Diagnosis
library(popbio)
logi.hist.plot(bc.boolean$smoothness_mean, bc.boolean$diag_bool, boxp = F, type = "hist")
```

**Code: Setting up 5-fold cross-validation**

```
ctrl <- trainControl(method = "cv",
                     number = 5)
```

**Code: Function for plotting confusion matrices**

```
cm_plot <- function(ml, title) {
  confusionMatrix(ml)$table %>%
    round(1) %>%
    fourfoldplot(
      color = c("#CC6666", "#99CC99"),
      main=title,
      conf.level=0,
      margin=1
    )
}
```

**Code: Logistic Regression [Predictive w/ PCA Components]**

```
library(e1071)
logit.ml <- train(pc_wdbc_c~., full_wdbc, method = "glm", family = "binomial", trControl =ctrl)
logit.cm <- confusionMatrix(logit.ml)
cm_plot(logit.ml, "Logistic Regression")
logit.metrics <- data.frame (
  "Model" = "Logistic Regression",
  "Accuracy" = (logit.cm$table[1,1] + logit.cm$table[2,2])/100,
  "Recall" = logit.cm$table[2,2] / (logit.cm$table[2,2] + logit.cm$table[1,2]),
  "Precision" = logit.cm$table[2,2] / (logit.cm$table[2,1] + logit.cm$table[2,2]),
  "FNR" = (logit.cm$table[1,2] / (logit.cm$table[2,2] + logit.cm$table[1,2])),
  "Fscore" = (2 * logit.cm$table[2,2]) / (2 * logit.cm$table[2,2] + logit.cm$table[1,2] + logit.cm$table[2,1])
)
logit.metrics
```

**Code: k-Nearest Neighbors**

```
knn.ml <- train(pc_wdbc_c~., full_wdbc, method = "knn", trControl =ctrl)
knn.cm <- confusionMatrix(knn.ml)
cm_plot(knn.ml, "kNN")
knn.metrics <- data.frame (
  "Model" = "k-NN",
  "Accuracy" = (knn.cm$table[1,1] + knn.cm$table[2,2])/100,
  "Recall" = knn.cm$table[2,2] / (knn.cm$table[2,2] + knn.cm$table[1,2]),
  "Precision" = knn.cm$table[2,2] / (knn.cm$table[2,1] + knn.cm$table[2,2]),
  "FNR" = (knn.cm$table[1,2] / (knn.cm$table[2,2] + knn.cm$table[1,2])),
  "Fscore" = (2 * knn.cm$table[2,2]) / (2 * knn.cm$table[2,2] + knn.cm$table[1,2] + knn.cm$table[2,1])
)
knn.metrics
```

**Code: Random Forest**

```
rf.ml <- train(pc_wdbc_c~., full_wdbc, method = "rf", trControl =ctrl)
rf.cm <- confusionMatrix(rf.ml)
cm_plot(rf.ml, "Random Forest")
rf.metrics <- data.frame (
  "Model" = "Random Forest",
  "Accuracy" = (rf.cm$table[1,1] + rf.cm$table[2,2])/100,
  "Recall" = rf.cm$table[2,2] / (rf.cm$table[2,2] + rf.cm$table[1,2]),
  "Precision" = rf.cm$table[2,2] / (rf.cm$table[2,1] + rf.cm$table[2,2]),
  "FNR" = (rf.cm$table[1,2] / (rf.cm$table[2,2] + rf.cm$table[1,2])),
  "Fscore" = (2 * rf.cm$table[2,2]) / (2 * rf.cm$table[2,2] + rf.cm$table[1,2] + rf.cm$table[2,1])
)
rf.metrics
```

**Code: Model Performance - Confusion Matrices**

```
#Take a look at all confusion matrices:
par(mfrow=c(1,3))
cm_plot(knn.ml, "k-NN")
cm_plot(logit.ml, "Logistic Regression")
cm_plot(rf.ml, "Random Forest")
```

**Code: Model Performance - Metrics:**

```
metrics1 <- rbind(knn.metrics,logit.metrics, rf.metrics)
metrics1 # Taking a look at everything together
ggplot(metrics1, aes(Model, Accuracy)) + geom_bar(stat="identity", aes(fill=Model)) +
coord_cartesian(ylim=c(0.9,1)) + ggtitle("Accuracy")
ggplot(metrics1, aes(Model, Recall)) + geom_bar(stat="identity", aes(fill=Model)) +
coord_cartesian(ylim=c(0.9,1)) + ggtitle("Recall")
ggplot(metrics1, aes(Model, Precision)) + geom_bar(stat="identity", aes(fill=Model)) +
coord_cartesian(ylim=c(0.8,1)) + ggtitle("Precision")
ggplot(metrics1, aes(Model, FNR)) + geom_bar(stat="identity", aes(fill=Model)) +
coord_cartesian(ylim=c(0,0.05)) + ggtitle("False Negative Rate")
ggplot(metrics1, aes(Model, Fscore)) + geom_bar(stat="identity", aes(fill=Model)) +
coord_cartesian(ylim=c(0.9,1)) + ggtitle("F score")
```