# Breast_Cancer_Diagnosis

November 15, 2022

## 1 Overview

This is my solution from the course project of IBM Supervised Machine Learning: Classification course. The Dataset used was the Breast Cancer Wisconsin (Diagnostic) downloaded from Kaggle.

The dataset contains characteristics of cell nuclei obtained from digitized images of breast masses which are: - radius (mean of distances from center to points on the perimeter - texture (standard deviation of gray-scale values) - perimeter - area - smoothness (local variation in radius lengths) - compactness (perimeter^2 / area - 1.0) - concavity (severity of concave portions of the contour) - concave points (number of concave portions of the contour) - symmetry - fractal dimension ("coastline approximation" - 1)

For each feature was computed the mean, standard error, and "worst" or largest (mean of the three largest values). In addition, the dataset contains an ID for each patient and the type of cancer (M = malignant, B = benign).

The main objective is: **train a classification model to predict the cancer diagnosis based on these cell characteristics**. I also interested on interpretability to understand which features contributes to a better diagnosis.

These and other analyzes related to the IBM Machine Learning Professional Certificate can be accessed in this repository.

## 2 Necessary packages

[ ]:
```
#Core
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import os

#Auto EDA -- !pip install dataprep --
#from dataprep.eda import create_report

#Machine Learning
from sklearn.model_selection import train_test_split, StratifiedKFold,␣
↪cross_val_score
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegressionCV, LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.pipeline import make_pipeline
from sklearn.metrics import roc_auc_score, classification_report,␣
 ↪confusion_matrix, ConfusionMatrixDisplay
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.ensemble import RandomForestClassifier
import xgboost as xgb

#Options
pd.set_option('display.max_columns', None)
pd.set_option('display.precision', 3)
```

## 3 Glimpse on Data

[ ]:
```
#loading dataframe
PATH = "data/data.csv"
df_raw = pd.read_csv(os.path.join(PATH))

#create a copy to avoid edit raw data
df = df_raw.copy()
```

[ ]:
```
df.head()
```

[ ]:
```
         id diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean  \
0    842302         M        17.99         10.38          122.80     1001.0
1    842517         M        20.57         17.77          132.90     1326.0
2  84300903         M        19.69         21.25          130.00     1203.0
3  84348301         M        11.42         20.38           77.58      386.1
4  84358402         M        20.29         14.34          135.10     1297.0

   smoothness_mean  compactness_mean  concavity_mean  concave points_mean  \
0            0.118             0.278           0.300                0.147
1            0.085             0.079           0.087                0.070
2            0.110             0.160           0.197                0.128
3            0.142             0.284           0.241                0.105
4            0.100             0.133           0.198                0.104

   symmetry_mean  fractal_dimension_mean  radius_se  texture_se  perimeter_se  \
0          0.242                   0.079      1.095       0.905         8.589
1          0.181                   0.057      0.543       0.734         3.398
2          0.207                   0.060      0.746       0.787         4.585
3          0.260                   0.097      0.496       1.156         3.445
4          0.181                   0.059      0.757       0.781         5.438

   area_se  smoothness_se  compactness_se  concavity_se  concave points_se  \
0   153.40          0.006           0.049         0.054                0.016
1    74.08          0.005           0.013         0.019                0.013
2    94.03          0.006           0.040         0.038                0.021
3    27.23          0.009           0.075         0.057                0.019
4    94.44          0.011           0.025         0.057                0.019

   symmetry_se  fractal_dimension_se  radius_worst  texture_worst  \
0        0.030                 0.006         25.38          17.33
1        0.014                 0.004         24.99          23.41
2        0.022                 0.005         23.57          25.53
3        0.060                 0.009         14.91          26.50
4        0.018                 0.005         22.54          16.67

   perimeter_worst  area_worst  smoothness_worst  compactness_worst  \
0           184.60      2019.0             0.162              0.666
1           158.80      1956.0             0.124              0.187
2           152.50      1709.0             0.144              0.424
3            98.87       567.7             0.210              0.866
4           152.20      1575.0             0.137              0.205

   concavity_worst  concave points_worst  symmetry_worst  \
0            0.712                 0.265           0.460
1            0.242                 0.186           0.275
2            0.450                 0.243           0.361
3            0.687                 0.258           0.664
4            0.400                 0.163           0.236

   fractal_dimension_worst  Unnamed: 32
0                    0.119          NaN
1                    0.089          NaN
2                    0.088          NaN
3                    0.173          NaN
4                    0.077          NaN
```

```
[ ]: df.tail()
```

```
[ ]:          id diagnosis  radius_mean  texture_mean  perimeter_mean  area_mean  \
     564  926424         M        21.56         22.39          142.00     1479.0
     565  926682         M        20.13         28.25          131.20     1261.0
     566  926954         M        16.60         28.08          108.30      858.1
     567  927241         M        20.60         29.33          140.10     1265.0
     568   92751         B         7.76         24.54           47.92      181.0

          smoothness_mean  compactness_mean  concavity_mean  concave points_mean  \
     564            0.111             0.116           0.244                0.139
     565            0.098             0.103           0.144                0.098
     566            0.085             0.102           0.093                0.053
```

```
567          0.118            0.277           0.351                0.152
568          0.053            0.044           0.000                0.000

     symmetry_mean  fractal_dimension_mean  radius_se  texture_se  \
564          0.173                   0.056      1.176       1.256
565          0.175                   0.055      0.765       2.463
566          0.159                   0.056      0.456       1.075
567          0.240                   0.070      0.726       1.595
568          0.159                   0.059      0.386       1.428

     perimeter_se  area_se  smoothness_se  compactness_se  concavity_se  \
564         7.673   158.70          0.010           0.029         0.052
565         5.203    99.04          0.006           0.024         0.040
566         3.425    48.55          0.006           0.037         0.047
567         5.772    86.22          0.007           0.062         0.071
568         2.548    19.15          0.007           0.005         0.000

     concave points_se  symmetry_se  fractal_dimension_se  radius_worst  \
564              0.025        0.011                 0.004        25.450
565              0.017        0.019                 0.002        23.690
566              0.016        0.013                 0.004        18.980
567              0.017        0.023                 0.006        25.740
568              0.000        0.027                 0.003         9.456

     texture_worst  perimeter_worst  area_worst  smoothness_worst  \
564          26.40           166.10      2027.0             0.141
565          38.25           155.00      1731.0             0.117
566          34.12           126.70      1124.0             0.114
567          39.42           184.60      1821.0             0.165
568          30.37            59.16       268.6             0.090

     compactness_worst  concavity_worst  concave points_worst  symmetry_worst  \
564              0.211            0.411                 0.222           0.206
565              0.192            0.322                 0.163           0.257
566              0.309            0.340                 0.142           0.222
567              0.868            0.939                 0.265           0.409
568              0.064            0.000                 0.000           0.287

     fractal_dimension_worst  Unnamed: 32
564                    0.071          NaN
565                    0.066          NaN
566                    0.078          NaN
567                    0.124          NaN
568                    0.070          NaN
```

[ ]:
```
df.shape
```

```
[ ]: (569, 33)
```

```
[ ]: df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 33 columns):
 #   Column                   Non-Null Count  Dtype
---  ------                   --------------  -----
 0   id                       569 non-null    int64
 1   diagnosis                569 non-null    object
 2   radius_mean              569 non-null    float64
 3   texture_mean             569 non-null    float64
 4   perimeter_mean           569 non-null    float64
 5   area_mean                569 non-null    float64
 6   smoothness_mean          569 non-null    float64
 7   compactness_mean         569 non-null    float64
 8   concavity_mean           569 non-null    float64
 9   concave points_mean      569 non-null    float64
 10  symmetry_mean            569 non-null    float64
 11  fractal_dimension_mean   569 non-null    float64
 12  radius_se                569 non-null    float64
 13  texture_se               569 non-null    float64
 14  perimeter_se             569 non-null    float64
 15  area_se                  569 non-null    float64
 16  smoothness_se            569 non-null    float64
 17  compactness_se           569 non-null    float64
 18  concavity_se             569 non-null    float64
 19  concave points_se        569 non-null    float64
 20  symmetry_se              569 non-null    float64
 21  fractal_dimension_se     569 non-null    float64
 22  radius_worst             569 non-null    float64
 23  texture_worst            569 non-null    float64
 24  perimeter_worst          569 non-null    float64
 25  area_worst               569 non-null    float64
 26  smoothness_worst         569 non-null    float64
 27  compactness_worst        569 non-null    float64
 28  concavity_worst          569 non-null    float64
 29  concave points_worst     569 non-null    float64
 30  symmetry_worst           569 non-null    float64
 31  fractal_dimension_worst  569 non-null    float64
 32  Unnamed: 32              0 non-null      float64
dtypes: float64(31), int64(1), object(1)
memory usage: 146.8+ KB
```

```
[ ]: #checking id
     len(df.id.unique()) == df.shape[0]
```

[ ]: 
```
True
```

[ ]:
```
#checking diagnosis
df.diagnosis.unique()
```

[ ]: 
```
array(['M', 'B'], dtype=object)
```

- Id contains a unique value for each observation. This kind of feature is not useful for Machine Learning models. I delete it.
- Diagnosis is the unique not numerical feature. I encode it with 0 mean "B" and 1 mean "M".
- Unnamed: 32 has only missing data.

[ ]:
```
#preprocessing
df = df.drop(["id","Unnamed: 32"], axis = 1)
df.diagnosis = df.diagnosis.map({"B":0, "M":1})
```

I always like to start the analysis with an auto EDA tool to give a first look on data and and get quick insights. Here I use dataprep for this purpose.

[ ]:
```
#this code export a html file with dataprep output which can be opened locally␣
↪by any browser
report = create_report(df, title='Cancer Detection')
report.save("Cancer Detection.html")
```

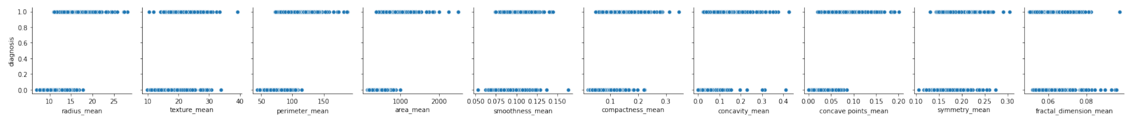
```
Report has been saved to Cancer Detection.html!
```

Here are some discoveries: - The target class is unbalanced (62.74% Benign and 37.26% Malign) - There are many features with skewness. - There are several features (Radius, Perimeter, Area, Compactness, Concavity) that seem to separate the classe well. I could bet that a simple linear classifier like a Logistic Regression would do a good job devide the the separability of classes. - For that features a great value in them are associated to malign cancer. - Many features with high degree of correlation (>70%) with target - There are high degree of multicolinearity between predictor features. Eliminate them could lead to a more simple model and simple to interpret due to the fewer features. - There are some outilers, two observation in concavity worst for example are very far from others

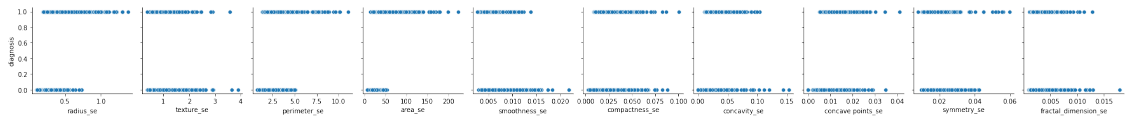
## 4 Exploratory Data Analysis

### 4.1 Bivariate Analysis

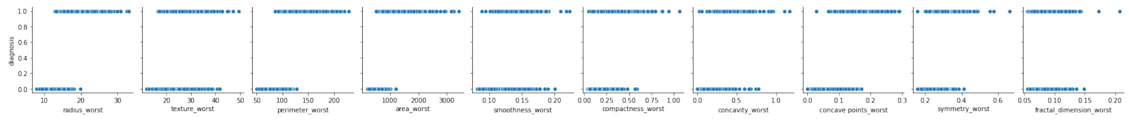
[ ]:
```
#_mean pairplot
sns.pairplot(data = df , x_vars =[i for i in df.columns if "mean" in i], ␣
↪y_vars = ["diagnosis"]);
```



[ ]:
```
#_se pairplot
sns.pairplot(data = df , x_vars =[i for i in df.columns if "_se" in i],  y_vars␣
↪= ["diagnosis"]);
```



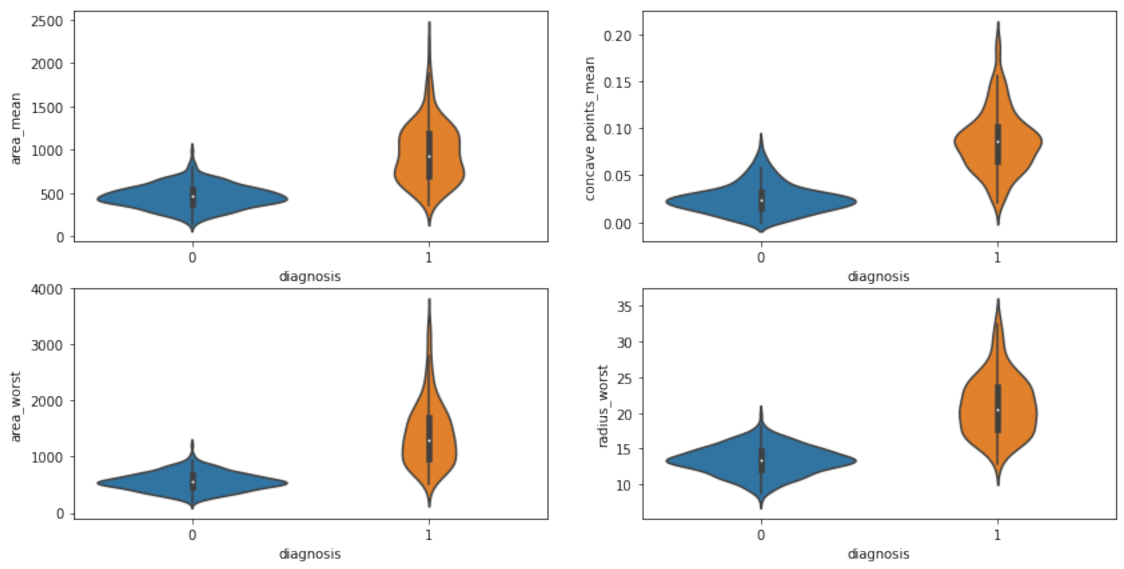
[ ]:
```
#_worst pairplot
sns.pairplot(data = df , x_vars =[i for i in df.columns if "_worst" in i], ␣
↪y_vars = ["diagnosis"]);
```



The pairplot confirm the separability between classes usually with large values leading to a malign cancer. **"area_mean"**, **"concave_points_mean"**, **"area_worst"**, **"radius_worst"** seem to separate the classes very well.

Also, we can see in the _se pairplot that there are two points that are very far from each other.

[ ]:
```
to_plot = ["area_mean", "concave points_mean", "area_worst", "radius_worst"]

fig, ax = plt.subplots(2,2, figsize = (14,7))

for i, var in enumerate(to_plot):
  sns.violinplot(data = df, x = "diagnosis", y = var, ax = ax.flat[i])
```



Again, we can see that those features have lower median and mean to Benign and in Benign the concentration of values are in lower values

## 4.2 Dealing With Outliers on _SE features

Here, I manually looked for the outliers based on pairplot

```
[ ]: df.query("radius_se > 2 and perimeter_se > 15 and area_se > 400" ).index
```

```
[ ]: Int64Index([212, 461], dtype='int64')
```

```
[ ]: df.query("smoothness_se > 0.02 and diagnosis == 1").index
```

```
[ ]: Int64Index([122, 213], dtype='int64')
```

```
[ ]: df.query("texture_se > 4").index
```

```
[ ]: Int64Index([192], dtype='int64')
```

```
[ ]: df.query("compactness_se > 0.12").index
```

```
[ ]: Int64Index([190], dtype='int64')
```

```
[ ]: df.query("concavity_se > 0.3").index
```

```
[ ]: Int64Index([68, 152], dtype='int64')
```

```
[ ]: df[df["concave points_se"] > 0.05].index
```

[ ]: Int64Index([152], dtype='int64')

[ ]:
```
df.query("(symmetry_se > 0.06 and diagnosis == 0) or symmetry_se > 0.065" ).
 ↪index
```

[ ]: Int64Index([78, 314], dtype='int64')

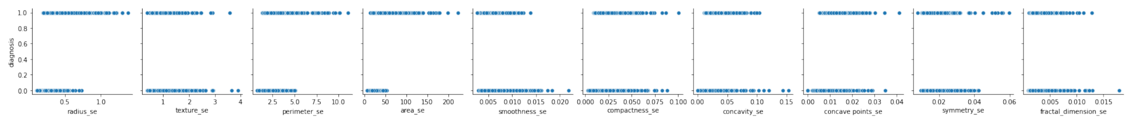
[ ]:
```
df.query("fractal_dimension_se > 0.02").index
```

[ ]: Int64Index([71, 152, 290], dtype='int64')

[ ]:
```
outliers = [212,461,122,192,213,190,68,152,78,314,71,152,290]
```

[ ]:
```
df = df.drop(outliers, axis = 0)
df = df.reset_index(drop = True)
```

[ ]:
```
# re-plot the _se pairplot
sns.pairplot(data = df , x_vars =[i for i in df.columns if "_se" in i],  y_vars␣
 ↪= ["diagnosis"]);
```

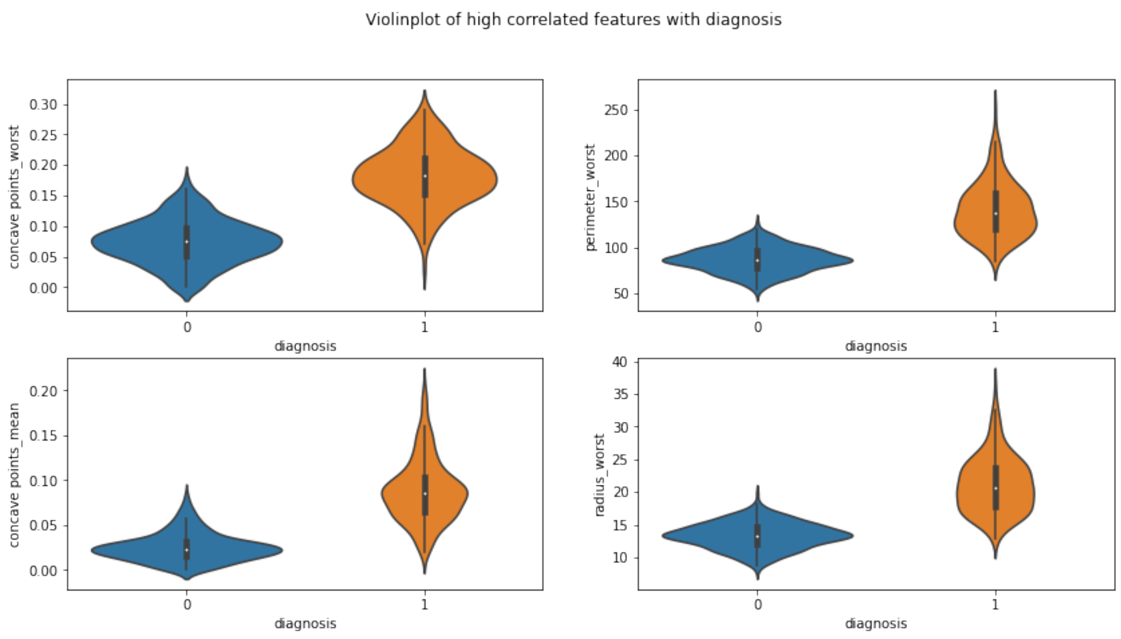


## 4.3 Correlation

[ ]:
```
corr = abs(df.corr()['diagnosis'].sort_values(ascending = False)[1:])
corr[corr > 0.75]
```

[ ]:
```
concave points_worst    0.797
perimeter_worst         0.787
concave points_mean     0.784
radius_worst            0.779
Name: diagnosis, dtype: float64
```

[ ]:
```
fig, ax = plt.subplots(2,2, figsize = (14,7))

for i, var in enumerate(corr[corr > 0.75].index):
  sns.violinplot(data = df, x = "diagnosis", y = var, ax = ax.flat[i])

fig.suptitle("Violinplot of high correlated features with diagnosis");
```



## 5 Create a Baseline

I will create a simple baseline with logistic regression regularizated (Lasso) to deal with multicollinearity.

As lasso regularization tends to zero the coefficients without importance I will use the results to get some insights.

The evaluation is done in a 4 fold cross validation with the choice of best regulatrization term (C) done from default options of LogisticRegressionCV class. The metric evaluated is the ROC auc since the desbalance between the classes it's not extreme.

```
[ ]: X = df.drop("diagnosis", axis = 1)
     y = df["diagnosis"]

     X_train, X_test, y_train, y_test = train_test_split(X,y, random_state=42,␣
      ↪shuffle=True, stratify=y)
     cv = StratifiedKFold(n_splits = 4, shuffle=True, random_state=42)
```

```
[ ]: #Need to scale because regularization. For that, I chained the scaller and␣
      ↪estimator inisde a Pipeline
     logit_base = LogisticRegressionCV(solver = "liblinear", cv =cv, penalty = "l1",␣
      ↪scoring = "roc_auc", max_iter = 1000, random_state = 42)
     baseline = make_pipeline(StandardScaler(), logit_base)
```

```
[ ]: #need to fit to get the coeficietns and C value
     baseline.fit(X_train,y_train)
```

```
[ ]: Pipeline(steps=[('standardscaler', StandardScaler()),
                     ('logisticregressioncv',
                      LogisticRegressionCV(cv=StratifiedKFold(n_splits=4,
     random_state=42, shuffle=True),
                                           max_iter=1000, penalty='l1',
                                           random_state=42, scoring='roc_auc',
                                           solver='liblinear'))])
```

```
[ ]: print(f"Baseline ROC auc: {baseline[1].scores_[1][0:,4].mean()}")
     print(f"Best C: {baseline[1].C_[0]}")
```

```
Baseline ROC auc: 0.9942542444060662
Best C: 2.782559402207126
```

This is a very good cross validation score. We could suspect overfitting but as the validation was correctly done it is more likely that this high score is due to the linear separability of the classes Malign and Benign.

## 6 Model Selection

I also evaluated three other models (Decision Tree, Random Forest and XGboost).

For the first I use some arbitraty hyperparameters to prune the tree. As in random forest the trees are independent, a high number of estimators tends to more stable predictions (the bagging nature also contribute to that). This does not occur in boosting models like XGBoost, in which case the trees are trained in a subsequent way and each one learns from the mistakes of the previous one. In this case, a greater number of estimators tends to overfitting.

```
[ ]: #decision tree - prune the tree to avoid "infinite" growing
     dt = DecisionTreeClassifier(max_depth = 4, min_samples_leaf = 40, random_state=␣
      ↪42)
     dt_cross_val = cross_val_score(dt, X_train, y_train, cv = cv, scoring =␣
      ↪"roc_auc")

     print(f"Decision Tree ROC auc: {np.mean(dt_cross_val)}")
```

```
Decision Tree ROC auc: 0.943455970480262
```

```
[ ]: #random forest - high n_estimators is better
     rf = RandomForestClassifier(n_estimators = 1000 , random_state= 42)
     rf_cross_val = cross_val_score(rf, X_train, y_train, cv = cv, scoring =␣
      ↪"roc_auc")

     print(f"Random Forest ROC auc: {np.mean(rf_cross_val)}")
```

```
Random Forest ROC auc: 0.9883828160143949
```

```
[ ]: #XGBoost - in opposite to Random Forest here more trees tend to overfit
     xgb = xgb.XGBClassifier(n_estimators = 100, random_state = 42)
     xgb_cross_val = cross_val_score(xgb, X_train, y_train, cv = cv, scoring =␣
      ↪"roc_auc")

     print(f"XGBoost ROC auc: {np.mean(rf_cross_val)}")
```

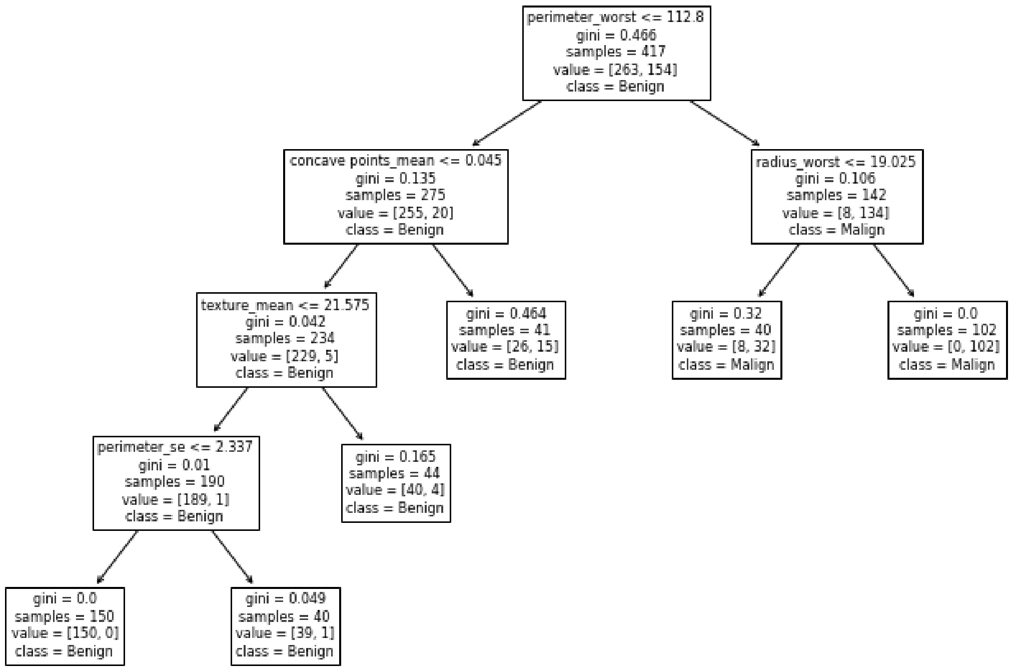
```
XGBoost ROC auc: 0.9883828160143949
```

Curiously none of them (including two complex ensemble models) could beat the baseline, a simple Logistic Regression.

## 7 Model Interpretability

As the decision tree has been pruned, it is easy to interpret the decisions made by the model.

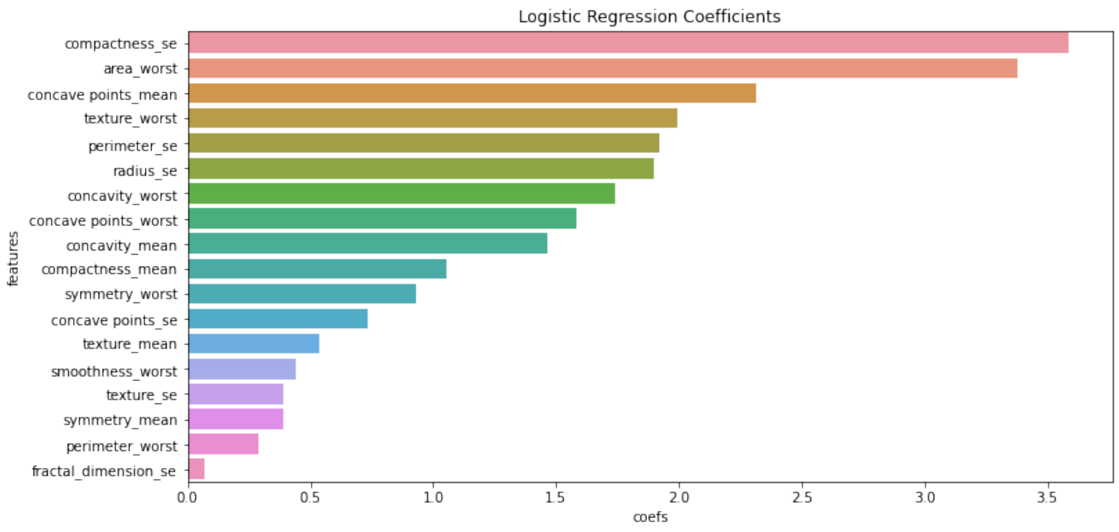
```
[ ]: #fitting estimator
     dt.fit(X_train, y_train)

     #plotting the tree
     feat_dt = ["perimeter_worst", "concave points_mean", "texture_mean", "concave␣
      ↪points_worst"]
     fig, ax = plt.subplots(figsize = (12,8))
     plot_tree(dt, feature_names = X_train.columns, class_names =␣
      ↪["Benign","Malign"]);
```



For example, a cell with perimeter_worst >= 112.8 and a radius_worst >= 19.025 has a 100% chance of being malignant based on 102 observations from training data.

```
[ ]: #Logistic regression Coefficients
     coefs = pd.DataFrame({'features':X_train.columns,
                  'coefs': abs(baseline[1].coef_[0])})
```

```
[ ]: fig, ax = plt.subplots(figsize = (12,6))
     sns.barplot(data = coefs.query('coefs > 0').sort_values(by = 'coefs', ascending␣
      ↪= False),
                 x='coefs',
                 y='features')
     ax.set_title('Logistic Regression Coefficients');
```



Lasso regularization zeroed the coefficients from 9 features. Logistic Regression give too much importance to compactness_se and area_worst. We can interpret this as the following: the greater the variation in compactness between different images of the same nucleus, the greater the tendency for the cancer to be malignant. The same can be said for the area measurement.

## 8 Final Evaluation on Test

To evaluate on test I instantiated a new object from the class LogisticRegression with the C value defined latter on cross validationn and fitted it again on entire train set.

```
[ ]: logit = LogisticRegression(C=2.782559402207126, solver = "liblinear", penalty =␣
      ↪"l1", max_iter = 1000, random_state = 42)
     final_model = make_pipeline(StandardScaler(), logit)
```

[ ]:
```
final_model.fit(X_train, y_train)
```

[ ]:
```
Pipeline(steps=[('standardscaler', StandardScaler()),
                ('logisticregression',
                 LogisticRegression(C=2.782559402207126, max_iter=1000,
                                    penalty='l1', random_state=42,
                                    solver='liblinear'))])
```

[ ]:
```
yhat = final_model.predict(X_test)
```

[ ]:
```
roc_auc_score(y_test, yhat)
```

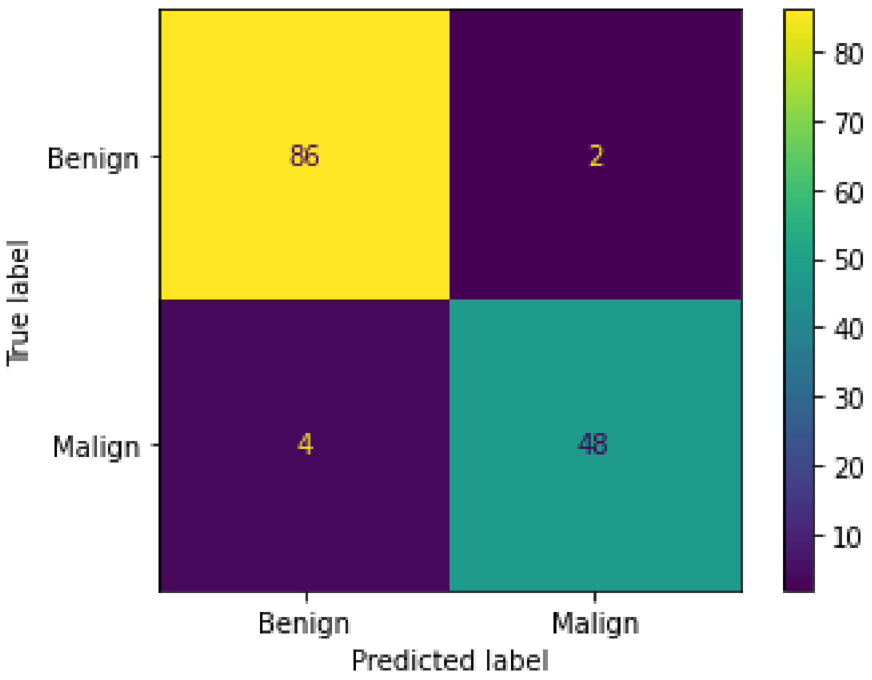
[ ]:
```
0.9501748251748252
```

We successfully managed to avoid overfitting on training since the difference in the metric was not that high

[ ]:
```
print(classification_report(y_test, yhat))
```

```
              precision    recall  f1-score   support

           0       0.96      0.98      0.97        88
           1       0.96      0.92      0.94        52

    accuracy                           0.96       140
   macro avg       0.96      0.95      0.95       140
weighted avg       0.96      0.96      0.96       140
```

[ ]:
```
cm = confusion_matrix(y_test, yhat, labels = final_model[1].classes_)
disp = ConfusionMatrixDisplay(cm,  display_labels = ['Benign','Malign'])
disp.plot();
```



The final result apoints to a good others metrics like f1, recall and precision for boths classes. Also, the model makes few mistakes only 4 False Negatives and 2 False Positive

## 9 Future Perspectives

This model can be applied to help automate the diagnosis of breast cancer as it has excellent metrics, is easily interpretable and the classes are easily distinguishable.

There are some measures that can be taken to improve it: - Treat the asymmetry in the data making them more normal. This would increase the reliability of the coefficients by improving the interpretation, although it does not affect the predictive ability. - Here I only treat outliers on the se_ features. An alternative would be to look at the restants features. - Optimize the model to avoid false negatives by increasing the recall of class 1. This is important because this type of error is very harmful (model identifies as benign when in fact it is malignant)